Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 02:32 pm GMT

PDB ID	:	5NB4
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 following versions of software and data (see references ⓘ) were used in the production of this report:

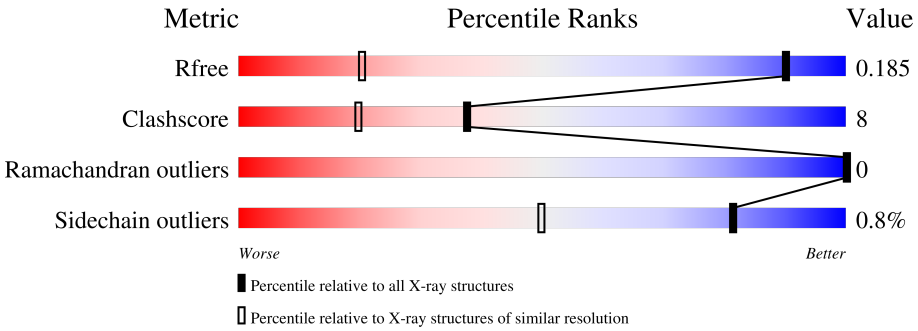
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1492 (1.18-1.10)
Clashscore	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	164	92% 7% •
1	B	164	94% 6%
1	C	164	91% 9%
1	D	164	95% 5%
1	E	164	94% 6%
1	F	164	86% 13% •
1	G	164	93% 7%

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Mol	Chain	Length	Quality of chain
1	H	164	92% 8%
1	I	164	91% 8%
1	J	164	92% 8%
1	K	164	95%
1	L	164	92% 7%
2	M	184	95%
2	N	184	90% 8%
2	O	184	91% 8%
2	P	184	91% 8%
2	Q	184	91% 8%
2	R	184	90% 10%
2	S	184	91% 8%
2	T	184	88% 11%
2	U	184	88% 12%
2	V	184	92% 7%
2	W	184	89% 11%
2	X	184	91% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PI	A	204	-	-	X	-
5	PI	H	203	-	-	X	-
7	MPD	O	204	-	-	X	-
7	MPD	P	204	-	-	X	-
7	MPD	Q	204	-	-	X	-
7	MPD	R	204	-	-	X	-
7	MPD	S	204	-	-	X	-
7	MPD	U	204	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MPD	W	204	-	-	X	-
7	MPD	X	204	-	-	X	-
8	MRD	T	204	-	-	X	-
8	MRD	V	204	-	-	X	-

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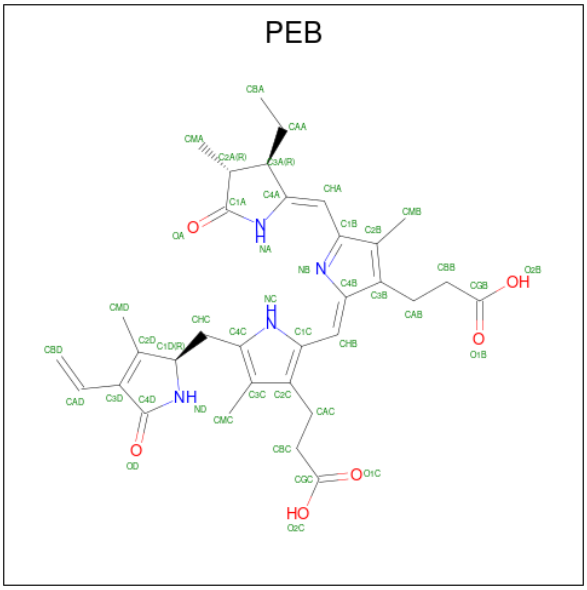
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	184	Total	C	N	O	S	0	9	0
			1400	867	252	268	13			
2	P	184	Total	C	N	O	S	0	11	0
			1401	865	249	273	14			
2	Q	184	Total	C	N	O	S	0	10	0
			1394	862	248	271	13			
2	R	184	Total	C	N	O	S	0	10	0
			1402	867	251	271	13			
2	S	184	Total	C	N	O	S	0	12	0
	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

- Molecule 3 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$).



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

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

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

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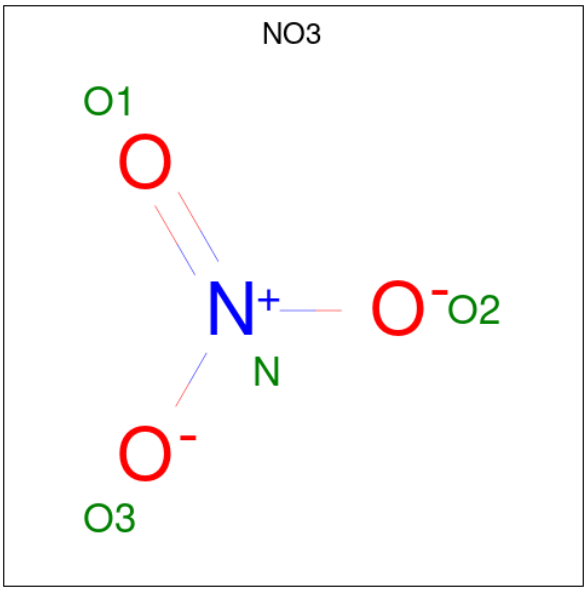
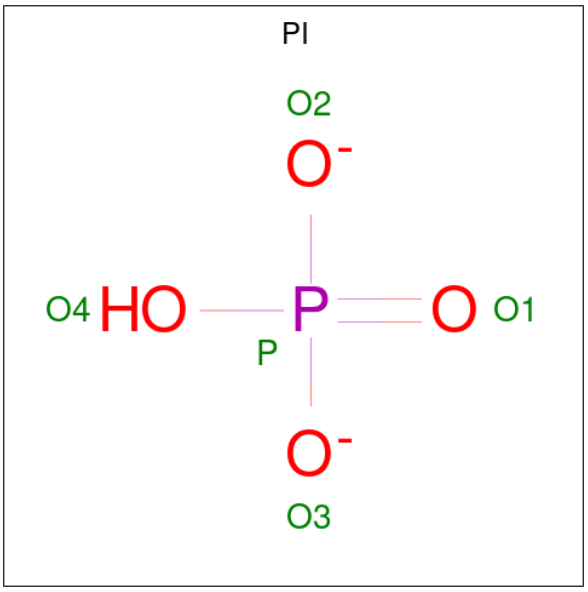
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	S	1	Total	C	N	O	0	0
			43	33	4	6		
3	S	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	U	1	Total	C	N	O	0	0
			43	33	4	6		
3	U	1	Total	C	N	O	0	0
			43	33	4	6		
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 (three-letter code: NO3) (formula: NO_3).



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

- Molecule 5 is HYDROGENPHOSPHATE ION (three-letter code: PI) (formula: HO_4P).



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

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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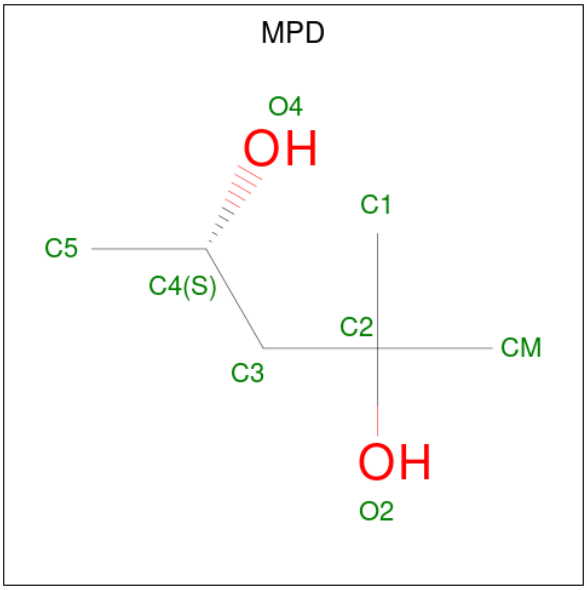
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total Na 1 1	0	0
6	K	1	Total Na 1 1	0	0
6	L	1	Total Na 1 1	0	0
6	N	1	Total Na 1 1	0	0
6	S	1	Total Na 1 1	0	0
6	V	1	Total Na 1 1	0	0
6	W	1	Total Na 1 1	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

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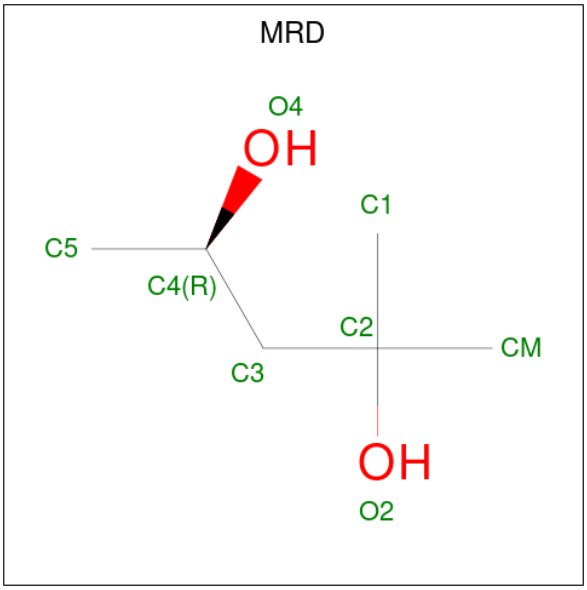
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Q	1	Total C O 8 6 2	0	0
7	R	1	Total C O 8 6 2	0	0
7	S	1	Total C O 8 6 2	0	0
7	U	1	Total C O 8 6 2	0	0
7	W	1	Total C O 8 6 2	0	0
7	X	1	Total C O 8 6 2	0	0

- Molecule 8 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



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

- Molecule 9 is water.

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

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

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

3 Residue-property plots (i)

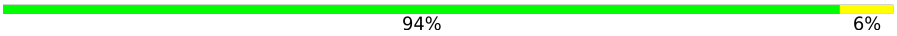
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

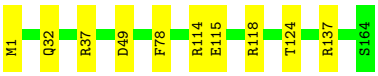
• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain A:

• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

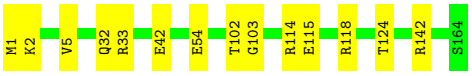
Chain B:





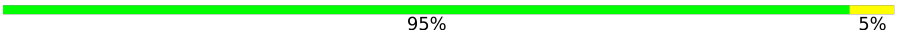
• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain C:



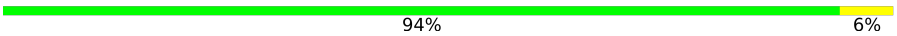
• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain D:



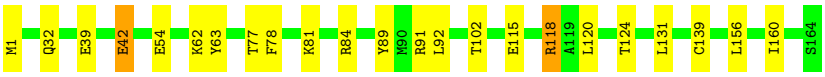
• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain E:



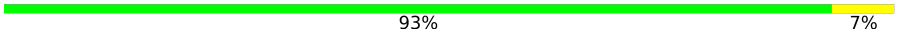
• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain F:



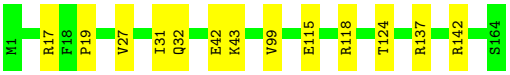
• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain G:



• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain H:



• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

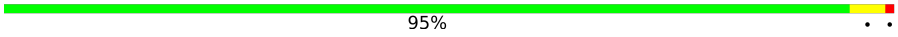
Chain I:

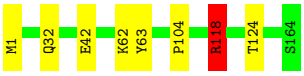
• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain J:

• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

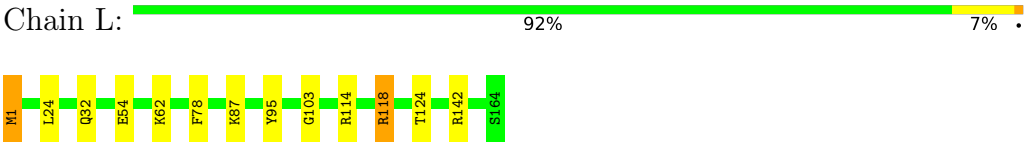
Chain K:





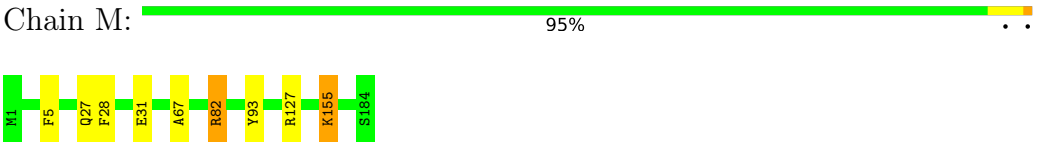
• Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain L:



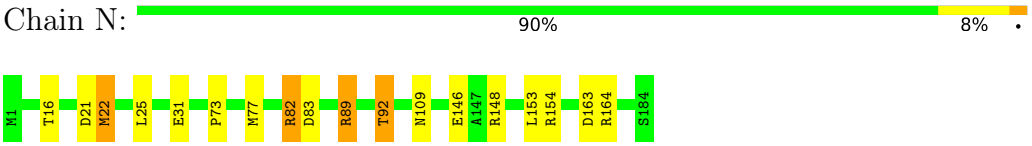
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain M:



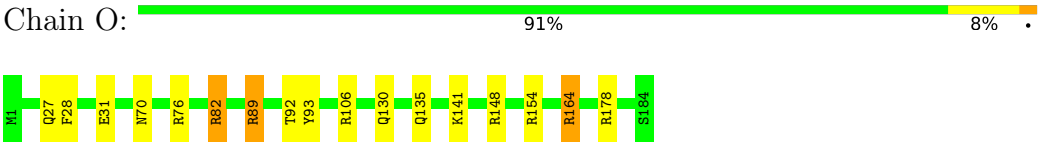
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain N:



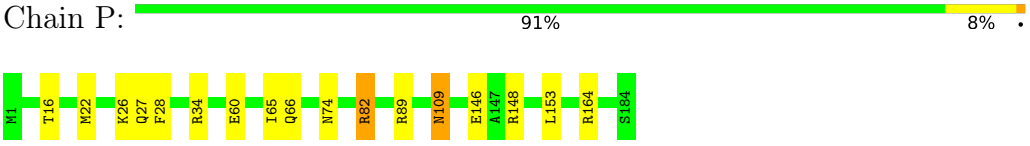
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain O:



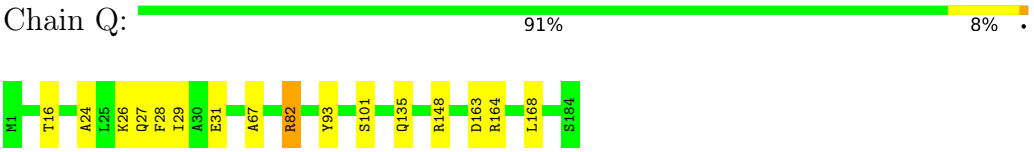
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain P:



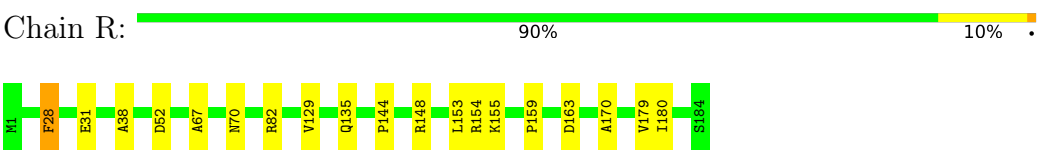
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain Q:



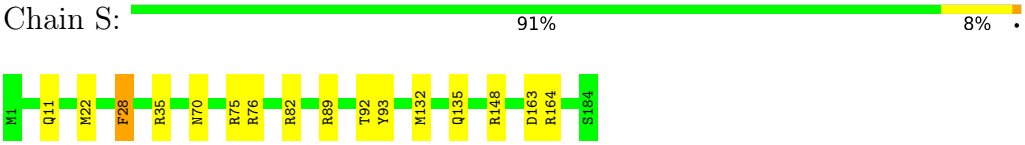
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain R:



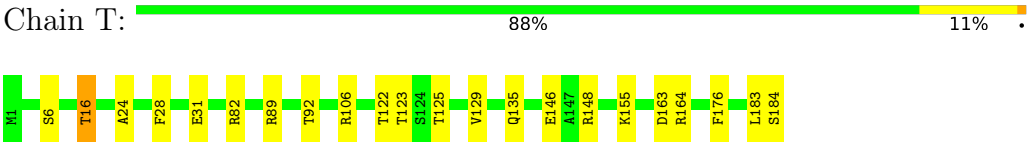
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain S:



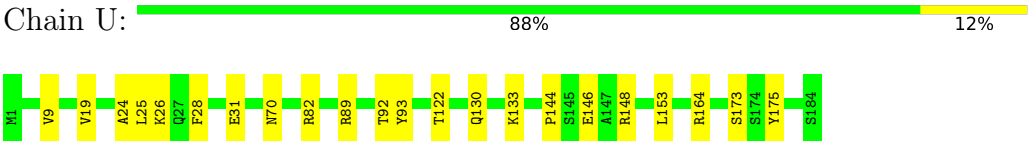
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain T:



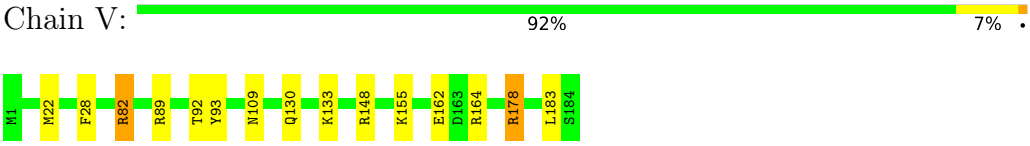
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain U:



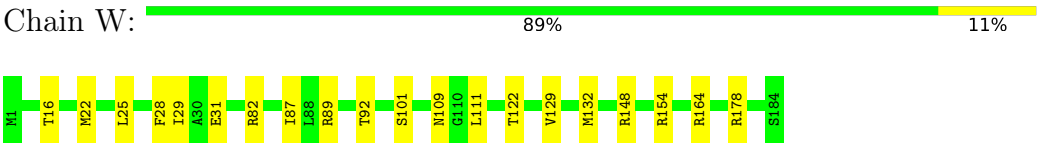
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain V:



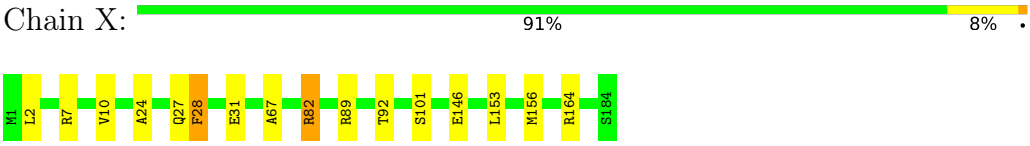
• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain W:



• Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain X:



4 Data and refinement statistics (i)

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 94.59 – 1.14	Depositor EDS
% Data completeness (in resolution range)	93.8 (94.62-1.14) 93.8 (94.59-1.14)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	79188 reflections (5.03%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.014 for h-k,-k,-l	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.85	1/1344 (0.1%)	0.99	7/1816 (0.4%)
1	B	0.74	0/1327	0.92	6/1795 (0.3%)
1	C	0.80	1/1336 (0.1%)	0.90	2/1806 (0.1%)
1	D	0.76	0/1364	0.90	1/1841 (0.1%)
1	E	0.74	1/1327 (0.1%)	0.88	1/1795 (0.1%)
1	F	0.82	0/1354	0.92	2/1830 (0.1%)
1	G	0.77	2/1336 (0.1%)	0.92	2/1806 (0.1%)
1	H	0.70	0/1354	0.88	5/1830 (0.3%)
1	I	0.79	0/1365	0.92	4/1843 (0.2%)
1	J	0.79	1/1344 (0.1%)	0.92	5/1817 (0.3%)
1	K	0.81	0/1342	1.01	4/1814 (0.2%)
1	L	0.81	1/1338 (0.1%)	0.98	10/1808 (0.6%)
2	M	0.82	0/1455	0.96	5/1959 (0.3%)
2	N	0.76	0/1439	1.00	9/1937 (0.5%)
2	O	0.74	0/1427	1.00	9/1921 (0.5%)
2	P	0.84	1/1434 (0.1%)	1.00	6/1933 (0.3%)
2	Q	0.75	0/1427	0.95	6/1925 (0.3%)
2	R	0.73	0/1432	0.92	2/1929 (0.1%)
2	S	0.72	0/1443	1.05	8/1945 (0.4%)
2	T	0.71	0/1442	0.91	3/1942 (0.2%)
2	U	0.82	0/1488	0.99	5/2002 (0.2%)
2	V	0.79	0/1478	0.89	5/1989 (0.3%)
2	W	0.77	0/1464	0.92	3/1971 (0.2%)
2	X	0.73	0/1437	0.94	3/1937 (0.2%)
All	All	0.77	8/33497 (0.0%)	0.95	113/45191 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	GLU	CD-OE2	-8.60	1.16	1.25
1	A	54	GLU	CD-OE2	-6.46	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	54	GLU	CD-OE2	-6.04	1.19	1.25
1	L	54	GLU	CD-OE2	-5.53	1.19	1.25
1	G	39	GLU	CD-OE2	-5.51	1.19	1.25
1	E	117	TYR	CG-CD1	5.44	1.46	1.39
2	P	60	GLU	CD-OE2	5.21	1.31	1.25
1	G	131	LEU	C-O	5.04	1.32	1.23

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	82[A]	ARG	NE-CZ-NH2	-11.16	114.72	120.30
2	S	82[B]	ARG	NE-CZ-NH2	-11.16	114.72	120.30
2	O	164	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	K	118[A]	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	K	118[B]	ARG	NE-CZ-NH2	-9.68	115.46	120.30
2	N	163	ASP	CB-CG-OD1	9.63	126.97	118.30
1	K	118[A]	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	K	118[B]	ARG	NE-CZ-NH1	9.46	125.03	120.30
2	P	164	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	S	82[A]	ARG	NE-CZ-NH1	9.33	124.96	120.30
2	S	82[B]	ARG	NE-CZ-NH1	9.33	124.96	120.30
2	U	164	ARG	NE-CZ-NH1	9.14	124.87	120.30
2	S	163	ASP	CB-CG-OD1	8.93	126.34	118.30
2	X	82[A]	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	X	82[B]	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	V	164	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	D	142	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	J	37	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	T	163	ASP	CB-CG-OD1	7.58	125.12	118.30
2	O	89	ARG	NE-CZ-NH2	-7.54	116.53	120.30
2	P	164	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	F	84	ARG	NE-CZ-NH2	-7.37	116.61	120.30
2	Q	82[A]	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	Q	82[B]	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	R	154	ARG	NE-CZ-NH2	-7.31	116.64	120.30
2	U	164	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	L	95	TYR	CB-CG-CD1	7.13	125.28	121.00
2	P	34	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	I	37	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	O	82[A]	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	O	82[B]	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	O	164	ARG	NE-CZ-NH2	-6.83	116.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	W	154	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	H	137	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	S	93	TYR	CB-CG-CD1	6.74	125.04	121.00
1	A	37	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	N	22[A]	MET	CG-SD-CE	6.71	110.94	100.20
2	N	22[B]	MET	CG-SD-CE	6.71	110.94	100.20
2	Q	163	ASP	CB-CG-OD1	6.69	124.32	118.30
2	O	89	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	N	164	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	142	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	M	82[A]	ARG	NE-CZ-NH2	-6.39	117.11	120.30
2	M	82[B]	ARG	NE-CZ-NH2	-6.39	117.11	120.30
2	M	82[C]	ARG	NE-CZ-NH2	-6.39	117.11	120.30
2	O	106	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	L	114	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	B	37	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	W	164	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	X	164	ARG	NE-CZ-NH1	6.21	123.41	120.30
2	N	89	ARG	NE-CZ-NH2	-6.13	117.23	120.30
2	Q	164	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	V	93	TYR	CB-CG-CD1	6.06	124.64	121.00
1	J	95	TYR	CB-CG-CD2	-6.05	117.37	121.00
2	S	93	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	H	142	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	N	21	ASP	CB-CG-OD1	5.87	123.58	118.30
2	R	154	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	U	175	TYR	CZ-CE2-CD2	-5.81	114.57	119.80
2	M	93	TYR	CB-CG-CD1	5.79	124.47	121.00
1	B	78	PHE	CB-CG-CD2	-5.77	116.76	120.80
2	O	93	TYR	CB-CG-CD1	5.74	124.44	121.00
2	N	82[A]	ARG	NE-CZ-NH2	-5.73	117.44	120.30
2	N	82[B]	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	137	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	78	PHE	CB-CG-CD1	5.65	124.76	120.80
2	O	154	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	H	142	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	C	142	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	P	82[A]	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	P	82[B]	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	V	82[A]	ARG	NE-CZ-NH2	-5.47	117.57	120.30
2	V	82[B]	ARG	NE-CZ-NH2	-5.47	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	137	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	P	34	ARG	CG-CD-NE	-5.46	100.34	111.80
1	L	142	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	J	95	TYR	CB-CG-CD1	5.33	124.20	121.00
2	W	164	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	J	142	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	M	127	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	L	78	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	G	37	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	F	84	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	Q	93	TYR	CB-CG-CD2	-5.28	117.83	121.00
2	S	164	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	N	154	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	95	TYR	CB-CG-CD1	5.24	124.14	121.00
1	A	114[A]	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	114[B]	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	G	49	ASP	CB-CG-OD1	5.22	122.99	118.30
1	H	137	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	L	78	PHE	CB-CG-CD1	5.20	124.44	120.80
2	U	93	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	E	17	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	114	ARG	NE-CZ-NH2	-5.15	117.72	120.30
2	U	93	TYR	CB-CG-CD1	5.14	124.09	121.00
1	I	137	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	V	133	LYS	CD-CE-NZ	-5.10	99.96	111.70
2	T	106	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	J	17	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	L	118[A]	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	L	118[B]	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	L	118[C]	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	H	17	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	Q	164	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	T	164	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	49	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	142	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	I	118[A]	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	I	118[B]	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	L	1[A]	MET	CG-SD-CE	5.01	108.22	100.20
1	L	1[B]	MET	CG-SD-CE	5.01	108.22	100.20

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	27	0
1	B	1292	0	1289	11	0
1	C	1298	0	1301	17	0
1	D	1314	0	1339	21	0
1	E	1292	0	1289	12	0
1	F	1316	0	1314	35	0
1	G	1301	0	1300	19	0
1	H	1316	0	1316	20	0
1	I	1315	0	1334	17	0
1	J	1306	0	1311	15	0
1	K	1304	0	1305	22	0
1	L	1300	0	1307	15	0
2	M	1416	0	1462	11	0
2	N	1411	0	1444	16	0
2	O	1400	0	1443	16	0
2	P	1401	0	1432	14	0
2	Q	1394	0	1428	27	0
2	R	1402	0	1439	30	0
2	S	1410	0	1439	20	0
2	T	1407	0	1443	27	0
2	U	1441	0	1488	25	0
2	V	1437	0	1476	18	0
2	W	1423	0	1466	29	0
2	X	1401	0	1437	21	0
3	A	86	0	74	2	0
3	B	86	0	74	1	0
3	C	86	0	74	2	0
3	D	86	0	74	1	0
3	E	86	0	74	2	0
3	F	86	0	74	3	0
3	G	86	0	74	2	0
3	H	86	0	74	2	0
3	I	86	0	74	1	0
3	J	86	0	74	1	0
3	K	86	0	74	1	0
3	L	86	0	74	2	0
3	M	129	0	110	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	129	0	110	6	0
3	O	129	0	110	6	0
3	P	129	0	110	6	0
3	Q	129	0	110	8	0
3	R	129	0	111	10	0
3	S	135	0	87	3	0
3	T	129	0	110	8	0
3	U	129	0	110	6	0
3	V	129	0	110	5	0
3	W	129	0	110	6	0
3	X	129	0	110	8	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	11	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	1	0
5	E	5	0	0	0	0
5	F	5	0	0	1	0
5	G	5	0	0	0	0
5	H	5	0	0	2	0
5	I	5	0	0	0	0
5	J	5	0	0	0	0
5	K	5	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	0
7	M	8	0	12	4	0
7	O	8	0	10	9	0
7	P	8	0	11	6	0
7	Q	8	0	11	11	0
7	R	8	0	14	15	0
7	S	8	0	14	8	0
7	U	8	0	12	8	0
7	W	8	0	11	7	0
7	X	8	0	14	8	0
8	T	8	0	11	10	0
8	V	8	0	11	10	0
9	A	356	0	0	8	0
9	B	312	0	0	10	0
9	C	341	0	0	9	0
9	D	363	0	0	15	1
9	E	319	0	0	8	0
9	F	345	0	0	27	0
9	G	350	0	0	11	0
9	H	324	0	0	11	0
9	I	351	0	0	15	0
9	J	345	0	0	12	0
9	K	319	0	0	9	0
9	L	355	0	0	6	0
9	M	362	0	0	2	1
9	N	359	0	0	6	1
9	O	362	0	0	7	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	330	0	0	5	0
9	Q	322	0	0	11	0
9	R	297	0	0	11	1
9	S	318	0	0	9	0
9	T	312	0	0	13	1
9	U	340	0	0	17	0
9	V	361	0	0	5	0
9	W	368	0	0	13	1
9	X	357	0	0	11	1
All	All	43607	0	35446	544	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 8.

All (544) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:28[A]:PHE:CE1	8:V:204:MRD:H5C2	1.27	1.59
2:V:28[A]:PHE:CD1	8:V:204:MRD:C5	1.83	1.57
2:V:28[A]:PHE:CD1	8:V:204:MRD:H5C2	1.03	1.56
2:X:28[A]:PHE:HE2	7:X:204:MPD:C1	1.18	1.54
2:O:28[B]:PHE:CD1	7:O:204:MPD:C5	1.76	1.51
2:Q:28[A]:PHE:CD1	7:Q:204:MPD:H4	1.53	1.42
2:Q:28[A]:PHE:CE1	7:Q:204:MPD:H4	1.56	1.40
2:X:28[A]:PHE:CE2	7:X:204:MPD:C1	2.01	1.40
2:X:28[A]:PHE:CE2	7:X:204:MPD:H12	1.57	1.39
1:A:114[B]:ARG:HG2	5:A:204:PI:P	1.62	1.38
2:S:28[A]:PHE:HE2	7:S:204:MPD:C1	1.39	1.33
1:K:118[B]:ARG:NE	9:K:303:HOH:O	1.57	1.32
2:S:28[A]:PHE:CE2	7:S:204:MPD:C1	2.16	1.27
2:N:109[A]:ASN:ND2	9:N:301:HOH:O	1.64	1.26
2:O:28[B]:PHE:HD1	7:O:204:MPD:C5	1.20	1.26
1:A:114[B]:ARG:HD2	5:A:204:PI:O4	1.14	1.24
2:Q:28[A]:PHE:CE1	7:Q:204:MPD:C4	2.16	1.23
2:S:11[B]:GLN:NE2	9:S:304:HOH:O	1.68	1.23
7:B:203:MPD:H52	9:B:311:HOH:O	1.33	1.23
5:K:203:PI:O3	9:K:302:HOH:O	1.53	1.21
2:R:28[A]:PHE:HE2	7:R:204:MPD:C1	1.53	1.21
2:T:28[A]:PHE:CE1	8:T:204:MRD:H4	1.75	1.21
2:V:28[A]:PHE:CE1	8:V:204:MRD:C5	2.07	1.20
1:K:118[B]:ARG:CZ	9:K:303:HOH:O	1.85	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:11[A]:GLN:OE1	9:S:303:HOH:O	1.58	1.20
2:N:31[B]:GLU:HG3	9:N:311:HOH:O	1.41	1.19
1:B:115[A]:GLU:OE1	9:M:301:HOH:O	1.60	1.19
9:D:511:HOH:O	7:P:204:MPD:H32	1.01	1.19
1:C:32[A]:GLN:HG3	1:F:32[A]:GLN:HG3	1.20	1.19
2:T:28[A]:PHE:CD1	8:T:204:MRD:H4	1.78	1.18
2:W:31[B]:GLU:HG3	9:W:364:HOH:O	1.41	1.18
2:V:28[A]:PHE:HD1	8:V:204:MRD:C5	1.30	1.17
1:A:114[B]:ARG:CG	5:A:204:PI:P	2.33	1.17
2:Q:31[B]:GLU:HG3	9:Q:307:HOH:O	1.45	1.16
7:B:203:MPD:C4	9:B:311:HOH:O	1.93	1.15
2:R:28[A]:PHE:CD2	7:R:204:MPD:H52	1.80	1.15
1:A:114[B]:ARG:CD	5:A:204:PI:O4	1.94	1.14
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
2:R:28[A]:PHE:CE2	7:R:204:MPD:C1	2.31	1.14
1:B:32[A]:GLN:HG3	1:E:32[A]:GLN:HG3	1.24	1.14
7:U:204:MPD:H31	9:U:317:HOH:O	0.97	1.14
1:L:62[A]:LYS:NZ	9:L:304:HOH:O	1.81	1.13
2:P:109[B]:ASN:ND2	9:P:301:HOH:O	1.69	1.12
1:A:32[A]:GLN:HG3	1:D:32[A]:GLN:HG3	1.25	1.12
1:H:118[B]:ARG:NH2	9:H:304:HOH:O	1.82	1.12
1:K:118[B]:ARG:NH2	9:K:303:HOH:O	1.80	1.12
2:U:130[B]:GLN:OE1	9:U:302:HOH:O	1.65	1.12
1:A:114[B]:ARG:HG2	5:A:204:PI:O2	1.48	1.11
1:F:118[B]:ARG:NH2	9:F:303:HOH:O	1.80	1.10
2:R:28[A]:PHE:HD2	7:R:204:MPD:C5	1.65	1.09
1:C:118[B]:ARG:HD3	9:E:354:HOH:O	1.51	1.09
1:J:124[A]:THR:HG21	9:J:312:HOH:O	1.51	1.08
2:W:28[A]:PHE:CE1	7:W:204:MPD:H4	1.89	1.08
7:B:203:MPD:C5	9:B:311:HOH:O	1.87	1.07
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
8:V:204:MRD:O4	9:V:301:HOH:O	1.72	1.06
2:R:28[A]:PHE:HE2	7:R:204:MPD:H12	1.16	1.06
1:C:32[A]:GLN:CG	1:F:32[A]:GLN:HG3	1.85	1.06
7:O:204:MPD:HM1	7:O:204:MPD:O4	1.50	1.06
2:P:28[A]:PHE:CD1	7:P:204:MPD:H4	1.91	1.06
2:U:130[A]:GLN:NE2	9:U:301:HOH:O	1.86	1.06
2:R:28[A]:PHE:CE2	7:R:204:MPD:H12	1.91	1.05
2:R:28[A]:PHE:HD2	7:R:204:MPD:H52	1.09	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:204:MPD:O4	7:O:204:MPD:CM	2.05	1.04
2:X:28[A]:PHE:CE2	7:X:204:MPD:H11	1.89	1.04
2:V:130[A]:GLN:OE1	9:V:302:HOH:O	1.75	1.04
2:W:122[A]:THR:HG22	9:W:491:HOH:O	1.56	1.04
2:U:130[A]:GLN:NE2	9:U:303:HOH:O	1.81	1.04
2:W:28[A]:PHE:CD1	7:W:204:MPD:H4	1.92	1.03
1:A:32[A]:GLN:HG3	1:D:32[A]:GLN:CG	1.88	1.03
1:D:114[B]:ARG:NH2	9:D:306:HOH:O	1.89	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:C:42[A]:GLU:OE2	9:C:303:HOH:O	1.76	1.01
9:G:397:HOH:O	1:L:124[A]:THR:HG21	1.60	1.01
2:O:130[A]:GLN:OE1	9:O:301:HOH:O	1.78	1.01
1:B:32[A]:GLN:CG	1:E:32[A]:GLN:HG3	1.90	0.99
2:S:28[A]:PHE:CE2	7:S:204:MPD:H12	1.93	0.99
2:V:28[A]:PHE:HD1	8:V:204:MRD:H5C3	1.27	0.99
1:A:32[A]:GLN:CG	1:D:32[A]:GLN:HG3	1.92	0.99
2:Q:28[A]:PHE:CD1	9:Q:316:HOH:O	2.15	0.99
2:N:82[B]:ARG:NH1	9:N:302:HOH:O	1.96	0.97
1:K:42[A]:GLU:CG	2:W:22[A]:MET:HG3	1.94	0.97
1:H:115[A]:GLU:OE2	9:H:303:HOH:O	1.80	0.97
2:M:28[A]:PHE:CD1	7:M:204:MPD:H4	2.00	0.97
9:I:579:HOH:O	3:X:187:PEB:HAD1	1.63	0.96
2:U:130[A]:GLN:OE1	9:U:303:HOH:O	1.83	0.96
2:X:24:ALA:HB3	9:X:307:HOH:O	1.65	0.96
2:M:28[A]:PHE:CE1	7:M:204:MPD:H4	2.00	0.96
1:H:32[A]:GLN:HG3	1:K:32[A]:GLN:CG	1.96	0.95
2:S:28[A]:PHE:HE2	7:S:204:MPD:H13	1.29	0.95
2:X:28[A]:PHE:HE2	7:X:204:MPD:H12	0.78	0.95
1:A:118[B]:ARG:HD2	9:F:377:HOH:O	1.67	0.94
1:I:124[A]:THR:HG21	9:I:367:HOH:O	1.65	0.93
2:P:28[A]:PHE:CE1	7:P:204:MPD:H4	2.02	0.93
2:S:28[A]:PHE:CE2	7:S:204:MPD:H11	2.02	0.93
2:Q:28[A]:PHE:CE1	9:Q:316:HOH:O	2.21	0.93
1:C:124[A]:THR:HG21	9:C:428:HOH:O	1.66	0.93
9:G:321:HOH:O	1:L:118[B]:ARG:HD2	1.69	0.93
2:Q:28[A]:PHE:HE1	7:Q:204:MPD:HO4	1.16	0.93
1:G:120:LEU:HA	9:G:313:HOH:O	1.67	0.93
2:Q:28[A]:PHE:HE1	7:Q:204:MPD:O4	1.52	0.93
1:D:114[B]:ARG:HG3	1:D:114[B]:ARG:HH11	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:124[A]:THR:HG21	9:B:371:HOH:O	1.70	0.92
2:T:28[A]:PHE:CE1	8:T:204:MRD:C4	2.45	0.91
2:Q:28[A]:PHE:HE1	7:Q:204:MPD:C4	1.62	0.91
1:K:124[A]:THR:HG21	9:K:398:HOH:O	1.68	0.91
2:Q:28[A]:PHE:HD1	7:Q:204:MPD:H4	1.36	0.91
1:F:62[A]:LYS:NZ	9:F:305:HOH:O	2.03	0.90
2:V:28[A]:PHE:CD1	8:V:204:MRD:H5C3	2.01	0.90
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:31[B]:GLU:CG	9:N:311:HOH:O	2.04	0.90
1:K:124[A]:THR:CG2	9:K:398:HOH:O	2.20	0.90
7:R:204:MPD:H52	7:R:204:MPD:H12	1.55	0.89
2:N:16[B]:THR:HG21	9:N:440:HOH:O	1.72	0.89
1:G:118[A]:ARG:NE	9:G:304:HOH:O	2.04	0.89
1:J:124[A]:THR:CG2	9:J:312:HOH:O	2.11	0.89
2:O:141[B]:LYS:NZ	9:O:302:HOH:O	1.99	0.89
2:S:22[B]:MET:HA	2:S:22[B]:MET:HE2	1.55	0.88
1:G:124[A]:THR:HG23	4:L:203:NO3:O2	1.73	0.88
1:K:118[A]:ARG:HD3	9:K:389:HOH:O	1.74	0.88
3:R:188:PEB:HBA1	9:R:330:HOH:O	1.74	0.88
7:Q:204:MPD:HM2	9:Q:500:HOH:O	1.74	0.87
1:F:78:PHE:HA	9:F:513:HOH:O	1.70	0.87
2:P:28[A]:PHE:CE1	7:P:204:MPD:C4	2.55	0.87
1:H:118[A]:ARG:NH2	9:H:305:HOH:O	1.99	0.87
1:J:32[B]:GLN:NE2	9:J:304:HOH:O	2.08	0.87
7:W:204:MPD:O4	9:W:302:HOH:O	1.92	0.87
2:T:146[B]:GLU:OE1	9:T:302:HOH:O	1.92	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
1:A:118[B]:ARG:CD	9:F:377:HOH:O	2.18	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:W:122[A]:THR:CG2	9:W:491:HOH:O	2.18	0.86
1:F:118[A]:ARG:NE	9:F:304:HOH:O	1.96	0.85
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:D:124[A]:THR:HG21	9:D:459:HOH:O	1.77	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:129:VAL:HG13	9:T:467:HOH:O	1.78	0.83
2:R:28[A]:PHE:CE2	7:R:204:MPD:H11	2.11	0.83
2:R:28[A]:PHE:CD2	7:R:204:MPD:C5	2.51	0.83
7:R:204:MPD:C1	7:R:204:MPD:H52	2.08	0.83
2:W:28[A]:PHE:CE1	7:W:204:MPD:C4	2.58	0.83
2:U:130[B]:GLN:CD	9:U:302:HOH:O	2.06	0.83
1:A:114[B]:ARG:HG2	5:A:204:PI:O1	1.77	0.82
2:Q:28[A]:PHE:CD1	7:Q:204:MPD:C4	2.48	0.82
1:A:114[B]:ARG:CD	5:A:204:PI:P	2.67	0.81
1:D:113:GLN:HE21	1:D:114[B]:ARG:HH12	1.23	0.81
9:D:511:HOH:O	7:P:204:MPD:C3	1.77	0.81
2:W:111:LEU:HD21	9:W:344:HOH:O	1.79	0.81
2:U:130[A]:GLN:CD	9:U:301:HOH:O	2.12	0.81
1:H:43[B]:LYS:NZ	9:H:306:HOH:O	2.01	0.81
2:S:28[A]:PHE:CD2	7:S:204:MPD:C1	2.64	0.81
2:M:82[C]:ARG:NH1	9:M:302:HOH:O	2.14	0.80
1:H:118[B]:ARG:CD	9:J:383:HOH:O	2.29	0.80
1:I:154:ALA:HB1	9:I:458:HOH:O	1.80	0.80
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
2:P:28[A]:PHE:HD1	7:P:204:MPD:H4	1.46	0.78
1:D:114[C]:ARG:HG3	5:D:204:PI:O4	1.84	0.77
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
2:W:31[B]:GLU:CG	9:W:364:HOH:O	2.14	0.76
1:B:124[A]:THR:CG2	9:B:371:HOH:O	2.30	0.76
4:A:203:NO3:O2	1:F:118[A]:ARG:NH2	2.19	0.76
1:F:124[A]:THR:HG21	9:F:474:HOH:O	1.86	0.76
2:S:28[A]:PHE:CD2	7:S:204:MPD:H12	2.21	0.76
9:I:390:HOH:O	1:K:118[B]:ARG:HD2	1.86	0.75
2:P:82[A]:ARG:NH1	3:P:186:PEB:O2C	2.16	0.75
1:B:118[A]:ARG:NH2	9:B:303:HOH:O	2.04	0.75
3:R:187:PEB:HBA2	9:R:354:HOH:O	1.87	0.75
2:M:28[A]:PHE:CE1	7:M:204:MPD:C4	2.66	0.75
2:N:83:ASP:HB3	9:N:320:HOH:O	1.86	0.75
2:Q:31[B]:GLU:CG	9:Q:307:HOH:O	2.14	0.75
7:B:203:MPD:H4	9:B:311:HOH:O	1.70	0.75
2:T:28[A]:PHE:HD1	8:T:204:MRD:H4	1.44	0.74
2:V:28[A]:PHE:CE1	8:V:204:MRD:C4	2.50	0.74
3:Q:187:PEB:HNA	3:Q:187:PEB:HMB2	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:89:ARG:O	2:U:92[B]:THR:HG22	1.88	0.74
1:A:114[B]:ARG:CG	5:A:204:PI:O2	2.32	0.73
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:G:62[B]:LYS:NZ	9:G:305:HOH:O	2.22	0.72
1:A:118[A]:ARG:NH2	9:A:303:HOH:O	1.84	0.72
1:F:115[B]:GLU:HG3	1:F:118[B]:ARG:HH22	1.55	0.72
1:I:87[B]:LYS:NZ	9:I:304:HOH:O	2.19	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
3:T:187:PEB:HMB2	3:T:187:PEB:HNA	1.55	0.72
1:A:114[B]:ARG:CG	5:A:204:PI:O1	2.32	0.72
1:B:118[B]:ARG:NE	9:D:307:HOH:O	2.22	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
3:O:187:PEB:HNA	3:O:187:PEB:HMB2	1.55	0.71
1:I:159:ALA:HB3	9:I:309:HOH:O	1.88	0.71
3:N:187:PEB:HMB2	3:N:187:PEB:HNA	1.56	0.71
1:I:118[B]:ARG:HD2	9:K:325:HOH:O	1.91	0.71
1:H:118[B]:ARG:HD2	9:J:383:HOH:O	1.90	0.70
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
2:T:28[A]:PHE:HE1	8:T:204:MRD:C4	1.75	0.70
1:A:124[A]:THR:HG21	9:A:486:HOH:O	1.90	0.70
9:I:390:HOH:O	1:K:118[B]:ARG:CD	2.37	0.70
1:K:118[A]:ARG:CD	9:K:389:HOH:O	2.36	0.70
5:F:203:PI:O4	9:F:301:HOH:O	0.70	0.70
1:G:118[B]:ARG:CD	9:L:318:HOH:O	2.40	0.70
3:W:187:PEB:HMB2	3:W:187:PEB:HNA	1.56	0.70
2:X:82[A]:ARG:NH1	3:X:186:PEB:O2C	2.23	0.70
9:G:397:HOH:O	1:L:124[A]:THR:CG2	2.30	0.69
1:H:118[B]:ARG:HD3	9:J:383:HOH:O	1.89	0.69
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:54[B]:GLU:HG2	9:F:461:HOH:O	1.93	0.67
1:F:89:TYR:HB2	9:F:532:HOH:O	1.93	0.67
2:W:28[A]:PHE:HD1	7:W:204:MPD:H4	1.54	0.67
2:W:109[B]:ASN:OD1	9:W:303:HOH:O	2.13	0.67
1:G:118[B]:ARG:HD3	9:L:318:HOH:O	1.94	0.67
2:S:28[A]:PHE:CD2	7:S:204:MPD:H11	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124[A]:THR:CG2	9:I:367:HOH:O	2.32	0.67
2:P:65:ILE:O	9:P:302:HOH:O	2.13	0.67
3:S:187:PEB:HNA	3:S:187:PEB:HMB2	1.60	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
3:M:187:PEB:HNA	3:M:187:PEB:HMB2	1.60	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
9:A:307:HOH:O	2:O:82[B]:ARG:HD3	1.94	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
2:O:130[B]:GLN:OE1	9:O:303:HOH:O	2.13	0.66
1:G:28:GLN:HG2	9:S:503:HOH:O	1.96	0.66
3:X:187:PEB:HNA	3:X:187:PEB:HMB2	1.61	0.65
3:U:187:PEB:HNA	3:U:187:PEB:HMB2	1.60	0.65
3:P:187:PEB:HNA	3:P:187:PEB:HMB2	1.60	0.65
2:R:28[A]:PHE:CE2	7:R:204:MPD:H52	2.30	0.65
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
1:H:124[A]:THR:HG21	9:H:422:HOH:O	1.98	0.64
2:T:148:ARG:NH1	9:T:305:HOH:O	2.29	0.64
2:V:89:ARG:O	2:V:92[B]:THR:HG22	1.97	0.64
7:O:204:MPD:HM1	7:O:204:MPD:HO4	1.63	0.64
5:H:203:PI:O2	9:H:301:HOH:O	0.64	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:U:122[A]:THR:HG22	9:U:528:HOH:O	1.96	0.64
1:A:118[A]:ARG:NH1	9:A:304:HOH:O	2.29	0.64
2:R:155[B]:LYS:HE2	2:R:155[B]:LYS:CA	2.28	0.64
7:U:204:MPD:HM1	7:U:204:MPD:O4	1.97	0.64
1:F:131:LEU:HB3	9:F:347:HOH:O	1.98	0.63
8:T:204:MRD:H5C3	8:T:204:MRD:O2	1.97	0.63
1:E:118[A]:ARG:NH2	9:E:305:HOH:O	2.12	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
3:V:187:PEB:HMB2	3:V:187:PEB:HNA	1.63	0.63
2:M:28[A]:PHE:HD1	7:M:204:MPD:H4	1.60	0.63
2:W:22[A]:MET:SD	2:W:25:LEU:HD12	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:204:MPD:C3	9:U:317:HOH:O	1.79	0.63
3:A:167:PEB:HNA	3:A:167:PEB:HMB2	1.64	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:V:28[A]:PHE:HE1	8:V:204:MRD:C4	1.70	0.62
2:U:82[A]:ARG:NH1	3:U:186:PEB:O2C	2.24	0.62
2:W:28[A]:PHE:HE1	7:W:204:MPD:C4	1.88	0.62
3:Q:186:PEB:HNA	3:Q:186:PEB:HMB2	1.65	0.62
2:X:28[A]:PHE:CD2	7:X:204:MPD:H12	2.30	0.61
3:J:167:PEB:HNA	3:J:167:PEB:HMB2	1.65	0.61
3:R:187:PEB:HNA	3:R:187:PEB:HMB2	1.66	0.61
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:X:28[A]:PHE:CD2	7:X:204:MPD:C1	2.78	0.60
2:O:141[B]:LYS:HE3	2:O:164:ARG:HB2	1.82	0.60
1:G:118[A]:ARG:CZ	9:G:304:HOH:O	2.48	0.60
3:L:167:PEB:HNA	3:L:167:PEB:HMB2	1.66	0.60
1:J:102:THR:N	9:J:305:HOH:O	2.34	0.60
3:I:167:PEB:HNA	3:I:167:PEB:HMB2	1.67	0.60
1:F:124[A]:THR:CG2	9:F:474:HOH:O	2.48	0.60
1:D:114[B]:ARG:CZ	9:D:301:HOH:O	2.49	0.60
2:U:28[A]:PHE:CD2	7:U:204:MPD:H32	2.37	0.59
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:B:118[A]:ARG:NE	9:B:303:HOH:O	2.31	0.59
8:T:204:MRD:HMC2	9:T:517:HOH:O	2.02	0.59
3:E:167:PEB:HMB2	3:E:167:PEB:HNA	1.68	0.58
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
1:G:118[B]:ARG:HD2	9:L:318:HOH:O	2.04	0.58
3:G:167:PEB:HMB2	3:G:167:PEB:HNA	1.68	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:V:130[B]:GLN:NE2	9:V:303:HOH:O	2.24	0.58
1:G:115[C]:GLU:CD	2:U:82[C]:ARG:NH2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:204:MPD:O4	7:O:204:MPD:HM2	2.00	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
1:C:124[A]:THR:CG2	9:C:428:HOH:O	2.37	0.57
2:U:9:VAL:HG23	9:U:369:HOH:O	2.04	0.57
3:K:167:PEB:HNA	3:K:167:PEB:HMB2	1.69	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
3:H:167:PEB:HNA	3:H:167:PEB:HMB2	1.70	0.57
1:A:118[B]:ARG:HD3	9:F:377:HOH:O	1.96	0.57
1:I:115[B]:GLU:CD	9:I:303:HOH:O	2.43	0.56
7:B:203:MPD:C3	9:B:311:HOH:O	2.38	0.56
2:R:28[A]:PHE:CD2	7:R:204:MPD:C1	2.87	0.56
7:U:204:MPD:C4	9:U:317:HOH:O	2.35	0.56
1:I:118[B]:ARG:NH2	9:I:303:HOH:O	2.35	0.56
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
3:B:167:PEB:HMB2	3:B:167:PEB:HNA	1.71	0.55
8:T:204:MRD:O2	8:T:204:MRD:C5	2.54	0.55
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
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
3:W:186:PEB:HNA	3:W:186:PEB:HMB2	1.72	0.55
3:F:167:PEB:HNA	3:F:167:PEB:HMB2	1.71	0.55
2:Q:29:ILE:HD13	7:Q:204:MPD:H52	1.89	0.55
1:A:114[B]:ARG:HG3	5:A:204:PI:O1	2.07	0.55
3:C:167:PEB:HNA	3:C:167:PEB:HMB2	1.72	0.55
1:D:124[A]:THR:CG2	9:D:459:HOH:O	2.46	0.55
1:H:124[A]:THR:CG2	9:H:422:HOH:O	2.54	0.54
2:W:132:MET:HB2	9:W:307:HOH:O	2.05	0.54
1:C:33:ARG:HG2	9:F:366:HOH:O	2.08	0.54
1:I:30[B]:SER:OG	7:U:204:MPD:H51	2.07	0.54
3:U:186:PEB:HMB2	3:U:186:PEB:HNA	1.72	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:T:146[B]:GLU:HG2	9:T:301:HOH:O	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:186:PEB:HNA	3:T:186:PEB:HMB2	1.74	0.53
1:D:114[C]:ARG:HG3	9:D:301:HOH:O	2.07	0.53
2:R:28[B]:PHE:HA	2:R:31[B]:GLU:HG2	1.89	0.53
3:R:186:PEB:HNA	3:R:186:PEB:HMB2	1.73	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
2:U:28[A]:PHE:CD2	7:U:204:MPD:C3	2.92	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
7:U:204:MPD:O4	7:U:204:MPD:CM	2.58	0.52
2:U:148:ARG:NH1	3:U:188:PEB:HND	2.07	0.52
2:Q:26:LYS:NZ	9:Q:302:HOH:O	2.42	0.52
2:R:163:ASP:HB3	9:R:443:HOH:O	2.10	0.52
3:M:186:PEB:HMB2	3:M:186:PEB:HNA	1.75	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:S:22[B]:MET:CE	2:S:22[B]:MET:CA	2.83	0.51
3:W:187:PEB:HMB2	3:W:187:PEB:NA	2.25	0.51
2:X:28[A]:PHE:CD2	7:X:204:MPD:H11	2.41	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
3:N:186:PEB:HMB2	3:N:186:PEB:HNA	1.74	0.51
2:R:28[A]:PHE:CD2	7:R:204:MPD:H12	2.41	0.51
1:A:128:VAL:CG1	9:A:390:HOH:O	2.59	0.51
2:N:22[A]:MET:HE2	2:N:25:LEU:HD12	1.93	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
3:P:186:PEB:HNA	3:P:186:PEB:HMB2	1.77	0.50
3:O:186:PEB:HNA	3:O:186:PEB:HMB2	1.75	0.50
3:S:188:PEB:HNA	3:S:188:PEB:HMB3	1.76	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
2:T:31[A]:GLU:OE1	9:T:303:HOH:O	2.20	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:W:101[A]:SER:HB2	9:W:322:HOH:O	2.11	0.50
1:C:115[A]:GLU:HG3	5:C:204:PI:O1	2.12	0.49
3:D:167:PEB:HNA	3:D:167:PEB:HMB2	1.76	0.49
1:D:114[B]:ARG:CZ	9:D:306:HOH:O	2.47	0.49
1:I:115[B]:GLU:OE2	9:I:303:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:390:HOH:O	1:K:118[B]:ARG:HD3	2.06	0.49
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
2:R:28[A]:PHE:CD2	7:R:204:MPD:H11	2.47	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
3:X:188:PEB:HNA	3:X:188:PEB:HMB3	1.76	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
3:Q:188:PEB:HNA	3:Q:188:PEB:HMB3	1.78	0.49
3:V:186:PEB:HMB2	3:V:186:PEB:HNA	1.78	0.49
1:H:118[A]:ARG:NH1	1:J:124[A]:THR:OG1	2.46	0.49
3:R:188:PEB:HNA	3:R:188:PEB:HMB3	1.77	0.49
9:I:579:HOH:O	3:X:187:PEB:HMD1	2.12	0.49
1:B:118[B]:ARG:HD2	9:D:307:HOH:O	2.13	0.49
1:F:54[B]:GLU:CG	9:F:461:HOH:O	2.55	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
1:B:118[B]:ARG:CD	9:D:307:HOH:O	2.61	0.48
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
2:Q:101[A]:SER:HB2	9:Q:337:HOH:O	2.12	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
3:X:186:PEB:HNA	3:X:186:PEB:HMB2	1.79	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:K:1[A]:MET:HE1	1:K:104:PRO:HG3	1.95	0.47
3:R:187:PEB:HBA3	3:R:187:PEB:HHA1	1.96	0.47
1:J:43[B]:LYS:NZ	9:J:307:HOH:O	2.47	0.47
3:H:167:PEB:HMB2	3:H:167:PEB:NA	2.29	0.47
2:X:101[A]:SER:HB2	9:X:318:HOH:O	2.13	0.47
2:T:28[B]:PHE:HA	2:T:31[B]:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:GLN:HG3	1:J:32[B]:GLN:HG2	1.97	0.46
3:N:188:PEB:HNA	3:N:188:PEB:HMB3	1.81	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
1:F:115[B]:GLU:HG3	9:F:303:HOH:O	2.15	0.46
2:U:144:PRO:HG2	2:U:153[B]:LEU:HD21	1.97	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
2:T:28[A]:PHE:HE1	8:T:204:MRD:C5	2.26	0.45
1:H:43[A]:LYS:HD3	9:H:492:HOH:O	2.16	0.45
2:P:22[A]:MET:HE2	2:P:22[A]:MET:HA	1.99	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:T:28[A]:PHE:CE1	8:T:204:MRD:C5	2.99	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
2:Q:148:ARG:NH1	3:Q:188:PEB:HND	2.14	0.45
3:W:188:PEB:HMB3	3:W:188:PEB:HNA	1.82	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:U:130[A]:GLN:CD	9:U:303:HOH:O	2.05	0.45
3:U:188:PEB:HNA	3:U:188:PEB:HMB3	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
1:A:121:GLY:HA2	9:A:394:HOH:O	2.16	0.44
1:G:163:LEU:O	1:L:118[A]:ARG:HD2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:125:THR:HG21	2:T:183:LEU:HD13	1.99	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:O:130[B]:GLN:NE2	9:O:305:HOH:O	2.31	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
3:M:187:PEB:HMB2	3:M:187:PEB:NA	2.31	0.43
3:O:188:PEB:HNA	3:O:188:PEB:HMB3	1.83	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
3:T:188:PEB:HNA	3:T:188:PEB:HMB3	1.83	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:X:188:PEB:HMC1	9:X:316:HOH:O	2.19	0.43
3:P:187:PEB:HBA3	3:P:187:PEB:HHA1	2.00	0.43
3:V:188:PEB:HNA	3:V:188:PEB:HMB3	1.83	0.43
1:A:114[B]:ARG:CG	5:A:204:PI:O4	2.45	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
3:E:167:PEB:HMB2	3:E:167:PEB:NA	2.32	0.43
2:O:31:GLU:HB3	9:O:358:HOH:O	2.18	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
1:K:42[A]:GLU:CD	2:W:22[A]:MET:HG3	2.39	0.42
3:L:167:PEB:HMB2	3:L:167:PEB:NA	2.34	0.42
3:G:167:PEB:HMB2	3:G:167:PEB:NA	2.34	0.42
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
2:S:22[B]:MET:HA	2:S:22[B]:MET:HE3	1.95	0.41
9:S:418:HOH:O	2:T:16:THR:HG21	2.19	0.41
3:C:166:PEB:HMC2	2:N:77:MET:HG2	2.01	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
3:T:187:PEB:HMB2	3:T:187:PEB:NA	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:188:PEB:HNA	3:M:188:PEB:HMB3	1.84	0.41
3:P:188:PEB:HMB3	3:P:188:PEB:HNA	1.85	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:N:187:PEB:HMB2	3:N:187:PEB:NA	2.29	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
3:X:187:PEB:HMB2	3:X:187:PEB:NA	2.30	0.41
1:D:114[A]:ARG:HG2	9:D:459:HOH:O	2.21	0.41
3:F:167:PEB:HMB2	3:F:167:PEB:NA	2.36	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
2:W:122[A]:THR:HG21	9:W:491:HOH:O	2.06	0.41
9:C:342:HOH:O	7:O:204:MPD:HM3	2.20	0.40
1:G:35:ALA:HB1	9:G:580:HOH:O	2.22	0.40
3:Q:187:PEB:HMB2	3:Q:187:PEB:NA	2.27	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
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	137/127 (108%)	137 (100%)	0	100 100
1	B	135/127 (106%)	133 (98%)	2 (2%)	65 27
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%)	135 (100%)	0	100 100
1	F	138/127 (109%)	132 (96%)	6 (4%)	29 3
1	G	136/127 (107%)	136 (100%)	0	100 100
1	H	138/127 (109%)	138 (100%)	0	100 100
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%)	135 (98%)	2 (2%)	65 27
1	L	136/127 (107%)	136 (100%)	0	100 100
2	M	151/138 (109%)	149 (99%)	2 (1%)	69 32
2	N	150/138 (109%)	147 (98%)	3 (2%)	55 15
2	O	147/138 (106%)	146 (99%)	1 (1%)	84 55
2	P	149/138 (108%)	145 (97%)	4 (3%)	44 8
2	Q	148/138 (107%)	148 (100%)	0	100 100
2	R	148/138 (107%)	146 (99%)	2 (1%)	67 29
2	S	150/138 (109%)	148 (99%)	2 (1%)	69 32
2	T	150/138 (109%)	145 (97%)	5 (3%)	38 5
2	U	155/138 (112%)	152 (98%)	3 (2%)	57 17
2	V	154/138 (112%)	148 (96%)	6 (4%)	32 4
2	W	153/138 (111%)	152 (99%)	1 (1%)	84 55
2	X	149/138 (108%)	147 (99%)	2 (1%)	69 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3448/3180 (108%)	3407 (99%)	41 (1%)	81 35

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1[A]	MET
1	B	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	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	O	178	ARG
2	P	26	LYS
2	P	27	GLN
2	P	109[A]	ASN
2	P	109[B]	ASN
2	R	28[A]	PHE
2	R	28[B]	PHE
2	S	28[A]	PHE
2	S	28[B]	PHE
2	T	16	THR
2	T	123	THR
2	T	155	LYS
2	T	184[A]	SER
2	T	184[B]	SER
2	U	25	LEU
2	U	26[A]	LYS
2	U	26[B]	LYS
2	V	109[A]	ASN
2	V	109[B]	ASN
2	V	155	LYS
2	V	162	GLU
2	V	178[A]	ARG

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Mol	Chain	Res	Type
2	V	178[B]	ARG
2	W	178	ARG
2	X	28[A]	PHE
2	X	28[B]	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	D	61	GLN
1	D	113	GLN
1	I	61	GLN
2	M	27	GLN
2	P	27	GLN
2	R	11	GLN
2	R	62	GLN
2	X	11	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	X	70	2	7,8,9	0.46	0	6,9,11	0.52	0
2	MEN	N	70	2	7,8,9	0.64	0	6,9,11	0.64	0
2	MEN	R	70	2	7,8,9	0.48	0	6,9,11	1.70	2 (33%)
2	MEN	M	70	2	7,8,9	0.44	0	6,9,11	0.50	0
2	MEN	U	70	2	7,8,9	0.76	0	6,9,11	1.48	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	O	70	2	7,8,9	0.46	0	6,9,11	1.18	1 (16%)
2	MEN	Q	70	2	7,8,9	0.44	0	6,9,11	0.93	0
2	MEN	P	70	2	7,8,9	0.58	0	6,9,11	0.69	0
2	MEN	T	70	2	7,8,9	0.46	0	6,9,11	0.69	0
2	MEN	V	70	2	7,8,9	0.68	0	6,9,11	0.80	0
2	MEN	W	70	2	7,8,9	0.67	0	6,9,11	0.42	0
2	MEN	S	70	2	7,8,9	0.35	0	6,9,11	1.61	1 (16%)

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	X	70	2	-	3/7/8/10	-
2	MEN	N	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	U	70	2	-	3/7/8/10	-
2	MEN	O	70	2	-	3/7/8/10	-
2	MEN	Q	70	2	-	4/7/8/10	-
2	MEN	P	70	2	-	3/7/8/10	-
2	MEN	T	70	2	-	4/7/8/10	-
2	MEN	V	70	2	-	3/7/8/10	-
2	MEN	W	70	2	-	3/7/8/10	-
2	MEN	S	70	2	-	3/7/8/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	70	MEN	OD1-CG-CB	-3.35	116.59	121.50
2	R	70	MEN	OD1-CG-CB	-3.19	116.83	121.50
2	U	70	MEN	CB-CA-C	2.73	116.58	111.47
2	R	70	MEN	CB-CG-ND2	2.53	118.89	115.48
2	O	70	MEN	OD1-CG-CB	-2.09	118.44	121.50

There are no chirality outliers.

All (38) 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	V	70	MEN	N-CA-CB-CG
2	X	70	MEN	N-CA-CB-CG
2	T	70	MEN	CA-CB-CG-OD1
2	V	70	MEN	CA-CB-CG-OD1
2	O	70	MEN	CA-CB-CG-OD1
2	Q	70	MEN	CA-CB-CG-OD1
2	M	70	MEN	CA-CB-CG-OD1
2	N	70	MEN	CA-CB-CG-OD1
2	P	70	MEN	CA-CB-CG-OD1
2	R	70	MEN	CA-CB-CG-OD1
2	S	70	MEN	CA-CB-CG-OD1
2	W	70	MEN	CA-CB-CG-OD1
2	X	70	MEN	CA-CB-CG-OD1
2	P	70	MEN	CA-CB-CG-ND2
2	Q	70	MEN	CA-CB-CG-ND2
2	U	70	MEN	CA-CB-CG-ND2
2	Q	70	MEN	C-CA-CB-CG
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	T	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	M	70	MEN	N-CA-CB-CG
2	P	70	MEN	N-CA-CB-CG
2	R	70	MEN	N-CA-CB-CG
2	U	70	MEN	CA-CB-CG-OD1
2	N	70	MEN	N-CA-CB-CG
2	S	70	MEN	N-CA-CB-CG
2	U	70	MEN	N-CA-CB-CG
2	W	70	MEN	N-CA-CB-CG
2	T	70	MEN	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	PEB	N	187	2	37,46,46	2.18	7 (18%)	39,67,67	1.50	6 (15%)
3	PEB	L	166	1	37,46,46	2.26	6 (16%)	39,67,67	2.17	12 (30%)
3	PEB	S	187	2	37,46,46	2.62	8 (21%)	39,67,67	1.64	8 (20%)
7	MPD	W	204	2	7,7,7	0.21	0	9,10,10	1.05	0
3	PEB	Q	188	2	37,46,46	2.11	7 (18%)	39,67,67	1.65	8 (20%)
3	PEB	S	188	2	37,46,46	2.71	9 (24%)	39,67,67	1.44	7 (17%)
3	PEB	M	186	2	37,46,46	2.90	9 (24%)	39,67,67	1.98	10 (25%)
5	PI	E	203	-	4,4,4	0.83	0	6,6,6	0.69	0
3	PEB	M	187	2	37,46,46	2.31	9 (24%)	39,67,67	1.55	6 (15%)
3	PEB	A	166	1	37,46,46	1.95	4 (10%)	39,67,67	1.88	6 (15%)
5	PI	S	205	-	4,4,4	0.81	0	6,6,6	0.39	0
3	PEB	U	186	2	37,46,46	2.62	8 (21%)	39,67,67	2.18	11 (28%)
3	PEB	N	188	2	37,46,46	2.65	6 (16%)	39,67,67	1.71	9 (23%)
3	PEB	M	188	2	37,46,46	2.40	8 (21%)	39,67,67	1.60	8 (20%)
3	PEB	T	187	2	37,46,46	2.48	10 (27%)	39,67,67	1.93	10 (25%)
5	PI	R	205	-	4,4,4	0.67	0	6,6,6	0.62	0
3	PEB	K	166	1	37,46,46	2.57	10 (27%)	39,67,67	2.11	8 (20%)
7	MPD	P	204	2	7,7,7	0.28	0	9,10,10	0.90	0
3	PEB	I	167	1	37,46,46	2.27	11 (29%)	39,67,67	1.58	11 (28%)
3	PEB	B	167	1	37,46,46	2.30	10 (27%)	39,67,67	1.71	10 (25%)
3	PEB	H	166	1	37,46,46	2.80	7 (18%)	39,67,67	2.35	11 (28%)
5	PI	Q	205	-	4,4,4	0.88	0	6,6,6	1.17	0
5	PI	U	205	-	4,4,4	1.30	1 (25%)	6,6,6	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PEB	T	186	2	37,46,46	2.93	8 (21%)	39,67,67	2.10	14 (35%)
8	MRD	T	204	2	7,7,7	0.46	0	9,10,10	0.55	0
3	PEB	C	167	1	37,46,46	2.27	9 (24%)	39,67,67	2.16	12 (30%)
5	PI	G	203	-	4,4,4	0.94	0	6,6,6	0.83	0
3	PEB	G	166	1	37,46,46	2.09	8 (21%)	39,67,67	2.19	10 (25%)
3	PEB	W	188	2	37,46,46	2.93	6 (16%)	39,67,67	1.75	9 (23%)
3	PEB	X	186	2	37,46,46	2.57	7 (18%)	39,67,67	1.72	9 (23%)
5	PI	K	203	-	4,4,4	1.02	0	6,6,6	0.90	0
7	MPD	M	204	2	7,7,7	0.19	0	9,10,10	1.17	1 (11%)
5	PI	M	205	-	4,4,4	1.09	0	6,6,6	1.13	0
3	PEB	V	188	2	37,46,46	2.48	10 (27%)	39,67,67	1.52	8 (20%)
7	MPD	X	204	-	7,7,7	0.36	0	9,10,10	0.87	1 (11%)
3	PEB	X	187	2	37,46,46	2.32	7 (18%)	39,67,67	1.50	6 (15%)
4	NO3	D	203	-	1,3,3	2.20	1 (100%)	0,3,3	-	-
5	PI	V	205	-	4,4,4	0.80	0	6,6,6	0.85	0
3	PEB	J	167	1	37,46,46	2.39	8 (21%)	39,67,67	1.94	11 (28%)
3	PEB	T	188	2	37,46,46	2.44	10 (27%)	39,67,67	1.98	14 (35%)
3	PEB	S	186[B]	-	37,46,46	2.85	8 (21%)	39,67,67	2.18	14 (35%)
5	PI	J	204	-	4,4,4	1.19	0	6,6,6	0.70	0
5	PI	H	203	-	4,4,4	1.36	0	6,6,6	1.15	0
4	NO3	L	203	-	1,3,3	1.88	0	0,3,3	-	-
3	PEB	U	187	2	37,46,46	2.72	7 (18%)	39,67,67	1.62	11 (28%)
3	PEB	D	166	1	37,46,46	2.56	9 (24%)	39,67,67	1.98	9 (23%)
7	MPD	O	204	2	7,7,7	0.91	0	9,10,10	1.35	1 (11%)
3	PEB	L	167	1	37,46,46	2.03	9 (24%)	39,67,67	1.60	7 (17%)
3	PEB	K	167	1	37,46,46	2.65	9 (24%)	39,67,67	1.74	8 (20%)
3	PEB	E	166	1	37,46,46	3.41	10 (27%)	39,67,67	2.25	10 (25%)
5	PI	F	203	-	4,4,4	1.03	0	6,6,6	0.49	0
3	PEB	V	186	2	37,46,46	2.37	6 (16%)	39,67,67	1.89	8 (20%)
3	PEB	P	188	2	37,46,46	2.32	7 (18%)	39,67,67	1.74	12 (30%)
4	NO3	A	203	-	1,3,3	1.78	0	0,3,3	-	-
8	MRD	V	204	2	7,7,7	0.28	0	9,10,10	1.16	1 (11%)
3	PEB	H	167	1	37,46,46	2.38	8 (21%)	39,67,67	1.62	5 (12%)
3	PEB	E	167	1	37,46,46	2.65	9 (24%)	39,67,67	1.36	4 (10%)
5	PI	B	204	-	4,4,4	1.20	0	6,6,6	1.86	2 (33%)
3	PEB	A	167	1	37,46,46	1.99	8 (21%)	39,67,67	1.49	8 (20%)
3	PEB	G	167	1	37,46,46	2.70	13 (35%)	39,67,67	1.44	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MPD	B	203	-	7,7,7	0.61	0	9,10,10	1.72	2 (22%)
3	PEB	Q	186	2	37,46,46	2.86	8 (21%)	39,67,67	1.82	11 (28%)
5	PI	C	204	-	4,4,4	1.15	0	6,6,6	1.43	1 (16%)
3	PEB	F	167	1	37,46,46	2.51	11 (29%)	39,67,67	1.71	9 (23%)
5	PI	A	204	-	4,4,4	1.10	0	6,6,6	0.94	0
3	PEB	J	166	1	37,46,46	2.23	5 (13%)	39,67,67	1.81	7 (17%)
3	PEB	R	187	2	37,46,46	2.97	8 (21%)	39,67,67	1.82	12 (30%)
7	MPD	Q	204	2	7,7,7	0.60	0	9,10,10	0.98	0
3	PEB	W	186	2	37,46,46	2.91	10 (27%)	39,67,67	1.94	13 (33%)
7	MPD	U	204	2	7,7,7	0.34	0	9,10,10	0.95	0
3	PEB	O	186	2	37,46,46	2.54	6 (16%)	39,67,67	1.82	9 (23%)
5	PI	T	205	-	4,4,4	0.87	0	6,6,6	1.33	0
3	PEB	N	186	2	37,46,46	2.68	8 (21%)	39,67,67	1.89	11 (28%)
3	PEB	W	187	2	37,46,46	2.43	7 (18%)	39,67,67	1.51	9 (23%)
3	PEB	O	187	2	37,46,46	2.69	9 (24%)	39,67,67	1.41	6 (15%)
3	PEB	S	186[A]	-	37,46,46	2.87	8 (21%)	39,67,67	2.19	13 (33%)
5	PI	N	204	-	4,4,4	0.75	0	6,6,6	1.28	1 (16%)
3	PEB	X	188	2	37,46,46	2.49	8 (21%)	39,67,67	1.84	14 (35%)
3	PEB	P	186	2	37,46,46	3.22	10 (27%)	39,67,67	1.74	10 (25%)
5	PI	W	205	-	4,4,4	0.97	0	6,6,6	1.12	0
3	PEB	P	187	2	37,46,46	2.30	8 (21%)	39,67,67	1.62	10 (25%)
5	PI	I	204	-	4,4,4	1.06	0	6,6,6	1.08	0
4	NO3	I	203	-	1,3,3	1.85	0	0,3,3	-	-
3	PEB	D	167	1	37,46,46	2.12	11 (29%)	39,67,67	1.51	7 (17%)
3	PEB	R	186	2	37,46,46	2.99	10 (27%)	39,67,67	2.10	12 (30%)
3	PEB	O	188	2	37,46,46	2.49	13 (35%)	39,67,67	1.46	5 (12%)
5	PI	L	204	-	4,4,4	1.10	0	6,6,6	0.89	0
3	PEB	V	187	2	37,46,46	2.66	5 (13%)	39,67,67	1.60	7 (17%)
3	PEB	R	188	2	37,46,46	2.58	9 (24%)	39,67,67	1.45	5 (12%)
5	PI	P	205	-	4,4,4	0.46	0	6,6,6	1.34	1 (16%)
5	PI	D	204	-	4,4,4	1.15	0	6,6,6	0.45	0
5	PI	O	205	-	4,4,4	0.90	0	6,6,6	1.02	0
3	PEB	B	166	1	37,46,46	2.50	8 (21%)	39,67,67	2.05	8 (20%)
3	PEB	Q	187	2	37,46,46	2.61	8 (21%)	39,67,67	1.69	8 (20%)
7	MPD	S	204	-	7,7,7	0.25	0	9,10,10	0.72	0
5	PI	X	205	-	4,4,4	0.81	0	6,6,6	0.78	0
7	MPD	R	204	-	7,7,7	0.17	0	9,10,10	1.62	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PEB	C	166	1	37,46,46	3.12	9 (24%)	39,67,67	2.26	11 (28%)
3	PEB	I	166	1	37,46,46	2.99	9 (24%)	39,67,67	2.07	9 (23%)
3	PEB	U	188	2	37,46,46	2.46	8 (21%)	39,67,67	1.53	8 (20%)
4	NO3	C	203	-	1,3,3	1.36	0	0,3,3	-	-
4	NO3	J	203	-	1,3,3	1.63	0	0,3,3	-	-
3	PEB	F	166	1	37,46,46	2.18	6 (16%)	39,67,67	2.05	8 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	P	186	2	-	2/20/74/74	0/4/4/4
3	PEB	E	166	1	-	2/20/74/74	0/4/4/4
8	MRD	T	204	2	-	1/5/5/5	-
3	PEB	N	187	2	-	3/20/74/74	0/4/4/4
3	PEB	L	166	1	-	2/20/74/74	0/4/4/4
3	PEB	C	167	1	-	2/20/74/74	0/4/4/4
3	PEB	S	187	2	-	4/20/74/74	0/4/4/4
3	PEB	P	187	2	-	3/20/74/74	0/4/4/4
7	MPD	W	204	2	-	0/5/5/5	-
3	PEB	Q	188	2	-	3/20/74/74	0/4/4/4
3	PEB	G	166	1	-	2/20/74/74	0/4/4/4
3	PEB	W	188	2	-	3/20/74/74	0/4/4/4
3	PEB	V	186	2	-	2/20/74/74	0/4/4/4
3	PEB	X	186	2	-	2/20/74/74	0/4/4/4
3	PEB	P	188	2	-	3/20/74/74	0/4/4/4
7	MPD	M	204	2	-	0/5/5/5	-
3	PEB	D	167	1	-	3/20/74/74	0/4/4/4
3	PEB	R	186	2	-	2/20/74/74	0/4/4/4
3	PEB	S	188	2	-	4/20/74/74	0/4/4/4
8	MRD	V	204	2	-	3/5/5/5	-
3	PEB	H	167	1	-	2/20/74/74	0/4/4/4
3	PEB	E	167	1	-	3/20/74/74	0/4/4/4
3	PEB	V	188	2	-	3/20/74/74	0/4/4/4
3	PEB	M	186	2	-	2/20/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	O	188	2	-	4/20/74/74	0/4/4/4
3	PEB	A	167	1	-	3/20/74/74	0/4/4/4
7	MPD	O	204	2	-	0/5/5/5	-
3	PEB	V	187	2	-	3/20/74/74	0/4/4/4
3	PEB	M	187	2	-	4/20/74/74	0/4/4/4
3	PEB	G	167	1	-	2/20/74/74	0/4/4/4
3	PEB	A	166	1	-	2/20/74/74	0/4/4/4
3	PEB	R	188	2	-	2/20/74/74	0/4/4/4
7	MPD	X	204	-	-	1/5/5/5	-
7	MPD	B	203	-	-	4/5/5/5	-
3	PEB	X	187	2	-	4/20/74/74	0/4/4/4
3	PEB	U	186	2	-	2/20/74/74	0/4/4/4
3	PEB	N	188	2	-	3/20/74/74	0/4/4/4
3	PEB	Q	186	2	-	2/20/74/74	0/4/4/4
3	PEB	F	167	1	-	2/20/74/74	0/4/4/4
3	PEB	M	188	2	-	3/20/74/74	0/4/4/4
3	PEB	T	187	2	-	4/20/74/74	0/4/4/4
3	PEB	B	166	1	-	2/20/74/74	0/4/4/4
3	PEB	J	167	1	-	2/20/74/74	0/4/4/4
3	PEB	L	167	1	-	3/20/74/74	0/4/4/4
3	PEB	T	188	2	-	3/20/74/74	0/4/4/4
3	PEB	J	166	1	-	2/20/74/74	0/4/4/4
3	PEB	K	166	1	-	2/20/74/74	0/4/4/4
3	PEB	Q	187	2	-	4/20/74/74	0/4/4/4
3	PEB	R	187	2	-	4/20/74/74	0/4/4/4
3	PEB	S	186[B]	-	-	2/20/74/74	0/4/4/4
7	MPD	S	204	-	-	1/5/5/5	-
7	MPD	Q	204	2	-	0/5/5/5	-
3	PEB	W	186	2	-	2/20/74/74	0/4/4/4
7	MPD	R	204	-	-	1/5/5/5	-
7	MPD	P	204	2	-	1/5/5/5	-
7	MPD	U	204	2	-	0/5/5/5	-
3	PEB	C	166	1	-	2/20/74/74	0/4/4/4
3	PEB	I	167	1	-	4/20/74/74	0/4/4/4
3	PEB	O	186	2	-	2/20/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	B	167	1	-	3/20/74/74	0/4/4/4
3	PEB	I	166	1	-	2/20/74/74	0/4/4/4
3	PEB	N	186	2	-	2/20/74/74	0/4/4/4
3	PEB	H	166	1	-	2/20/74/74	0/4/4/4
3	PEB	U	187	2	-	4/20/74/74	0/4/4/4
3	PEB	O	187	2	-	3/20/74/74	0/4/4/4
3	PEB	S	186[A]	-	-	3/20/74/74	0/4/4/4
3	PEB	D	166	1	-	2/20/74/74	0/4/4/4
3	PEB	U	188	2	-	3/20/74/74	0/4/4/4
3	PEB	W	187	2	-	3/20/74/74	0/4/4/4
3	PEB	X	188	2	-	3/20/74/74	0/4/4/4
3	PEB	F	166	1	-	2/20/74/74	0/4/4/4
3	PEB	T	186	2	-	2/20/74/74	0/4/4/4
3	PEB	K	167	1	-	2/20/74/74	0/4/4/4

All (509) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	166	PEB	CHB-C4B	16.56	1.49	1.35
3	C	166	PEB	CHB-C4B	15.44	1.48	1.35
3	P	186	PEB	CHB-C4B	14.76	1.47	1.35
3	W	186	PEB	CHB-C4B	14.35	1.47	1.35
3	S	186[A]	PEB	CHB-C4B	14.19	1.47	1.35
3	S	186[B]	PEB	CHB-C4B	14.19	1.47	1.35
3	I	166	PEB	CHB-C4B	14.18	1.47	1.35
3	R	186	PEB	CHB-C4B	14.16	1.46	1.35
3	R	187	PEB	CHB-C4B	14.13	1.46	1.35
3	M	186	PEB	CHB-C4B	14.06	1.46	1.35
3	T	186	PEB	CHB-C4B	13.45	1.46	1.35
3	Q	186	PEB	CHB-C4B	13.22	1.46	1.35
3	N	186	PEB	CHB-C4B	13.20	1.46	1.35
3	W	188	PEB	CHB-C4B	13.19	1.46	1.35
3	S	188	PEB	CHB-C4B	12.67	1.45	1.35
3	H	166	PEB	CHB-C4B	12.60	1.45	1.35
3	Q	187	PEB	CHB-C4B	12.49	1.45	1.35
3	U	187	PEB	CHB-C4B	12.33	1.45	1.35
3	O	186	PEB	CHB-C4B	12.15	1.45	1.35
3	V	187	PEB	CHB-C4B	12.15	1.45	1.35
3	S	187	PEB	CHB-C4B	12.15	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	167	PEB	CHB-C4B	12.10	1.45	1.35
3	G	167	PEB	CHB-C4B	11.99	1.45	1.35
3	N	188	PEB	CHB-C4B	11.95	1.45	1.35
3	X	186	PEB	CHB-C4B	11.62	1.44	1.35
3	T	187	PEB	CHB-C4B	11.61	1.44	1.35
3	U	186	PEB	CHB-C4B	11.35	1.44	1.35
3	V	186	PEB	CHB-C4B	11.13	1.44	1.35
3	B	166	PEB	CHB-C4B	11.01	1.44	1.35
3	R	188	PEB	CHB-C4B	10.98	1.44	1.35
3	O	187	PEB	CHB-C4B	10.72	1.44	1.35
3	F	167	PEB	CHB-C4B	10.64	1.44	1.35
3	J	167	PEB	CHB-C4B	10.59	1.44	1.35
3	K	166	PEB	CHB-C4B	10.48	1.43	1.35
3	D	166	PEB	CHB-C4B	10.31	1.43	1.35
3	W	187	PEB	CHB-C4B	10.28	1.43	1.35
3	J	166	PEB	CHB-C4B	10.15	1.43	1.35
3	H	167	PEB	CHB-C4B	10.01	1.43	1.35
3	M	187	PEB	CHB-C4B	9.95	1.43	1.35
3	V	188	PEB	CHB-C4B	9.95	1.43	1.35
3	P	187	PEB	CHB-C4B	9.95	1.43	1.35
3	K	167	PEB	CHB-C4B	9.85	1.43	1.35
3	U	188	PEB	CHB-C4B	9.80	1.43	1.35
3	X	187	PEB	CHB-C4B	9.70	1.43	1.35
3	T	188	PEB	CHB-C4B	9.63	1.43	1.35
3	X	188	PEB	C2D-C3D	9.37	1.46	1.34
3	B	167	PEB	CHB-C4B	9.35	1.42	1.35
3	M	188	PEB	CHB-C4B	9.31	1.42	1.35
3	N	187	PEB	CHB-C4B	9.30	1.42	1.35
3	L	166	PEB	CHB-C4B	9.18	1.42	1.35
3	A	166	PEB	CHB-C4B	9.05	1.42	1.35
3	P	186	PEB	C2D-C3D	8.88	1.46	1.34
3	F	166	PEB	CHB-C4B	8.85	1.42	1.35
3	P	188	PEB	CHB-C4B	8.82	1.42	1.35
3	G	166	PEB	CHB-C4B	8.56	1.42	1.35
3	D	167	PEB	CHB-C4B	8.54	1.42	1.35
3	C	167	PEB	CHB-C4B	8.47	1.42	1.35
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	P	188	PEB	C2D-C3D	8.07	1.44	1.34
3	W	188	PEB	C2D-C3D	8.00	1.44	1.34
3	Q	188	PEB	CHB-C4B	7.95	1.41	1.35
3	X	188	PEB	CHB-C4B	7.93	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	167	PEB	CHB-C4B	7.81	1.41	1.35
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	L	167	PEB	CHB-C4B	7.67	1.41	1.35
3	O	188	PEB	CHB-C4B	7.61	1.41	1.35
3	N	188	PEB	C2D-C3D	7.53	1.44	1.34
3	I	167	PEB	CHB-C4B	7.48	1.41	1.35
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	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	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	M	186	PEB	C2D-C3D	6.37	1.42	1.34
3	I	167	PEB	C2D-C3D	6.33	1.42	1.34
3	Q	188	PEB	C2D-C3D	6.28	1.42	1.34
3	W	186	PEB	C2D-C3D	6.28	1.42	1.34
3	X	187	PEB	C2D-C3D	6.24	1.42	1.34
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	S	188	PEB	C2D-C3D	5.86	1.42	1.34
3	K	167	PEB	C1A-NA	-5.78	1.30	1.37
3	R	188	PEB	C2D-C3D	5.73	1.41	1.34
3	F	167	PEB	C2D-C3D	5.61	1.41	1.34
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	N	187	PEB	C2D-C3D	5.52	1.41	1.34
3	K	166	PEB	C2D-C3D	5.50	1.41	1.34
3	P	187	PEB	C2D-C3D	5.42	1.41	1.34
3	E	166	PEB	C3B-C2B	5.38	1.48	1.36
3	Q	187	PEB	C2D-C3D	5.29	1.41	1.34

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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	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	W	187	PEB	C2D-C3D	5.11	1.41	1.34
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	C3B-C2B	4.82	1.47	1.36
3	G	167	PEB	C2D-C3D	4.82	1.40	1.34
3	R	188	PEB	CHA-C1B	4.79	1.51	1.40
3	T	186	PEB	C3B-C2B	4.78	1.46	1.36
3	H	166	PEB	C3C-C4C	4.75	1.49	1.42
3	B	167	PEB	C1A-NA	-4.72	1.31	1.37
3	J	166	PEB	C3B-C2B	4.69	1.46	1.36
3	E	166	PEB	C3C-C4C	4.66	1.49	1.42
3	J	167	PEB	C2D-C3D	4.62	1.40	1.34
3	T	186	PEB	C3C-C4C	4.62	1.49	1.42
3	B	167	PEB	C2A-C1A	-4.52	1.48	1.52
3	R	187	PEB	C3B-C2B	4.48	1.46	1.36
3	D	166	PEB	C2A-C1A	-4.46	1.48	1.52
3	J	167	PEB	C3B-C2B	4.43	1.46	1.36
3	T	187	PEB	C2D-C3D	4.40	1.40	1.34
3	K	167	PEB	C2A-C1A	-4.39	1.48	1.52
3	U	187	PEB	C3A-C4A	4.38	1.57	1.50
3	C	167	PEB	C2D-C3D	4.37	1.40	1.34
3	W	188	PEB	C3B-C2B	4.34	1.46	1.36
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	X	188	PEB	C1A-NA	-4.31	1.32	1.37
3	N	188	PEB	C3B-C2B	4.28	1.45	1.36
3	T	188	PEB	CHA-C1B	4.26	1.50	1.40
3	R	186	PEB	C3C-C4C	4.23	1.48	1.42
3	N	186	PEB	CHA-C1B	4.17	1.50	1.40
3	H	166	PEB	C3B-C2B	4.16	1.45	1.36
3	U	186	PEB	C3B-C2B	4.15	1.45	1.36
3	I	167	PEB	CAC-C2C	-4.13	1.46	1.52
3	R	188	PEB	C3B-C2B	4.13	1.45	1.36
3	W	187	PEB	C1A-NA	-4.10	1.32	1.37
3	G	166	PEB	C3B-C2B	4.09	1.45	1.36
3	E	167	PEB	C1A-NA	-4.07	1.32	1.37
3	T	186	PEB	CHA-C1B	4.06	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	167	PEB	C1A-NA	-4.05	1.32	1.37
3	B	166	PEB	C3B-C2B	4.02	1.45	1.36
3	L	166	PEB	CHA-C1B	4.00	1.49	1.40
3	O	188	PEB	CHA-C1B	3.99	1.49	1.40
3	G	167	PEB	C1A-NA	-3.98	1.32	1.37
3	V	186	PEB	C2D-C3D	3.95	1.39	1.34
3	H	167	PEB	CHA-C1B	3.90	1.49	1.40
3	O	187	PEB	C1A-NA	-3.88	1.32	1.37
3	P	188	PEB	C3B-C2B	3.86	1.44	1.36
3	I	166	PEB	C3B-C2B	3.85	1.44	1.36
3	W	187	PEB	C3B-C2B	3.84	1.44	1.36
3	Q	186	PEB	CHA-C1B	3.82	1.49	1.40
3	A	167	PEB	C1A-NA	-3.82	1.32	1.37
3	L	166	PEB	C4B-C3B	-3.80	1.39	1.45
3	W	187	PEB	C3C-C4C	3.79	1.48	1.42
3	Q	186	PEB	C3B-C2B	3.79	1.44	1.36
3	U	187	PEB	CHA-C1B	3.78	1.49	1.40
3	L	166	PEB	C4D-ND	-3.78	1.29	1.35
3	S	186[A]	PEB	C3B-C2B	3.78	1.44	1.36
3	S	186[B]	PEB	C3B-C2B	3.78	1.44	1.36
3	J	167	PEB	C1A-NA	-3.78	1.32	1.37
3	K	166	PEB	C3B-C2B	3.75	1.44	1.36
3	L	167	PEB	C1A-NA	-3.74	1.32	1.37
3	R	186	PEB	C3B-C2B	3.74	1.44	1.36
3	X	187	PEB	C3B-C2B	3.71	1.44	1.36
3	O	186	PEB	C3B-C2B	3.69	1.44	1.36
3	A	167	PEB	C2D-C3D	3.68	1.39	1.34
3	N	187	PEB	CHA-C1B	3.67	1.49	1.40
3	O	187	PEB	C3B-C2B	3.66	1.44	1.36
3	S	188	PEB	C3B-C2B	3.65	1.44	1.36
3	B	167	PEB	C2D-C3D	3.65	1.39	1.34
3	T	188	PEB	C3B-C2B	3.64	1.44	1.36
3	P	187	PEB	CHA-C1B	3.64	1.48	1.40
3	X	188	PEB	C3B-C2B	3.63	1.44	1.36
3	U	188	PEB	CHA-C1B	3.62	1.48	1.40
3	M	188	PEB	C1A-NA	-3.62	1.32	1.37
3	O	186	PEB	C2A-C1A	-3.62	1.48	1.52
3	W	186	PEB	C3B-C2B	3.60	1.44	1.36
3	F	167	PEB	C3B-C2B	3.59	1.44	1.36
3	M	186	PEB	C3B-C2B	3.59	1.44	1.36
3	U	188	PEB	C1A-NA	-3.58	1.33	1.37
3	X	186	PEB	CHA-C1B	3.58	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	187	PEB	CHA-C1B	3.53	1.48	1.40
3	Q	187	PEB	C2A-C1A	-3.51	1.49	1.52
3	P	186	PEB	C3B-C2B	3.51	1.44	1.36
3	R	186	PEB	CHA-C1B	3.50	1.48	1.40
3	Q	187	PEB	CHA-C1B	3.50	1.48	1.40
3	C	167	PEB	CHA-C1B	3.49	1.48	1.40
3	W	188	PEB	CHA-C1B	3.48	1.48	1.40
3	U	187	PEB	C1A-NA	-3.48	1.33	1.37
3	D	167	PEB	C1A-NA	-3.48	1.33	1.37
3	R	188	PEB	C1A-NA	-3.47	1.33	1.37
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	T	187	PEB	CHA-C1B	3.47	1.48	1.40
3	O	188	PEB	C3B-C2B	3.46	1.44	1.36
3	W	188	PEB	C2C-C3C	3.44	1.47	1.37
3	M	186	PEB	CHA-C1B	3.44	1.48	1.40
3	D	167	PEB	C3B-C2B	3.44	1.44	1.36
3	O	188	PEB	C1D-ND	3.43	1.50	1.45
3	H	167	PEB	C2A-C1A	-3.42	1.49	1.52
3	E	166	PEB	C1A-NA	-3.40	1.33	1.37
3	G	167	PEB	C3B-C2B	3.40	1.43	1.36
3	D	166	PEB	C3B-C2B	3.39	1.43	1.36
3	P	187	PEB	C3B-C2B	3.39	1.43	1.36
3	J	166	PEB	C2D-C3D	3.38	1.39	1.34
3	D	166	PEB	C1A-NA	-3.36	1.33	1.37
3	C	167	PEB	C3C-C4C	3.36	1.47	1.42
3	Q	187	PEB	C3B-C2B	3.35	1.43	1.36
3	C	167	PEB	C3B-C2B	3.35	1.43	1.36
3	M	187	PEB	C3B-C2B	3.34	1.43	1.36
3	B	166	PEB	C1A-NA	-3.34	1.33	1.37
3	E	166	PEB	OD-C4D	3.33	1.29	1.23
3	I	167	PEB	C1A-NA	-3.32	1.33	1.37
3	F	167	PEB	C3C-C4C	3.31	1.47	1.42
3	A	167	PEB	CHA-C1B	3.30	1.48	1.40
3	H	166	PEB	CHA-C1B	3.29	1.48	1.40
3	U	187	PEB	C3B-C2B	3.28	1.43	1.36
3	U	188	PEB	C3B-C2B	3.28	1.43	1.36
3	B	166	PEB	C3C-C4C	3.27	1.47	1.42
3	N	187	PEB	C3B-C2B	3.27	1.43	1.36
3	C	167	PEB	C2C-C3C	3.26	1.47	1.37
3	B	166	PEB	CHA-C1B	3.25	1.48	1.40
3	O	187	PEB	CHA-C1B	3.24	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	188	PEB	C3B-C2B	3.24	1.43	1.36
3	V	186	PEB	CHA-C1B	3.24	1.48	1.40
3	K	166	PEB	OD-C4D	3.23	1.29	1.23
3	Q	188	PEB	C1A-NA	-3.22	1.33	1.37
3	S	186[A]	PEB	C2C-C3C	3.22	1.47	1.37
3	U	186	PEB	CHA-C1B	3.22	1.48	1.40
3	P	188	PEB	CHA-C1B	3.21	1.47	1.40
3	B	167	PEB	C3B-C2B	3.20	1.43	1.36
3	O	188	PEB	OD-C4D	3.19	1.29	1.23
3	D	166	PEB	CHA-C1B	3.19	1.47	1.40
3	C	166	PEB	C2A-C1A	-3.19	1.49	1.52
3	R	186	PEB	C2C-C3C	3.18	1.47	1.37
3	E	166	PEB	CHA-C1B	3.16	1.47	1.40
3	V	186	PEB	C3B-C2B	3.16	1.43	1.36
3	K	167	PEB	C2C-C3C	3.16	1.47	1.37
3	X	188	PEB	CHA-C1B	3.15	1.47	1.40
3	N	186	PEB	C3B-C2B	3.14	1.43	1.36
3	S	187	PEB	CHA-C1B	3.13	1.47	1.40
3	F	166	PEB	C3B-C2B	3.13	1.43	1.36
3	S	186[A]	PEB	CHA-C1B	3.12	1.47	1.40
3	S	186[B]	PEB	CHA-C1B	3.12	1.47	1.40
3	P	186	PEB	CMB-C2B	-3.11	1.44	1.50
3	D	167	PEB	C3C-C4C	3.10	1.46	1.42
3	Q	188	PEB	C3A-C4A	3.10	1.55	1.50
3	I	167	PEB	CHA-C1B	3.10	1.47	1.40
3	V	187	PEB	C3B-C2B	3.06	1.43	1.36
3	W	186	PEB	CHA-C1B	3.06	1.47	1.40
3	D	167	PEB	CHA-C1B	3.06	1.47	1.40
3	I	166	PEB	CHA-C1B	3.06	1.47	1.40
3	Q	188	PEB	C3B-C2B	3.05	1.43	1.36
3	K	167	PEB	C3C-C4C	3.04	1.46	1.42
3	C	167	PEB	C4A-NA	-3.04	1.31	1.37
3	J	166	PEB	C2A-C1A	-3.03	1.49	1.52
3	G	167	PEB	CHA-C1B	3.03	1.47	1.40
3	V	188	PEB	CHA-C1B	3.03	1.47	1.40
3	O	188	PEB	C4D-ND	-3.03	1.30	1.35
3	E	167	PEB	C3C-C4C	3.03	1.46	1.42
3	H	167	PEB	C2C-C3C	3.02	1.46	1.37
3	P	186	PEB	CHA-C1B	3.02	1.47	1.40
3	F	167	PEB	C2A-C1A	-3.02	1.49	1.52
3	F	166	PEB	C3C-C4C	3.00	1.46	1.42
3	K	166	PEB	CHA-C1B	2.99	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	187	PEB	CAC-C2C	-2.99	1.47	1.52
3	V	187	PEB	CHA-C1B	2.98	1.47	1.40
3	V	188	PEB	C1A-NA	-2.98	1.33	1.37
3	M	188	PEB	C3B-C2B	2.97	1.43	1.36
3	L	167	PEB	CHA-C1B	2.97	1.47	1.40
3	K	167	PEB	C3B-C2B	2.96	1.43	1.36
3	O	188	PEB	C1A-NA	-2.95	1.33	1.37
3	I	167	PEB	C3B-C2B	2.95	1.43	1.36
3	P	186	PEB	C2A-C1A	-2.95	1.49	1.52
3	R	186	PEB	C2A-C1A	-2.94	1.49	1.52
3	C	166	PEB	C1A-NA	-2.92	1.33	1.37
3	M	187	PEB	CHA-C1B	2.92	1.47	1.40
3	S	188	PEB	CAC-C2C	-2.90	1.47	1.52
3	S	188	PEB	CHA-C1B	2.89	1.47	1.40
3	X	186	PEB	C3B-C2B	2.88	1.42	1.36
3	N	188	PEB	C2C-C3C	2.88	1.46	1.37
3	W	186	PEB	OD-C4D	2.87	1.29	1.23
3	Q	188	PEB	OD-C4D	2.87	1.29	1.23
3	K	166	PEB	C3A-C4A	2.87	1.55	1.50
3	P	187	PEB	CAC-C2C	-2.86	1.47	1.52
3	E	167	PEB	CHA-C1B	2.85	1.47	1.40
3	A	166	PEB	CHA-C1B	2.85	1.47	1.40
3	O	188	PEB	C2C-C3C	2.85	1.46	1.37
3	W	187	PEB	C2A-C1A	-2.85	1.49	1.52
3	J	167	PEB	CHA-C1B	2.85	1.47	1.40
3	R	187	PEB	OD-C4D	2.85	1.29	1.23
3	R	186	PEB	OD-C4D	2.84	1.29	1.23
3	P	186	PEB	OD-C4D	2.83	1.29	1.23
3	P	186	PEB	C1D-ND	2.83	1.50	1.45
3	G	166	PEB	CAC-C2C	-2.83	1.47	1.52
3	S	186[A]	PEB	OD-C4D	2.83	1.29	1.23
3	S	186[B]	PEB	OD-C4D	2.83	1.29	1.23
3	Q	186	PEB	C2C-C3C	2.81	1.46	1.37
3	F	167	PEB	CHA-C1B	2.80	1.47	1.40
3	R	187	PEB	C2C-C3C	2.80	1.46	1.37
3	L	166	PEB	C2A-C1A	-2.79	1.49	1.52
3	P	188	PEB	OD-C4D	2.79	1.28	1.23
3	C	167	PEB	C4B-NB	-2.78	1.32	1.38
3	J	166	PEB	CHA-C1B	2.78	1.46	1.40
3	G	167	PEB	C4D-ND	-2.77	1.31	1.35
3	D	167	PEB	CAC-C2C	-2.77	1.48	1.52
3	H	167	PEB	C3B-C2B	2.76	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	167	PEB	OD-C4D	2.76	1.28	1.23
3	L	167	PEB	C3B-C2B	2.76	1.42	1.36
3	T	188	PEB	C2C-C3C	2.76	1.45	1.37
3	C	166	PEB	C3C-C4C	2.76	1.46	1.42
3	D	167	PEB	C2A-C1A	-2.75	1.49	1.52
3	T	187	PEB	C3B-C2B	2.74	1.42	1.36
3	D	166	PEB	C4B-C3B	-2.73	1.41	1.45
3	Q	186	PEB	C3C-C4C	2.72	1.46	1.42
3	Q	188	PEB	CHA-C1B	2.71	1.46	1.40
3	E	166	PEB	C2C-C3C	2.71	1.45	1.37
3	S	187	PEB	C1D-ND	2.70	1.49	1.45
3	P	186	PEB	C1A-NA	-2.70	1.34	1.37
3	I	166	PEB	C1D-ND	2.70	1.49	1.45
3	X	187	PEB	CHA-C1B	2.68	1.46	1.40
3	L	167	PEB	OD-C4D	2.68	1.28	1.23
3	T	187	PEB	C2C-C3C	2.68	1.45	1.37
3	M	188	PEB	CHA-C1B	2.67	1.46	1.40
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
3	H	167	PEB	C1A-NA	-2.66	1.34	1.37
3	E	167	PEB	C3B-C2B	2.66	1.42	1.36
3	L	167	PEB	C2D-C3D	2.66	1.38	1.34
3	S	187	PEB	C3B-C2B	2.66	1.42	1.36
3	U	186	PEB	C2C-C3C	2.65	1.45	1.37
3	T	187	PEB	CAC-C2C	-2.65	1.48	1.52
3	E	166	PEB	C4D-ND	-2.65	1.31	1.35
3	F	166	PEB	CHA-C1B	2.64	1.46	1.40
3	X	188	PEB	C2C-C3C	2.64	1.45	1.37
3	E	167	PEB	C2A-C1A	-2.64	1.49	1.52
3	L	167	PEB	C4D-ND	-2.63	1.31	1.35
3	T	186	PEB	C2C-C3C	2.63	1.45	1.37
3	I	166	PEB	C3C-C4C	2.62	1.46	1.42
3	Q	187	PEB	C1A-NA	-2.61	1.34	1.37
3	U	186	PEB	C3C-C4C	2.61	1.46	1.42
3	X	186	PEB	C2C-C3C	2.60	1.45	1.37
3	G	167	PEB	C3C-C4C	2.60	1.46	1.42
3	B	167	PEB	C2C-C3C	2.60	1.45	1.37
3	L	167	PEB	C1D-ND	2.60	1.49	1.45
3	T	186	PEB	OD-C4D	2.59	1.28	1.23
3	S	186[B]	PEB	C2C-C3C	2.59	1.45	1.37
3	F	166	PEB	CAC-C2C	-2.59	1.48	1.52
3	C	166	PEB	C4D-ND	-2.58	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	167	PEB	C4A-NA	-2.58	1.31	1.37
3	I	167	PEB	C3C-C4C	2.56	1.46	1.42
3	N	187	PEB	CAA-C3A	2.56	1.59	1.54
3	S	187	PEB	OD-C4D	2.55	1.28	1.23
3	W	188	PEB	OD-C4D	2.54	1.28	1.23
3	M	186	PEB	C1B-NB	2.52	1.42	1.36
3	I	167	PEB	C1D-ND	-2.52	1.42	1.45
3	S	186[A]	PEB	C1A-NA	-2.52	1.34	1.37
3	S	186[B]	PEB	C1A-NA	-2.52	1.34	1.37
3	X	187	PEB	C1A-NA	-2.52	1.34	1.37
3	J	167	PEB	C2A-C1A	-2.52	1.49	1.52
3	E	167	PEB	C2C-C3C	2.51	1.45	1.37
3	F	167	PEB	C1A-NA	-2.51	1.34	1.37
3	D	167	PEB	OD-C4D	2.50	1.28	1.23
3	W	186	PEB	C2C-C3C	2.50	1.45	1.37
3	F	167	PEB	C2C-C3C	2.50	1.45	1.37
3	S	188	PEB	OD-C4D	2.50	1.28	1.23
3	Q	186	PEB	OD-C4D	2.50	1.28	1.23
3	M	186	PEB	OD-C4D	2.49	1.28	1.23
3	N	188	PEB	C4A-NA	-2.48	1.32	1.37
3	W	186	PEB	C3C-C4C	2.48	1.45	1.42
3	V	188	PEB	C4D-ND	-2.48	1.31	1.35
3	B	167	PEB	C3C-C4C	2.47	1.45	1.42
3	K	166	PEB	C1A-NA	-2.47	1.34	1.37
3	D	166	PEB	C3C-C4C	2.47	1.45	1.42
3	L	167	PEB	C3C-C4C	2.47	1.45	1.42
3	N	188	PEB	CHA-C1B	2.45	1.46	1.40
3	V	188	PEB	C2C-C3C	2.44	1.44	1.37
3	R	187	PEB	C1A-NA	-2.43	1.34	1.37
3	H	166	PEB	CAC-C2C	-2.42	1.48	1.52
3	R	188	PEB	C3C-C4C	2.42	1.45	1.42
3	A	167	PEB	C2C-C3C	2.41	1.44	1.37
3	G	166	PEB	C4B-C3B	-2.40	1.41	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	G	167	PEB	CAC-C2C	-2.39	1.48	1.52
3	Q	186	PEB	C2A-C1A	-2.39	1.50	1.52
3	G	167	PEB	C4B-NB	-2.39	1.33	1.38
3	X	187	PEB	OD-C4D	2.39	1.28	1.23
3	S	187	PEB	C1A-NA	-2.38	1.34	1.37
3	G	166	PEB	CHA-C1B	2.38	1.46	1.40
3	O	186	PEB	C3C-C4C	2.38	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	167	PEB	C1D-ND	2.38	1.49	1.45
3	W	186	PEB	CMD-C2D	-2.38	1.46	1.50
3	M	187	PEB	C3C-C4C	2.37	1.45	1.42
5	U	205	PI	P-O1	2.37	1.56	1.50
3	R	187	PEB	C3C-C4C	2.36	1.45	1.42
3	X	187	PEB	CAC-C2C	-2.35	1.48	1.52
3	K	167	PEB	CHA-C1B	2.35	1.45	1.40
3	G	166	PEB	C3C-C4C	2.35	1.45	1.42
3	V	187	PEB	C4B-C3B	-2.35	1.42	1.45
3	T	188	PEB	C4B-NB	-2.34	1.33	1.38
3	D	167	PEB	C2D-C3D	2.33	1.37	1.34
3	A	167	PEB	C3C-C4C	2.33	1.45	1.42
3	X	186	PEB	OD-C4D	2.33	1.28	1.23
3	U	186	PEB	CHA-C4A	-2.33	1.32	1.36
3	M	187	PEB	C2A-C1A	-2.32	1.50	1.52
3	T	186	PEB	C1A-NA	-2.31	1.34	1.37
3	W	186	PEB	C1A-NA	-2.31	1.34	1.37
3	N	186	PEB	C1A-NA	-2.30	1.34	1.37
3	F	167	PEB	C4A-NA	-2.30	1.32	1.37
3	I	166	PEB	C2C-C3C	2.30	1.44	1.37
3	P	187	PEB	C2C-C3C	2.30	1.44	1.37
3	D	166	PEB	CMC-C3C	-2.28	1.46	1.51
3	J	167	PEB	C2C-C3C	2.28	1.44	1.37
3	B	166	PEB	C2A-C1A	-2.28	1.50	1.52
3	R	188	PEB	C4B-NB	-2.27	1.33	1.38
3	K	166	PEB	CAC-C2C	-2.27	1.48	1.52
3	V	188	PEB	CHA-C4A	-2.26	1.32	1.36
3	B	167	PEB	CAC-C2C	-2.26	1.48	1.52
3	O	187	PEB	C3C-C4C	2.26	1.45	1.42
3	M	187	PEB	C1A-NA	-2.26	1.34	1.37
3	M	188	PEB	C4D-ND	-2.26	1.31	1.35
3	U	186	PEB	C1A-NA	-2.26	1.34	1.37
3	R	186	PEB	C1A-NA	-2.25	1.34	1.37
3	I	167	PEB	C4D-ND	-2.25	1.31	1.35
3	U	188	PEB	C2C-C3C	2.24	1.44	1.37
3	M	186	PEB	C1A-NA	-2.24	1.34	1.37
3	S	187	PEB	C2C-C3C	2.23	1.44	1.37
3	I	166	PEB	C2A-C1A	-2.23	1.50	1.52
3	V	186	PEB	CMD-C2D	-2.23	1.46	1.50
3	I	167	PEB	C2A-C1A	-2.23	1.50	1.52
3	H	166	PEB	C2C-C3C	2.23	1.44	1.37
3	C	166	PEB	CHA-C1B	2.23	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	188	PEB	OD-C4D	2.23	1.27	1.23
3	N	187	PEB	CAC-C2C	-2.22	1.48	1.52
3	T	188	PEB	C3C-C4C	2.22	1.45	1.42
3	M	187	PEB	OD-C4D	2.22	1.27	1.23
3	F	167	PEB	OD-C4D	2.21	1.27	1.23
3	V	186	PEB	C2A-C1A	-2.21	1.50	1.52
3	V	188	PEB	C3A-C4A	2.21	1.54	1.50
3	T	188	PEB	OD-C4D	2.21	1.27	1.23
3	C	166	PEB	C2C-C3C	2.21	1.44	1.37
3	U	188	PEB	C3C-C4C	2.20	1.45	1.42
3	K	167	PEB	C1B-NB	-2.20	1.31	1.36
4	D	203	NO3	O1-N	2.20	1.34	1.24
3	O	188	PEB	CMD-C2D	2.20	1.54	1.50
3	H	167	PEB	C3C-C4C	2.20	1.45	1.42
3	S	188	PEB	C3C-C4C	2.19	1.45	1.42
3	Q	187	PEB	C2C-C3C	2.19	1.44	1.37
3	P	188	PEB	C3C-C4C	2.18	1.45	1.42
3	G	167	PEB	C4B-C3B	-2.18	1.42	1.45
3	P	187	PEB	C1D-ND	2.17	1.49	1.45
3	O	186	PEB	CHA-C1B	2.17	1.45	1.40
3	N	187	PEB	C2C-C3C	2.17	1.44	1.37
3	T	188	PEB	CAC-C2C	-2.17	1.48	1.52
3	R	186	PEB	C4B-NB	-2.16	1.33	1.38
3	O	187	PEB	OD-C4D	2.16	1.27	1.23
3	B	167	PEB	OD-C4D	2.15	1.27	1.23
3	V	188	PEB	CMD-C2D	2.15	1.54	1.50
3	P	187	PEB	C3A-C4A	2.15	1.54	1.50
3	M	188	PEB	OD-C4D	2.14	1.27	1.23
3	A	167	PEB	C3B-C2B	2.13	1.41	1.36
3	R	188	PEB	C1D-ND	2.13	1.48	1.45
3	X	186	PEB	C3C-C4C	2.12	1.45	1.42
3	A	166	PEB	OD-C4D	2.11	1.27	1.23
3	T	187	PEB	CMB-C2B	-2.10	1.46	1.50
3	O	188	PEB	C3C-C4C	2.10	1.45	1.42
3	M	188	PEB	C3C-C4C	2.10	1.45	1.42
3	R	188	PEB	OD-C4D	2.09	1.27	1.23
3	Q	187	PEB	C4B-NB	-2.09	1.34	1.38
3	D	167	PEB	C2C-C3C	2.08	1.43	1.37
3	I	167	PEB	C2C-C3C	2.08	1.43	1.37
3	P	188	PEB	C2C-C3C	2.08	1.43	1.37
3	J	167	PEB	C4B-NB	-2.08	1.34	1.38
3	N	186	PEB	C2C-C3C	2.08	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	188	PEB	CAC-C2C	-2.08	1.49	1.52
3	M	186	PEB	C2C-C3C	2.07	1.43	1.37
3	T	187	PEB	C3C-C4C	2.07	1.45	1.42
3	X	188	PEB	C3C-C4C	2.06	1.45	1.42
3	D	167	PEB	C3A-C4A	-2.06	1.47	1.50
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	T	187	PEB	C4B-NB	-2.05	1.34	1.38
3	N	186	PEB	C3C-C4C	2.04	1.45	1.42
3	M	187	PEB	CMC-C3C	-2.04	1.47	1.51
3	G	167	PEB	CMC-C3C	-2.04	1.47	1.51
3	U	188	PEB	C1D-ND	2.04	1.48	1.45
3	K	166	PEB	CAB-C3B	-2.03	1.46	1.51
3	W	187	PEB	CHA-C1B	2.03	1.45	1.40
3	P	186	PEB	C2C-C3C	2.03	1.43	1.37
3	T	188	PEB	C3A-C4A	2.02	1.53	1.50
3	B	166	PEB	CMB-C2B	-2.02	1.46	1.50
3	I	166	PEB	C1A-NA	-2.02	1.35	1.37
3	N	186	PEB	C2A-C1A	-2.02	1.50	1.52
3	O	188	PEB	C4B-C3B	-2.01	1.42	1.45
3	M	186	PEB	CMC-C3C	-2.01	1.47	1.51
3	B	167	PEB	CHA-C1B	2.01	1.45	1.40
3	W	186	PEB	C1D-ND	2.01	1.48	1.45
3	O	187	PEB	C4B-C3B	-2.01	1.42	1.45
3	S	188	PEB	C1A-NA	-2.00	1.35	1.37
3	G	166	PEB	C4D-ND	-2.00	1.32	1.35

All (569) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	166	PEB	CHA-C4A-NA	9.03	135.95	125.20
3	L	166	PEB	CHA-C4A-NA	7.94	134.64	125.20
3	I	166	PEB	CHA-C4A-NA	7.91	134.61	125.20
3	F	166	PEB	CHA-C4A-NA	7.69	134.35	125.20
3	H	166	PEB	CHA-C4A-NA	7.68	134.34	125.20
3	K	166	PEB	CHA-C4A-NA	7.45	134.06	125.20
3	C	166	PEB	CHA-C4A-NA	7.29	133.87	125.20
3	E	166	PEB	CHA-C4A-NA	7.08	133.62	125.20
3	B	166	PEB	CHA-C4A-NA	7.02	133.55	125.20
3	D	166	PEB	CHA-C4A-NA	6.90	133.41	125.20
3	V	186	PEB	CHA-C4A-NA	6.71	133.18	125.20
3	A	166	PEB	CHA-C4A-NA	5.81	132.11	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	186	PEB	CHA-C4A-NA	5.77	132.06	125.20
3	J	167	PEB	CMB-C2B-C1B	5.73	133.89	125.06
3	J	166	PEB	CHA-C1B-NB	-5.66	113.09	124.93
3	U	186	PEB	CHA-C4A-NA	5.52	131.77	125.20
3	H	166	PEB	CHA-C1B-NB	-5.46	113.52	124.93
3	J	166	PEB	CHA-C4A-NA	5.44	131.67	125.20
3	R	186	PEB	CHA-C4A-NA	5.35	131.57	125.20
3	C	167	PEB	CMB-C2B-C1B	5.31	133.24	125.06
3	C	166	PEB	CHA-C1B-NB	-5.27	113.91	124.93
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	C2A-C1A-NA	5.24	112.79	108.27
3	S	186[A]	PEB	CHA-C4A-NA	5.19	131.38	125.20
3	S	186[B]	PEB	CHA-C4A-NA	5.19	131.38	125.20
3	C	167	PEB	CHC-C1D-ND	-5.05	108.08	113.95
3	U	186	PEB	OA-C1A-C2A	-5.02	122.18	126.17
3	E	166	PEB	CHA-C1B-NB	-5.02	114.43	124.93
3	E	166	PEB	C1B-C2B-C3B	-4.91	100.87	106.51
3	Q	186	PEB	CHA-C4A-NA	4.88	131.01	125.20
3	E	166	PEB	CHC-C4C-C3C	-4.86	122.05	130.34
3	U	186	PEB	CMB-C2B-C1B	4.85	132.54	125.06
3	T	187	PEB	CHA-C4A-NA	4.77	130.87	125.20
3	A	166	PEB	CHA-C1B-NB	-4.76	114.98	124.93
3	T	186	PEB	CMB-C2B-C1B	4.74	132.37	125.06
3	W	188	PEB	CHC-C4C-C3C	-4.72	122.29	130.34
3	U	188	PEB	CAC-CBC-CGC	4.68	120.52	112.67
3	H	167	PEB	CMB-C2B-C1B	4.63	132.19	125.06
3	T	187	PEB	CHC-C1D-ND	-4.59	108.62	113.95
3	X	186	PEB	CMB-C2B-C1B	4.58	132.12	125.06
3	K	166	PEB	CHA-C1B-NB	-4.55	115.41	124.93
3	O	188	PEB	CHC-C1D-ND	-4.53	108.68	113.95
3	Q	187	PEB	CHC-C1D-ND	-4.52	108.70	113.95
3	M	186	PEB	CHA-C4A-NA	4.51	130.56	125.20
3	F	166	PEB	CHA-C1B-NB	-4.50	115.52	124.93
3	W	186	PEB	CHA-C4A-NA	4.47	130.53	125.20
3	I	166	PEB	CHA-C1B-NB	-4.46	115.61	124.93
3	M	186	PEB	CAC-CBC-CGC	4.42	120.09	112.67
3	F	167	PEB	CMB-C2B-C1B	4.40	131.84	125.06
3	X	187	PEB	CHC-C1D-ND	-4.37	108.87	113.95
3	K	166	PEB	C2A-C1A-NA	4.34	112.01	108.27
3	G	166	PEB	CHA-C1B-NB	-4.32	115.89	124.93
3	W	186	PEB	CHA-C1B-NB	-4.31	115.91	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	188	PEB	C2A-C1A-NA	4.31	111.99	108.27
3	O	186	PEB	CMB-C2B-C1B	4.31	131.70	125.06
3	M	186	PEB	CHA-C1B-NB	-4.29	115.96	124.93
3	S	186[A]	PEB	CHC-C1D-ND	-4.29	108.97	113.95
3	S	186[B]	PEB	CHC-C1D-ND	-4.29	108.97	113.95
3	C	166	PEB	CAB-C3B-C4B	4.29	132.59	125.01
3	R	186	PEB	OA-C1A-C2A	-4.26	122.78	126.17
3	A	166	PEB	CHA-C1B-C2B	4.24	135.82	124.90
3	T	187	PEB	CMB-C2B-C1B	4.22	131.57	125.06
3	D	166	PEB	CHA-C1B-NB	-4.21	116.12	124.93
3	H	166	PEB	CMB-C2B-C1B	4.19	131.52	125.06
3	X	188	PEB	OA-C1A-C2A	-4.19	122.84	126.17
3	K	167	PEB	CAB-C3B-C4B	4.18	132.40	125.01
3	G	167	PEB	CMB-C2B-C1B	4.17	131.48	125.06
3	R	187	PEB	C1C-CHB-C4B	4.16	133.78	128.81
3	B	166	PEB	CHA-C1B-NB	-4.14	116.27	124.93
3	P	186	PEB	CMB-C2B-C1B	4.14	131.44	125.06
3	T	188	PEB	C2A-C3A-C4A	4.13	107.53	101.34
3	B	167	PEB	CMB-C2B-C1B	4.12	131.41	125.06
3	V	187	PEB	CMB-C2B-C1B	4.12	131.41	125.06
3	T	186	PEB	OA-C1A-C2A	-4.12	122.90	126.17
3	V	187	PEB	C1C-CHB-C4B	4.10	133.71	128.81
3	B	166	PEB	CHC-C1D-ND	-4.10	109.19	113.95
3	L	166	PEB	CHA-C1B-NB	-4.10	116.36	124.93
3	D	167	PEB	OA-C1A-C2A	-4.07	122.94	126.17
3	N	186	PEB	CHA-C4A-NA	4.06	130.03	125.20
3	R	187	PEB	CMB-C2B-C1B	4.02	131.26	125.06
3	R	188	PEB	CHC-C4C-C3C	-4.01	123.50	130.34
3	P	188	PEB	CHC-C1D-ND	-4.00	109.30	113.95
3	N	188	PEB	CMD-C2D-C3D	-4.00	124.43	130.06
3	A	166	PEB	CHC-C1D-ND	-3.99	109.32	113.95
3	N	186	PEB	CHA-C1B-NB	-3.96	116.66	124.93
3	E	166	PEB	CMB-C2B-C1B	3.95	131.14	125.06
3	S	187	PEB	C4B-C3B-C2B	-3.95	102.42	106.78
3	P	188	PEB	CMD-C2D-C3D	-3.92	124.53	130.06
3	M	187	PEB	CHA-C4A-NA	3.91	129.86	125.20
3	O	187	PEB	C1C-CHB-C4B	3.89	133.46	128.81
3	U	186	PEB	CHA-C1B-NB	-3.88	116.82	124.93
3	U	187	PEB	C1C-CHB-C4B	3.86	133.42	128.81
3	V	186	PEB	CHA-C1B-C2B	3.86	134.82	124.90
3	Q	187	PEB	CHA-C4A-NA	3.85	129.79	125.20
3	K	167	PEB	C4B-C3B-C2B	-3.83	102.54	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	186	PEB	CHC-C1D-ND	-3.83	109.50	113.95
3	L	166	PEB	CHA-C1B-C2B	3.82	134.73	124.90
3	M	186	PEB	CMB-C2B-C1B	3.79	130.90	125.06
3	T	186	PEB	C2A-C1A-NA	3.79	111.54	108.27
3	U	186	PEB	CHC-C1D-ND	-3.78	109.56	113.95
3	C	166	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
3	R	186	PEB	C3D-C4D-ND	3.76	114.65	107.26
3	X	186	PEB	CHA-C4A-NA	3.75	129.66	125.20
3	T	187	PEB	C2A-C3A-C4A	3.74	106.94	101.34
3	Q	188	PEB	CHC-C1D-ND	-3.73	109.62	113.95
3	G	166	PEB	CHA-C1B-C2B	3.73	134.48	124.90
3	U	187	PEB	CAC-CBC-CGC	3.72	118.92	112.67
3	C	166	PEB	CHA-C1B-C2B	3.72	134.46	124.90
3	T	186	PEB	CHA-C4A-NA	3.70	129.61	125.20
3	B	167	PEB	CAB-C3B-C4B	3.69	131.53	125.01
3	C	167	PEB	CHC-C4C-C3C	-3.69	124.05	130.34
3	R	186	PEB	CMB-C2B-C1B	3.68	130.73	125.06
3	B	166	PEB	OA-C1A-C2A	-3.65	123.27	126.17
3	U	186	PEB	C2A-C3A-C4A	3.64	106.79	101.34
3	S	186[A]	PEB	CMB-C2B-C1B	3.62	130.64	125.06
3	S	186[B]	PEB	CMB-C2B-C1B	3.62	130.64	125.06
3	F	167	PEB	CHC-C1D-ND	-3.62	109.75	113.95
3	S	186[A]	PEB	C3D-C4D-ND	3.61	114.34	107.26
3	S	186[B]	PEB	C3D-C4D-ND	3.61	114.34	107.26
3	H	167	PEB	CAB-CBB-CGB	-3.61	106.61	112.67
3	E	166	PEB	CHC-C1D-ND	-3.60	109.76	113.95
3	W	186	PEB	CHC-C1D-ND	-3.59	109.78	113.95
3	R	186	PEB	CHC-C1D-ND	-3.58	109.79	113.95
3	H	166	PEB	OD-C4D-C3D	-3.56	121.39	129.46
3	M	188	PEB	OD-C4D-C3D	-3.55	121.41	129.46
3	T	187	PEB	CHC-C4C-C3C	-3.55	124.28	130.34
3	T	186	PEB	CHC-C4C-C3C	-3.55	124.29	130.34
3	P	186	PEB	C2A-C1A-NA	3.53	111.31	108.27
3	L	167	PEB	OD-C4D-ND	-3.50	120.74	125.93
3	J	167	PEB	OA-C1A-C2A	-3.50	123.39	126.17
3	M	188	PEB	C2A-C1A-NA	3.48	111.27	108.27
3	Q	186	PEB	CHA-C1B-NB	-3.47	117.68	124.93
3	Q	186	PEB	CHC-C1D-ND	-3.47	109.92	113.95
3	O	187	PEB	CMB-C2B-C1B	3.46	130.40	125.06
3	P	187	PEB	CMB-C2B-C1B	3.46	130.39	125.06
3	T	186	PEB	CHA-C1B-NB	-3.46	117.70	124.93
3	B	166	PEB	C2A-C1A-NA	3.46	111.25	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	167	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
3	H	167	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
3	J	166	PEB	CHA-C1B-C2B	3.45	133.78	124.90
3	S	187	PEB	CAB-C3B-C4B	3.45	131.11	125.01
3	C	167	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
3	F	167	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
3	N	188	PEB	CBC-CAC-C2C	-3.43	106.16	112.49
3	K	167	PEB	OD-C4D-ND	-3.42	120.87	125.93
3	V	186	PEB	CHA-C1B-NB	-3.42	117.79	124.93
3	H	166	PEB	C3D-C4D-ND	3.42	113.96	107.26
3	J	167	PEB	CHC-C1D-ND	-3.41	109.98	113.95
3	P	186	PEB	CHA-C1B-NB	-3.41	117.80	124.93
3	N	186	PEB	CAB-C3B-C4B	3.41	131.04	125.01
3	H	166	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
3	T	188	PEB	CHA-C4A-NA	3.37	129.21	125.20
3	R	186	PEB	CHA-C1B-NB	-3.36	117.90	124.93
3	C	167	PEB	CHB-C4B-NB	-3.35	124.18	128.83
3	A	167	PEB	C3D-C4D-ND	3.35	113.83	107.26
3	M	186	PEB	CHA-C1B-C2B	3.35	133.51	124.90
3	K	167	PEB	CHA-C4A-NA	3.35	129.18	125.20
3	I	166	PEB	CMB-C2B-C1B	3.34	130.21	125.06
3	G	167	PEB	CHC-C1D-ND	-3.34	110.06	113.95
3	L	167	PEB	CMB-C2B-C1B	3.31	130.16	125.06
3	H	166	PEB	CHB-C4B-NB	-3.31	124.24	128.83
3	B	166	PEB	CAC-CBC-CGC	-3.30	107.14	112.67
3	S	188	PEB	CMB-C2B-C1B	3.29	130.13	125.06
3	W	186	PEB	CMB-C2B-C1B	3.29	130.13	125.06
3	Q	187	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
3	R	187	PEB	CHA-C4A-NA	3.29	129.11	125.20
3	W	188	PEB	CAB-C3B-C4B	3.28	130.82	125.01
3	X	188	PEB	C2A-C1A-NA	3.28	111.10	108.27
3	D	166	PEB	CHA-C1B-C2B	3.28	133.34	124.90
3	K	166	PEB	CHA-C1B-C2B	3.27	133.31	124.90
3	X	188	PEB	CMB-C2B-C1B	3.27	130.10	125.06
3	H	167	PEB	CHC-C1D-ND	-3.26	110.16	113.95
3	L	167	PEB	CAB-C3B-C4B	3.22	130.70	125.01
3	K	166	PEB	OA-C1A-C2A	-3.22	123.62	126.17
3	W	186	PEB	CHA-C1B-C2B	3.21	133.15	124.90
3	V	188	PEB	OD-C4D-C3D	-3.21	122.20	129.46
3	Q	188	PEB	C2A-C1A-NA	3.18	111.02	108.27
3	O	186	PEB	CHC-C1D-ND	-3.17	110.26	113.95
3	M	186	PEB	OA-C1A-C2A	-3.16	123.66	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	166	PEB	CHB-C4B-NB	-3.15	124.46	128.83
3	S	186[A]	PEB	CAB-C3B-C4B	3.15	130.58	125.01
3	S	186[B]	PEB	CAB-C3B-C4B	3.15	130.58	125.01
5	B	204	PI	O2-P-O1	-3.14	99.41	110.89
3	N	186	PEB	CHB-C4B-C3B	-3.13	118.09	125.32
3	T	188	PEB	OD-C4D-ND	-3.13	121.30	125.93
3	C	166	PEB	CAC-CBC-CGC	-3.12	107.44	112.67
3	T	188	PEB	C3D-C4D-ND	3.12	113.38	107.26
3	N	188	PEB	OA-C1A-C2A	-3.11	123.70	126.17
3	P	188	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
3	P	187	PEB	CAC-CBC-CGC	3.10	117.87	112.67
3	D	166	PEB	CMB-C2B-C1B	3.10	129.84	125.06
3	X	188	PEB	CHC-C4C-C3C	-3.10	125.06	130.34
3	P	186	PEB	CHA-C1B-C2B	3.09	132.85	124.90
3	W	187	PEB	C2A-C1A-NA	3.09	110.94	108.27
3	M	187	PEB	CHC-C1D-ND	-3.09	110.36	113.95
3	B	166	PEB	CHA-C1B-C2B	3.08	132.83	124.90
3	N	186	PEB	CHA-C1B-C2B	3.08	132.83	124.90
3	A	167	PEB	OD-C4D-ND	-3.08	121.37	125.93
3	W	187	PEB	CMB-C2B-C1B	3.08	129.81	125.06
3	S	188	PEB	CHC-C4C-C3C	-3.08	125.09	130.34
3	L	166	PEB	CMA-C2A-C1A	-3.08	105.77	112.40
3	V	187	PEB	OA-C1A-C2A	3.07	128.62	126.17
3	K	166	PEB	CAC-CBC-CGC	-3.06	107.53	112.67
7	R	204	MPD	C5-C4-C3	-3.06	97.27	111.69
3	X	186	PEB	CAC-CBC-CGC	3.05	117.79	112.67
3	I	167	PEB	CHC-C4C-C3C	-3.05	125.14	130.34
3	T	188	PEB	CAB-C3B-C4B	3.04	130.39	125.01
3	F	166	PEB	CHA-C1B-C2B	3.04	132.72	124.90
3	J	167	PEB	OD-C4D-ND	-3.04	121.42	125.93
3	H	166	PEB	CHC-C4C-C3C	-3.04	125.16	130.34
3	D	167	PEB	CMB-C2B-C1B	3.02	129.72	125.06
3	T	186	PEB	OD-C4D-C3D	-3.02	122.61	129.46
3	U	187	PEB	CHA-C4A-NA	3.02	128.80	125.20
3	T	186	PEB	CAB-CBB-CGB	-3.02	107.60	112.67
3	M	188	PEB	OA-C1A-C2A	-3.01	123.78	126.17
3	I	166	PEB	CHA-C1B-C2B	3.01	132.65	124.90
3	L	167	PEB	C3D-C4D-ND	3.01	113.17	107.26
3	K	167	PEB	CMB-C2B-C1B	3.00	129.68	125.06
3	R	187	PEB	CAB-C3B-C4B	3.00	130.31	125.01
3	L	166	PEB	C1C-CHB-C4B	3.00	132.39	128.81
3	T	188	PEB	OA-C1A-NA	-2.98	121.34	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	186	PEB	C3D-C4D-ND	2.97	113.09	107.26
3	T	188	PEB	CHC-C4C-C3C	-2.96	125.28	130.34
3	J	166	PEB	CAB-C3B-C4B	2.96	130.25	125.01
3	S	186[A]	PEB	CHA-C1B-NB	-2.95	118.75	124.93
3	S	186[B]	PEB	CHA-C1B-NB	-2.95	118.75	124.93
3	F	166	PEB	CHB-C4B-NB	-2.95	124.73	128.83
3	M	188	PEB	CAB-C3B-C4B	2.94	130.21	125.01
3	W	188	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
3	S	188	PEB	OD-C4D-C3D	-2.94	122.81	129.46
3	N	187	PEB	C1C-CHB-C4B	2.93	132.31	128.81
3	N	188	PEB	OD-C4D-C3D	-2.91	122.86	129.46
3	O	187	PEB	CHA-C4A-NA	2.91	128.67	125.20
3	E	167	PEB	CHC-C1D-ND	-2.91	110.56	113.95
3	S	186[A]	PEB	OD-C4D-C3D	-2.91	122.86	129.46
3	S	186[B]	PEB	OD-C4D-C3D	-2.91	122.86	129.46
3	I	167	PEB	C2A-C1A-NA	2.91	110.78	108.27
3	I	166	PEB	CAC-CBC-CGC	-2.89	107.82	112.67
3	X	187	PEB	CMD-C2D-C3D	-2.88	126.00	130.06
3	J	167	PEB	CHC-C4C-C3C	-2.88	125.42	130.34
3	S	188	PEB	C3D-C4D-ND	2.88	112.91	107.26
3	P	186	PEB	CHA-C4A-NA	2.88	128.63	125.20
3	V	188	PEB	C2A-C1A-NA	2.87	110.74	108.27
3	W	187	PEB	OD-C4D-ND	-2.86	121.69	125.93
3	W	186	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
3	R	186	PEB	OD-C4D-ND	-2.85	121.70	125.93
3	R	186	PEB	CHC-C4C-C3C	-2.85	125.47	130.34
3	H	166	PEB	CHA-C1B-C2B	2.85	132.23	124.90
3	U	186	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
3	T	187	PEB	C1C-CHB-C4B	2.84	132.21	128.81
3	S	187	PEB	OA-C1A-C2A	-2.83	123.92	126.17
3	N	186	PEB	CMB-C2B-C1B	2.83	129.43	125.06
3	V	187	PEB	CHC-C4C-C3C	-2.83	125.51	130.34
3	A	166	PEB	CMA-C2A-C1A	-2.83	106.31	112.40
3	V	186	PEB	OD-C4D-ND	-2.82	121.75	125.93
3	S	187	PEB	CHC-C1D-ND	-2.82	110.67	113.95
3	C	167	PEB	CHA-C4A-NA	2.82	128.56	125.20
3	M	188	PEB	C3D-C4D-ND	2.82	112.79	107.26
3	O	187	PEB	CAC-CBC-CGC	2.82	117.39	112.67
3	P	187	PEB	OD-C4D-C3D	-2.81	123.09	129.46
3	W	187	PEB	CHC-C4C-C3C	-2.80	125.55	130.34
3	X	186	PEB	OD-C4D-C3D	-2.80	123.12	129.46
3	T	186	PEB	CHC-C1D-ND	-2.80	110.70	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	W	188	PEB	CMD-C2D-C3D	-2.78	126.14	130.06
3	Q	187	PEB	CMB-C2B-C1B	2.78	129.34	125.06
3	L	166	PEB	C4B-C3B-C2B	2.77	109.85	106.78
3	S	187	PEB	C3B-C4B-NB	2.77	114.08	110.05
3	E	167	PEB	CAB-C3B-C4B	2.77	129.91	125.01
3	P	188	PEB	CHC-C4C-C3C	-2.77	125.61	130.34
3	K	167	PEB	CBC-CAC-C2C	-2.77	107.38	112.49
7	B	203	MPD	O4-C4-C3	-2.77	100.19	111.36
3	N	187	PEB	C2A-C1A-NA	-2.77	105.89	108.27
3	K	166	PEB	CMA-C2A-C1A	-2.76	106.45	112.40
3	Q	188	PEB	CHA-C4A-NA	2.76	128.49	125.20
3	W	188	PEB	CBC-CAC-C2C	-2.76	107.39	112.49
3	R	187	PEB	OA-C1A-NA	2.76	128.28	124.94
3	E	166	PEB	OD-C4D-C3D	-2.76	123.21	129.46
3	N	187	PEB	CHC-C1D-ND	-2.75	110.75	113.95
3	M	188	PEB	CHC-C4C-C3C	-2.75	125.65	130.34
3	S	186[A]	PEB	OA-C1A-NA	2.74	128.26	124.94
3	S	186[B]	PEB	OA-C1A-NA	2.74	128.26	124.94
3	Q	188	PEB	CMB-C2B-C1B	2.74	129.28	125.06
3	D	167	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
3	F	167	PEB	OD-C4D-C3D	-2.74	123.26	129.46
7	B	203	MPD	C1-C2-C3	-2.73	97.24	109.96
3	V	188	PEB	CMB-C2B-C1B	2.73	129.27	125.06
3	P	187	PEB	C1C-CHB-C4B	2.72	132.06	128.81
3	G	167	PEB	CAB-C3B-C4B	2.72	129.82	125.01
3	R	186	PEB	OD-C4D-C3D	-2.72	123.30	129.46
3	P	187	PEB	CHC-C4C-C3C	-2.72	125.70	130.34
3	Q	187	PEB	C1C-CHB-C4B	2.72	132.05	128.81
3	I	167	PEB	CAB-C3B-C2B	-2.71	122.83	127.88
3	F	166	PEB	CMC-C3C-C2C	2.71	130.05	124.94
3	R	186	PEB	CHA-C1B-C2B	2.71	131.87	124.90
3	W	188	PEB	CBD-CAD-C3D	-2.71	114.15	127.62
3	N	186	PEB	OA-C1A-C2A	-2.70	124.02	126.17
3	X	187	PEB	CMB-C2B-C1B	2.69	129.21	125.06
3	P	188	PEB	CHA-C4A-NA	2.69	128.40	125.20
3	M	187	PEB	C1C-CHB-C4B	2.68	132.01	128.81
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	X	188	PEB	CHC-C1D-ND	-2.68	110.84	113.95
3	B	167	PEB	CMD-C2D-C3D	-2.68	126.29	130.06
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	166	PEB	CMB-C2B-C1B	2.67	129.17	125.06
3	V	188	PEB	CAB-CBB-CGB	2.66	117.13	112.67
3	W	186	PEB	CAB-C3B-C4B	2.66	129.71	125.01
3	F	167	PEB	CAB-C3B-C4B	2.65	129.69	125.01
3	P	186	PEB	CHC-C1D-ND	-2.65	110.88	113.95
3	U	186	PEB	OA-C1A-NA	2.64	128.14	124.94
3	R	188	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
3	M	187	PEB	CMB-C2B-C1B	2.64	129.12	125.06
3	C	166	PEB	OD-C4D-C3D	-2.63	123.50	129.46
3	C	167	PEB	C2A-C3A-C4A	2.62	105.27	101.34
3	P	188	PEB	CAB-C3B-C4B	2.62	129.65	125.01
3	G	166	PEB	CAC-CBC-CGC	-2.62	108.27	112.67
3	C	167	PEB	OA-C1A-NA	-2.62	121.77	124.94
5	C	204	PI	O3-P-O1	-2.62	101.32	110.89
3	A	167	PEB	OA-C1A-C2A	-2.61	124.10	126.17
3	E	166	PEB	CAC-CBC-CGC	-2.61	108.29	112.67
3	J	167	PEB	C3D-C4D-ND	2.61	112.37	107.26
3	X	188	PEB	OD-C4D-C3D	-2.61	123.56	129.46
3	X	186	PEB	CMD-C2D-C3D	-2.60	126.40	130.06
3	C	167	PEB	C3D-C4D-ND	2.60	112.36	107.26
3	B	167	PEB	CHB-C4B-C3B	-2.60	119.32	125.32
3	B	167	PEB	CHC-C4C-C3C	-2.60	125.91	130.34
3	S	187	PEB	CHB-C4B-C3B	-2.59	119.33	125.32
3	X	186	PEB	C3D-C4D-ND	2.59	112.33	107.26
3	R	187	PEB	OD-C4D-C3D	-2.58	123.61	129.46
3	S	186[A]	PEB	C4B-C3B-C2B	-2.58	103.93	106.78
3	S	186[B]	PEB	C4B-C3B-C2B	-2.58	103.93	106.78
3	O	186	PEB	CHA-C1B-C2B	2.58	131.53	124.90
3	O	188	PEB	OD-C4D-C3D	-2.58	123.63	129.46
3	U	187	PEB	C1B-C2B-C3B	-2.57	103.56	106.51
3	H	166	PEB	CHC-C1D-ND	-2.57	110.97	113.95
3	Q	186	PEB	C2A-C1A-NA	2.57	110.48	108.27
3	Q	186	PEB	CHA-C1B-C2B	2.56	131.50	124.90
3	N	188	PEB	CBD-CAD-C3D	-2.56	114.87	127.62
3	L	166	PEB	CHB-C4B-NB	-2.56	125.27	128.83
5	B	204	PI	O4-P-O3	2.56	116.19	107.97
3	R	187	PEB	OA-C1A-C2A	-2.56	124.14	126.17
3	T	188	PEB	C3B-C4B-NB	2.55	113.76	110.05
3	K	167	PEB	CHB-C4B-C3B	-2.55	119.43	125.32
3	P	187	PEB	C3D-C4D-ND	2.55	112.26	107.26
3	D	167	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
3	G	166	PEB	CMB-C2B-C1B	2.54	128.97	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	166	PEB	C3D-C4D-ND	2.53	112.23	107.26
3	R	186	PEB	CAB-CBB-CGB	-2.53	108.42	112.67
3	G	166	PEB	CHB-C4B-NB	-2.53	125.31	128.83
3	D	166	PEB	C1C-CHB-C4B	2.53	131.83	128.81
3	W	187	PEB	CMD-C2D-C3D	-2.53	126.50	130.06
3	U	186	PEB	CHA-C1B-C2B	2.52	131.39	124.90
3	T	186	PEB	CHB-C4B-C3B	-2.52	119.49	125.32
3	P	186	PEB	OA-C1A-C2A	-2.52	124.17	126.17
3	V	186	PEB	CMB-C2B-C1B	2.52	128.94	125.06
3	X	188	PEB	CMD-C2D-C3D	-2.51	126.53	130.06
3	Q	188	PEB	CMD-C2D-C3D	-2.51	126.53	130.06
3	V	186	PEB	C3D-C4D-ND	2.50	112.17	107.26
3	Q	186	PEB	C3D-C4D-ND	2.50	112.17	107.26
3	V	188	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
3	B	167	PEB	C1C-CHB-C4B	-2.49	125.83	128.81
3	I	167	PEB	CBC-CAC-C2C	-2.49	107.89	112.49
3	V	188	PEB	OA-C1A-C2A	-2.49	124.19	126.17
3	N	188	PEB	CMB-C2B-C1B	2.48	128.89	125.06
3	T	188	PEB	CBC-CAC-C2C	-2.48	107.91	112.49
3	W	186	PEB	OD-C4D-C3D	-2.48	123.84	129.46
3	Q	186	PEB	CMB-C2B-C1B	2.48	128.88	125.06
3	I	166	PEB	OD-C4D-C3D	-2.48	123.84	129.46
3	R	186	PEB	OA-C1A-NA	2.48	127.94	124.94
3	L	166	PEB	CHC-C4C-C3C	-2.48	126.11	130.34
3	P	187	PEB	CAB-CBB-CGB	-2.48	108.52	112.67
3	D	166	PEB	CAB-C3B-C4B	2.47	129.37	125.01
3	N	188	PEB	CHC-C4C-C3C	-2.46	126.14	130.34
3	G	166	PEB	CMC-C3C-C2C	2.46	129.58	124.94
3	J	167	PEB	C2A-C1A-NA	2.46	110.39	108.27
3	S	186[A]	PEB	CHA-C1B-C2B	2.46	131.22	124.90
3	S	186[B]	PEB	CHA-C1B-C2B	2.46	131.22	124.90
3	R	188	PEB	CMB-C2B-C1B	2.46	128.85	125.06
3	I	167	PEB	C4B-NB-C1B	2.45	111.12	106.51
3	Q	188	PEB	C3D-C4D-ND	2.44	112.04	107.26
3	P	188	PEB	C2A-C3A-C4A	2.43	104.98	101.34
3	N	187	PEB	C4B-C3B-C2B	-2.43	104.09	106.78
3	L	167	PEB	C2A-C1A-NA	2.43	110.37	108.27
3	F	166	PEB	CMA-C2A-C1A	-2.43	107.16	112.40
3	H	167	PEB	CHC-C4C-C3C	-2.43	126.20	130.34
3	I	167	PEB	CAB-C3B-C4B	2.43	129.30	125.01
3	G	167	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
3	O	186	PEB	C3D-C4D-ND	2.41	111.98	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	167	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
3	B	166	PEB	CHC-C4C-C3C	-2.40	126.24	130.34
5	P	205	PI	O3-P-O2	2.40	115.68	107.97
3	W	186	PEB	C3D-C4D-ND	2.39	111.95	107.26
3	C	167	PEB	C1C-CHB-C4B	2.39	131.66	128.81
3	W	188	PEB	C2A-C3A-C4A	2.39	104.91	101.34
3	O	186	PEB	OD-C4D-C3D	-2.38	124.07	129.46
3	R	187	PEB	CHC-C1D-ND	-2.38	111.19	113.95
3	U	187	PEB	CMB-C2B-C1B	2.37	128.71	125.06
7	M	204	MPD	CM-C2-C1	-2.36	105.65	110.57
3	N	187	PEB	CMB-C2B-C1B	2.36	128.70	125.06
3	F	166	PEB	CMB-C2B-C1B	2.36	128.70	125.06
3	A	167	PEB	CAB-C3B-C4B	2.36	129.18	125.01
3	D	166	PEB	CHC-C4C-C3C	-2.36	126.31	130.34
3	R	187	PEB	C2A-C3A-C4A	2.36	104.87	101.34
3	M	186	PEB	OD-C4D-C3D	-2.36	124.12	129.46
3	J	166	PEB	CHC-C4C-C3C	-2.35	126.32	130.34
3	Q	186	PEB	OD-C4D-ND	-2.35	122.44	125.93
3	O	186	PEB	CHB-C4B-NB	-2.35	125.56	128.83
3	B	167	PEB	OD-C4D-ND	-2.35	122.45	125.93
3	Q	188	PEB	CBD-CAD-C3D	-2.35	115.93	127.62
3	T	187	PEB	CAC-CBC-CGC	2.35	116.61	112.67
3	W	186	PEB	CHB-C4B-C3B	-2.35	119.90	125.32
3	X	186	PEB	CHA-C1B-NB	-2.35	120.03	124.93
3	B	167	PEB	C4B-C3B-C2B	-2.34	104.19	106.78
3	X	188	PEB	CAB-C3B-C4B	2.34	129.15	125.01
3	K	166	PEB	OD-C4D-ND	-2.34	122.46	125.93
3	U	188	PEB	CHC-C4C-C3C	-2.34	126.35	130.34
3	V	187	PEB	CMD-C2D-C3D	-2.34	126.77	130.06
3	W	187	PEB	CAB-CBB-CGB	-2.33	108.75	112.67
3	D	167	PEB	CAB-C3B-C4B	2.33	129.13	125.01
3	F	167	PEB	C2A-C1A-NA	-2.33	106.27	108.27
3	P	188	PEB	CAC-CBC-CGC	-2.33	108.77	112.67
3	O	186	PEB	CHA-C1B-NB	-2.33	120.07	124.93
3	U	188	PEB	C3D-C4D-ND	2.33	111.82	107.26
3	U	188	PEB	CBC-CAC-C2C	-2.32	108.20	112.49
3	G	166	PEB	CMD-C2D-C3D	-2.32	126.80	130.06
3	V	188	PEB	C3D-C4D-ND	2.31	111.79	107.26
3	X	188	PEB	CHA-C4A-NA	2.31	127.95	125.20
3	U	188	PEB	CMB-C2B-C1B	2.31	128.62	125.06
3	E	166	PEB	CHA-C1B-C2B	2.30	130.83	124.90
3	O	187	PEB	C1B-C2B-C3B	-2.30	103.86	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	188	PEB	C2A-C3A-C4A	2.30	104.78	101.34
3	R	187	PEB	CHA-C1B-NB	-2.30	120.12	124.93
3	W	186	PEB	CHC-C4C-C3C	-2.29	126.42	130.34
3	Q	188	PEB	OD-C4D-ND	-2.29	122.53	125.93
3	U	188	PEB	OD-C4D-C3D	-2.29	124.27	129.46
3	U	186	PEB	C3D-C4D-ND	2.28	111.74	107.26
3	V	187	PEB	CAC-CBC-CGC	2.28	116.50	112.67
3	H	166	PEB	C2C-C3C-C4C	-2.28	102.23	111.33
3	W	188	PEB	C3D-C4D-ND	2.28	111.73	107.26
3	M	186	PEB	C2A-C3A-C4A	2.28	104.75	101.34
3	V	187	PEB	CHC-C1D-ND	-2.28	111.30	113.95
3	L	166	PEB	C4B-NB-C1B	2.28	110.80	106.51
3	S	188	PEB	CAB-C3B-C4B	2.27	129.02	125.01
3	F	167	PEB	CHA-C4A-NA	2.27	127.90	125.20
3	T	186	PEB	CAC-CBC-CGC	2.27	116.47	112.67
3	O	188	PEB	CHC-C4C-C3C	-2.27	126.47	130.34
3	P	186	PEB	CHB-C4B-C3B	-2.26	120.11	125.32
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	A	167	PEB	C2A-C1A-NA	2.26	110.22	108.27
3	N	188	PEB	CAB-C3B-C4B	2.25	128.99	125.01
3	T	186	PEB	CHA-C1B-C2B	2.25	130.68	124.90
3	T	187	PEB	C1B-C2B-C3B	-2.24	103.93	106.51
3	O	188	PEB	CAB-C3B-C4B	2.24	128.98	125.01
3	G	166	PEB	C1C-CHB-C4B	2.24	131.49	128.81
3	I	167	PEB	OD-C4D-C3D	-2.24	124.38	129.46
3	R	188	PEB	C3D-C4D-ND	2.24	111.65	107.26
3	L	166	PEB	OD-C4D-C3D	-2.24	124.39	129.46
3	Q	187	PEB	CAC-CBC-CGC	2.24	116.42	112.67
3	E	166	PEB	C2C-C3C-C4C	-2.23	102.43	111.33
3	X	188	PEB	CHB-C4B-C3B	-2.23	120.17	125.32
3	A	167	PEB	CHB-C4B-NB	-2.23	125.73	128.83
3	Q	187	PEB	C2A-C3A-C4A	2.23	104.68	101.34
3	Q	187	PEB	CHA-C1B-NB	-2.22	120.28	124.93
3	T	188	PEB	CBD-CAD-C3D	-2.22	116.56	127.62
3	T	187	PEB	CAB-CBB-CGB	-2.22	108.95	112.67
3	K	167	PEB	C3D-C4D-ND	2.22	111.61	107.26
3	C	167	PEB	OD-C4D-C3D	-2.22	124.44	129.46
3	O	188	PEB	CBD-CAD-C3D	-2.21	116.63	127.62
3	X	188	PEB	C2C-C3C-C4C	-2.21	102.53	111.33
3	P	188	PEB	CHB-C4B-C3B	-2.20	120.23	125.32
3	F	167	PEB	CBC-CAC-C2C	-2.20	108.43	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	188	PEB	C1C-CHB-C4B	2.20	131.44	128.81
3	D	167	PEB	C3B-C4B-NB	2.20	113.25	110.05
3	S	186[B]	PEB	CAC-CBC-CGC	2.20	116.36	112.67
5	N	204	PI	O4-P-O1	-2.20	102.86	110.89
3	T	188	PEB	CHB-C4B-C3B	-2.19	120.26	125.32
7	O	204	MPD	O2-C2-C1	2.19	115.11	108.08
3	C	166	PEB	CHB-C4B-C3B	-2.19	120.26	125.32
3	P	186	PEB	C3D-C4D-ND	2.19	111.55	107.26
3	O	186	PEB	C1C-CHB-C4B	2.18	131.42	128.81
3	X	186	PEB	CHA-C1B-C2B	2.18	130.52	124.90
7	X	204	MPD	CM-C2-C1	-2.18	106.03	110.57
3	U	187	PEB	CBC-CAC-C2C	-2.18	108.47	112.49
3	T	186	PEB	C4B-C3B-C2B	-2.17	104.38	106.78
3	T	187	PEB	CAA-C3A-C2A	-2.17	108.84	114.26
3	U	187	PEB	CHA-C1B-NB	-2.17	120.39	124.93
3	V	186	PEB	OA-C1A-C2A	-2.17	124.45	126.17
3	W	187	PEB	OA-C1A-NA	-2.17	122.32	124.94
7	R	204	MPD	O2-C2-CM	2.17	115.03	108.08
3	J	167	PEB	C2A-C3A-C4A	2.17	104.58	101.34
3	M	187	PEB	CAB-C3B-C4B	2.16	128.84	125.01
3	U	187	PEB	OD-C4D-C3D	-2.16	124.56	129.46
3	Q	186	PEB	CAC-CBC-CGC	-2.16	109.05	112.67
3	R	187	PEB	C3D-C4D-ND	2.16	111.49	107.26
3	P	187	PEB	OA-C1A-C2A	-2.16	124.46	126.17
3	S	186[A]	PEB	OD-C4D-ND	-2.16	122.74	125.93
3	S	186[B]	PEB	OD-C4D-ND	-2.16	122.74	125.93
3	E	167	PEB	C4B-C3B-C2B	-2.15	104.40	106.78
3	U	187	PEB	OA-C1A-C2A	-2.15	124.46	126.17
3	T	186	PEB	C3D-C4D-ND	2.15	111.48	107.26
3	M	186	PEB	OD-C4D-ND	-2.15	122.74	125.93
3	I	166	PEB	CMA-C2A-C1A	-2.15	107.77	112.40
3	N	186	PEB	C2A-C3A-C4A	2.14	104.55	101.34
3	M	188	PEB	CAB-C3B-C2B	-2.14	123.89	127.88
3	L	167	PEB	CAB-C3B-C2B	-2.14	123.89	127.88
3	S	188	PEB	C2A-C1A-NA	2.14	110.11	108.27
3	W	187	PEB	CHB-C4B-C3B	-2.13	120.39	125.32
3	P	186	PEB	C4B-C3B-C2B	-2.13	104.42	106.78
3	B	167	PEB	CHC-C1D-ND	-2.13	111.47	113.95
3	X	187	PEB	OA-C1A-NA	2.13	127.53	124.94
3	I	167	PEB	CMB-C2B-C1B	2.13	128.34	125.06
3	A	166	PEB	OD-C4D-ND	-2.12	122.79	125.93
3	C	166	PEB	CMA-C2A-C1A	-2.12	107.83	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	204	MRD	CM-C2-C1	-2.12	106.16	110.57
3	X	188	PEB	CMC-C3C-C2C	2.11	128.92	124.94
3	R	188	PEB	CHC-C1D-ND	-2.10	111.50	113.95
3	W	188	PEB	CHC-C1D-ND	-2.10	111.51	113.95
3	T	188	PEB	CMB-C2B-C1B	2.10	128.30	125.06
3	W	186	PEB	OA-C1A-C2A	-2.10	124.50	126.17
3	A	167	PEB	CHA-C1B-NB	-2.10	120.54	124.93
3	X	187	PEB	OD-C4D-C3D	-2.10	124.70	129.46
3	I	167	PEB	OA-C1A-C2A	-2.09	124.51	126.17
3	N	187	PEB	OA-C1A-C2A	2.09	127.84	126.17
3	N	186	PEB	C4B-C3B-C2B	-2.09	104.47	106.78
3	U	187	PEB	CHC-C4C-C3C	-2.08	126.78	130.34
3	E	167	PEB	CMB-C2B-C1B	2.08	128.27	125.06
3	T	188	PEB	CHB-C4B-NB	-2.08	125.94	128.83
3	I	166	PEB	C3D-C4D-ND	2.08	111.33	107.26
3	V	186	PEB	CHB-C4B-C3B	-2.07	120.53	125.32
3	A	167	PEB	OD-C4D-C3D	-2.07	124.77	129.46
3	Q	186	PEB	CAB-C3B-C4B	2.07	128.67	125.01
3	U	186	PEB	OD-C4D-ND	-2.07	122.86	125.93
3	L	166	PEB	CAB-C3B-C2B	-2.07	124.03	127.88
3	U	188	PEB	CBD-CAD-C3D	-2.06	117.35	127.62
3	I	167	PEB	CAC-CBC-CGC	2.06	116.13	112.67
3	X	186	PEB	CAB-C3B-C4B	2.06	128.65	125.01
3	S	188	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
3	P	187	PEB	OA-C1A-NA	2.06	127.43	124.94
3	P	187	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
3	G	166	PEB	CHC-C4C-C3C	-2.05	126.83	130.34
3	V	188	PEB	CHC-C1D-ND	-2.05	111.56	113.95
3	W	187	PEB	CHA-C4A-NA	2.05	127.64	125.20
3	X	188	PEB	C1B-C2B-C3B	-2.04	104.16	106.51
3	L	167	PEB	CHB-C4B-NB	-2.04	125.99	128.83
3	B	167	PEB	C2A-C3A-C4A	2.04	104.40	101.34
3	F	166	PEB	CAB-C3B-C4B	2.04	128.61	125.01
3	L	166	PEB	CHC-C1D-ND	-2.03	111.58	113.95
3	M	188	PEB	CBC-CAC-C2C	2.03	116.23	112.49
3	U	187	PEB	C3D-C4D-ND	2.03	111.24	107.26
3	S	187	PEB	CMB-C2B-C1B	2.03	128.19	125.06
3	O	187	PEB	CAA-C3A-C2A	-2.03	109.19	114.26
3	P	188	PEB	OD-C4D-ND	-2.03	122.93	125.93
3	J	167	PEB	CHA-C4A-NA	2.03	127.61	125.20
3	N	186	PEB	C2A-C1A-NA	2.02	110.02	108.27
3	W	186	PEB	C2A-C1A-NA	2.02	110.01	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	188	PEB	C3D-C4D-ND	2.01	111.21	107.26
3	R	187	PEB	CHB-C4B-C3B	-2.01	120.67	125.32
3	J	167	PEB	CMA-C2A-C1A	2.01	116.74	112.40
3	S	187	PEB	CHA-C1B-NB	-2.01	120.72	124.93
3	X	188	PEB	C3D-C4D-ND	2.01	111.20	107.26
3	P	188	PEB	CAB-CBB-CGB	2.01	116.04	112.67
3	J	166	PEB	C2A-C1A-NA	2.01	110.00	108.27
3	F	167	PEB	CHB-C4B-C3B	-2.01	120.68	125.32
3	X	187	PEB	C1C-CHB-C4B	2.01	131.21	128.81
3	D	167	PEB	CHB-C4B-C3B	-2.00	120.70	125.32
3	M	187	PEB	CHB-C4B-C3B	-2.00	120.70	125.32

There are no chirality outliers.

All (174) 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

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Mol	Chain	Res	Type	Atoms
3	J	166	PEB	C2B-C1B-CHA-C4A
3	J	167	PEB	NB-C1B-CHA-C4A
3	J	167	PEB	C2B-C1B-CHA-C4A
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	C2C-CAC-CBC-CGC
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

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Mol	Chain	Res	Type	Atoms
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
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
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

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Mol	Chain	Res	Type	Atoms
3	U	186	PEB	NB-C1B-CHA-C4A
3	V	186	PEB	NB-C1B-CHA-C4A
3	W	186	PEB	NB-C1B-CHA-C4A
3	X	186	PEB	NB-C1B-CHA-C4A
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	O	188	PEB	C4D-C3D-CAD-CBD
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	S	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	Q	187	PEB	C2A-C3A-CAA-CBA
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
8	V	204	MRD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	T	188	PEB	C2D-C3D-CAD-CBD
8	V	204	MRD	C2-C3-C4-C5
3	M	187	PEB	C2A-C3A-CAA-CBA
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	B	167	PEB	C3B-CAB-CBB-CGB
3	S	188	PEB	C2B-C3B-CAB-CBB
3	T	187	PEB	C2A-C3A-CAA-CBA
7	B	203	MPD	O2-C2-C3-C4
3	I	167	PEB	C3B-CAB-CBB-CGB
3	L	167	PEB	C3B-CAB-CBB-CGB
7	B	203	MPD	C2-C3-C4-C5
8	T	204	MRD	C2-C3-C4-C5
3	D	167	PEB	C3B-CAB-CBB-CGB
3	R	187	PEB	C2A-C3A-CAA-CBA
3	S	187	PEB	C2A-C3A-CAA-CBA
3	U	187	PEB	C2A-C3A-CAA-CBA
3	X	187	PEB	C2A-C3A-CAA-CBA
7	P	204	MPD	C2-C3-C4-O4
7	S	204	MPD	C2-C3-C4-O4
7	X	204	MPD	C2-C3-C4-O4

There are no ring outliers.

69 monomers are involved in 218 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	187	PEB	2	0
3	S	187	PEB	1	0
7	W	204	MPD	7	0
3	Q	188	PEB	3	0
3	S	188	PEB	2	0
3	M	186	PEB	2	0
3	M	187	PEB	2	0
3	U	186	PEB	2	0
3	N	188	PEB	2	0
3	M	188	PEB	1	0
3	T	187	PEB	3	0
7	P	204	MPD	6	0
3	I	167	PEB	1	0
3	B	167	PEB	1	0
3	T	186	PEB	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	T	204	MRD	10	0
3	C	167	PEB	1	0
3	W	188	PEB	2	0
3	X	186	PEB	2	0
5	K	203	PI	1	0
7	M	204	MPD	4	0
3	V	188	PEB	2	0
7	X	204	MPD	8	0
3	X	187	PEB	4	0
3	J	167	PEB	1	0
3	T	188	PEB	3	0
5	H	203	PI	2	0
4	L	203	NO3	1	0
3	U	187	PEB	2	0
7	O	204	MPD	9	0
3	L	167	PEB	2	0
3	K	167	PEB	1	0
5	F	203	PI	1	0
3	V	186	PEB	2	0
3	P	188	PEB	2	0
4	A	203	NO3	1	0
8	V	204	MRD	10	0
3	H	167	PEB	2	0
3	E	167	PEB	2	0
3	A	167	PEB	2	0
3	G	167	PEB	2	0
7	B	203	MPD	5	0
3	Q	186	PEB	3	0
5	C	204	PI	1	0
3	F	167	PEB	3	0
5	A	204	PI	11	0
3	R	187	PEB	3	0
7	Q	204	MPD	11	0
3	W	186	PEB	2	0
7	U	204	MPD	8	0
3	O	186	PEB	2	0
3	N	186	PEB	2	0
3	W	187	PEB	2	0
3	O	187	PEB	1	0
3	X	188	PEB	2	0
3	P	186	PEB	2	0
3	P	187	PEB	2	0

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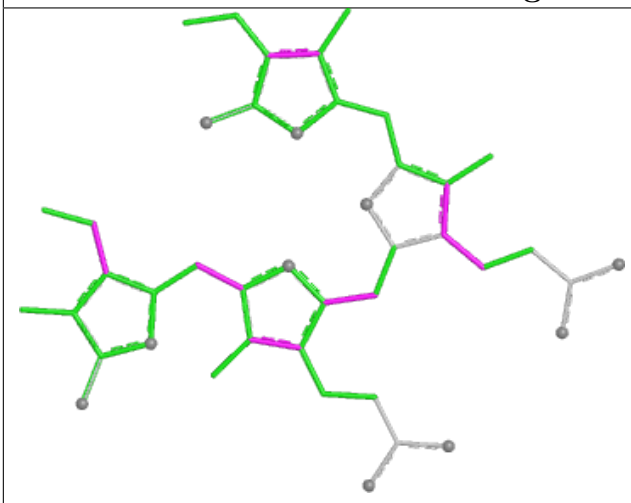
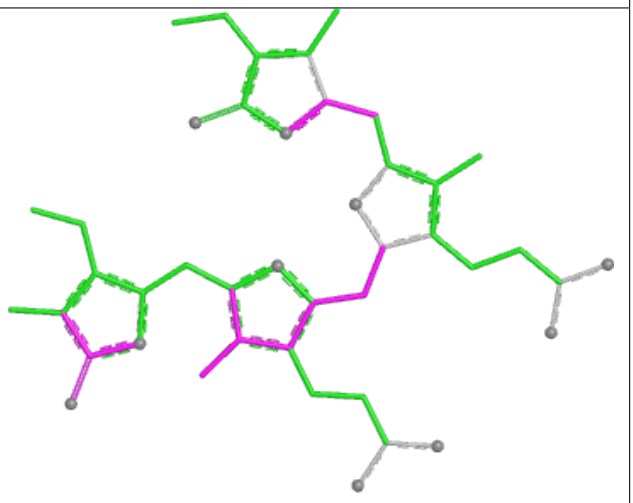
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	203	NO3	1	0
3	D	167	PEB	1	0
3	R	186	PEB	2	0
3	O	188	PEB	3	0
3	V	187	PEB	1	0
3	R	188	PEB	5	0
5	D	204	PI	1	0
3	Q	187	PEB	2	0
7	S	204	MPD	8	0
7	R	204	MPD	15	0
3	C	166	PEB	1	0
3	U	188	PEB	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

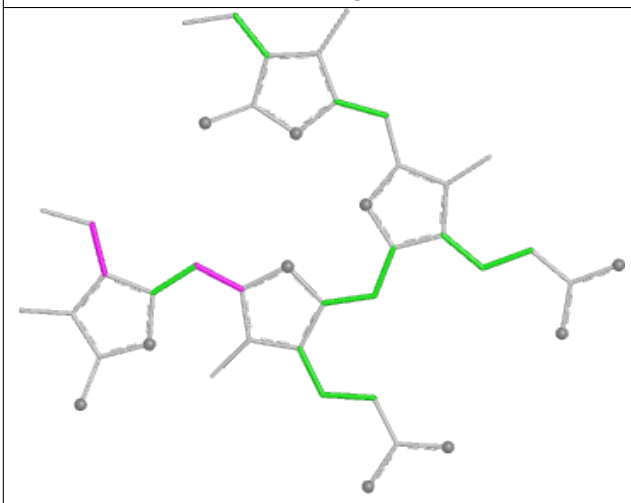
Ligand PEB N 187



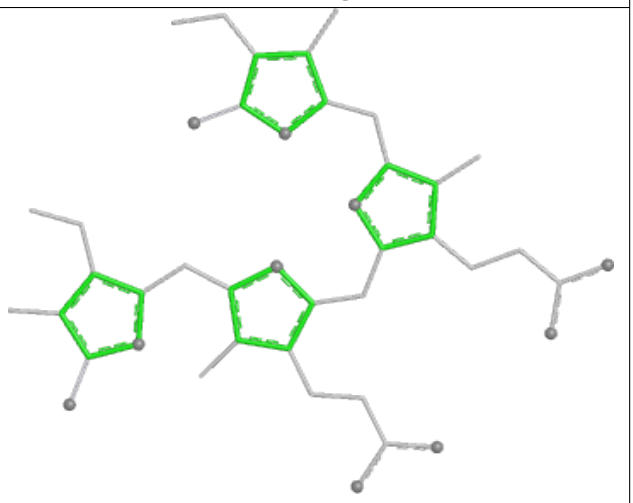
Bond lengths



Bond angles

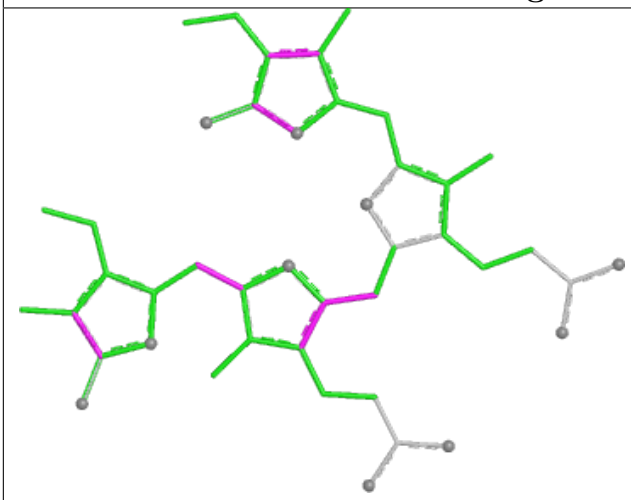


Torsions

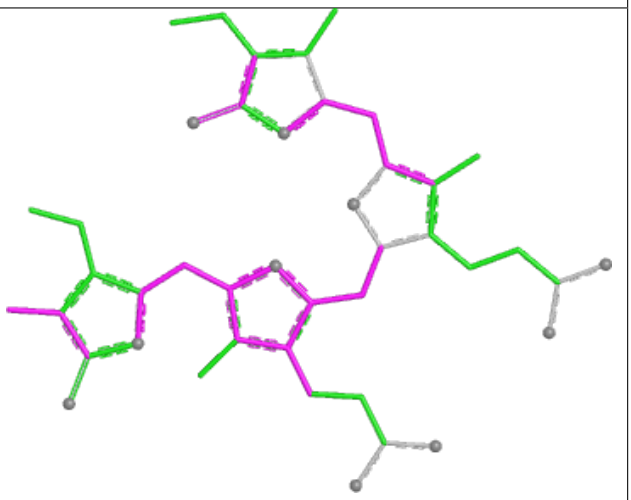


Rings

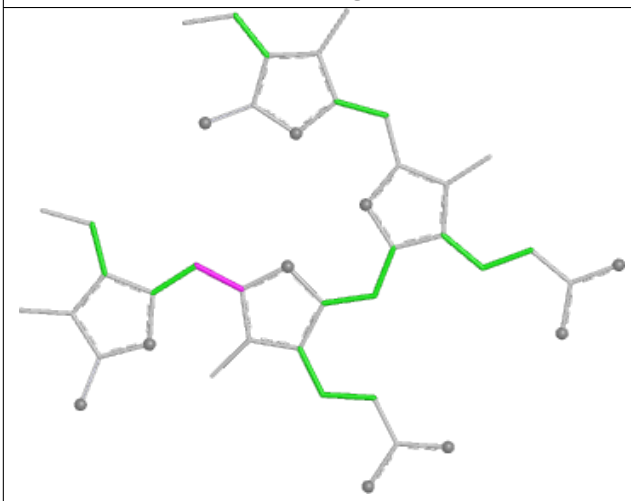
Ligand PEB L 166



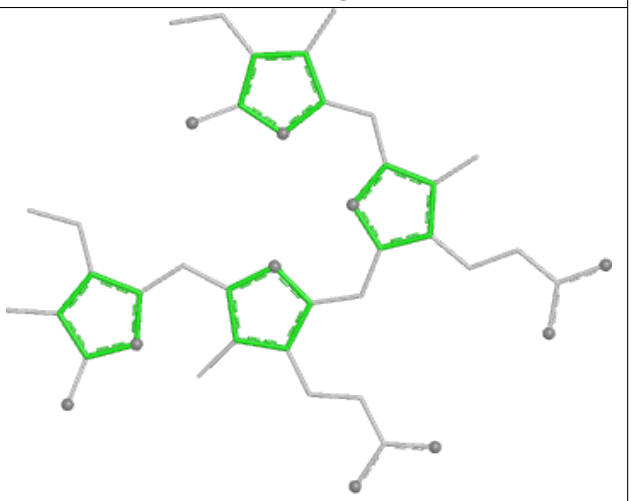
Bond lengths



Bond angles

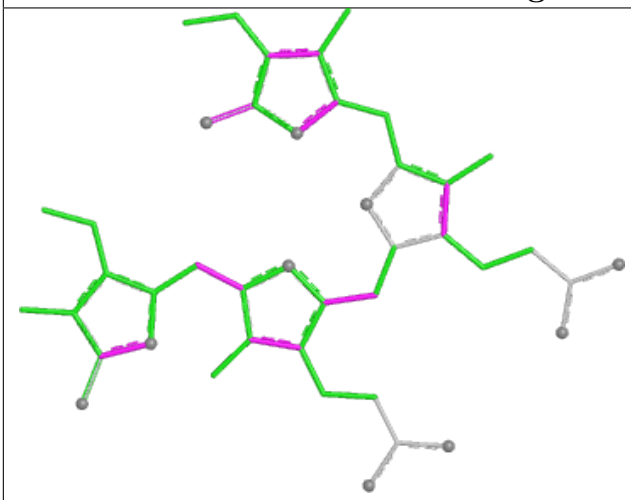


Torsions

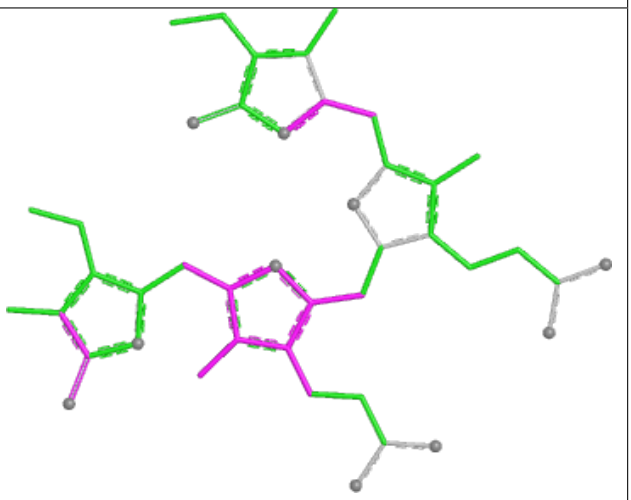


Rings

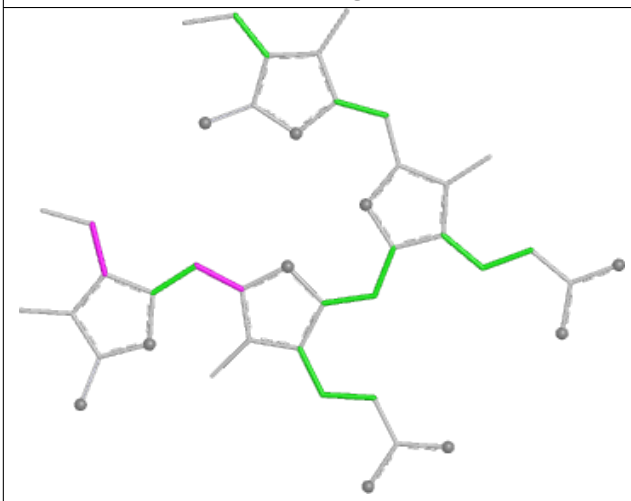
Ligand PEB S 187



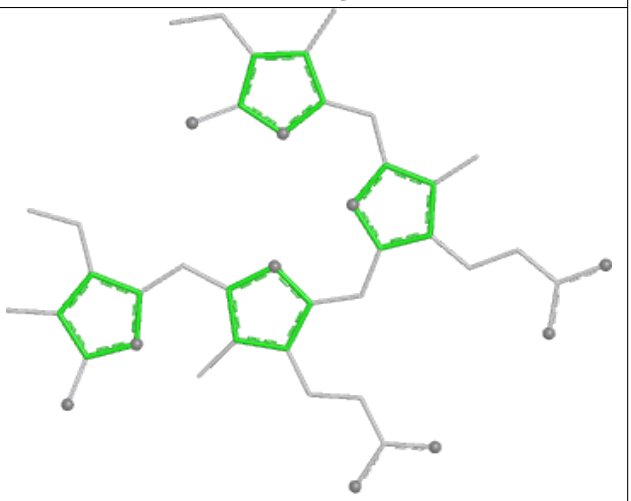
Bond lengths



Bond angles

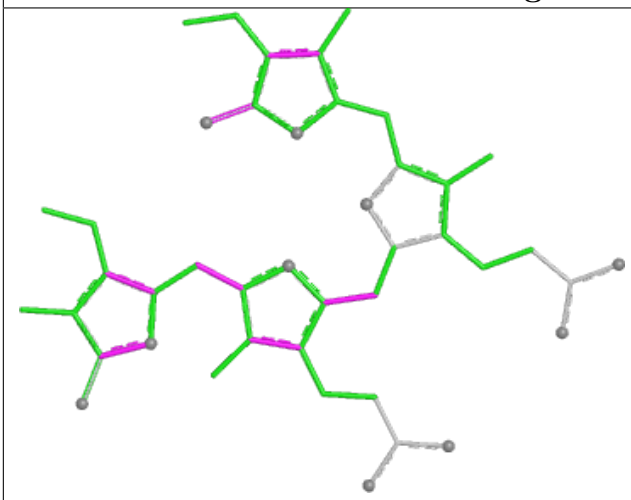


Torsions

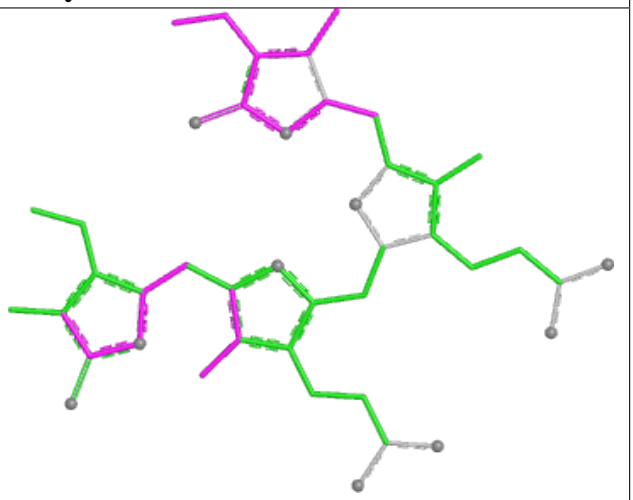


Rings

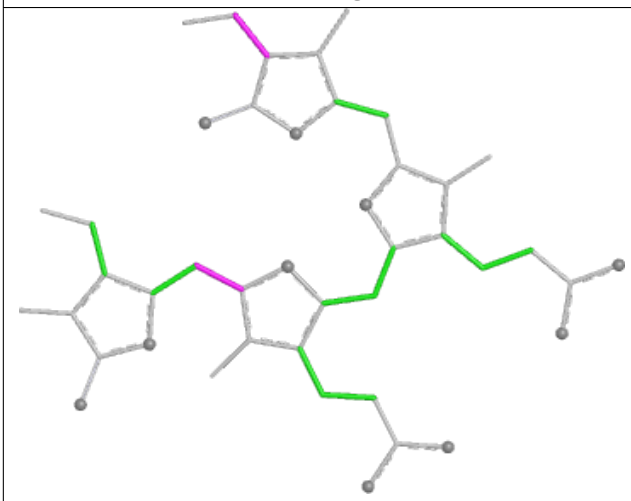
Ligand PEB Q 188



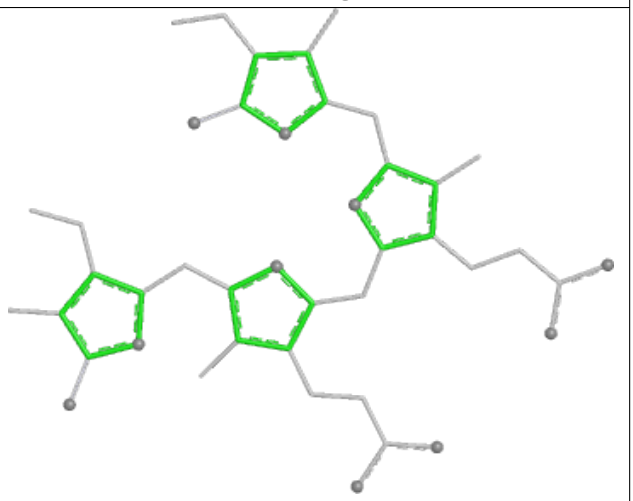
Bond lengths



Bond angles

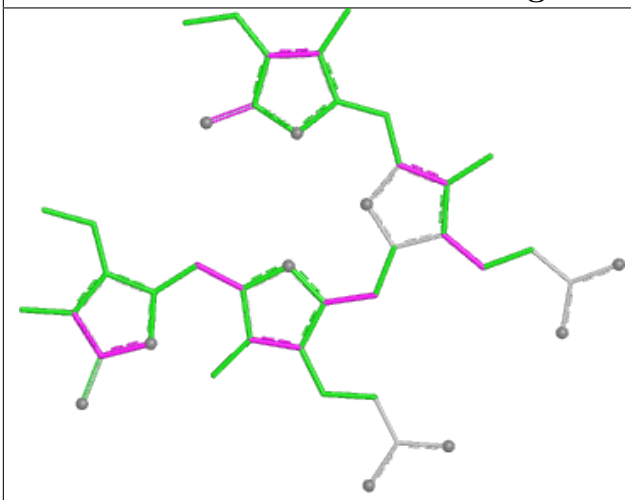


Torsions

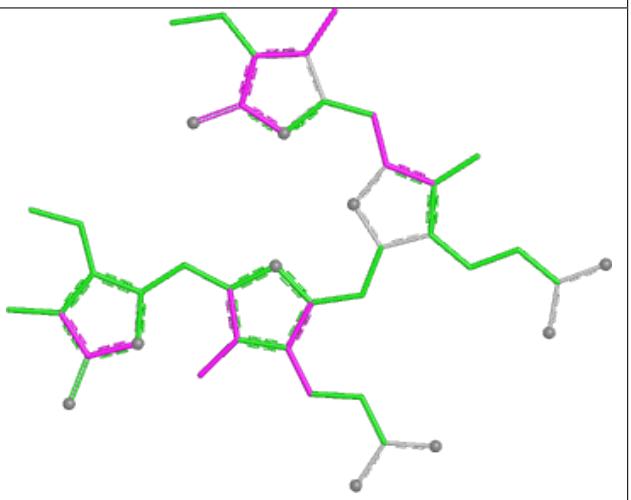


Rings

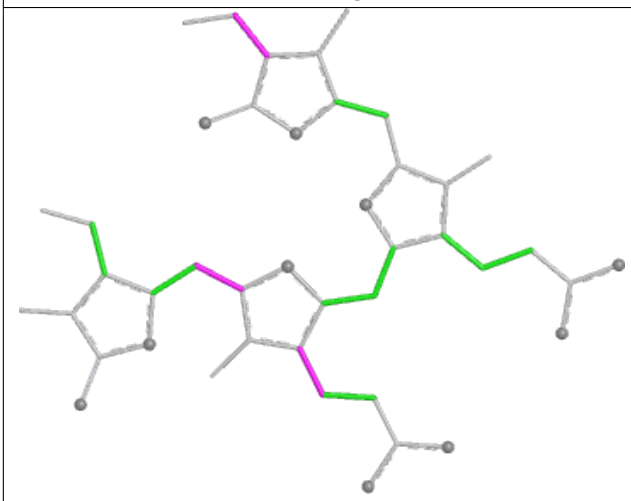
Ligand PEB S 188



Bond lengths



Bond angles



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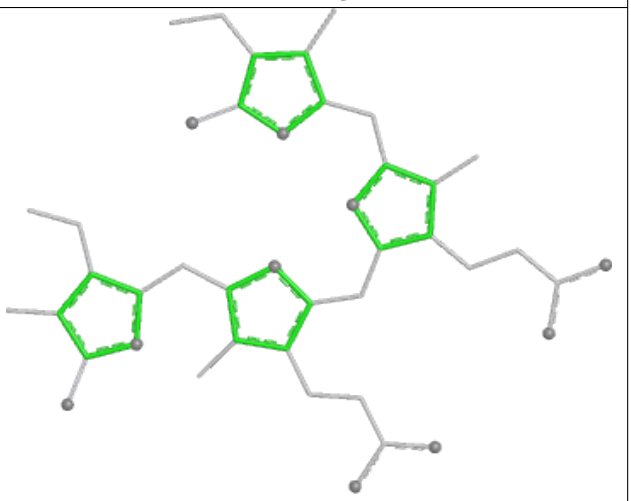
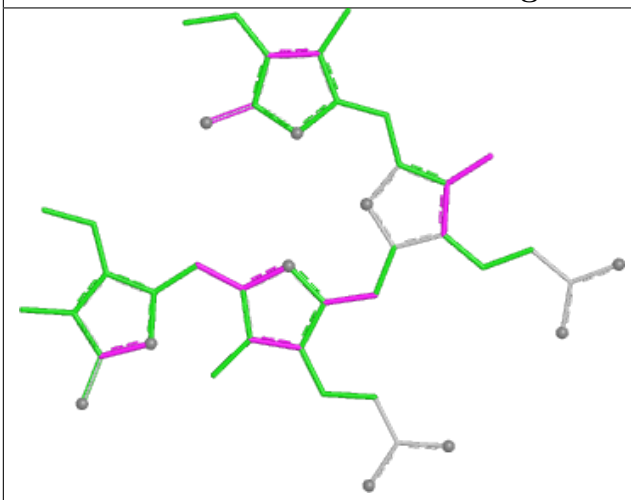


Rings

Ligand PEB M 186



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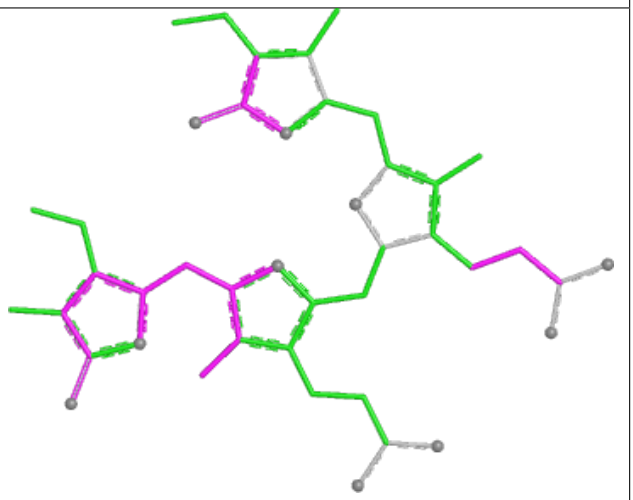
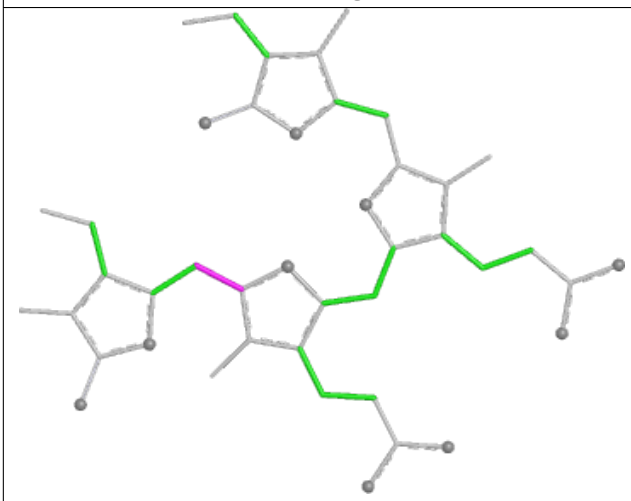
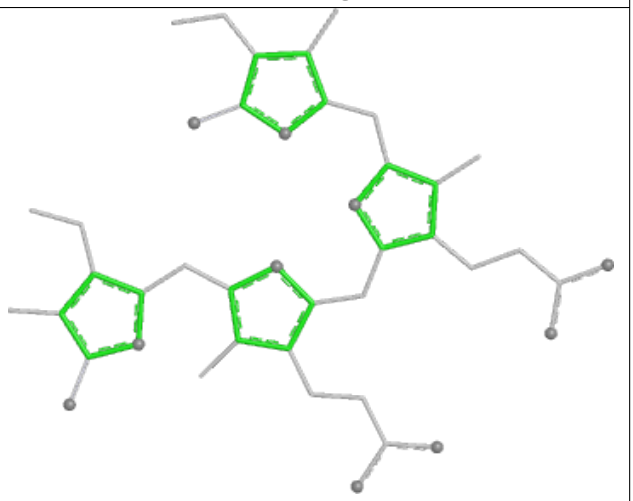


Bond angles

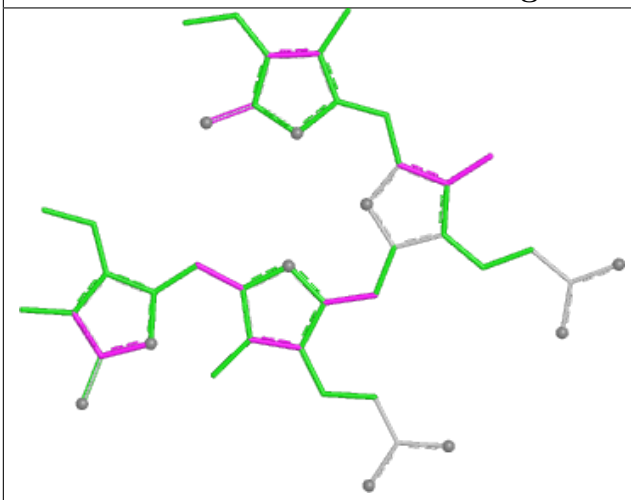


Torsions



Rings

Ligand PEB M 187



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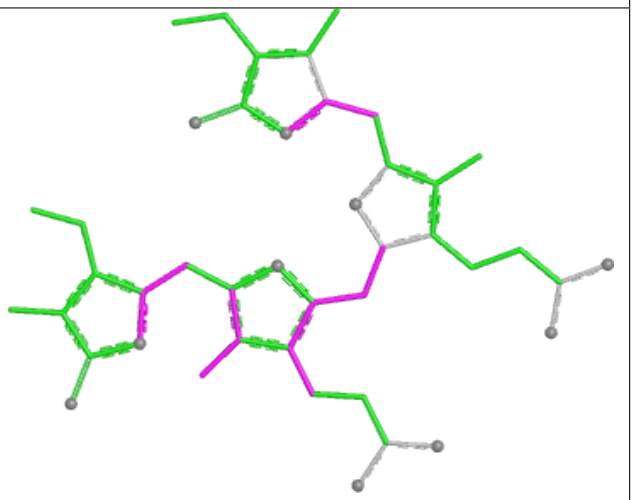

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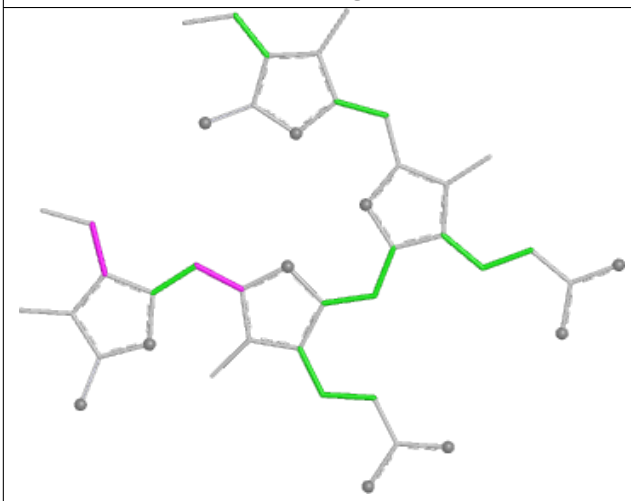

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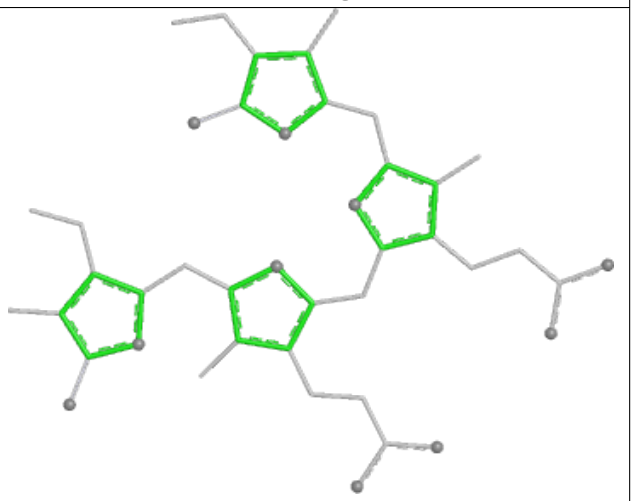
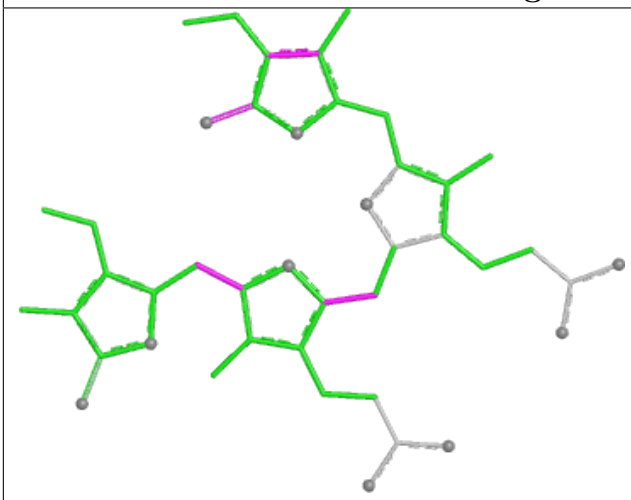


Rings

Ligand PEB A 166



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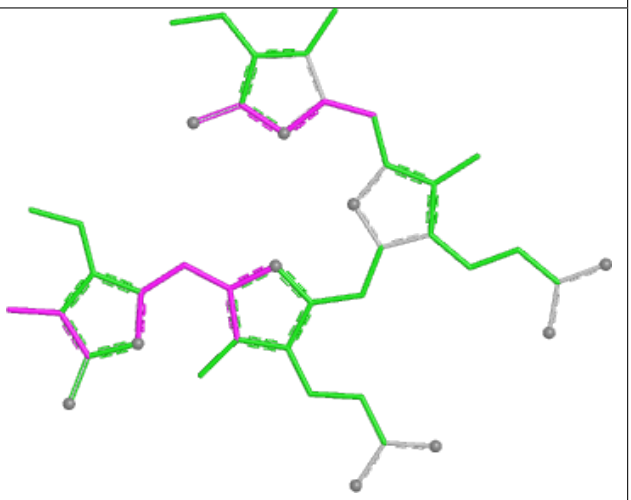
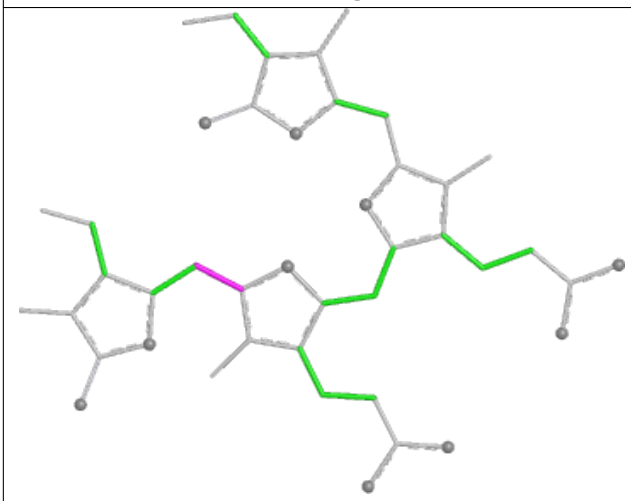


Bond angles



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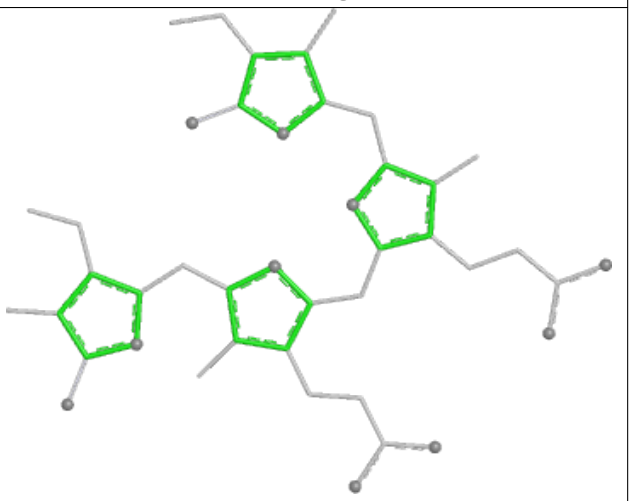
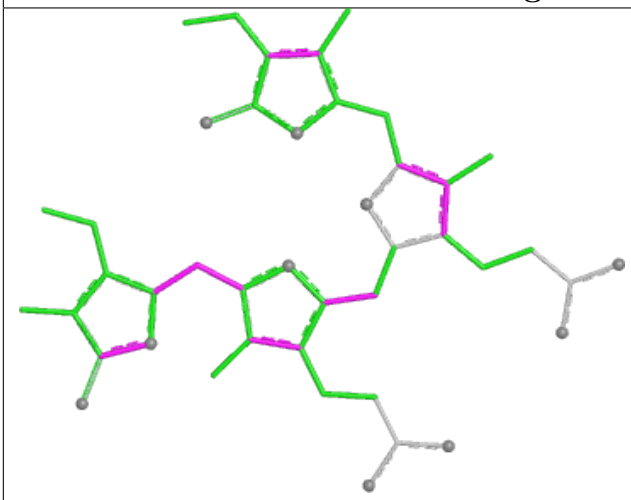


Rings

Ligand PEB U 186



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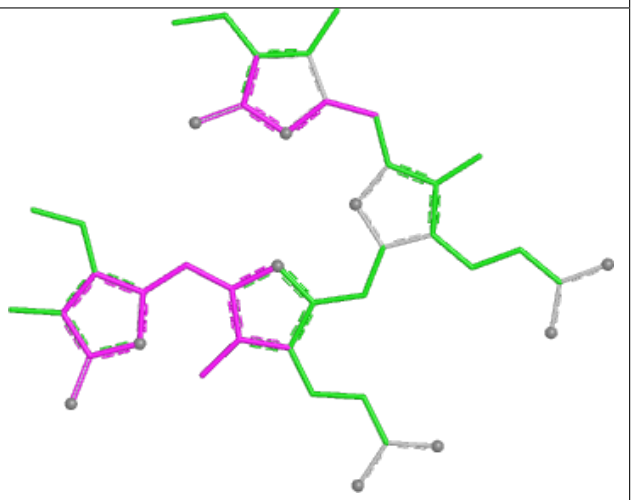
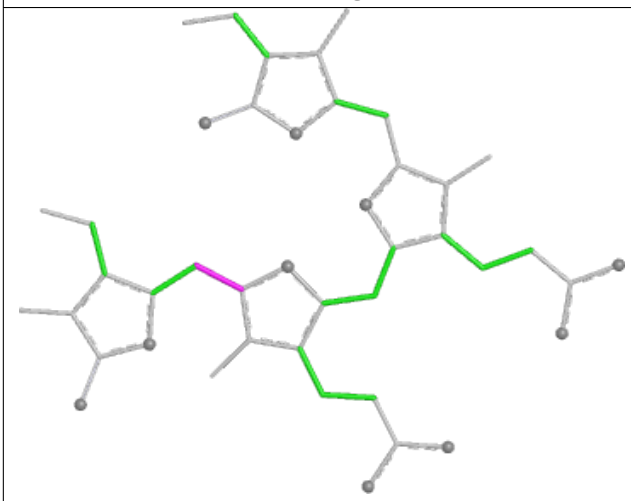
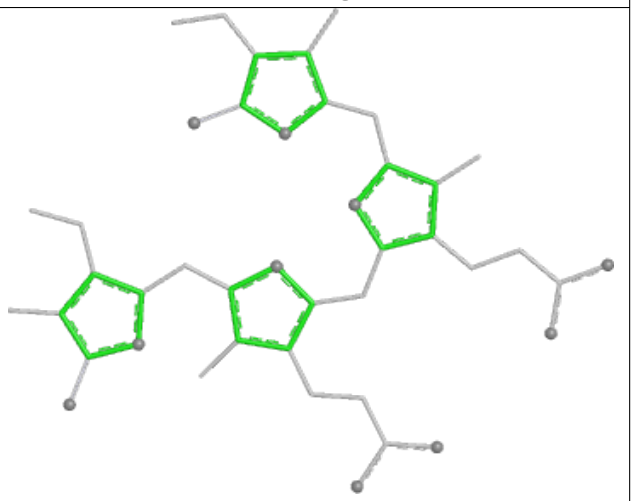


Bond angles

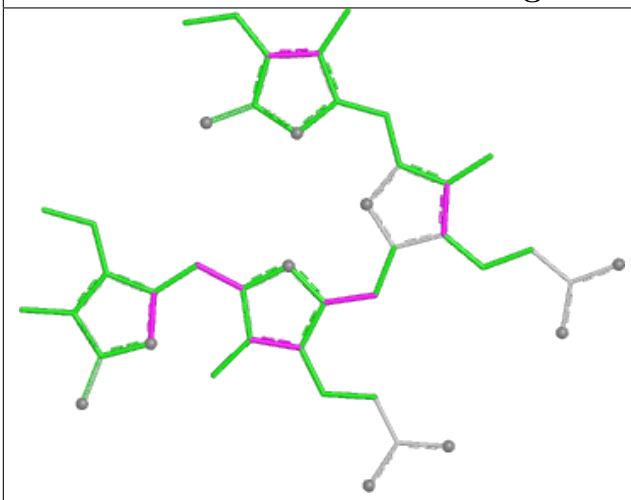


Torsions



Rings

Ligand PEB N 188



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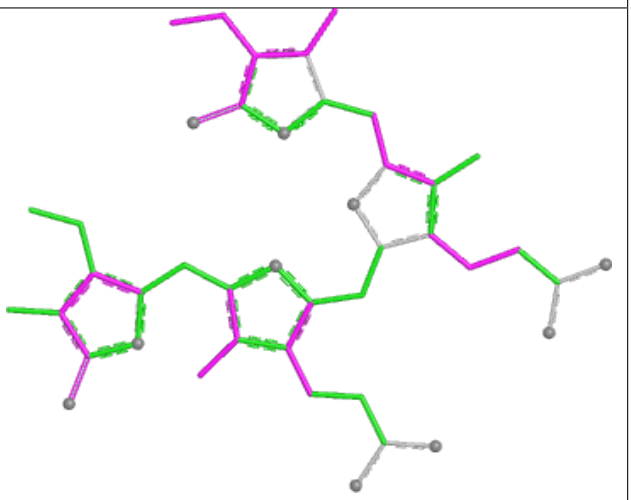
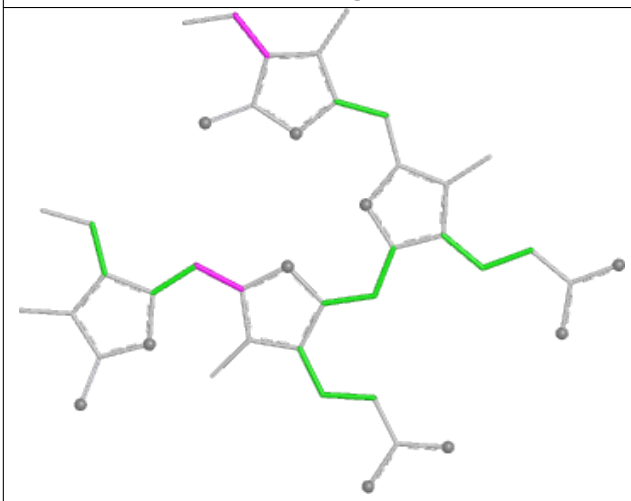


Bond angles



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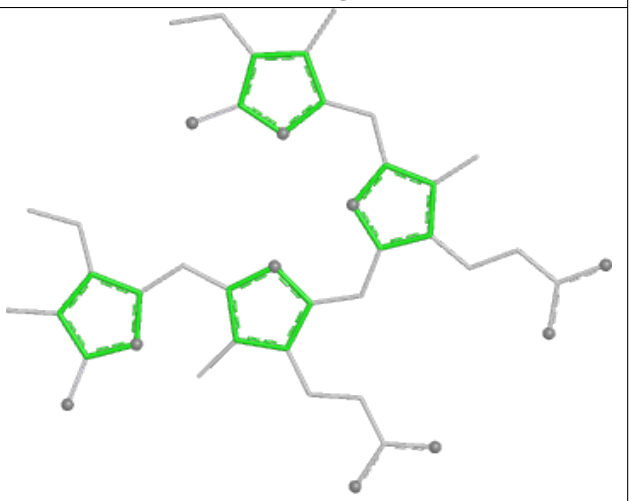
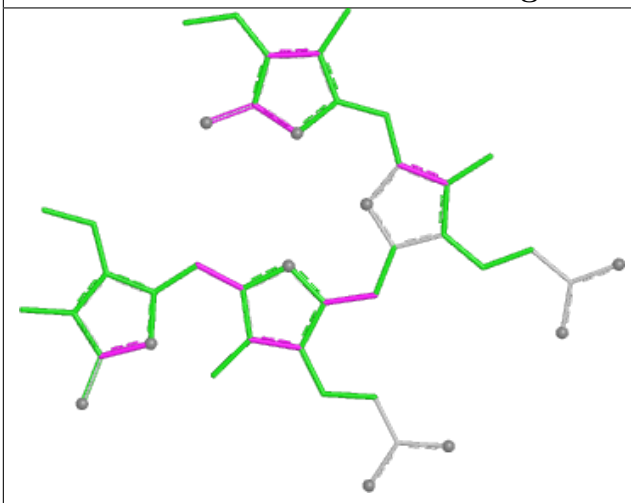


Rings

Ligand PEB M 188



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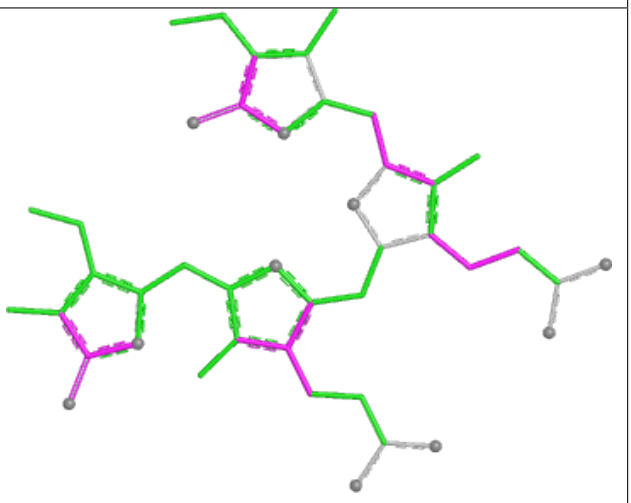
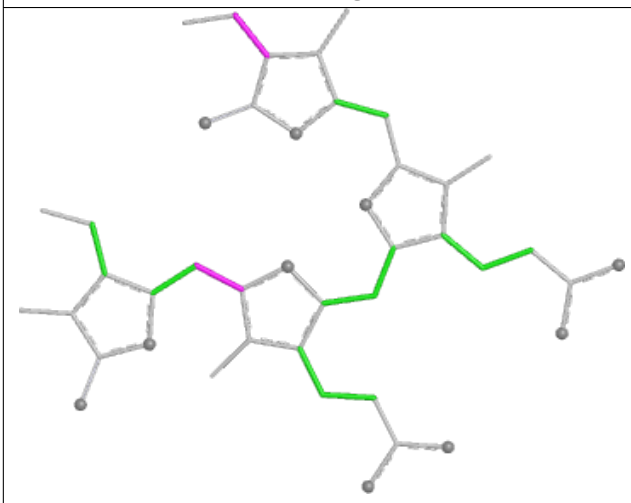
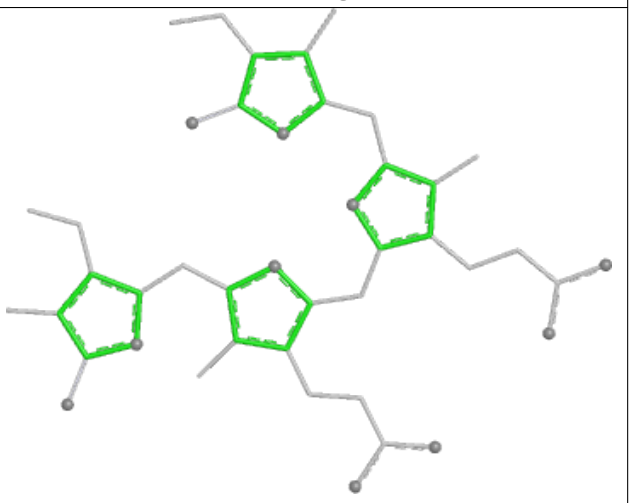


Bond angles

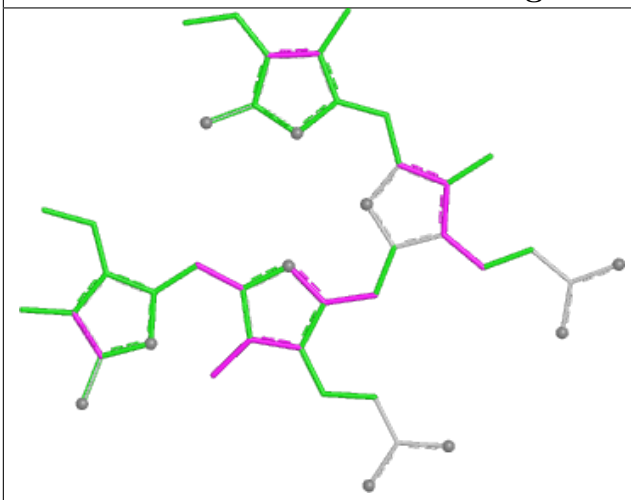


Torsions

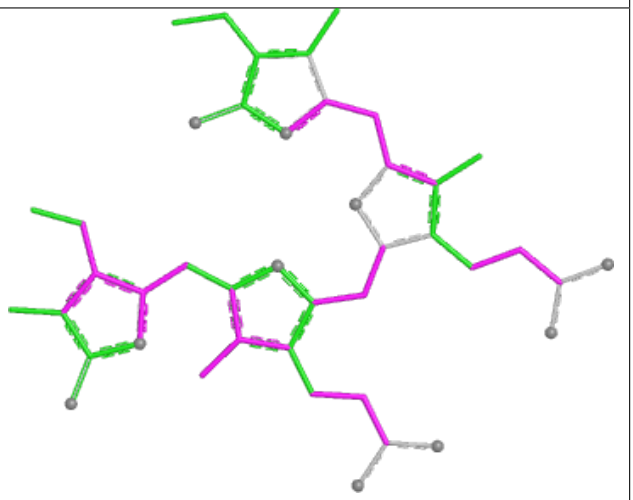


Rings

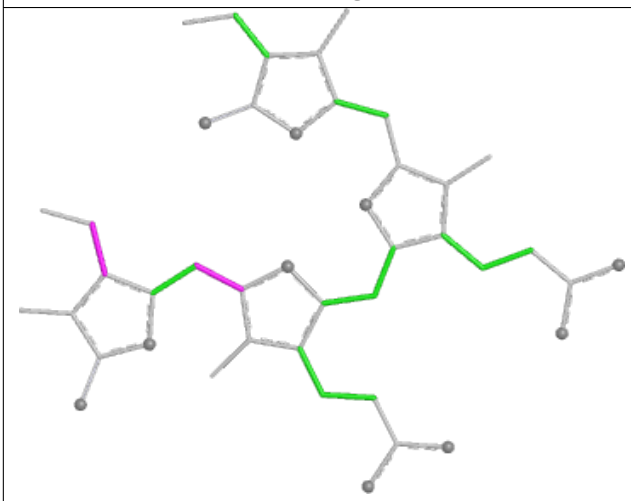
Ligand PEB T 187



Bond lengths



Bond angles



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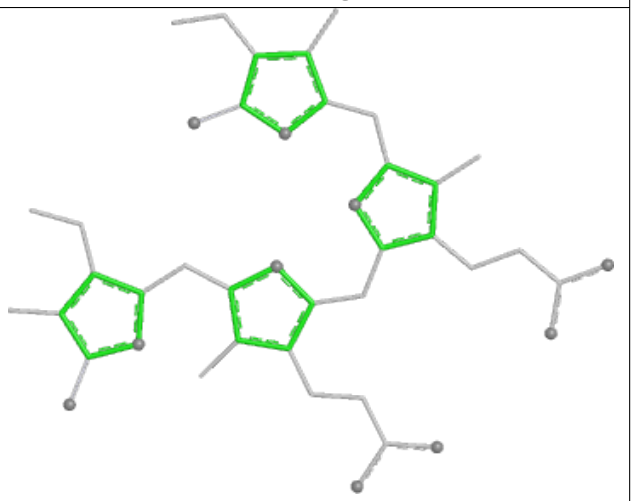
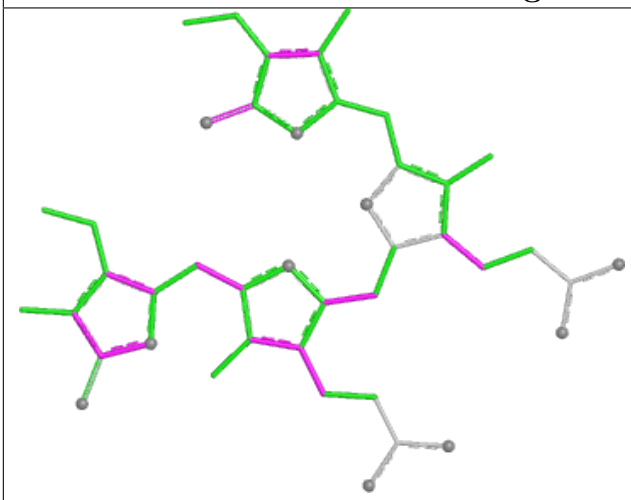
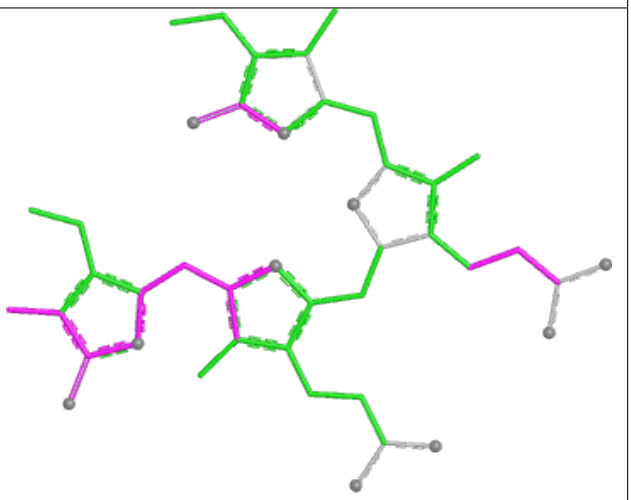


Rings

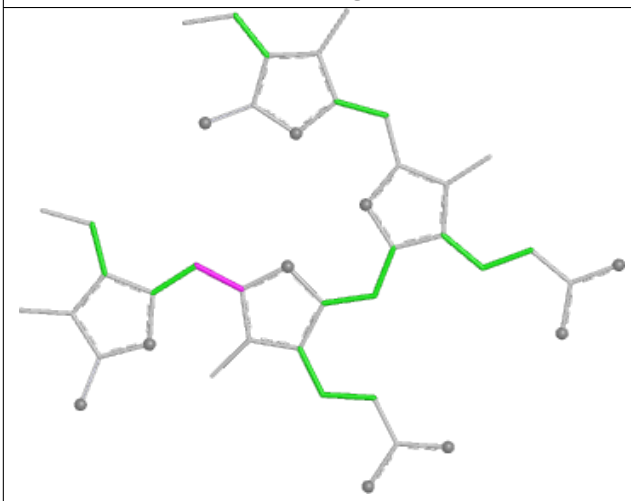
Ligand PEB K 166



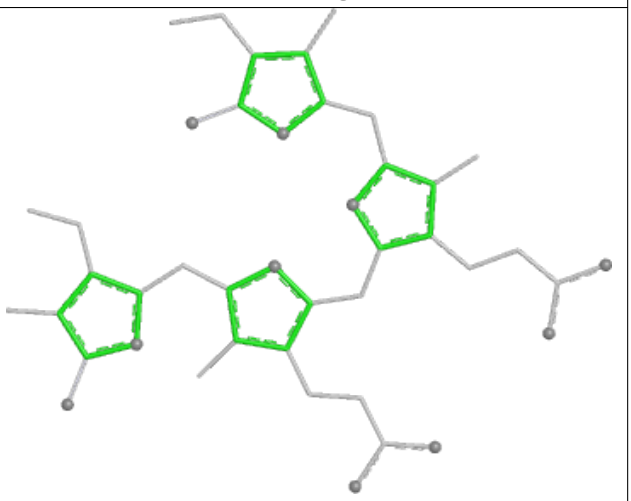
Bond lengths



Bond angles

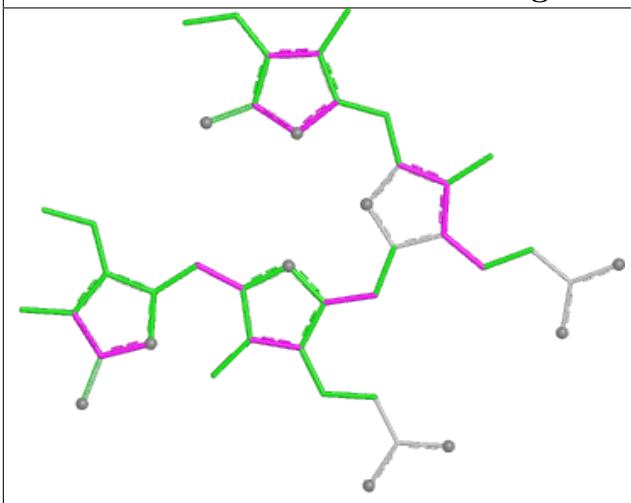


Torsions



Rings

Ligand PEB I 167



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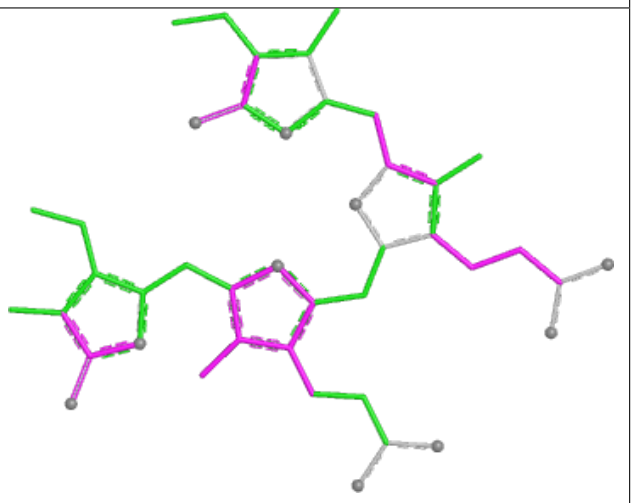
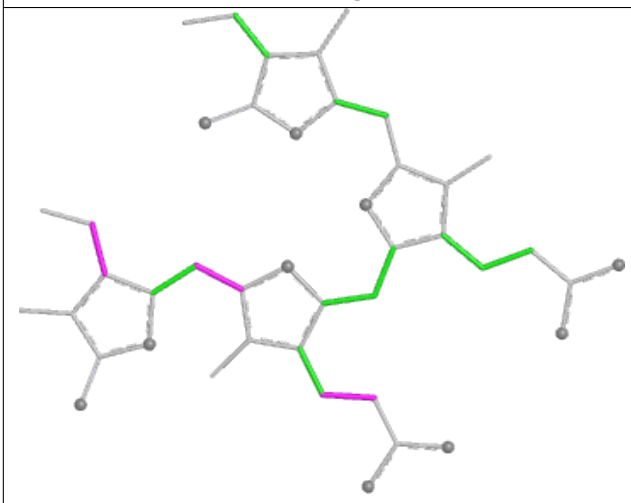
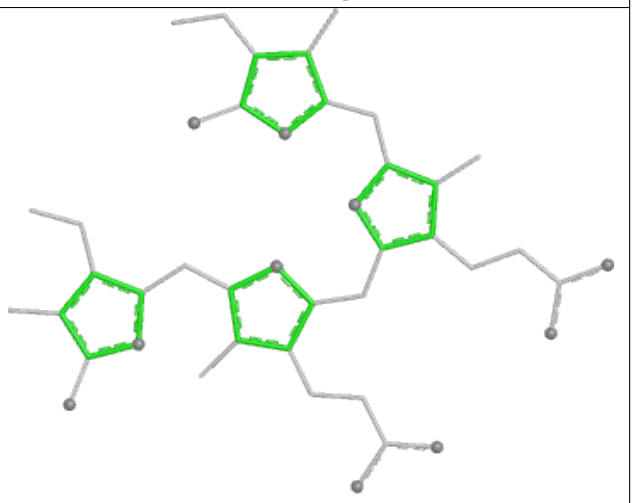


Bond angles

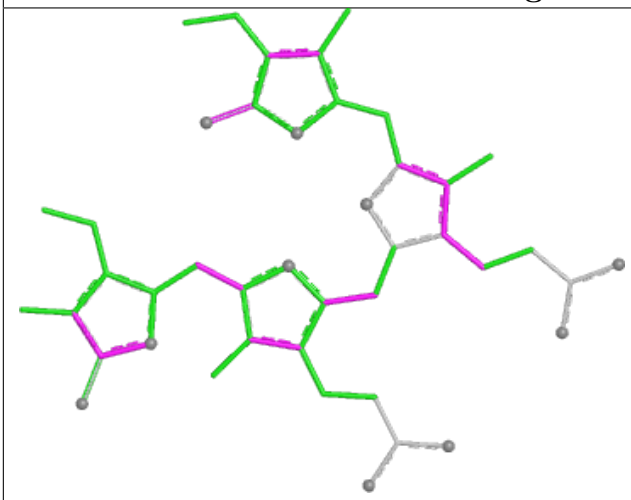


Torsions

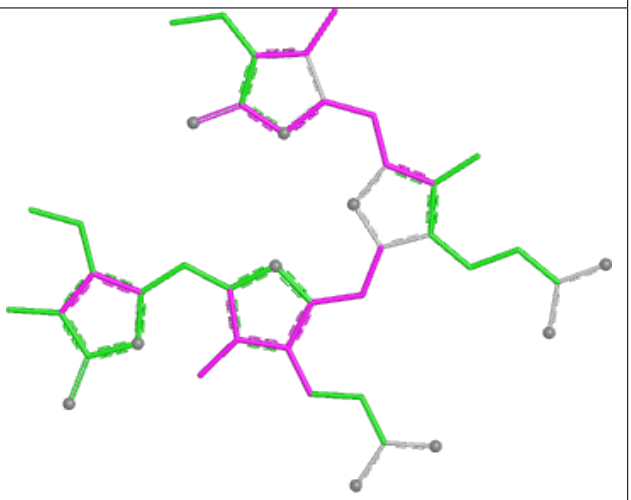


Rings

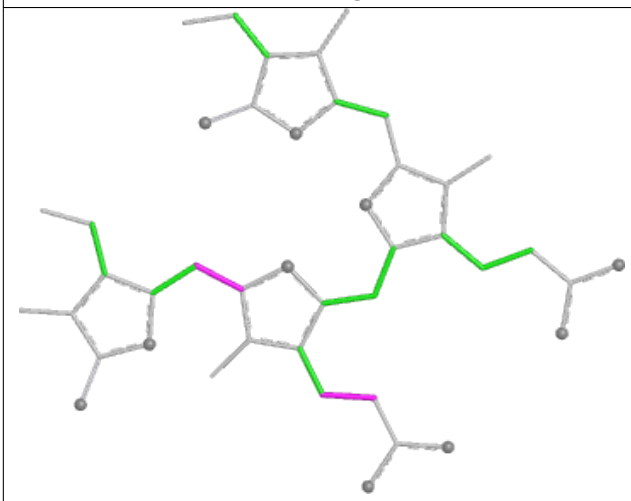
Ligand PEB B 167



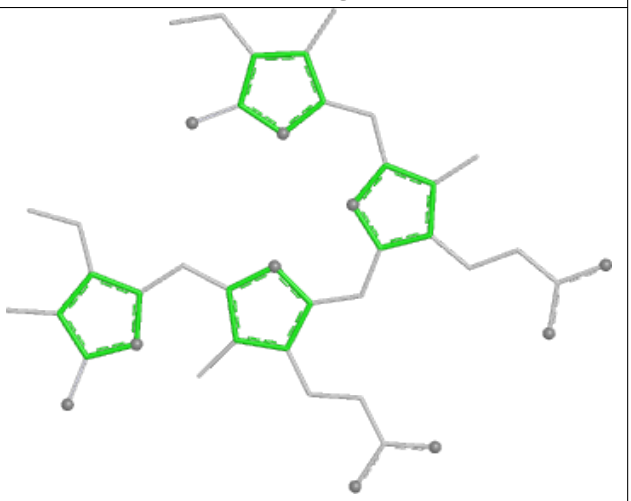
Bond lengths



Bond angles

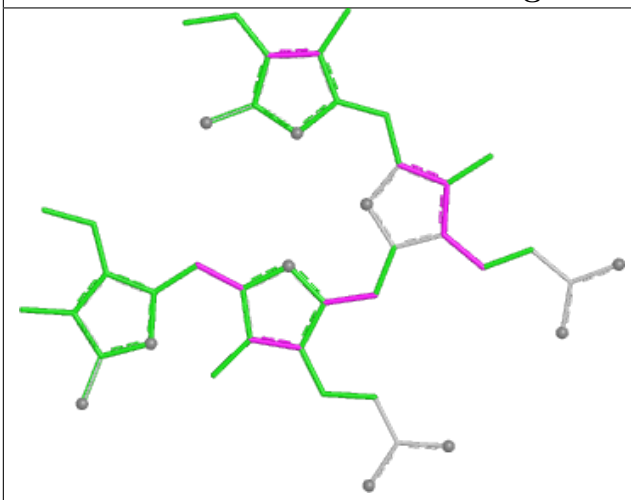


Torsions



Rings

Ligand PEB H 166



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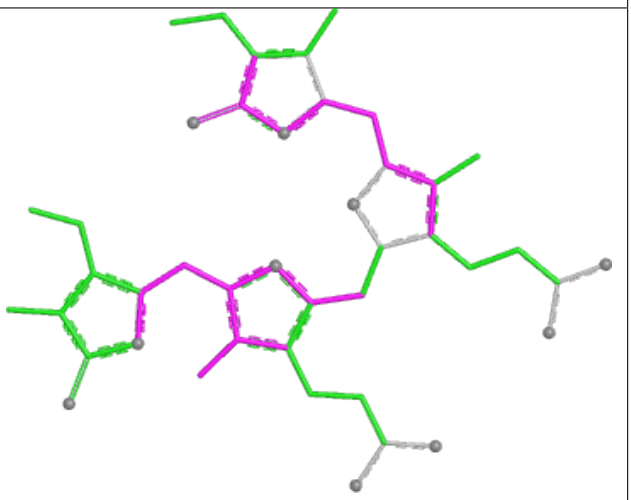
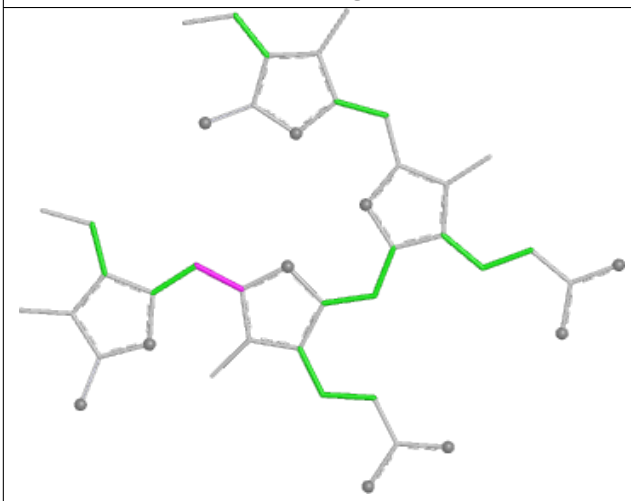


Bond angles



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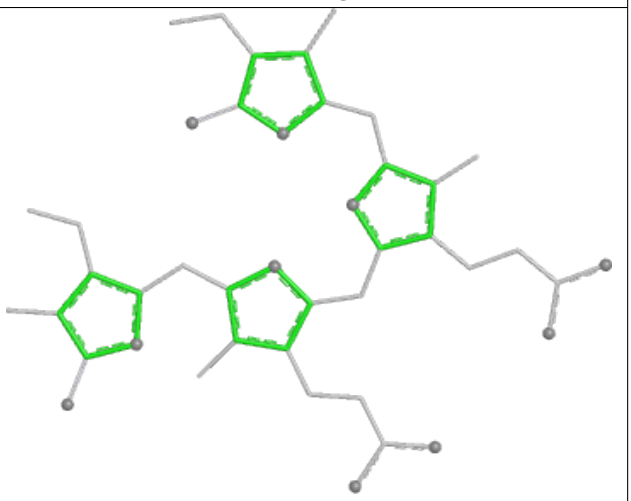
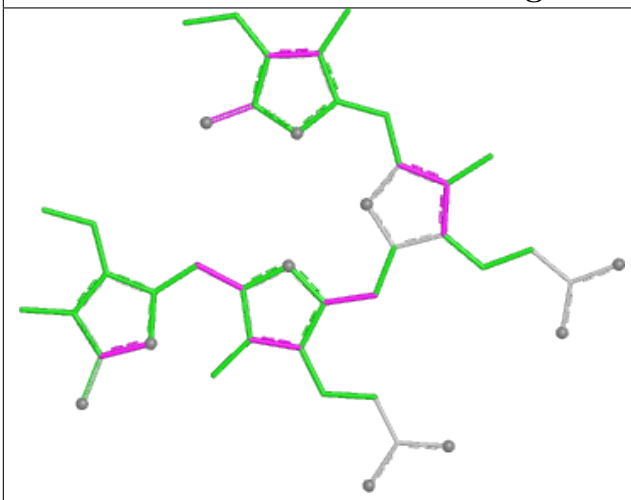


Rings

Ligand PEB T 186



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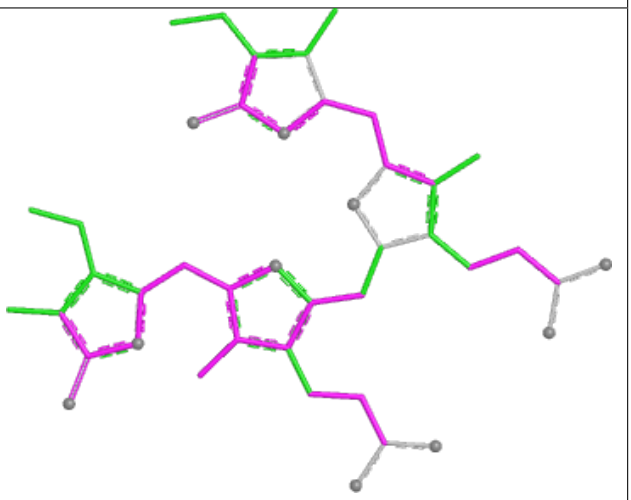
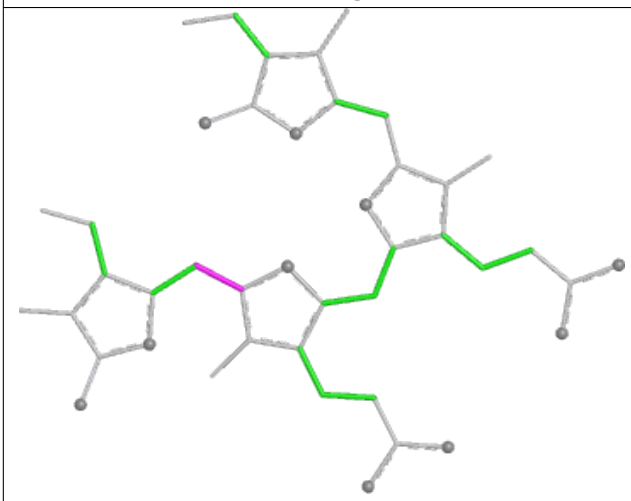


Bond angles



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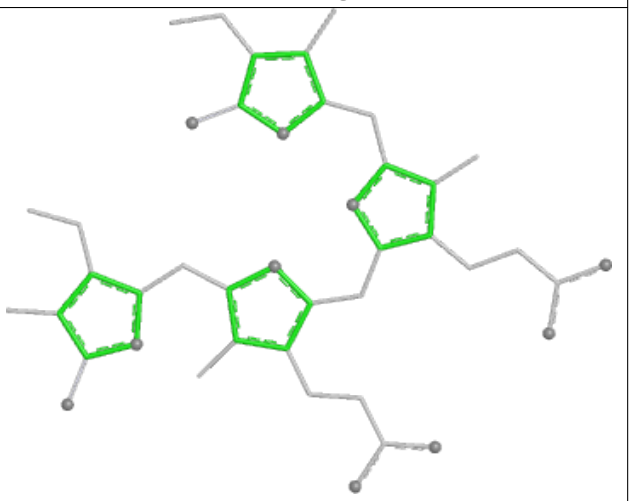
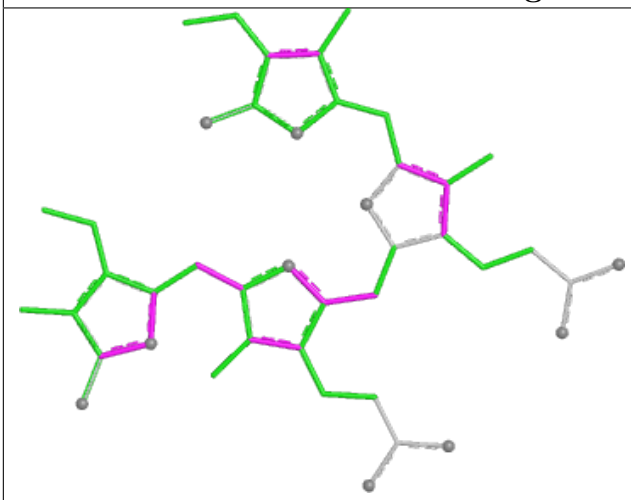


Rings

Ligand PEB C 167



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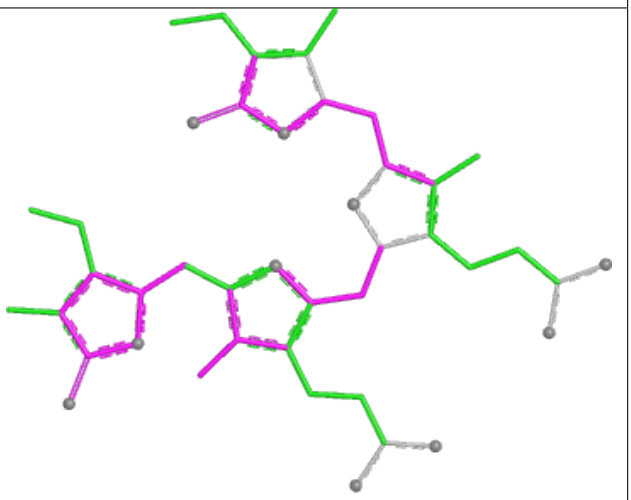
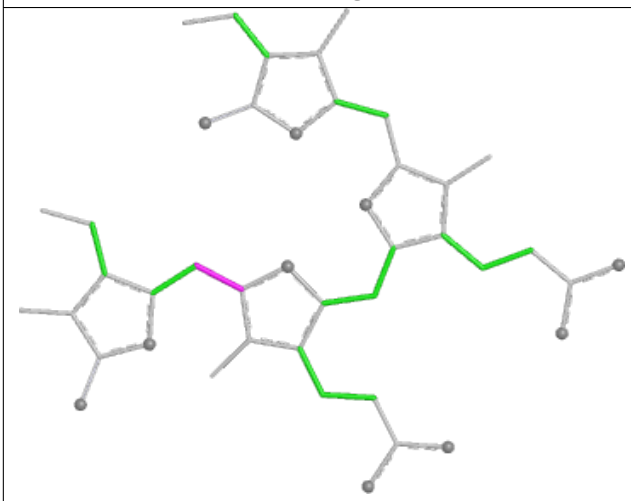


Bond angles



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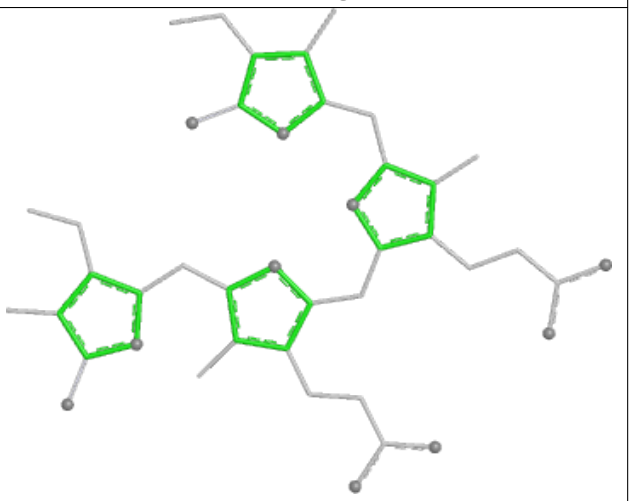
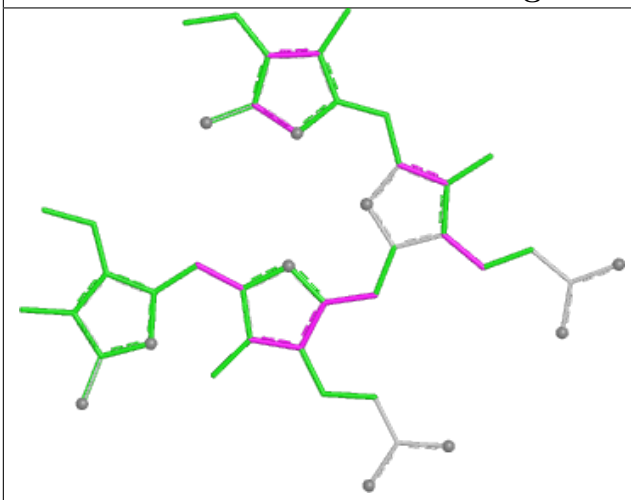


Rings

Ligand PEB G 166



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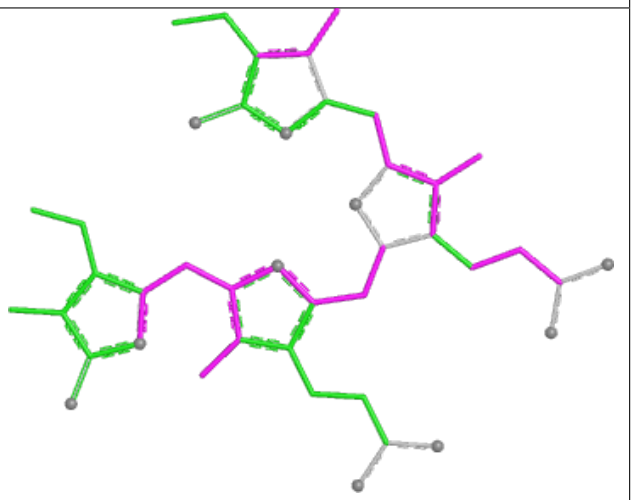

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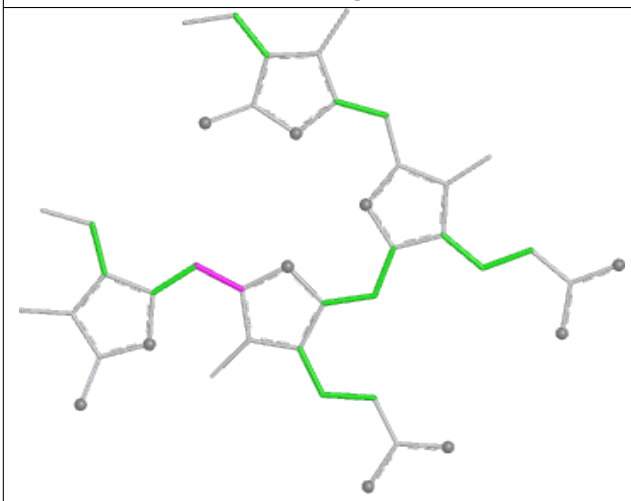

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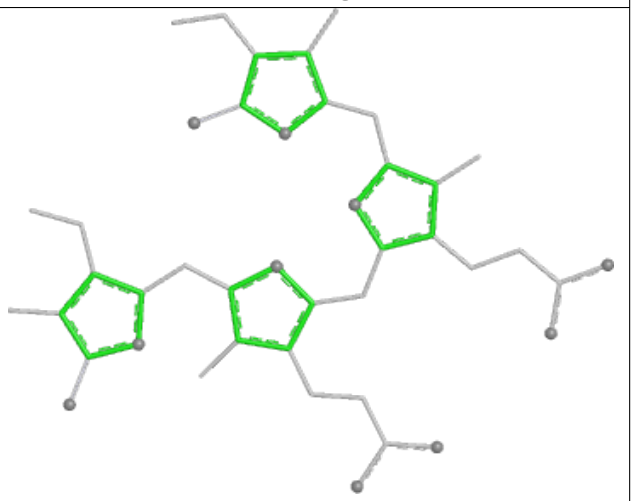
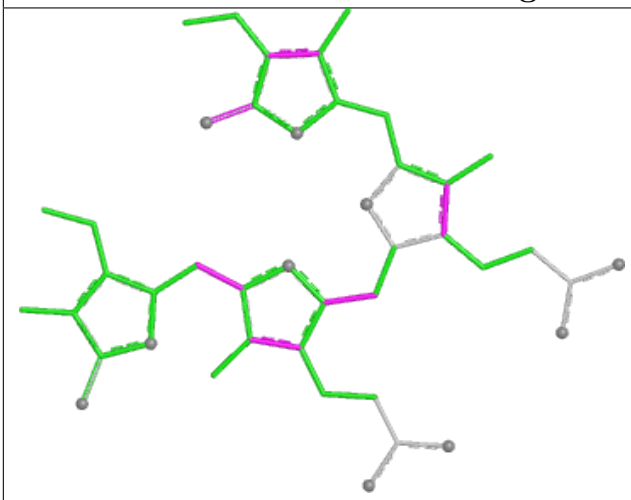


Rings

Ligand PEB W 188



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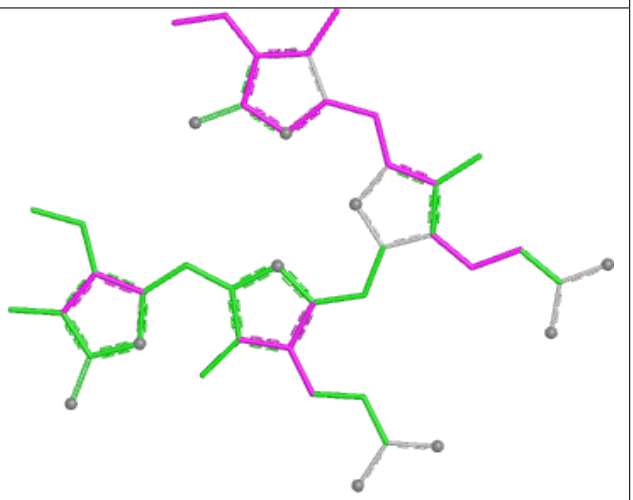
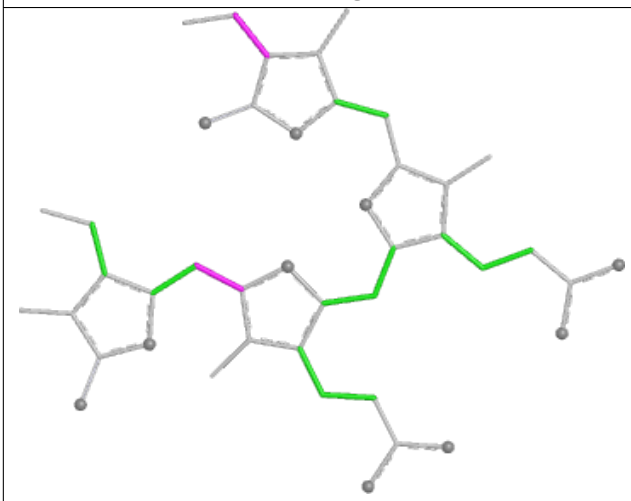


Bond angles



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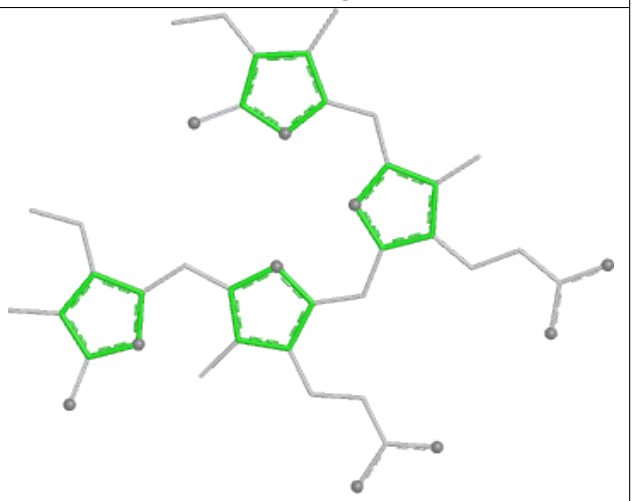
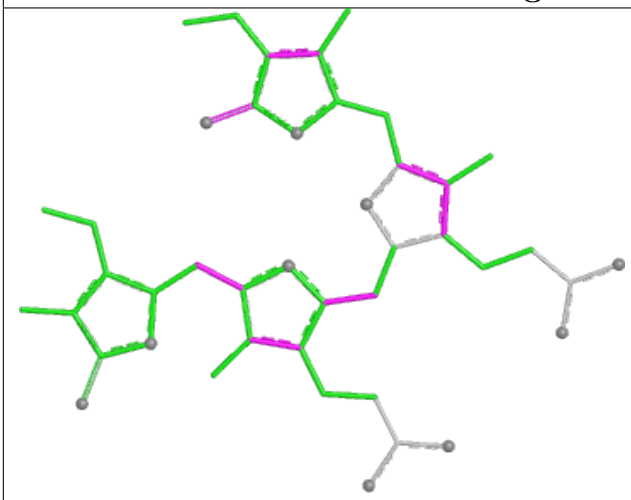


Rings

Ligand PEB X 186



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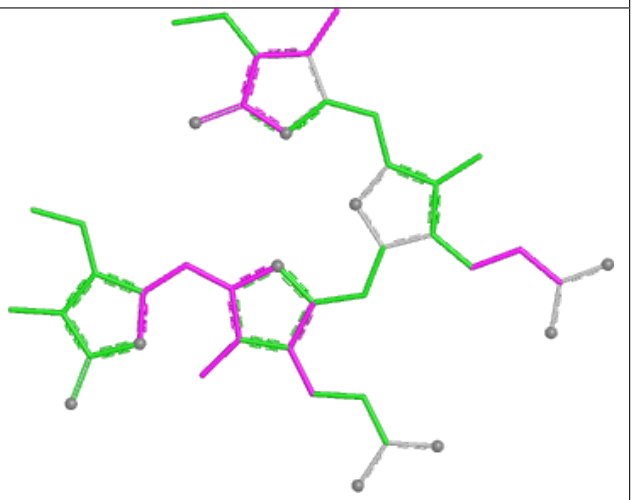
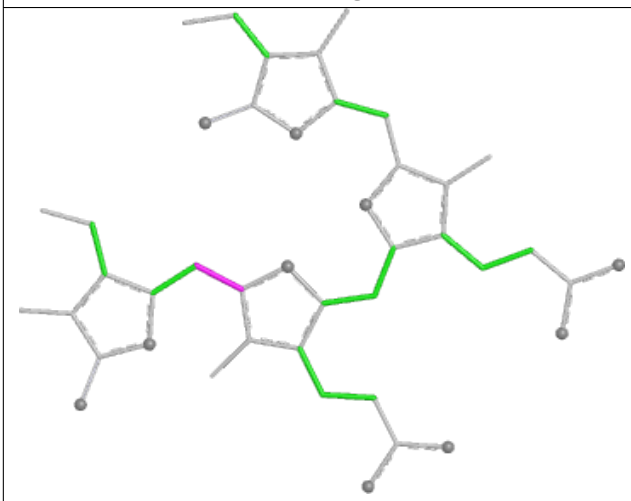


Bond angles



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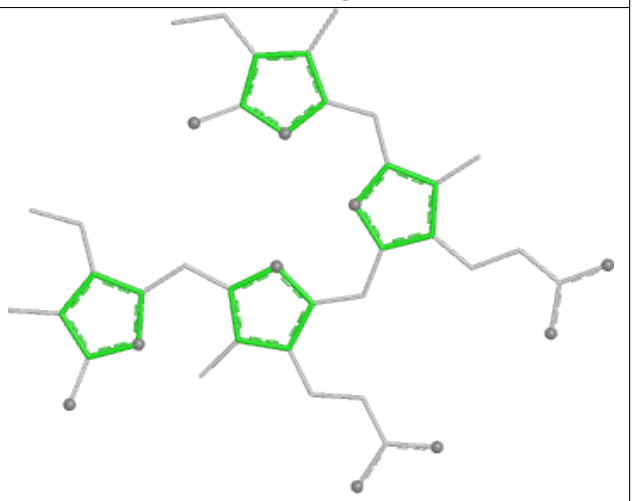
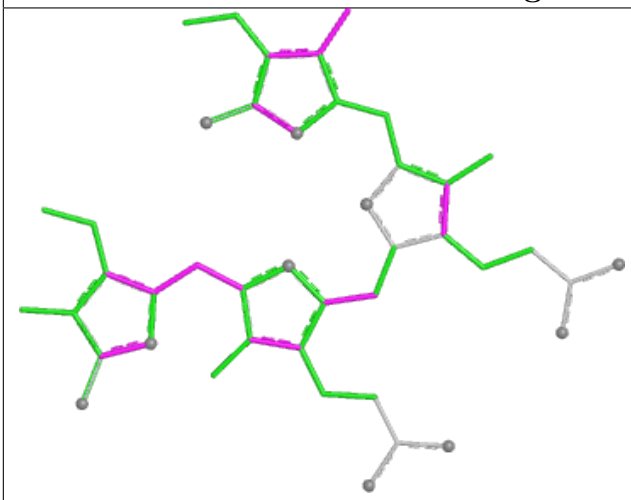


Rings

Ligand PEB V 188



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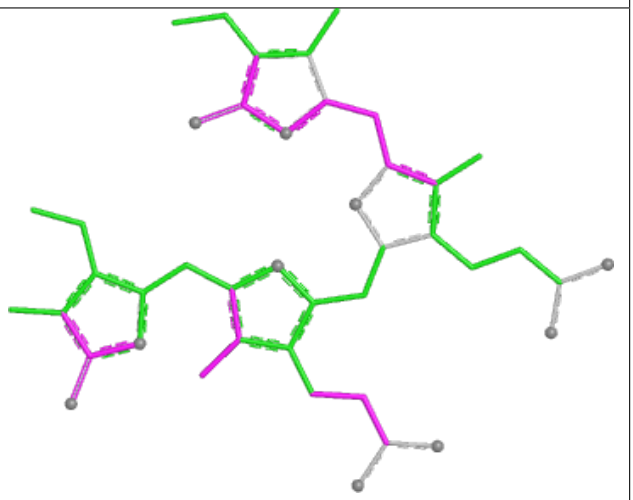
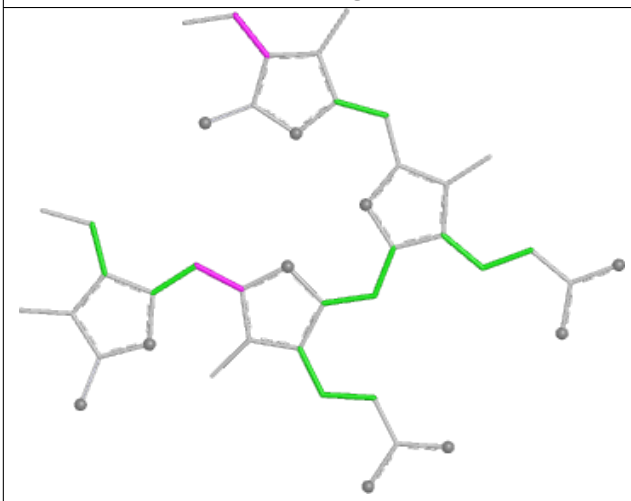


Bond angles



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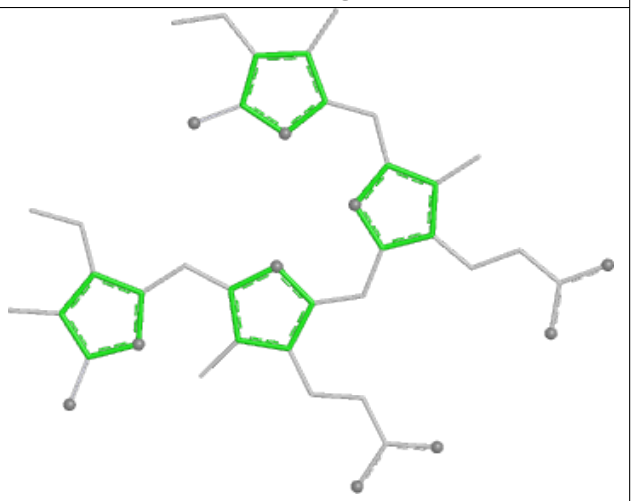
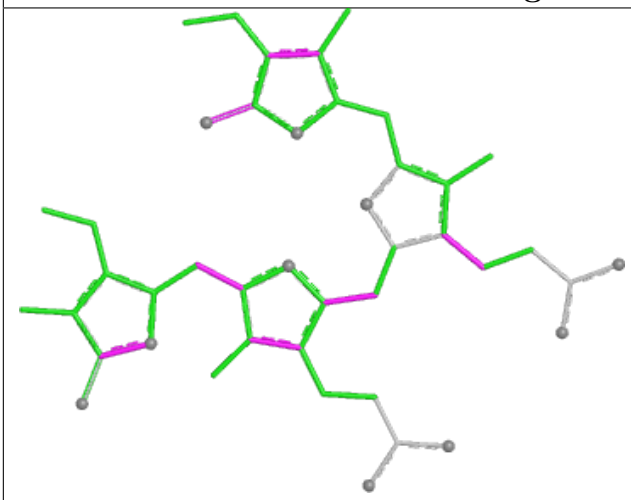


Rings

Ligand PEB X 187



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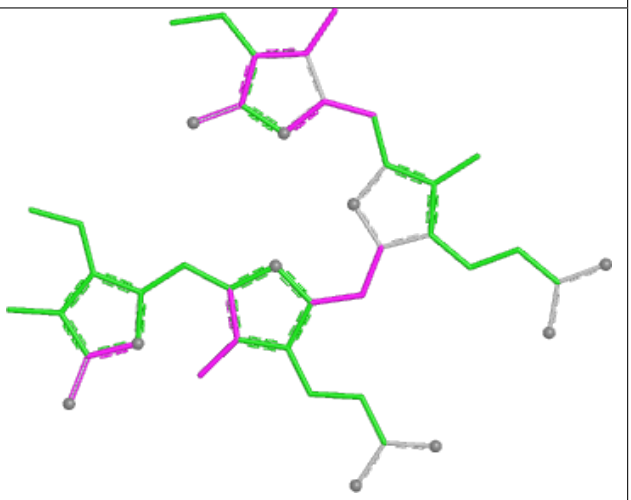
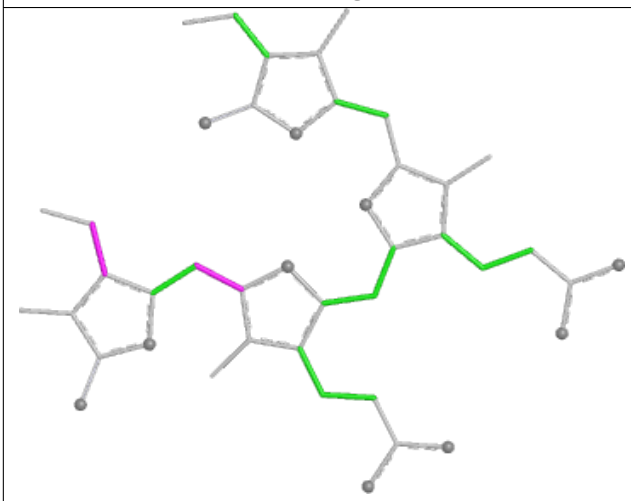
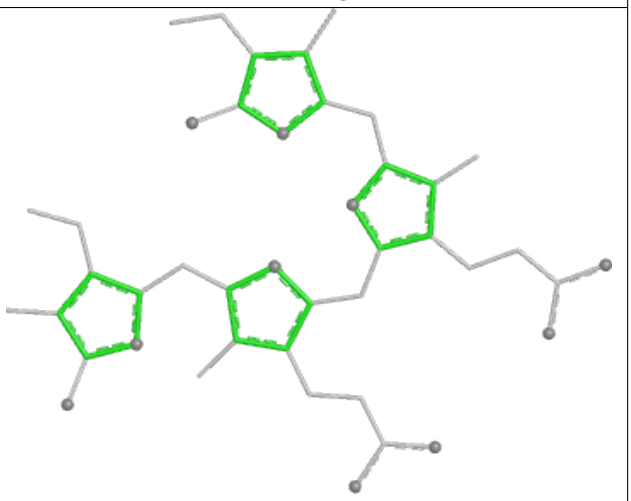


Bond angles

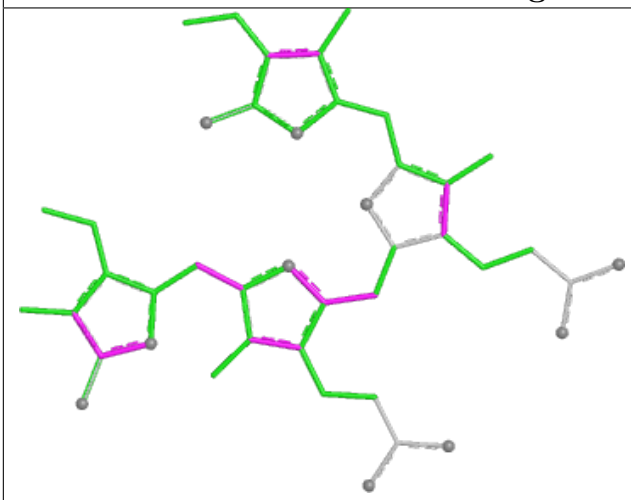


Torsions



Rings

Ligand PEB J 167



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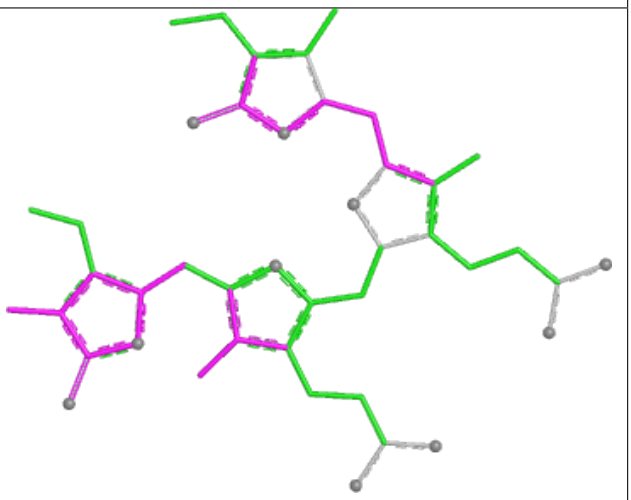
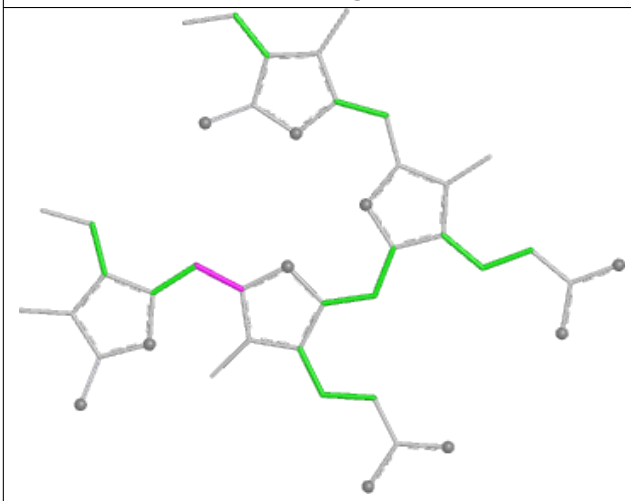
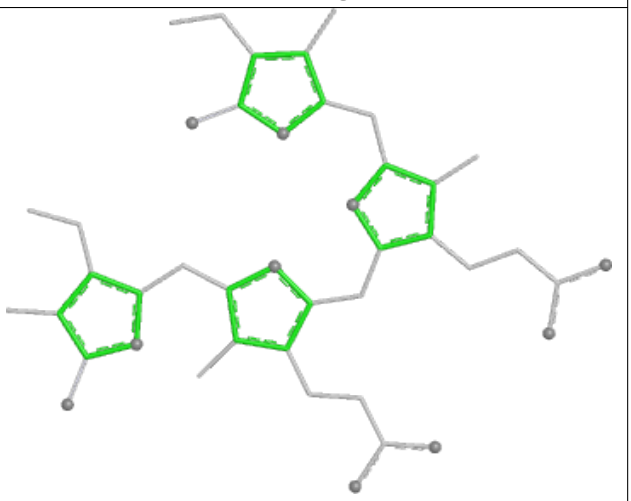


Bond angles

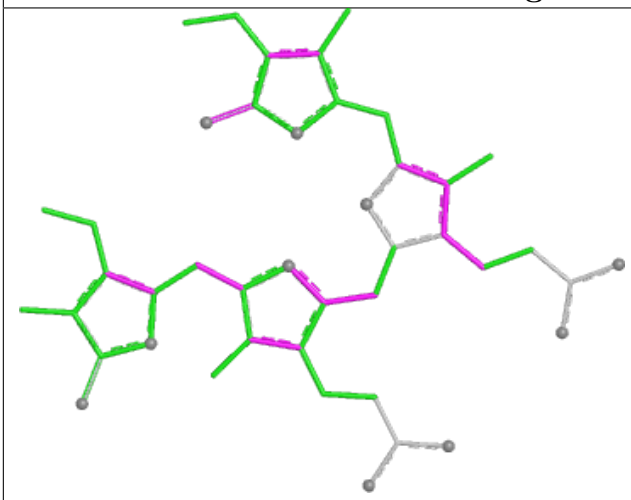


Torsions



Rings

Ligand PEB T 188



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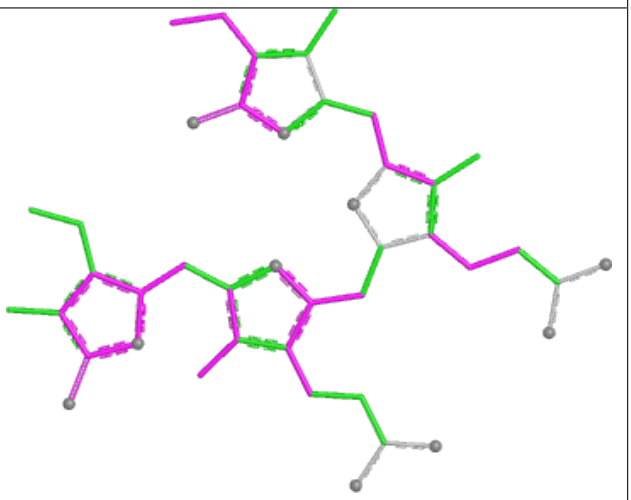
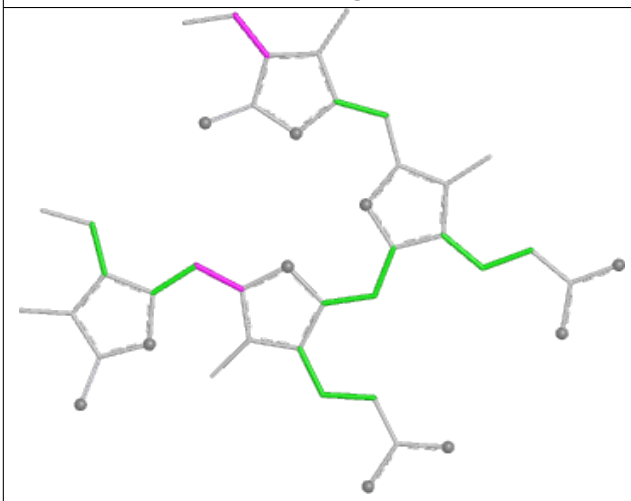


Bond angles



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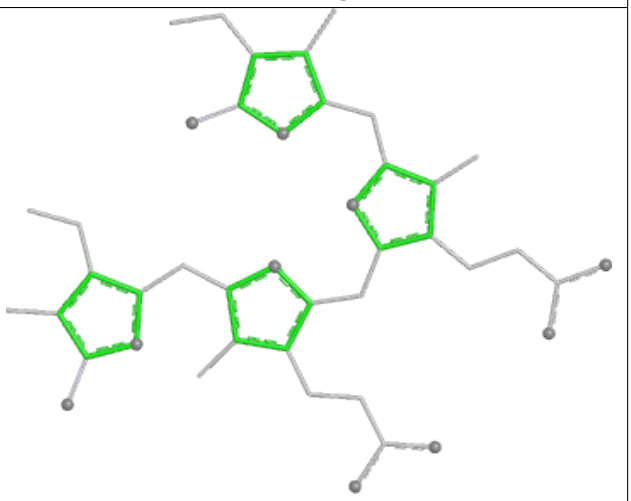
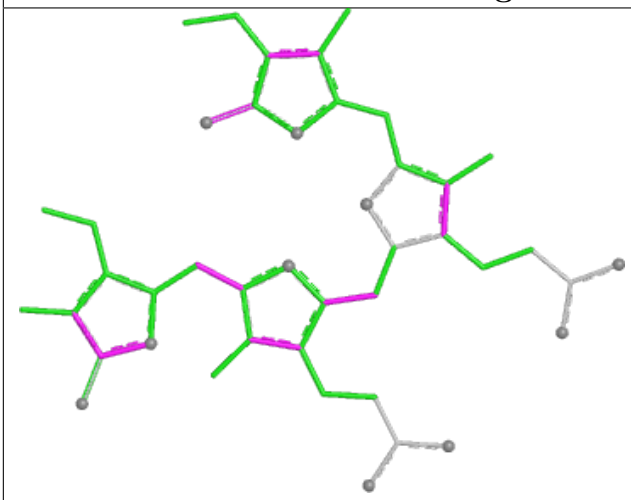
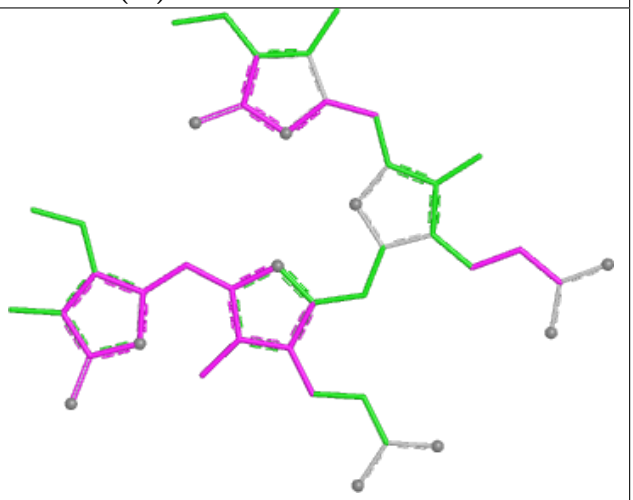


Rings

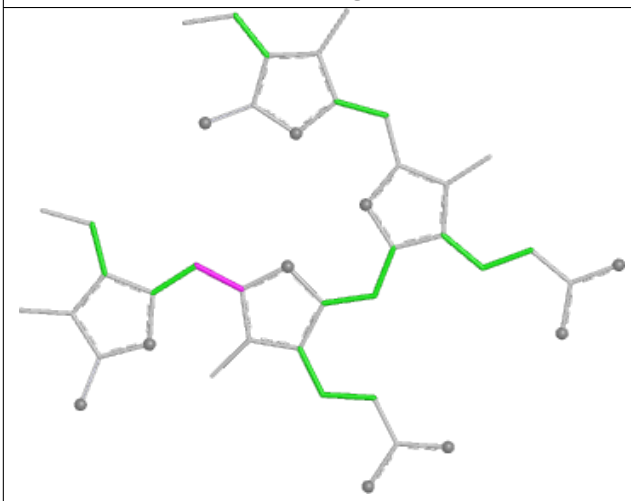
Ligand PEB S 186 (B)



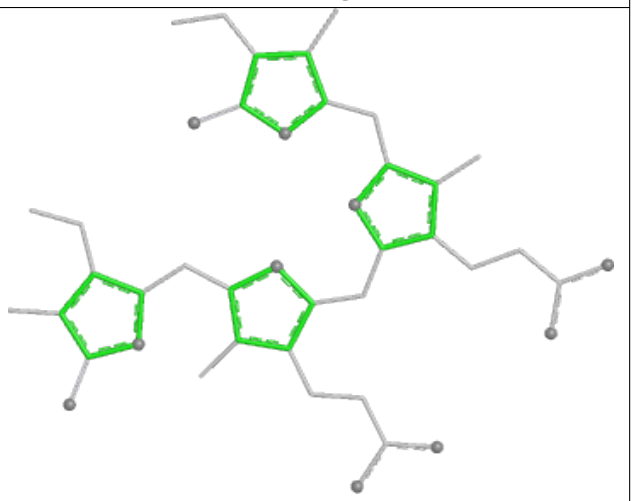
Bond lengths



Bond angles

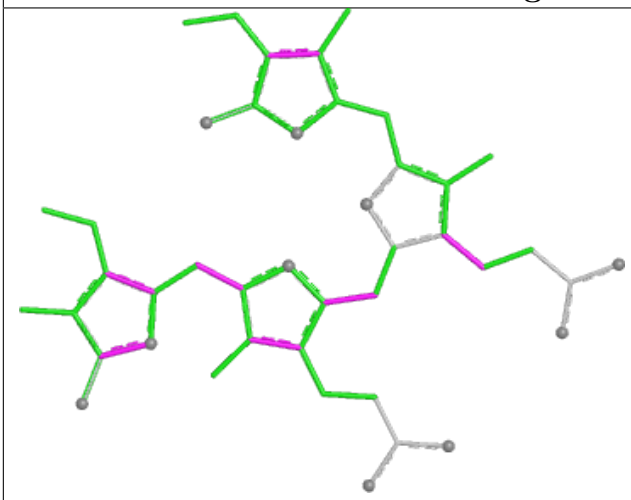


Torsions



Rings

Ligand PEB U 187



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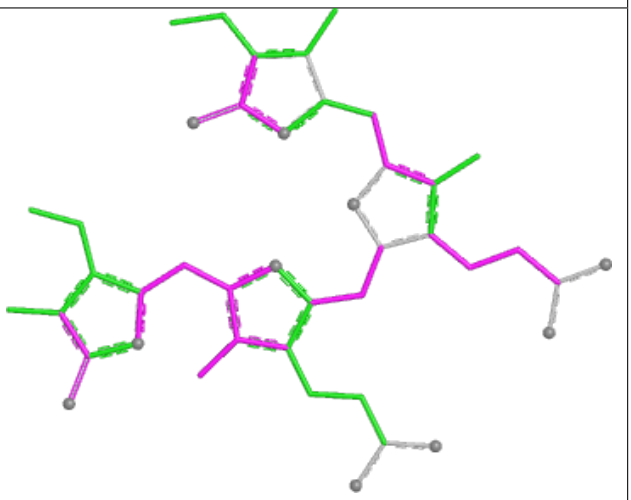
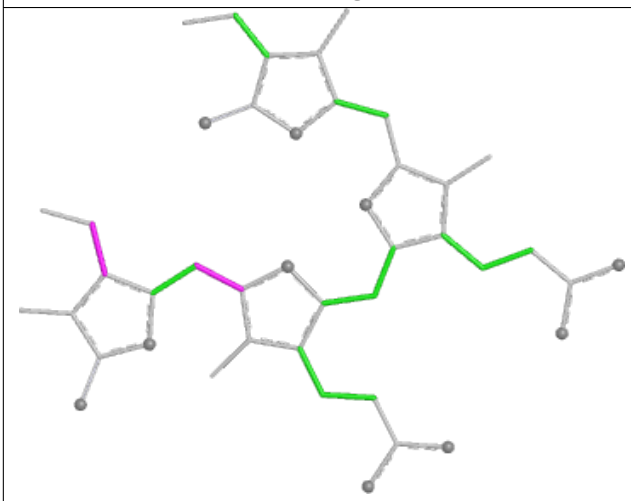
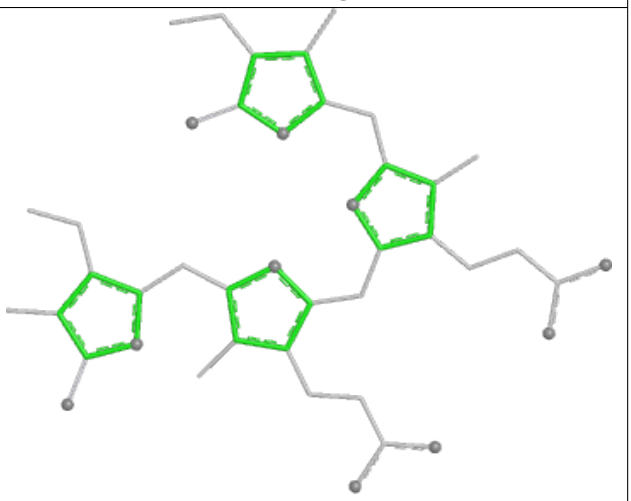


Bond angles

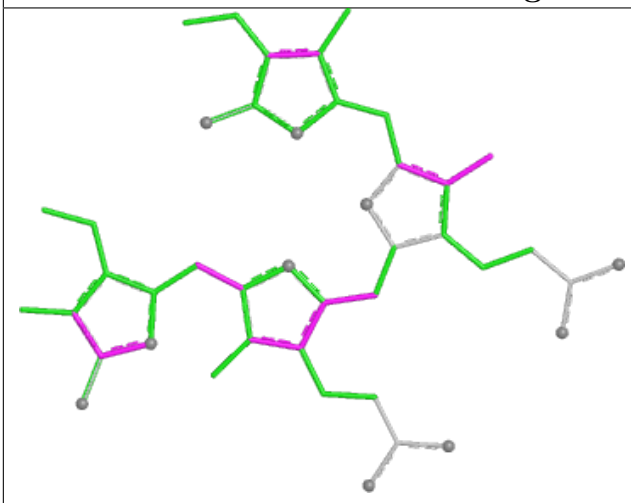


Torsions

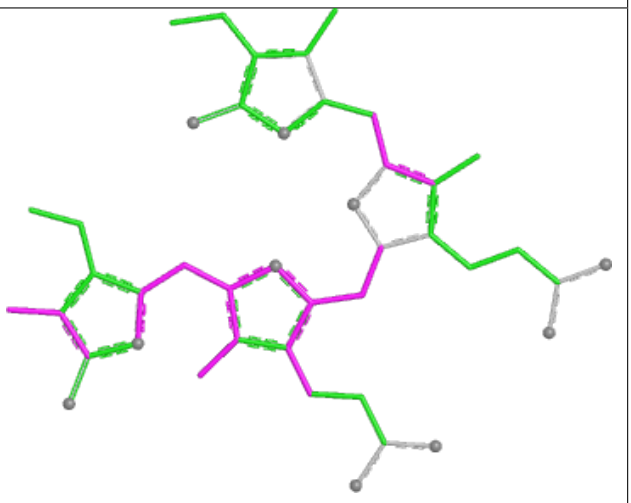


Rings

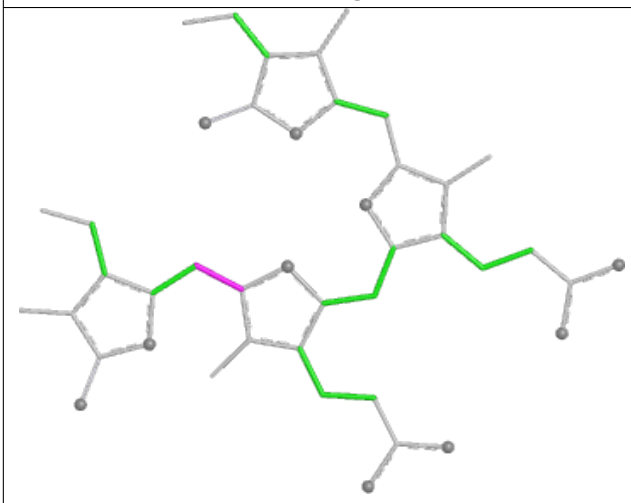
Ligand PEB D 166



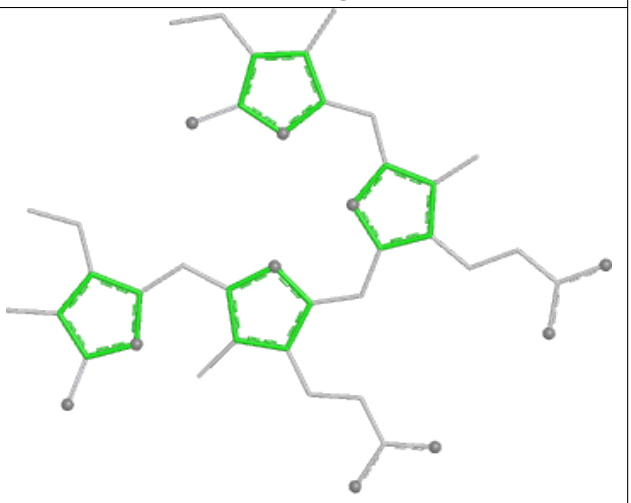
Bond lengths



Bond angles

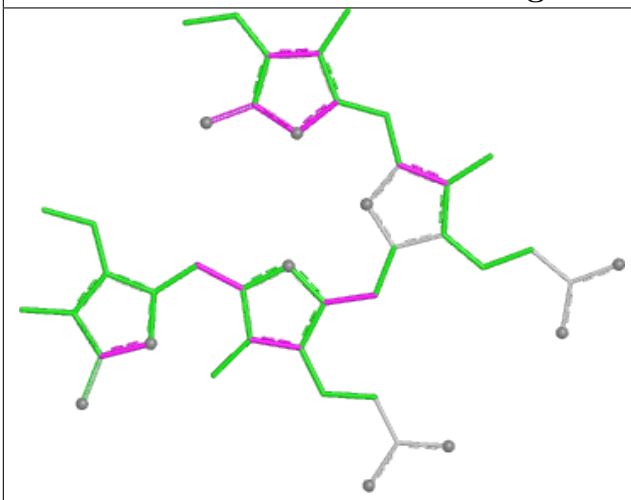


Torsions

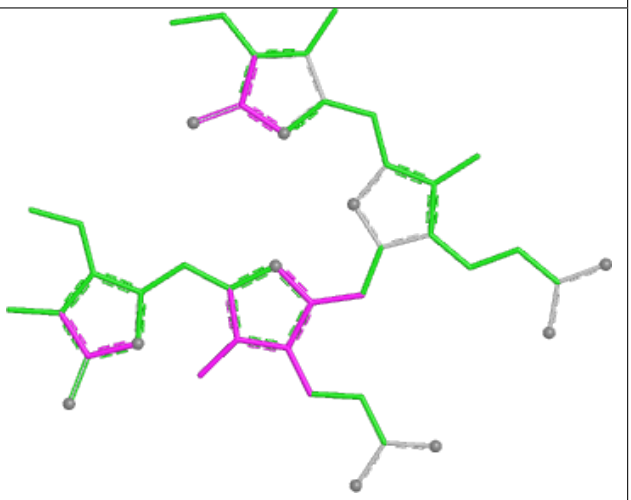


Rings

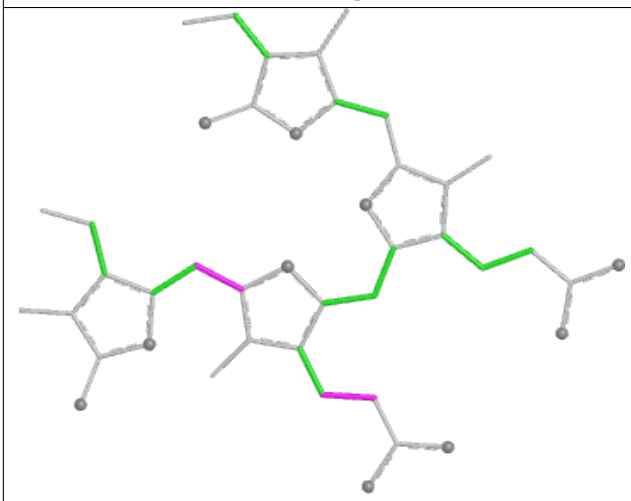
Ligand PEB L 167



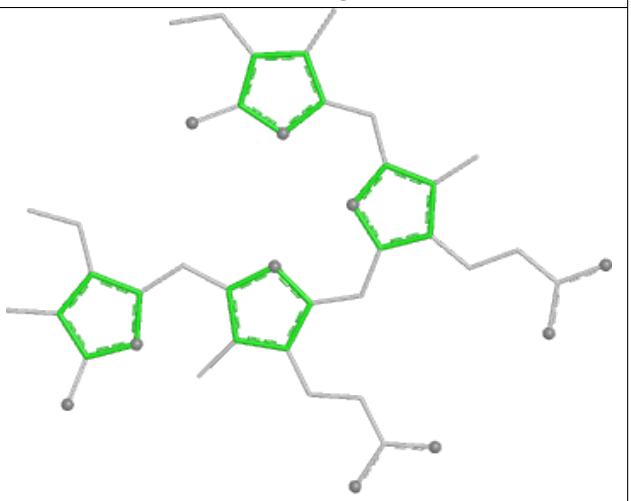
Bond lengths



Bond angles

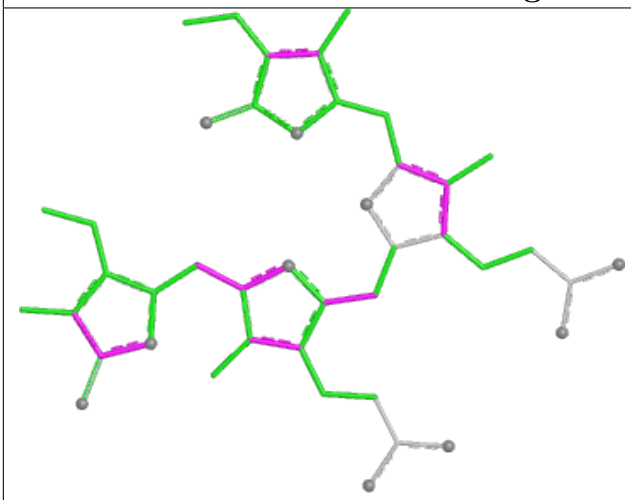


Torsions



Rings

Ligand PEB K 167



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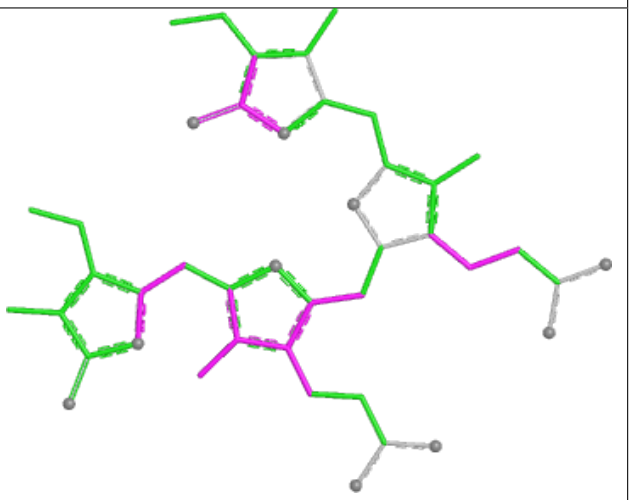

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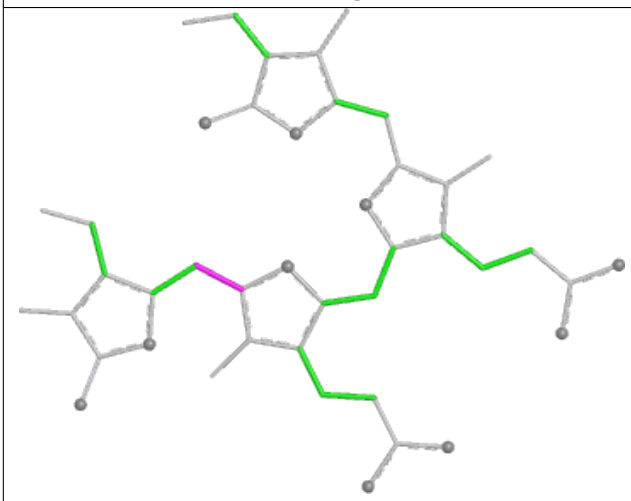

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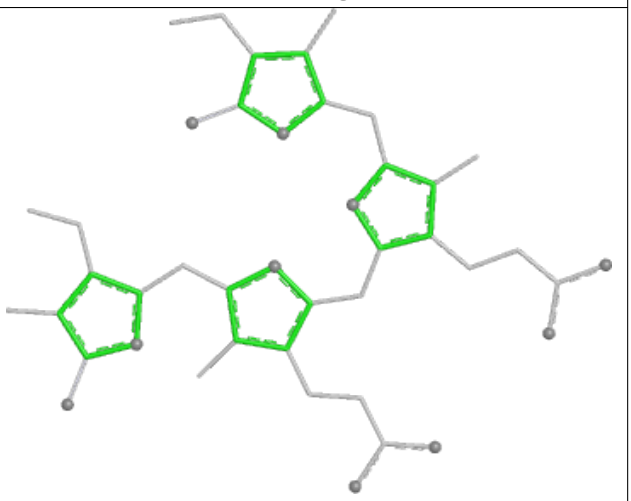
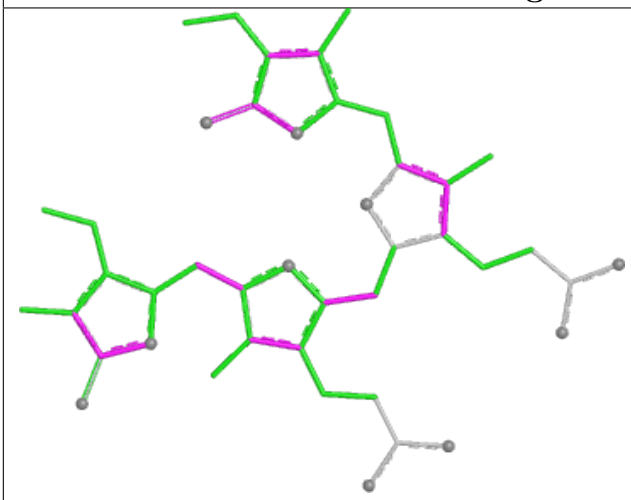


Rings

Ligand PEB E 166



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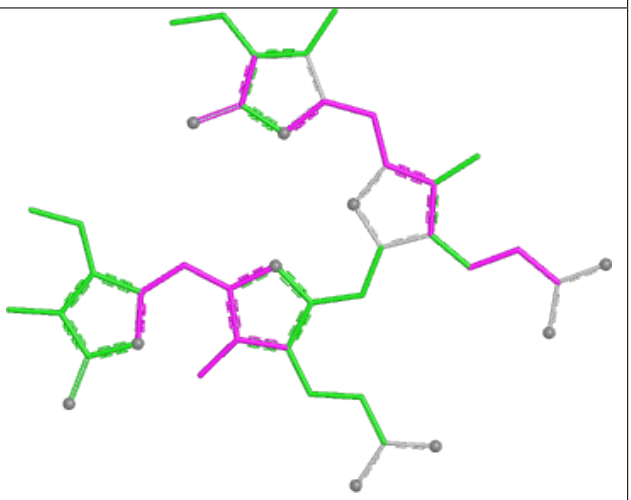

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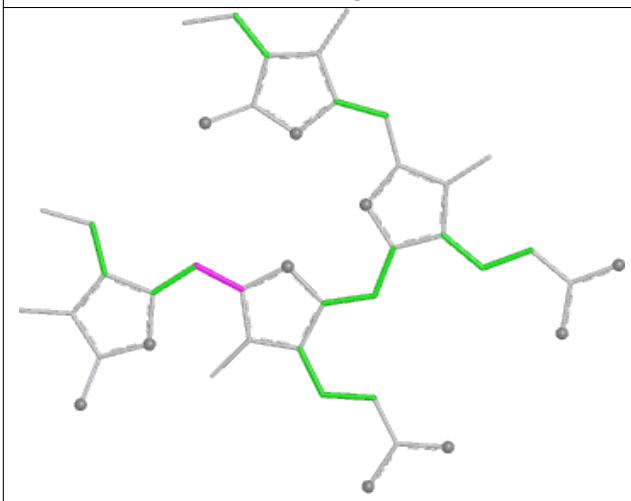

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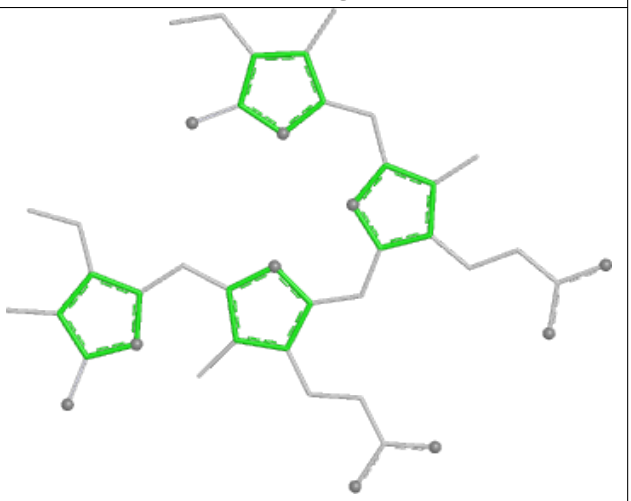
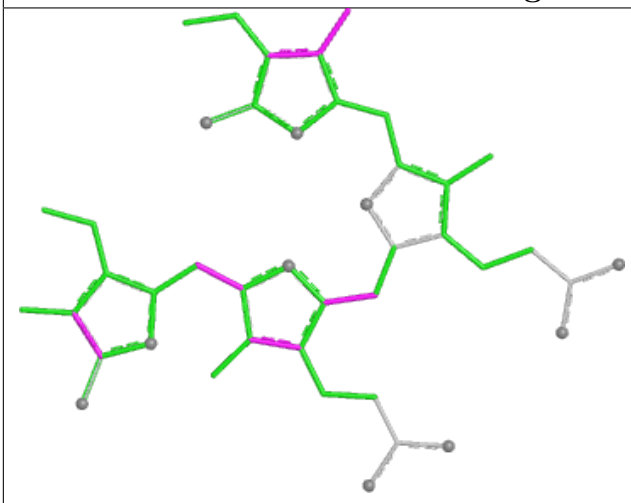


Rings

Ligand PEB V 186



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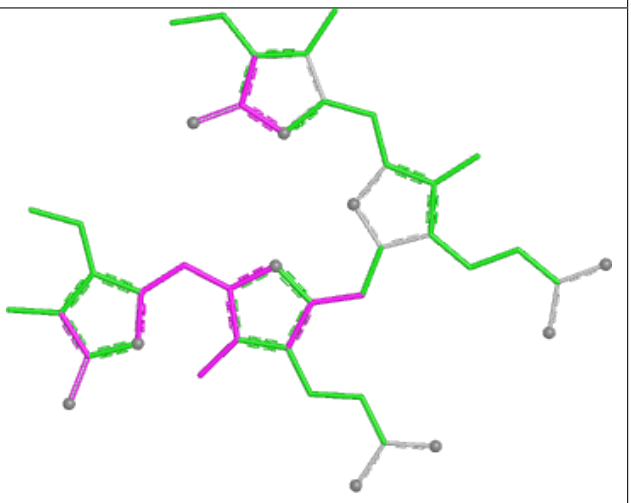

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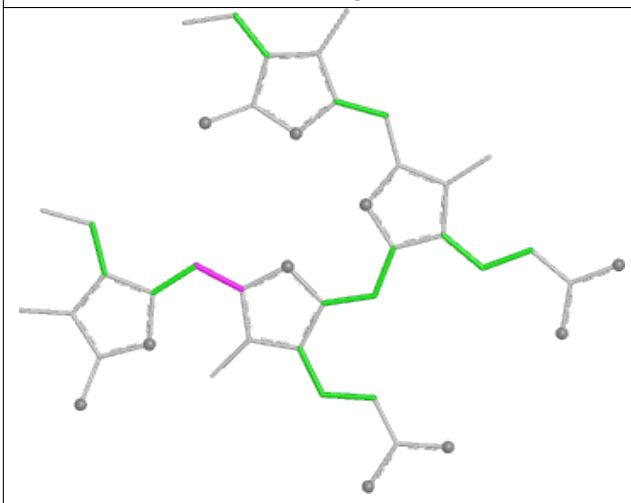

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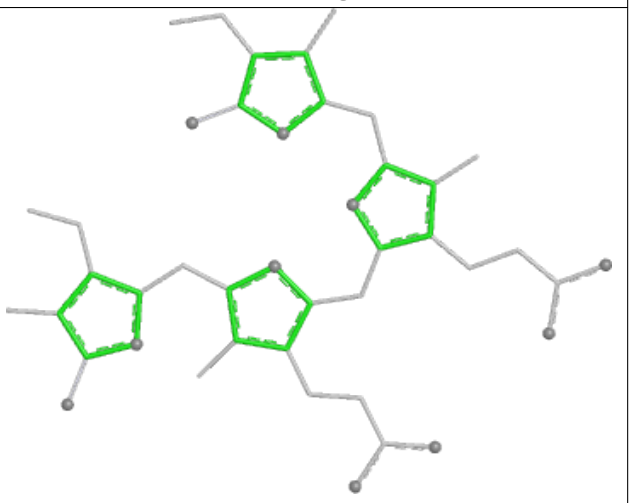
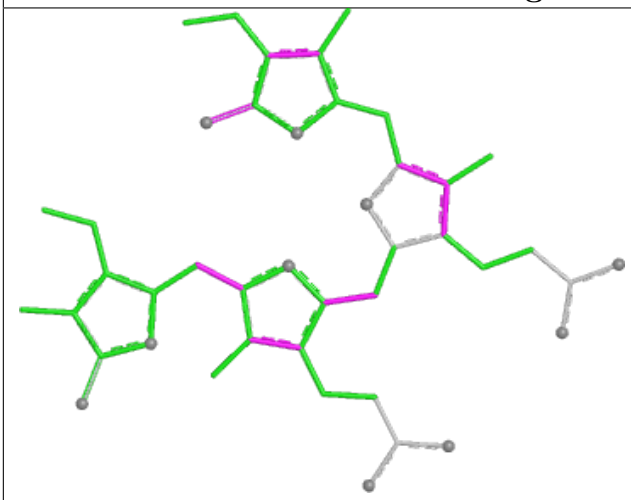


Rings

Ligand PEB P 188



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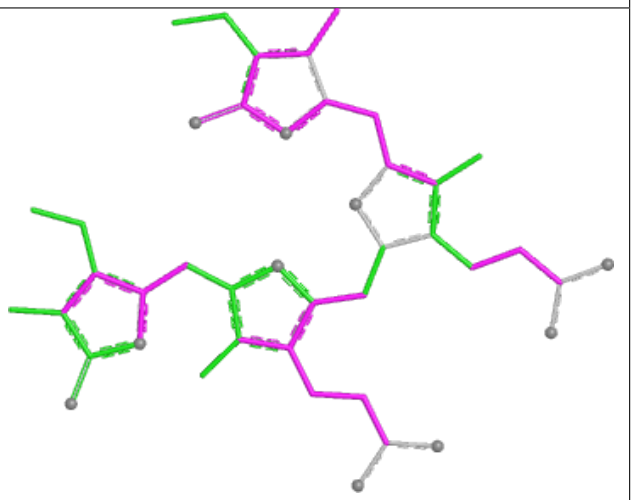

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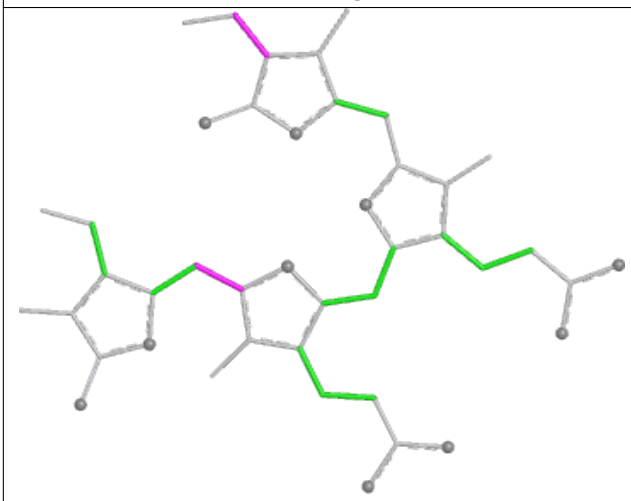

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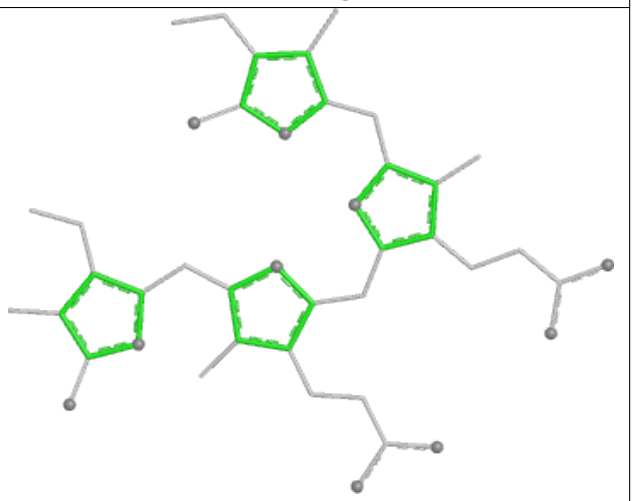
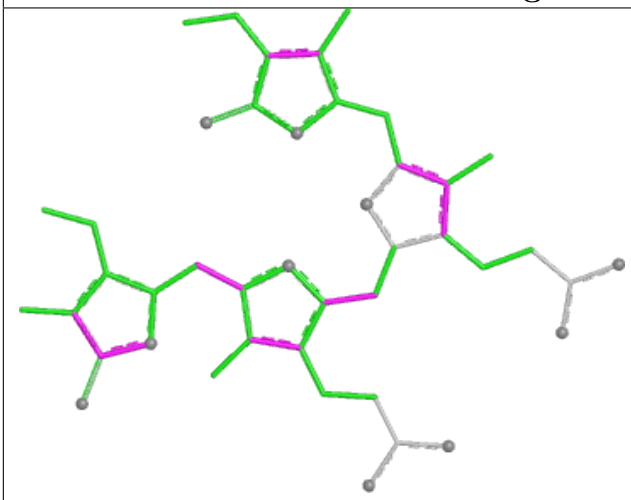


Rings

Ligand PEB H 167



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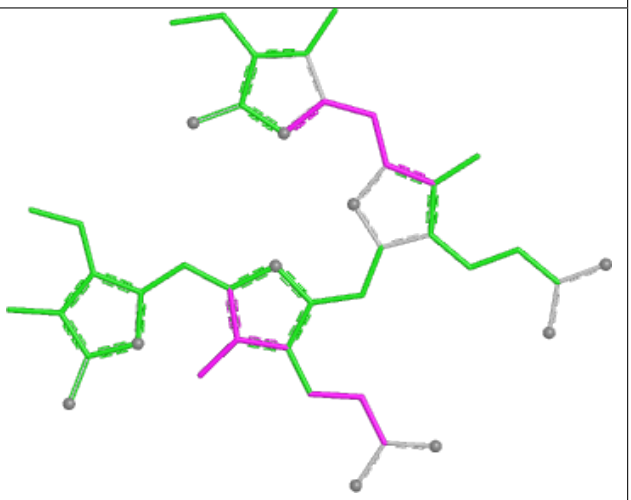

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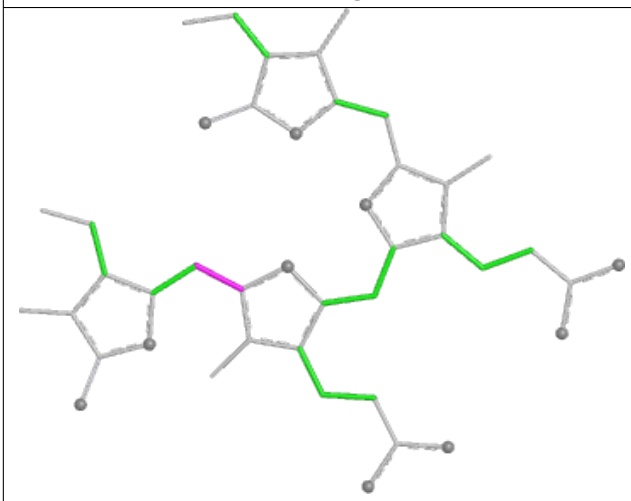

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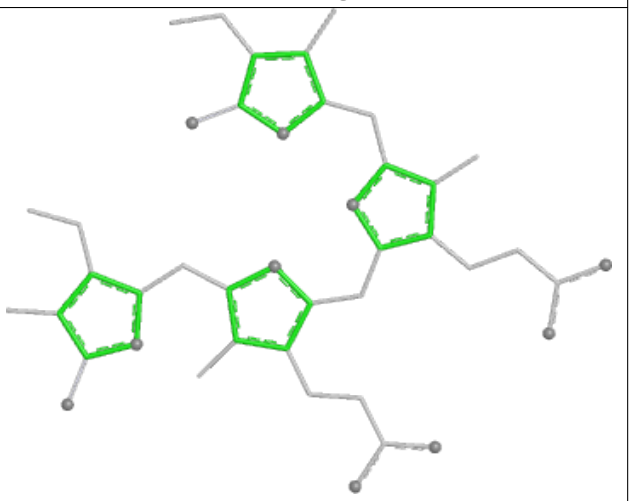
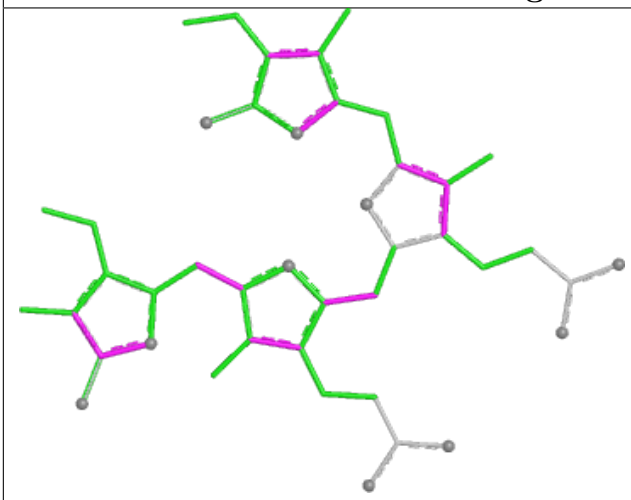


Rings

Ligand PEB E 167



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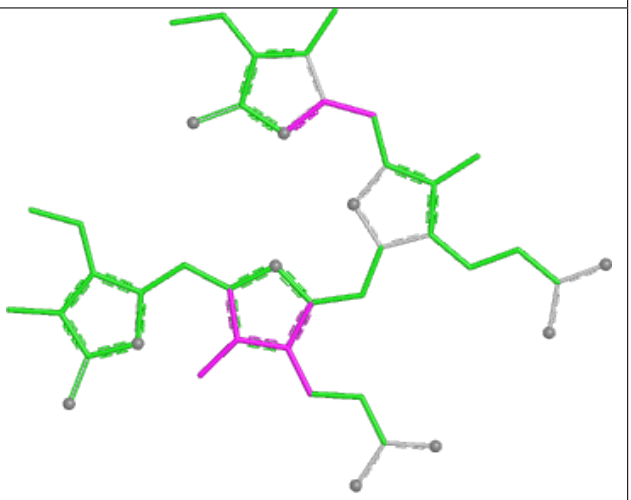
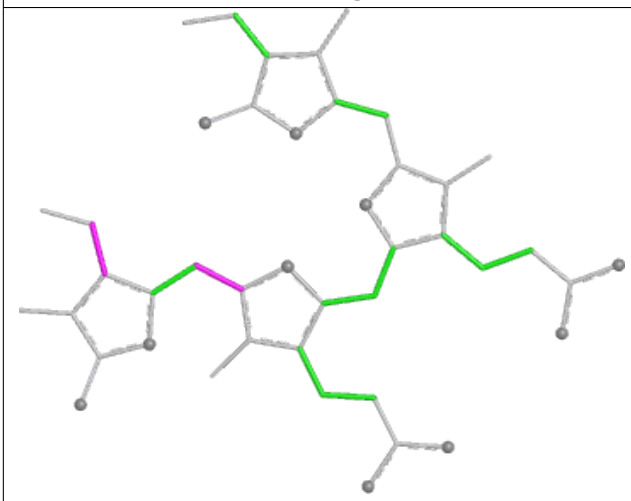


Bond angles



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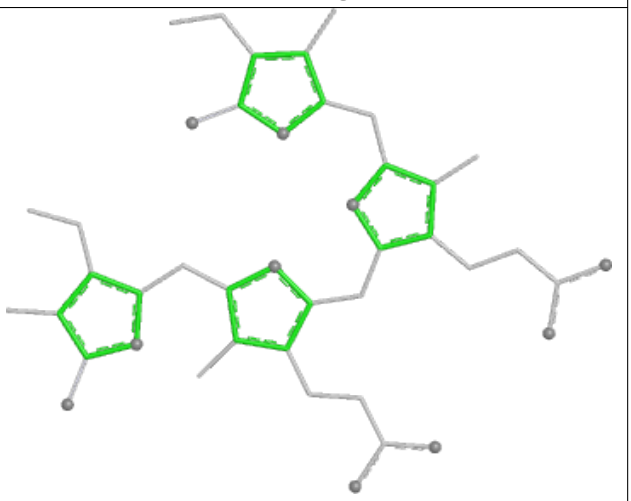
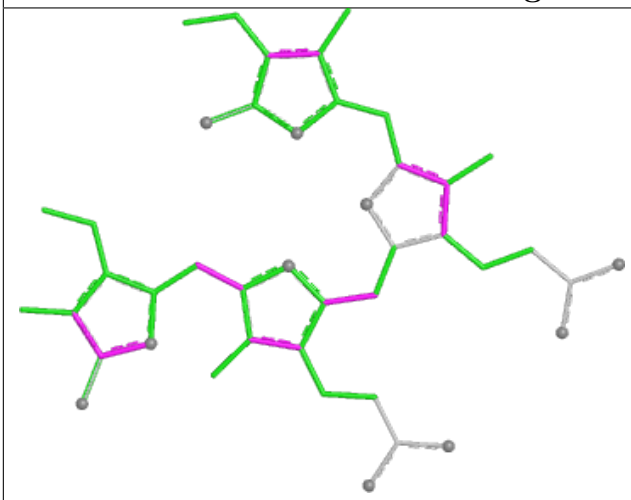


Rings

Ligand PEB A 167



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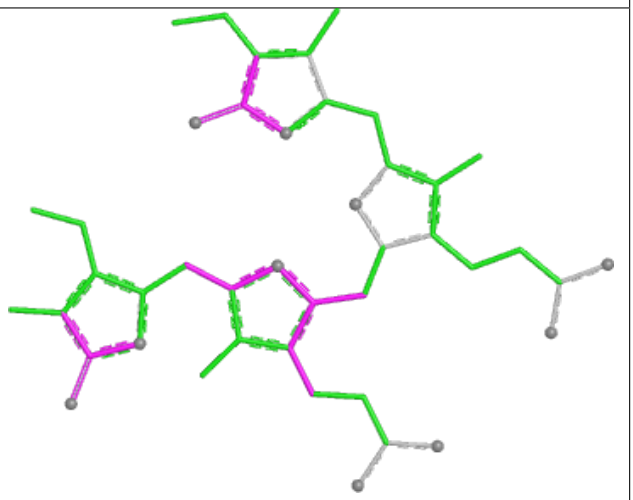

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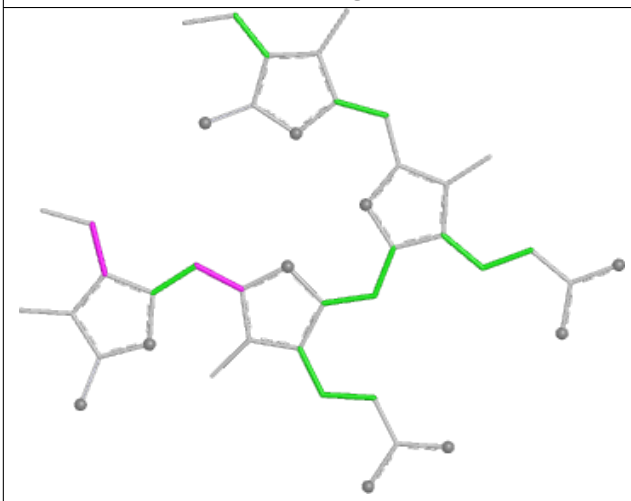

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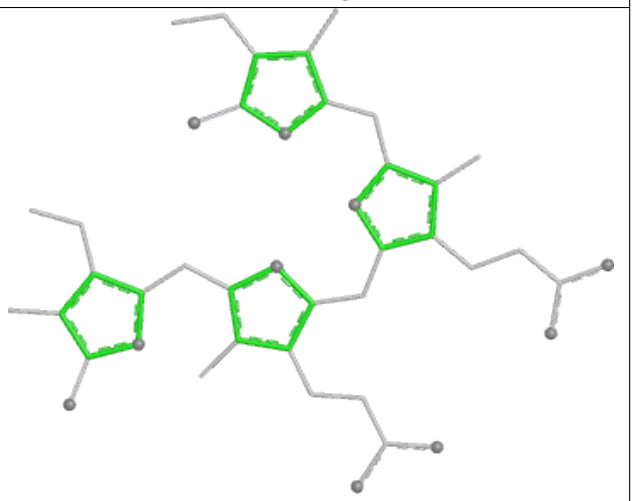
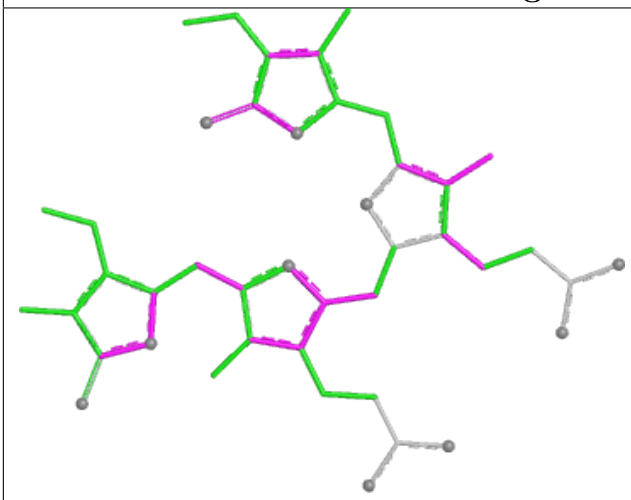


Rings

Ligand PEB G 167



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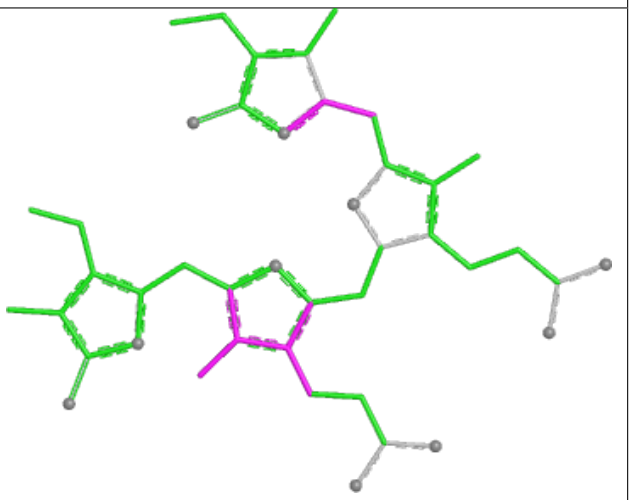

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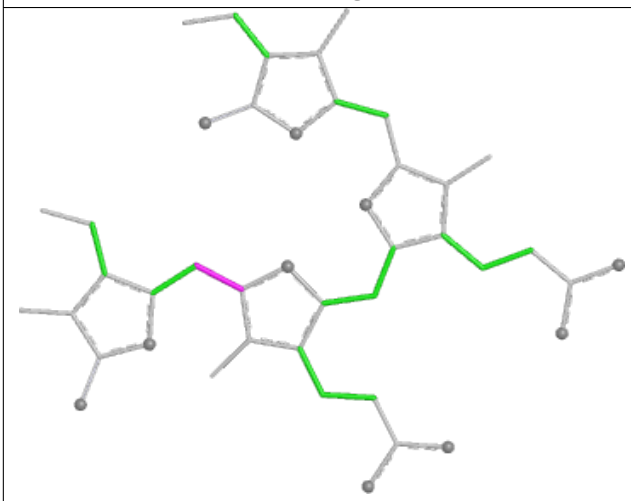

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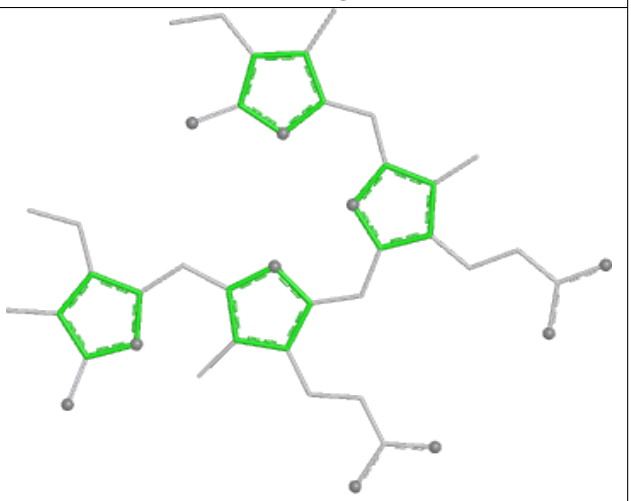
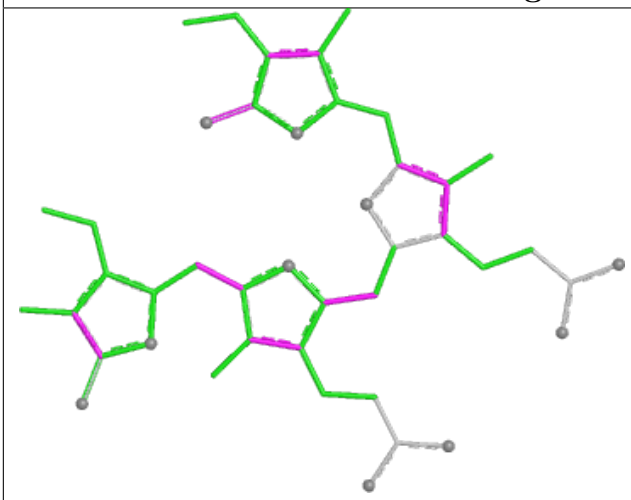


Rings

Ligand PEB Q 186



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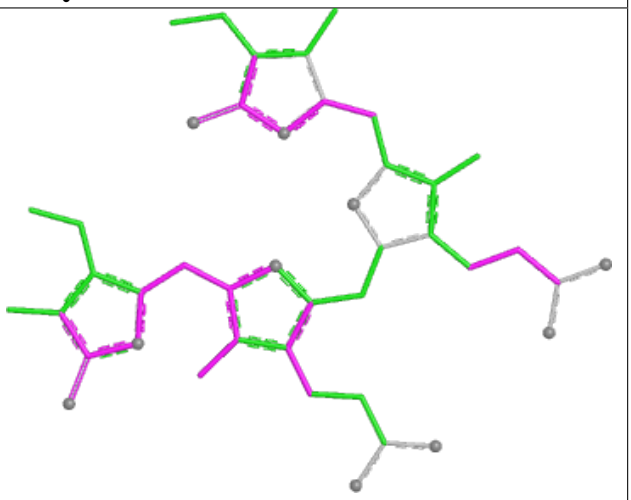

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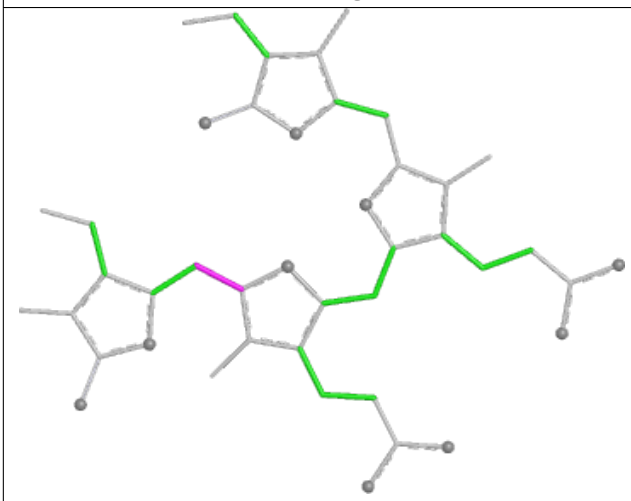

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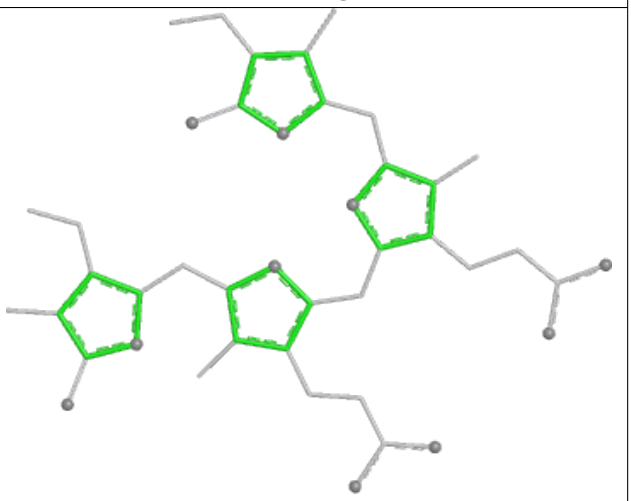
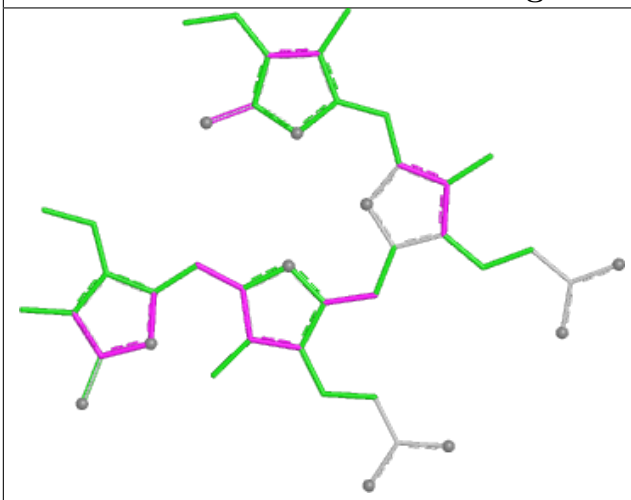


Rings

Ligand PEB F 167



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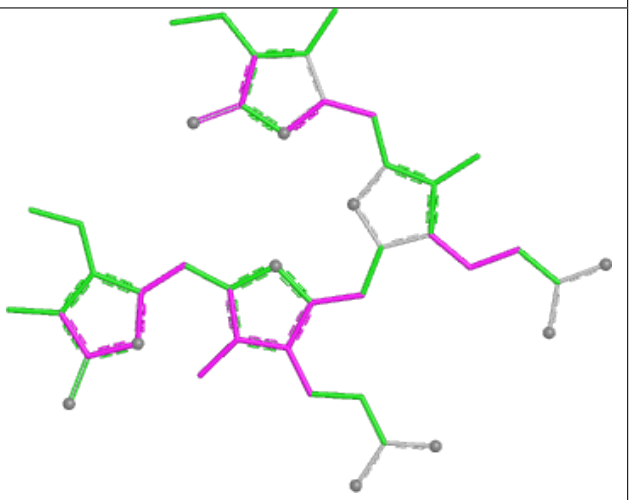
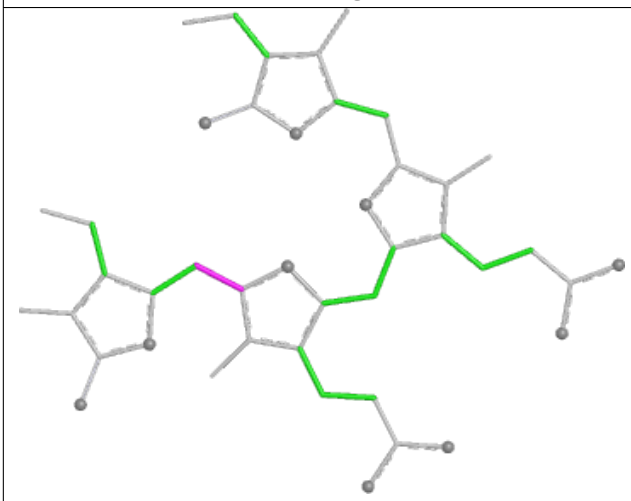


Bond angles



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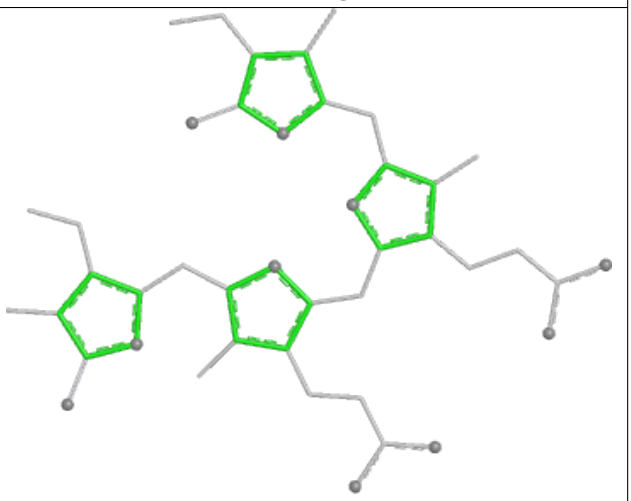
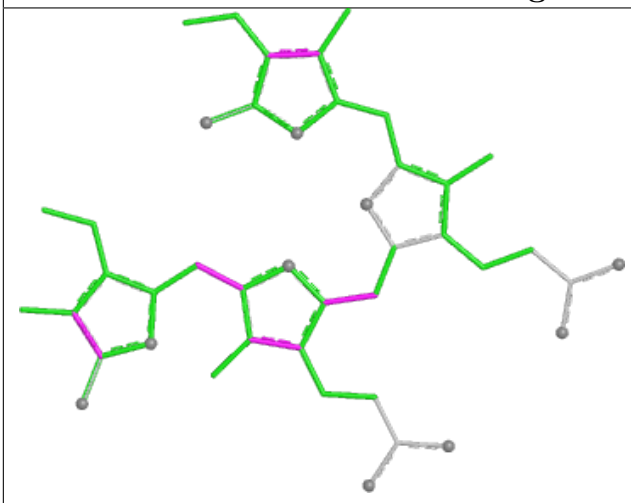


Rings

Ligand PEB J 166



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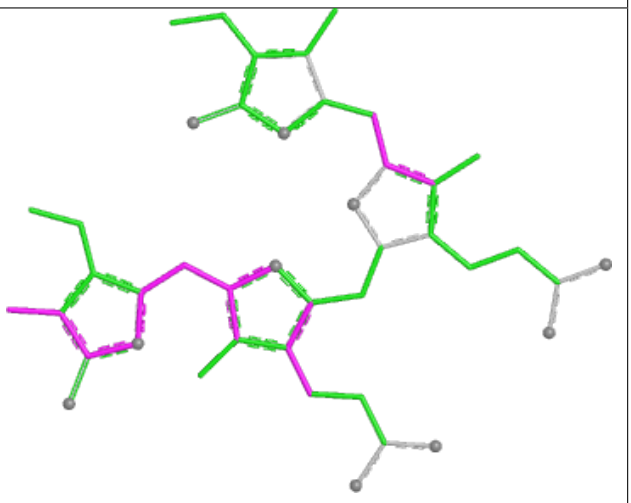
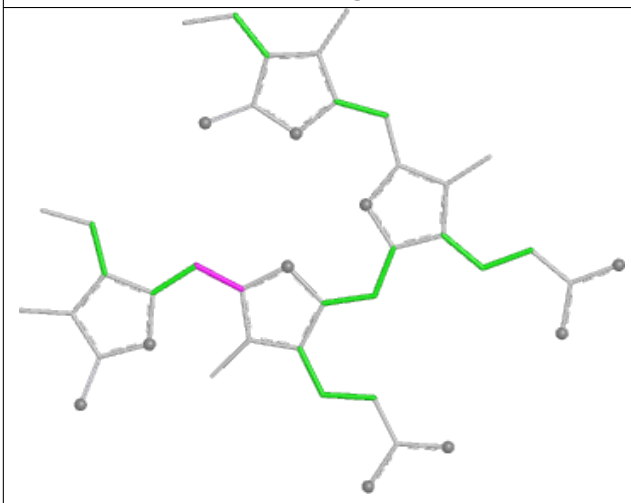


Bond angles



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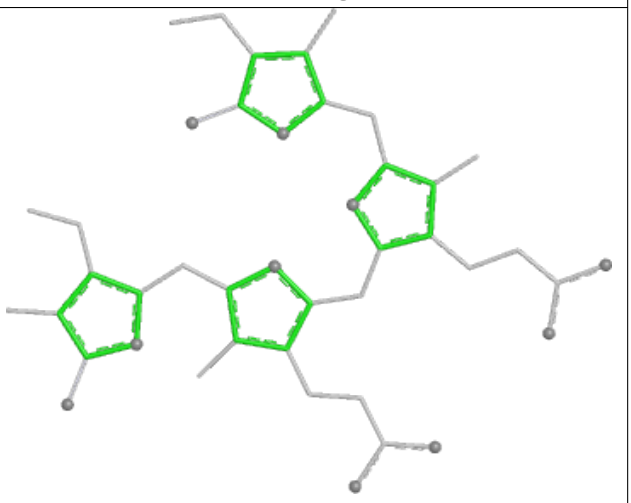
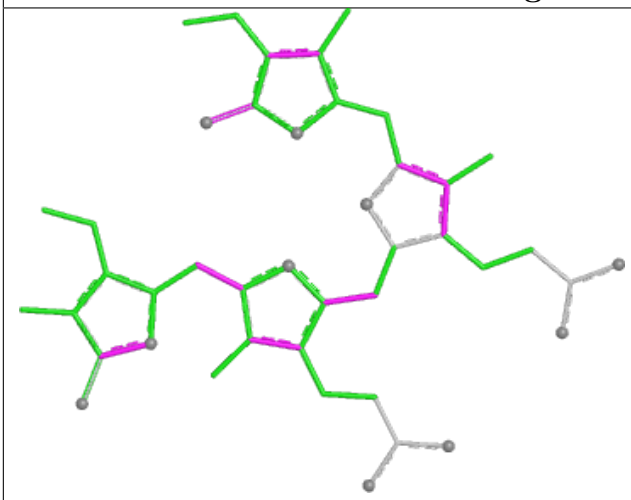


Rings

Ligand PEB R 187



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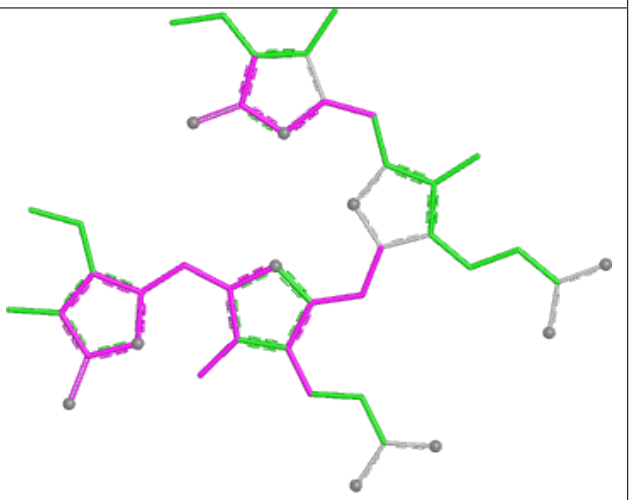
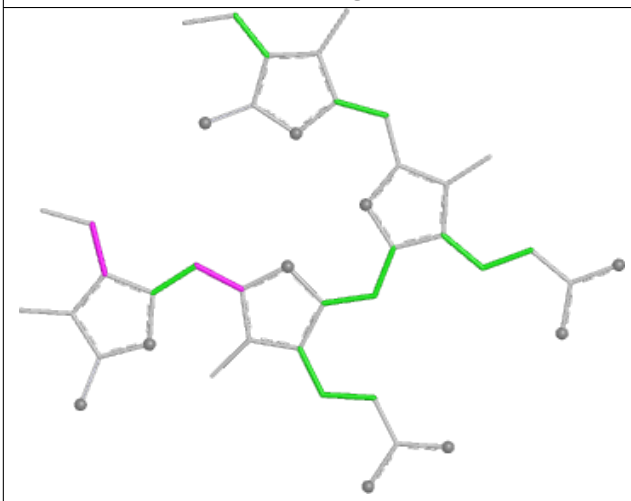


Bond angles



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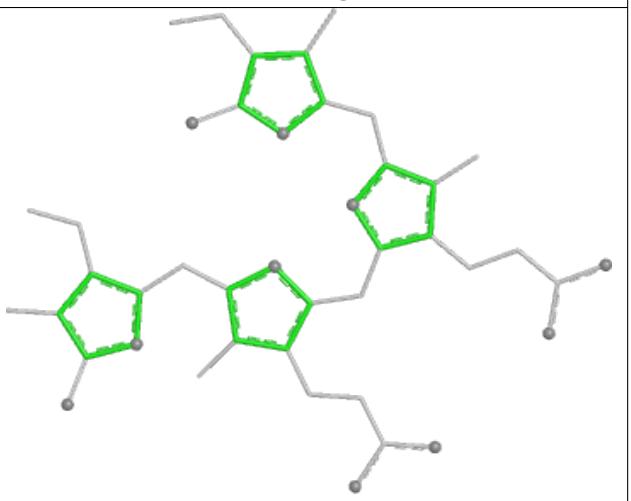
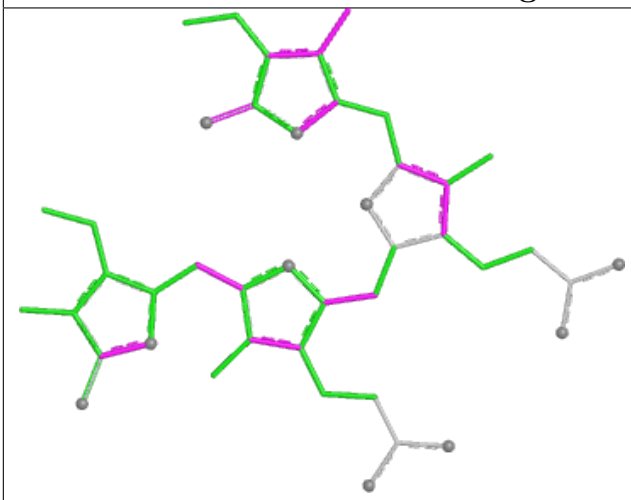


Rings

Ligand PEB W 186



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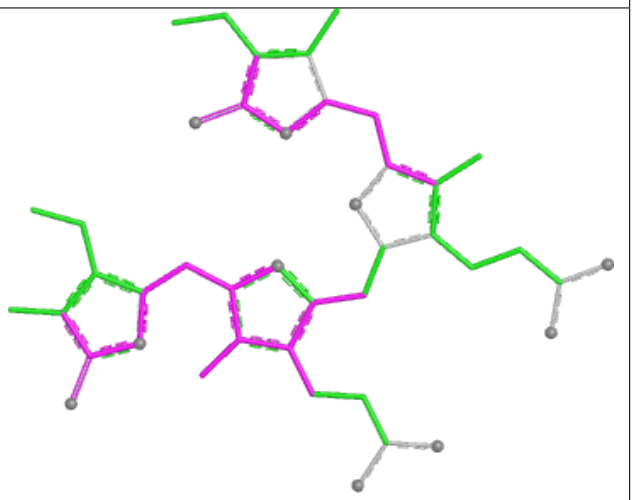
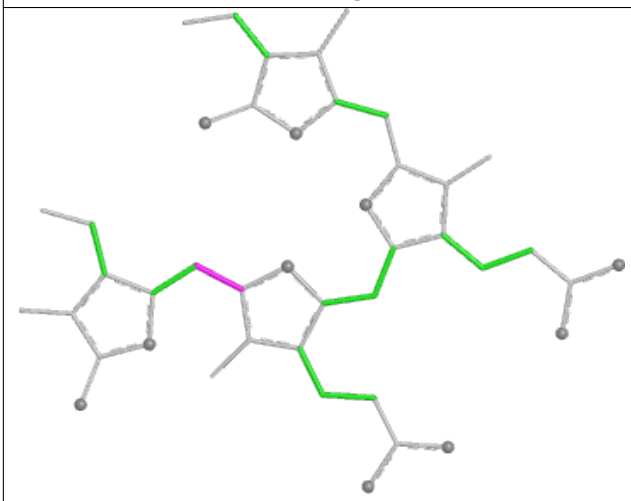


Bond angles



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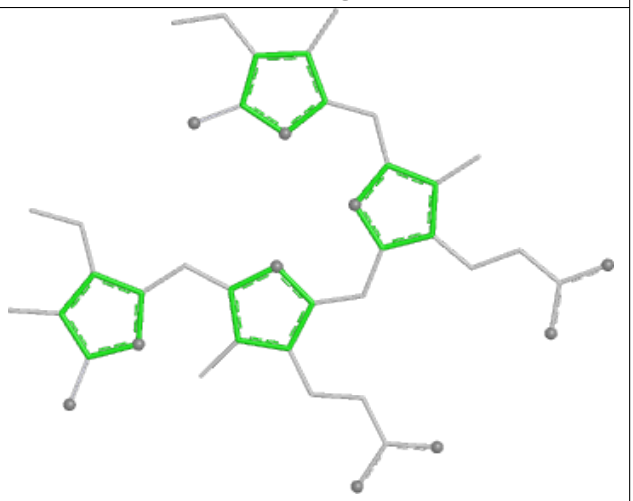
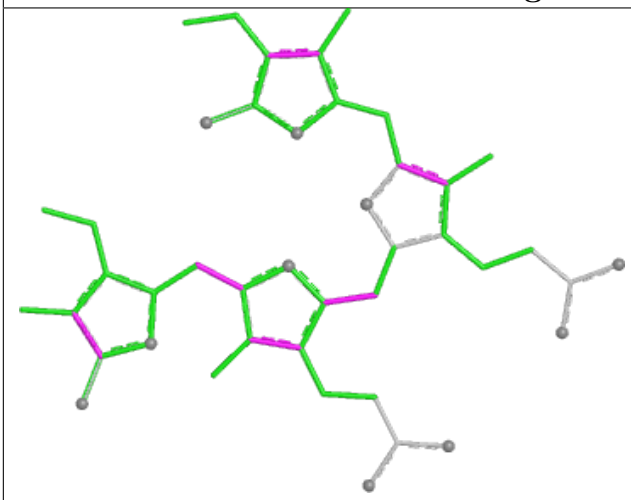


Rings

Ligand PEB O 186



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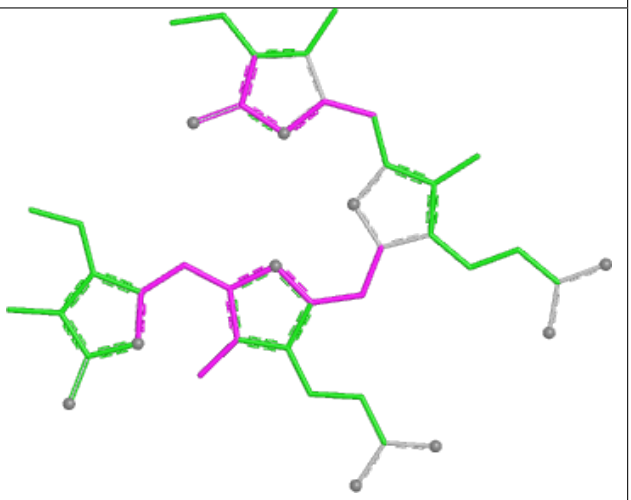
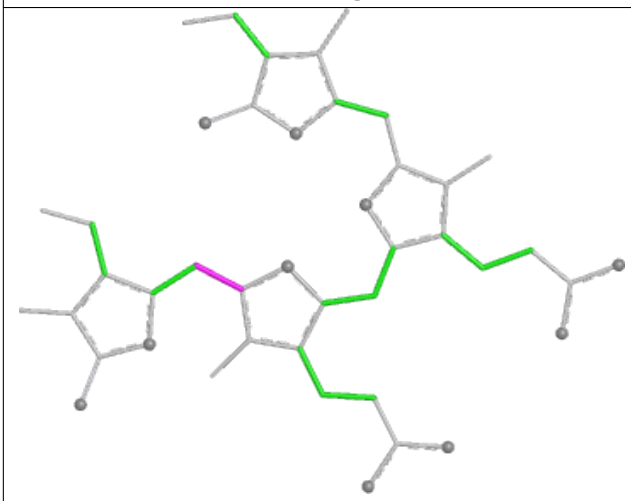


Bond angles



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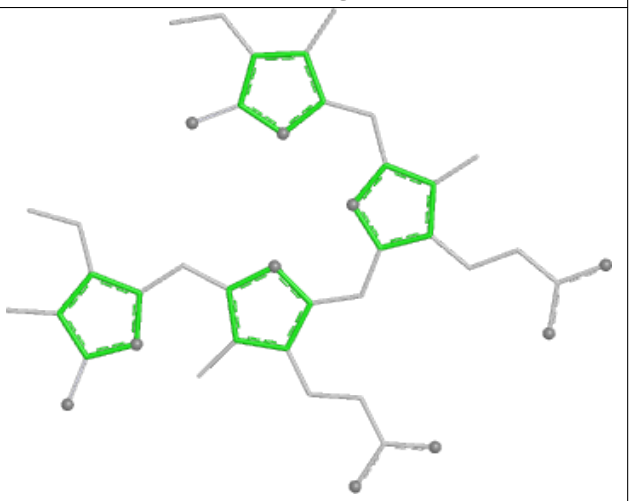
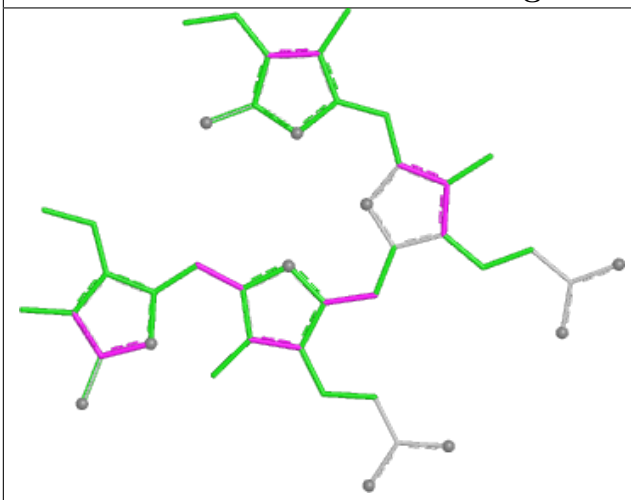
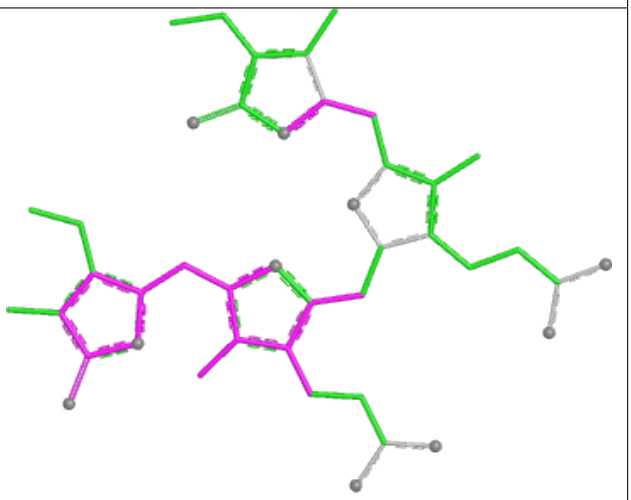


Rings

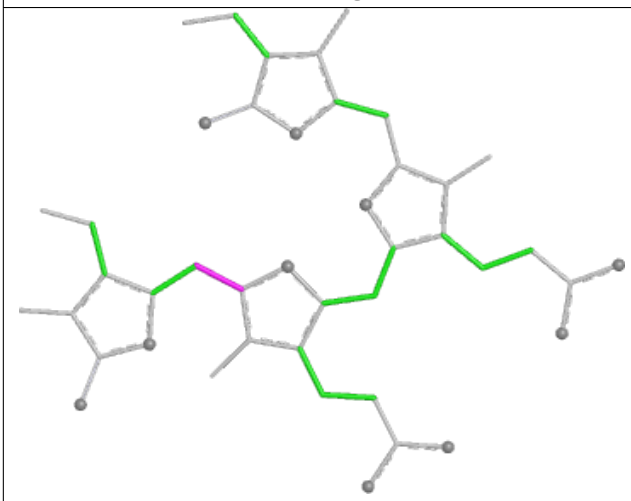
Ligand PEB N 186



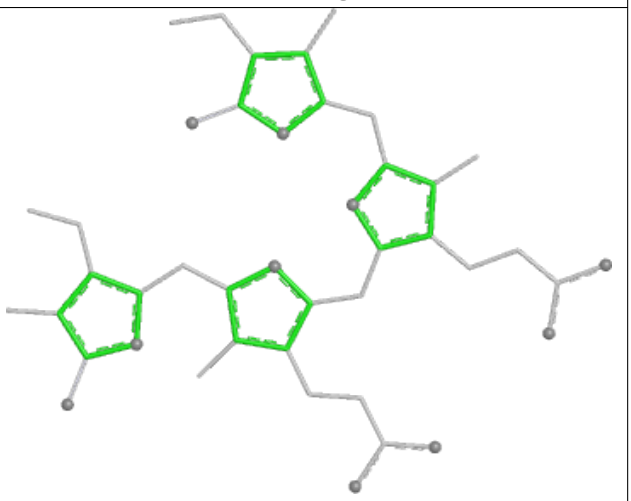
Bond lengths



Bond angles

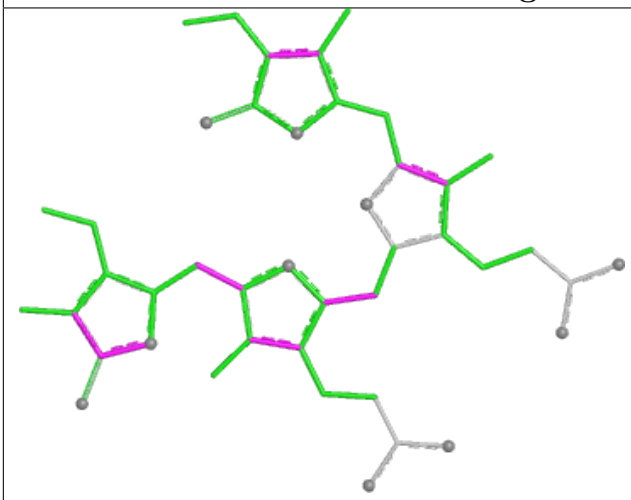


Torsions



Rings

Ligand PEB W 187



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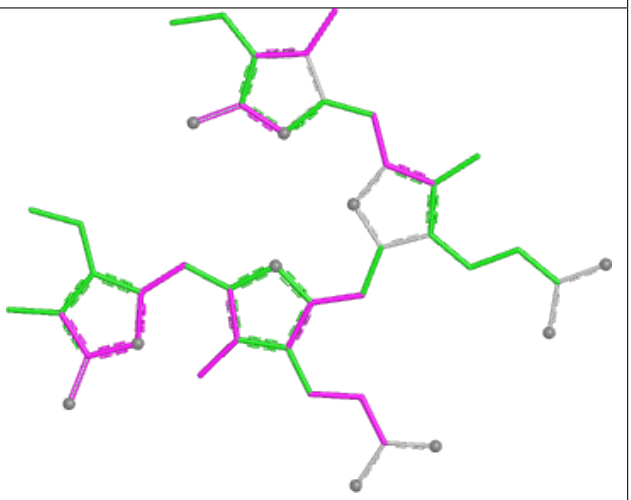
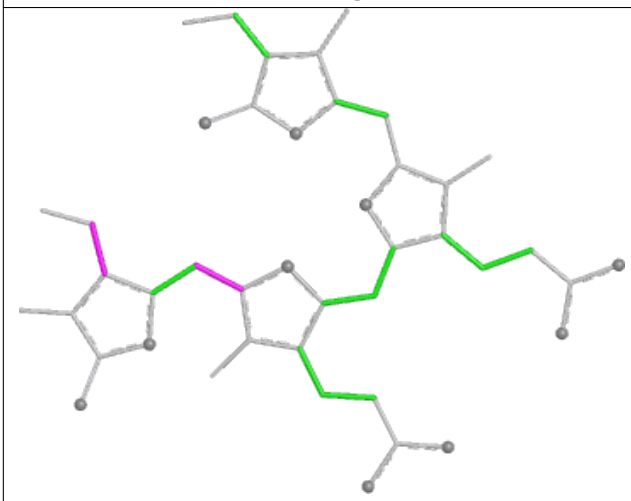


Bond angles



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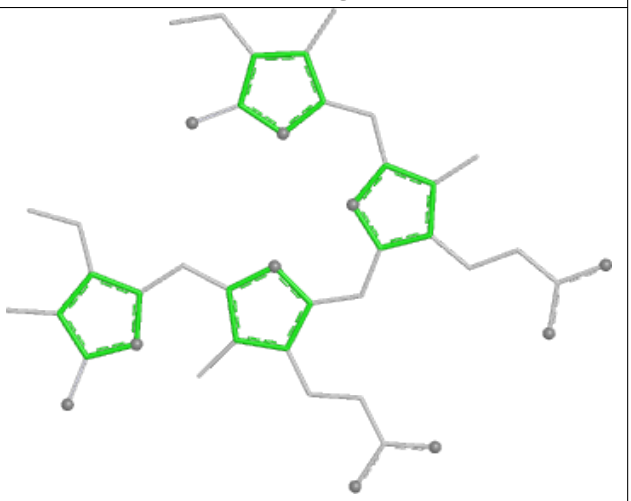
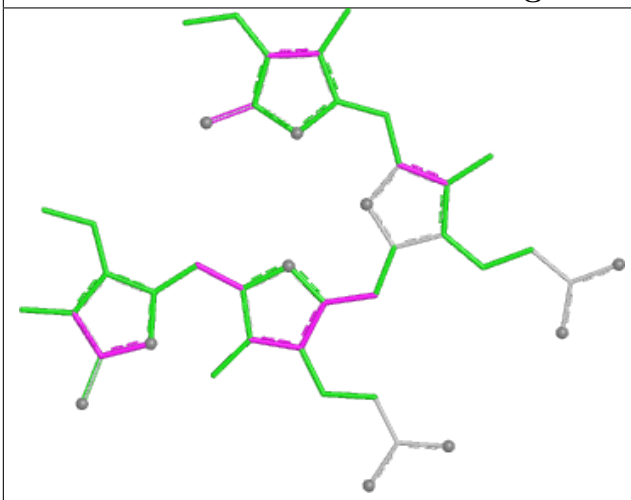


Rings

Ligand PEB O 187



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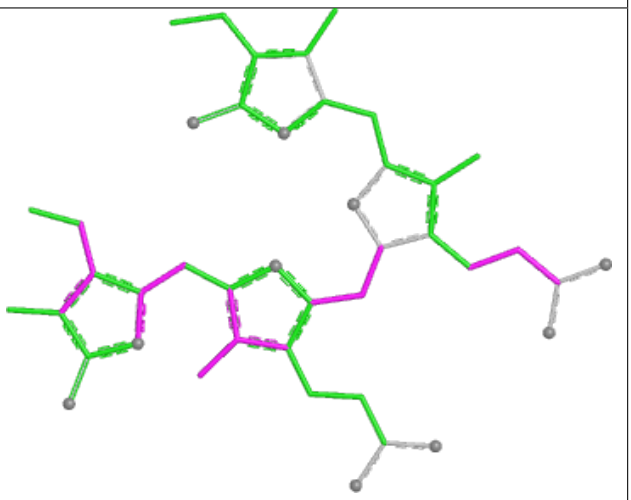
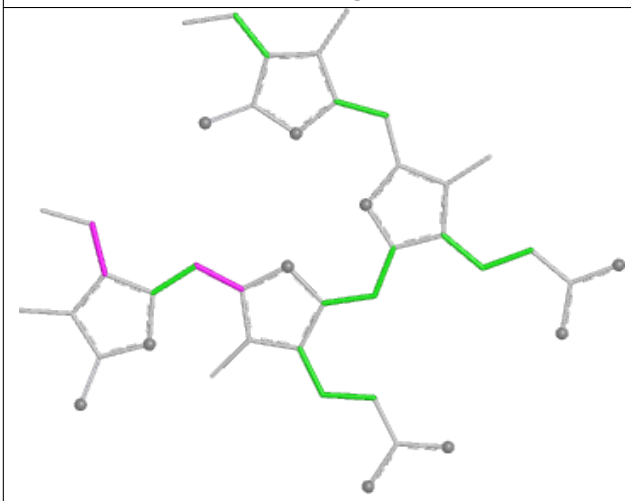


Bond angles



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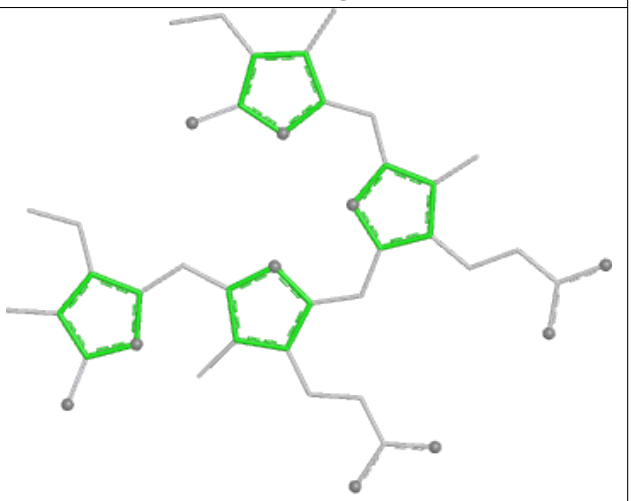
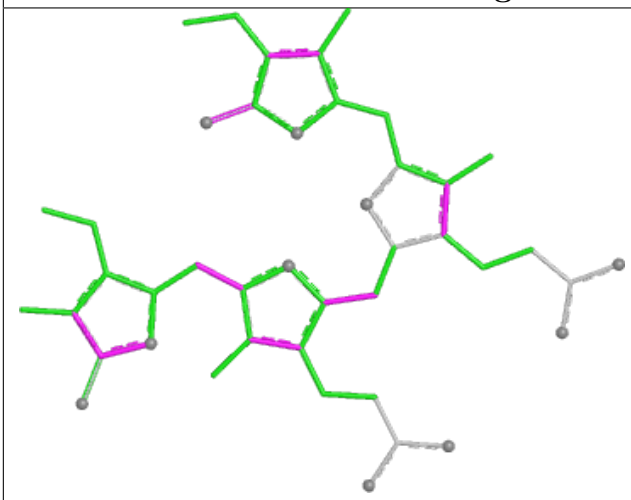


Rings

Ligand PEB S 186 (A)



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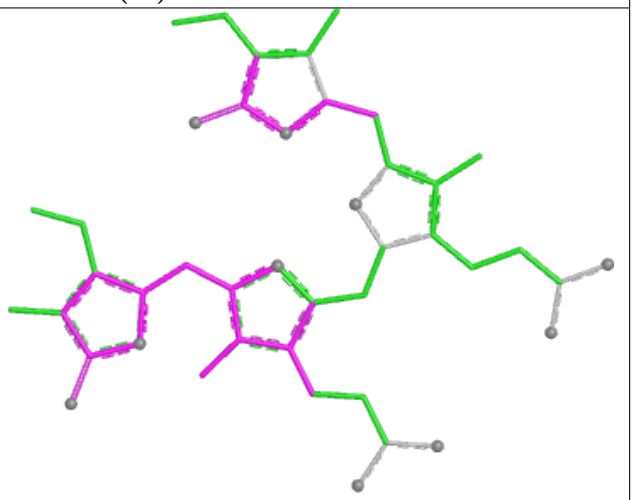
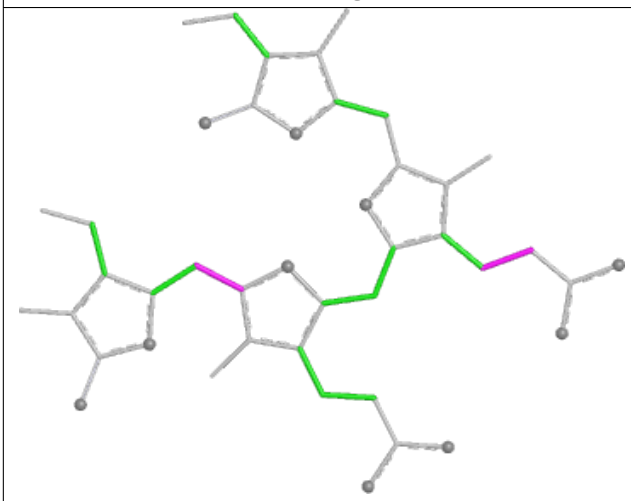


Bond angles



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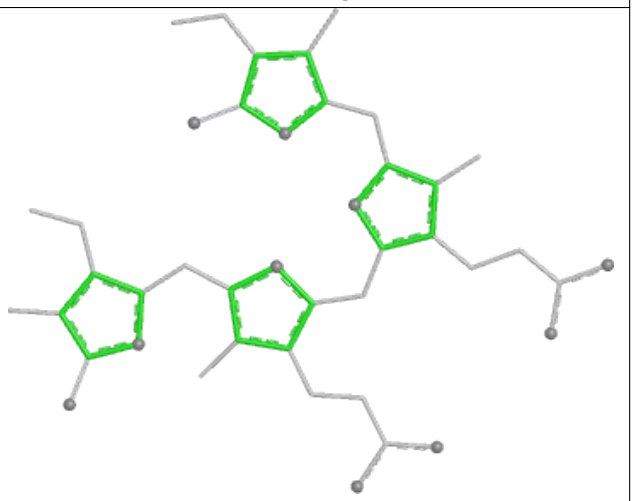
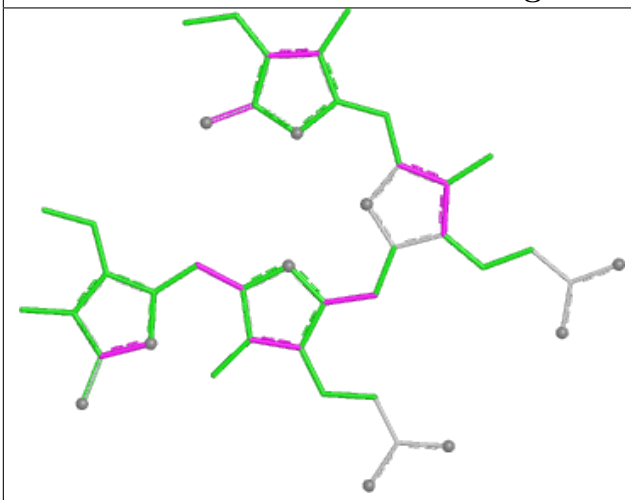


Rings

Ligand PEB X 188



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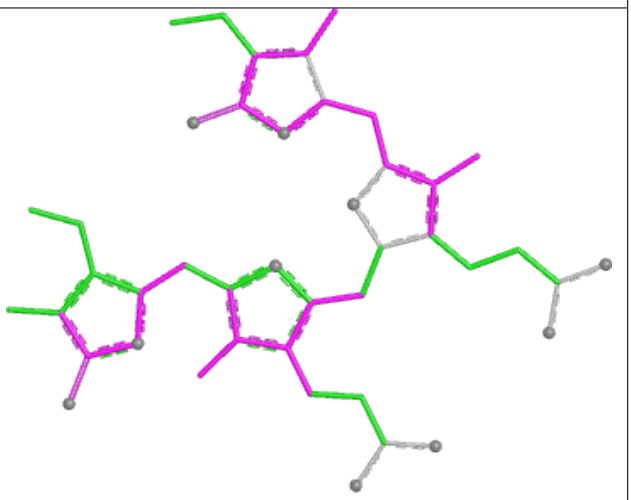
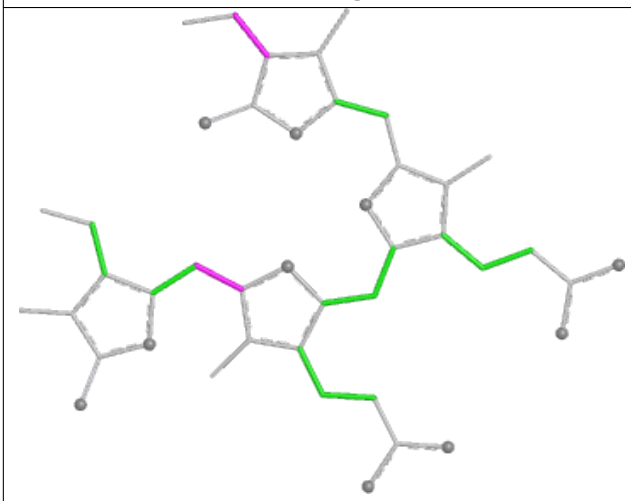


Bond angles



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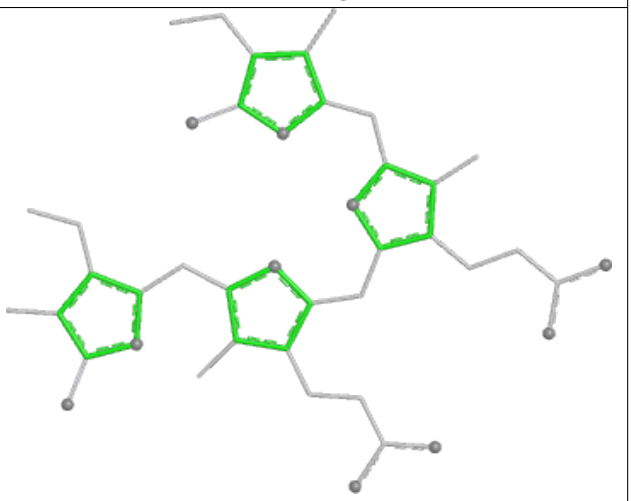
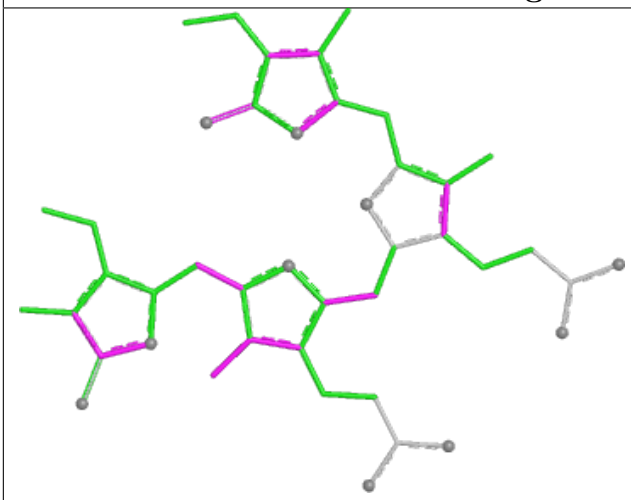


Rings

Ligand PEB P 186



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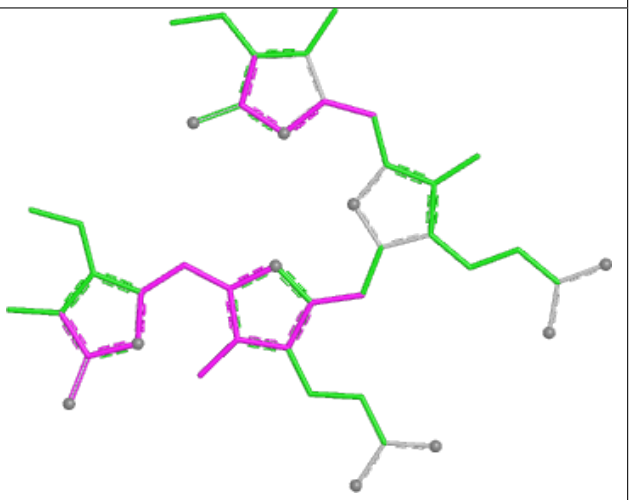
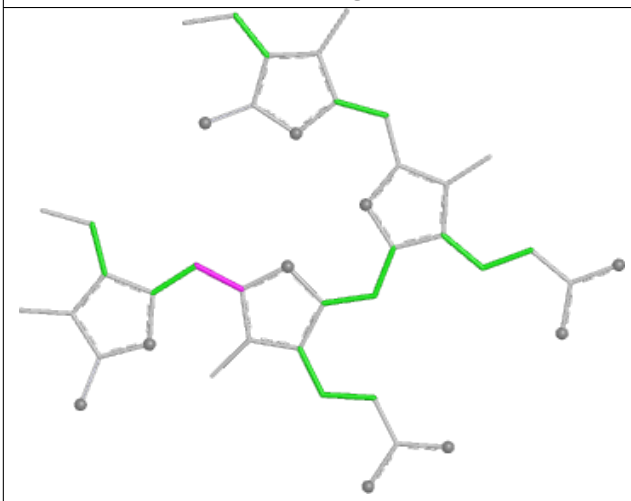


Bond angles



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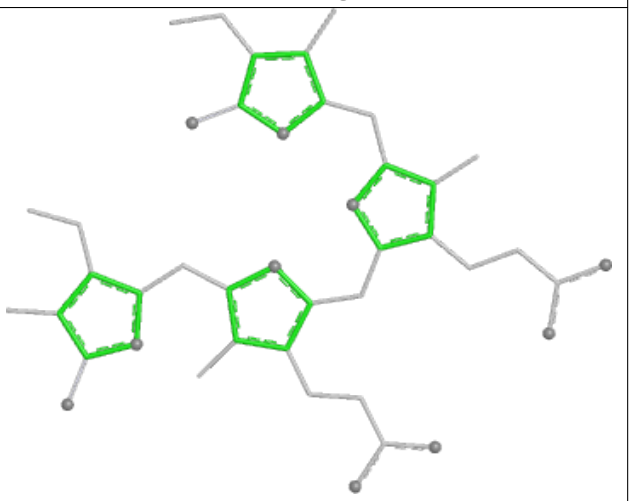
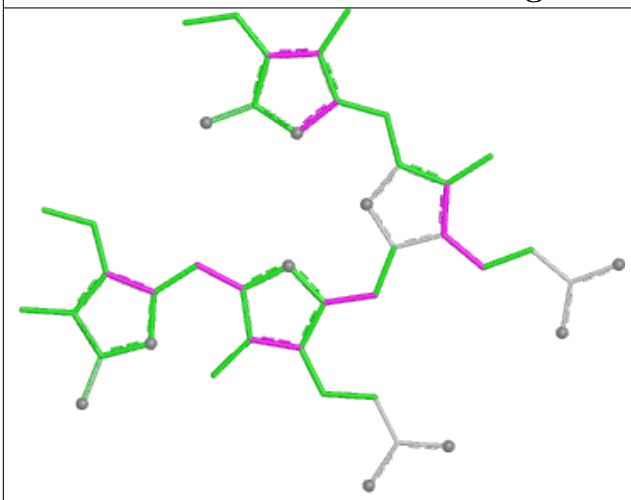


Rings

Ligand PEB P 187



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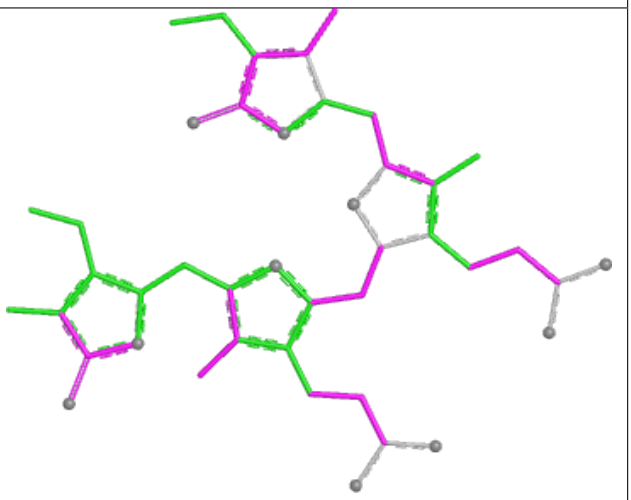

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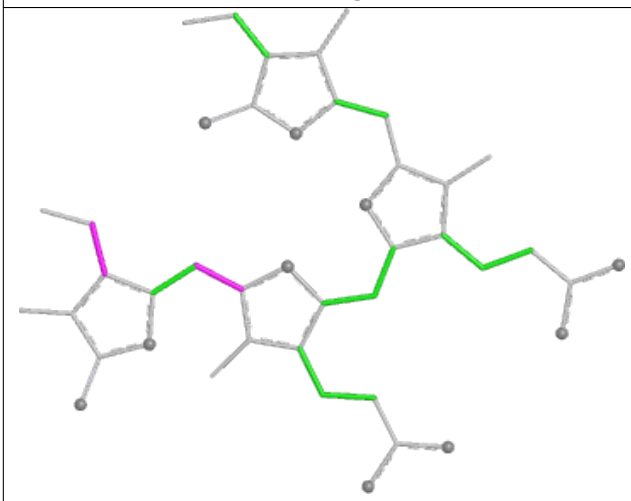

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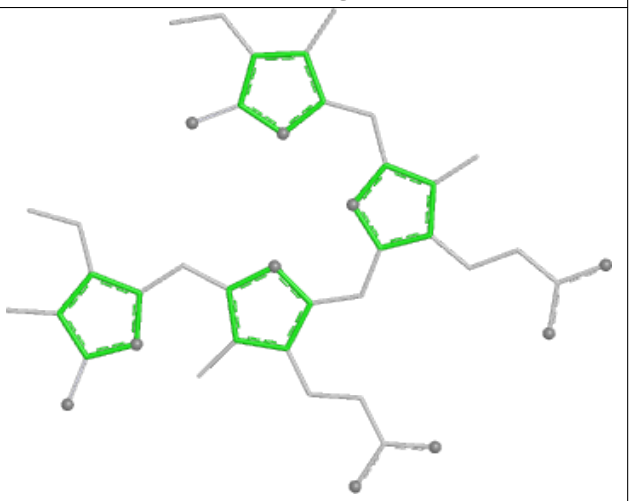
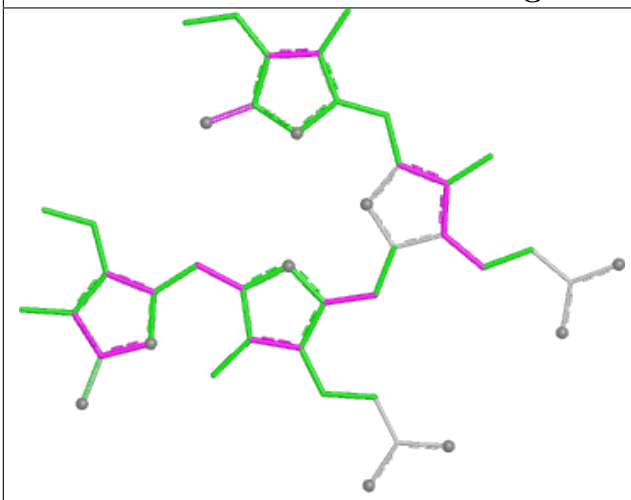


Rings

Ligand PEB D 167



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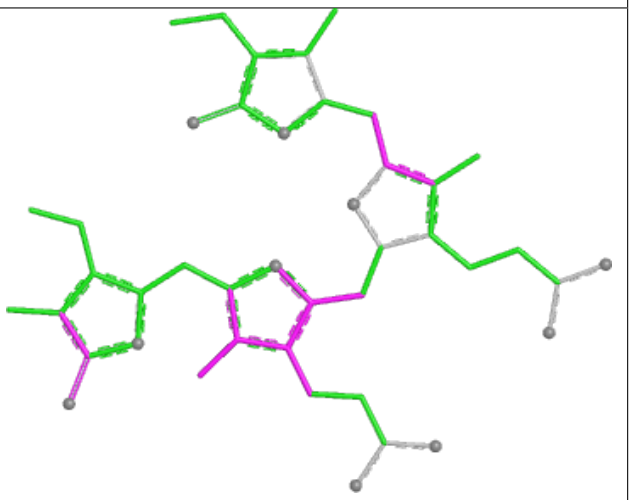
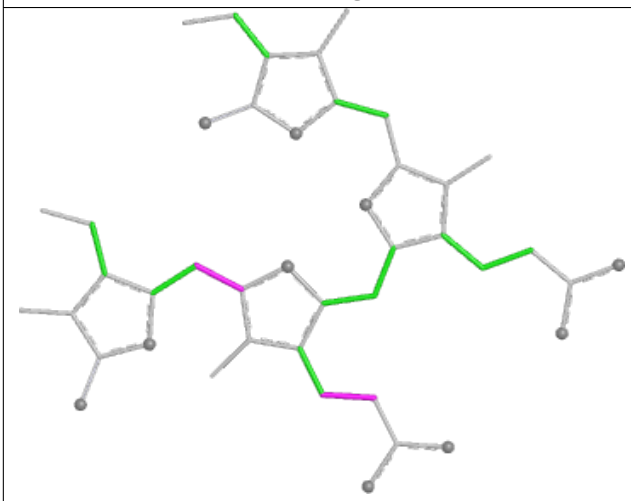


Bond angles



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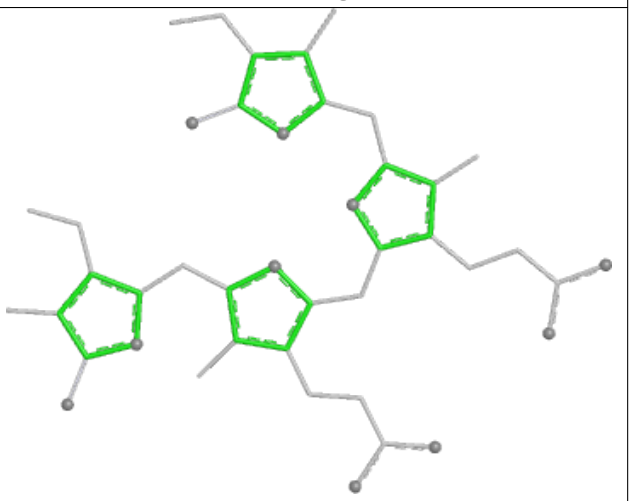
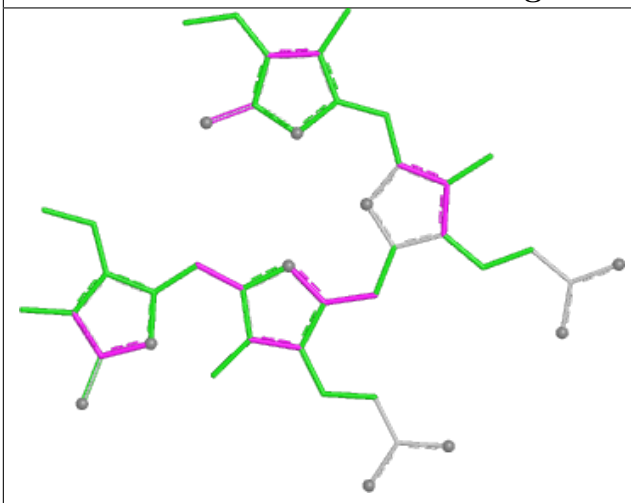


Rings

Ligand PEB R 186



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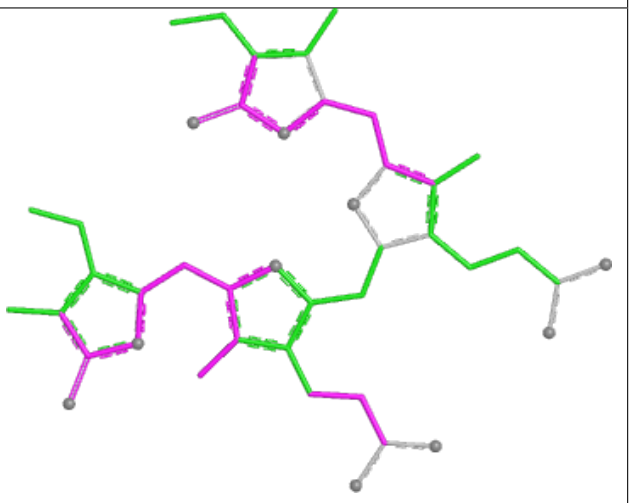
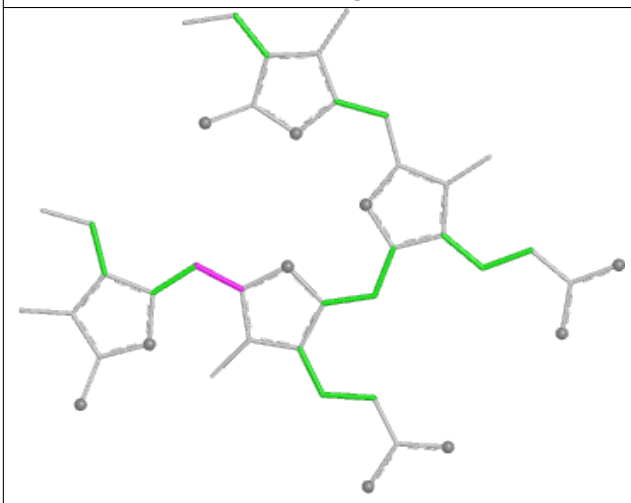


Bond angles



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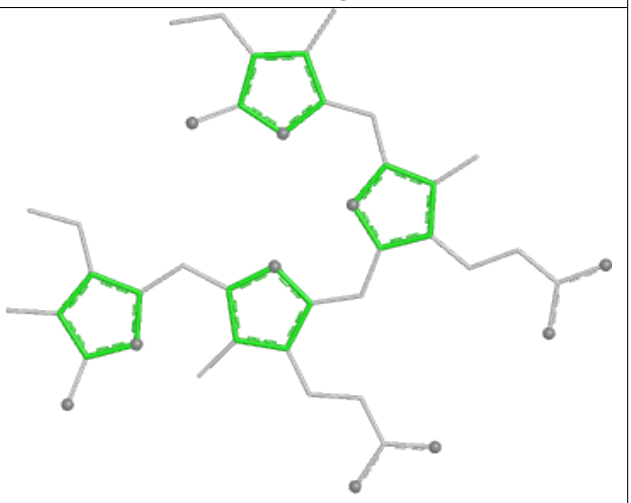
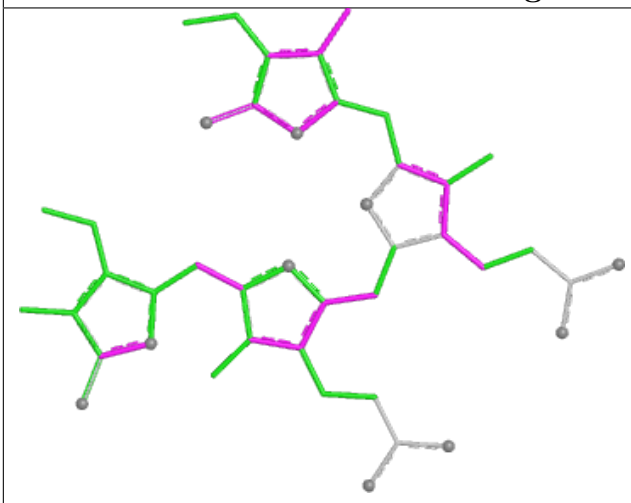


Rings

Ligand PEB O 188



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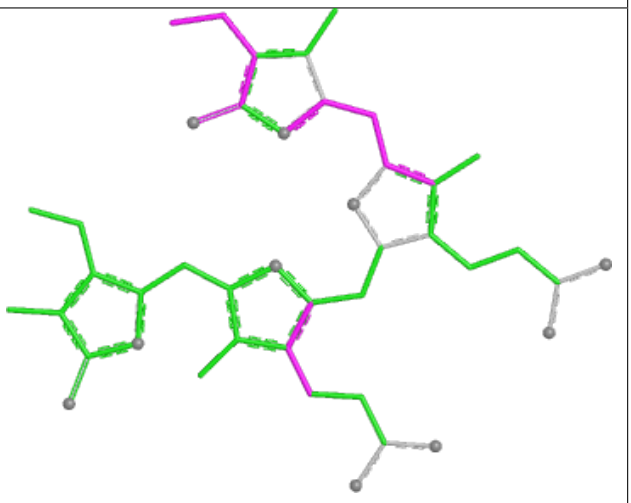
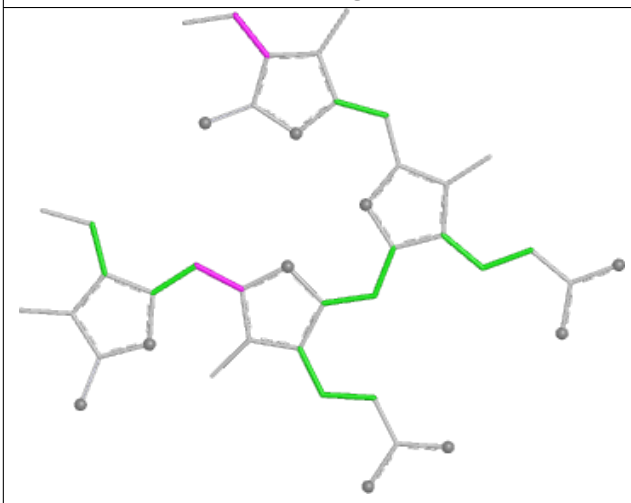


Bond angles



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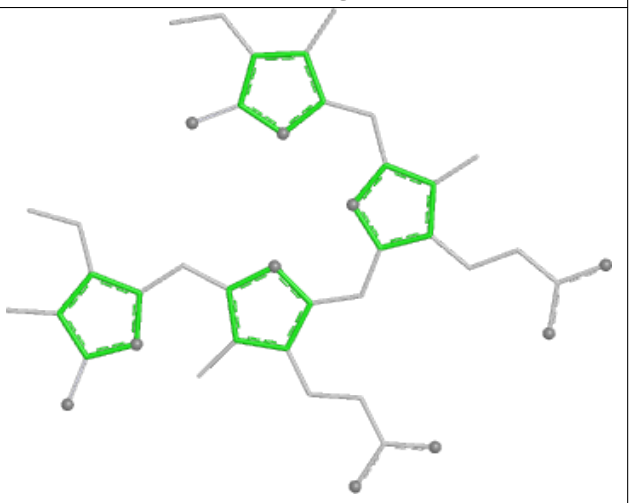
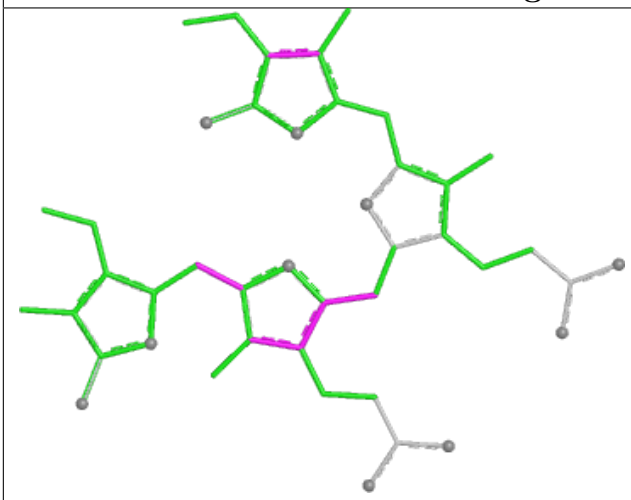


Rings

Ligand PEB V 187



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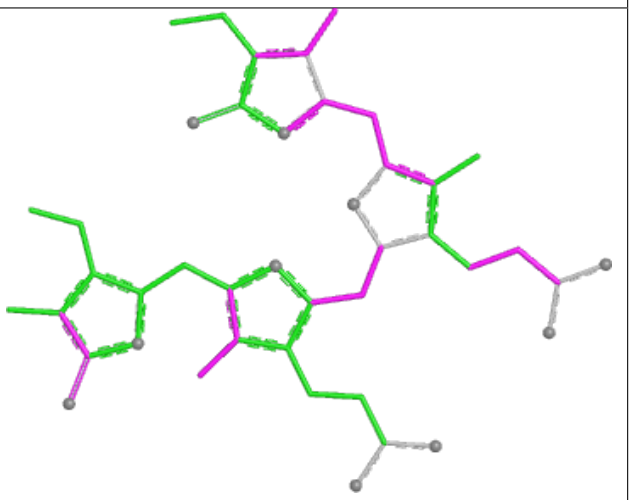
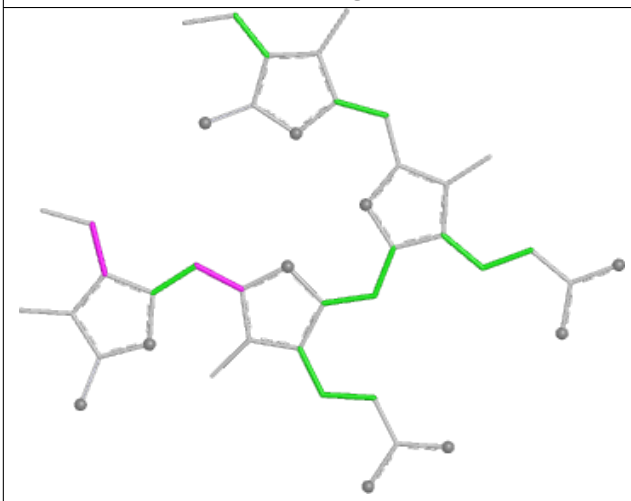


Bond angles



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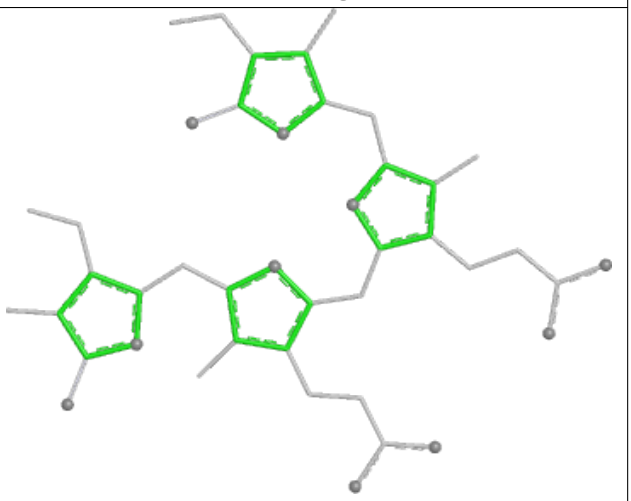
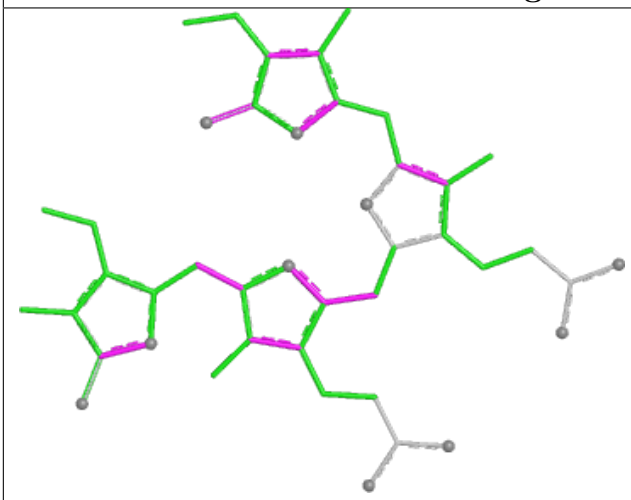


Rings

Ligand PEB R 188



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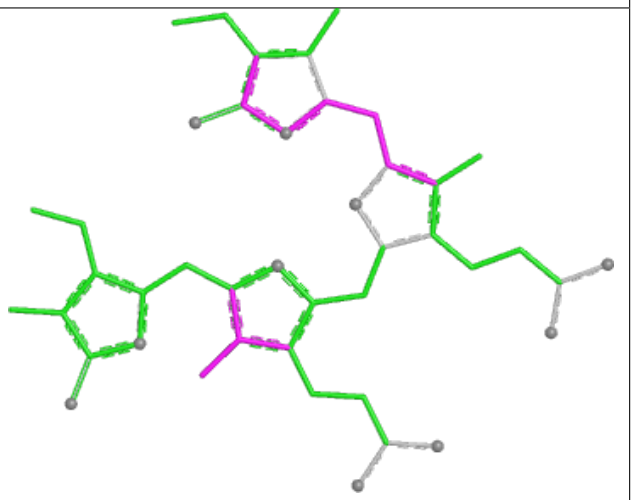
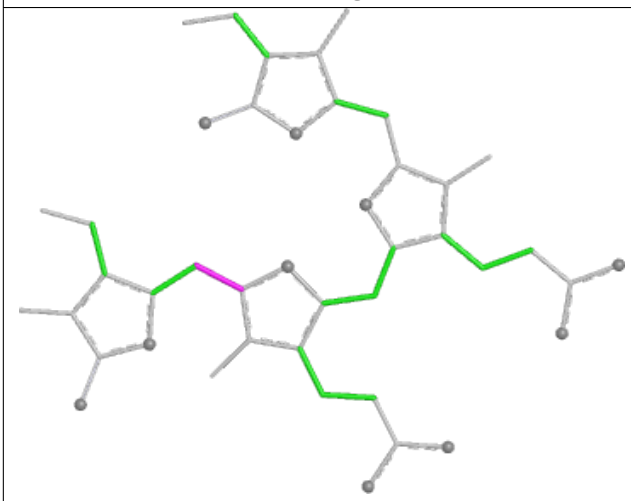
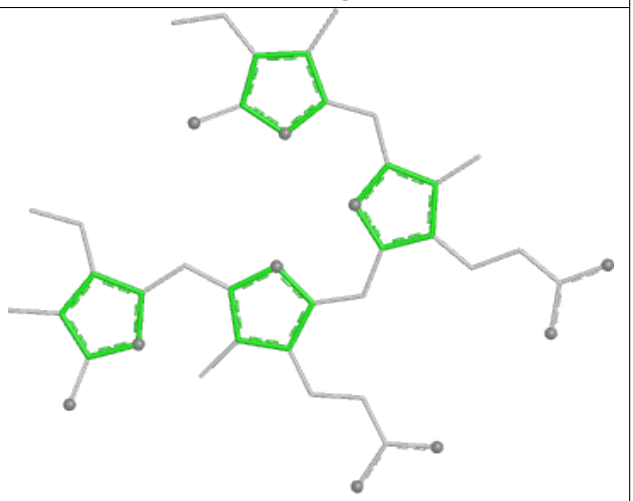


Bond angles

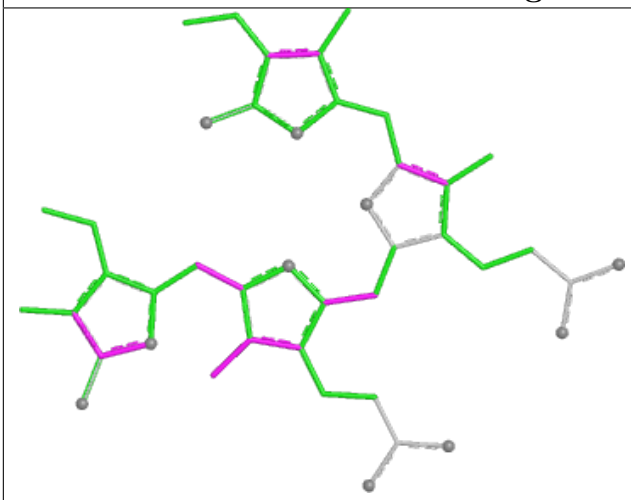


Torsions



Rings

Ligand PEB B 166



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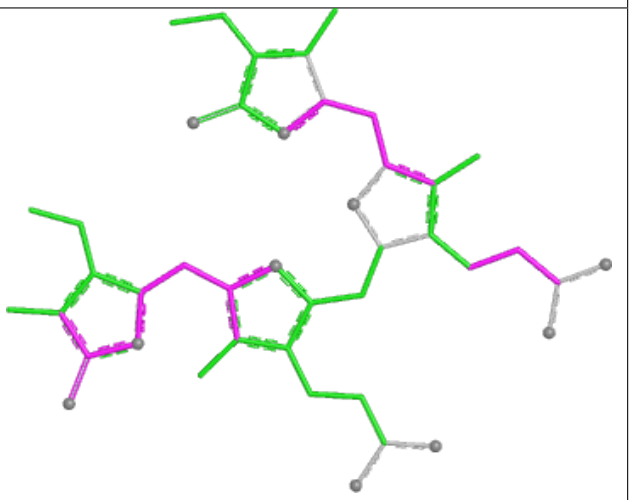
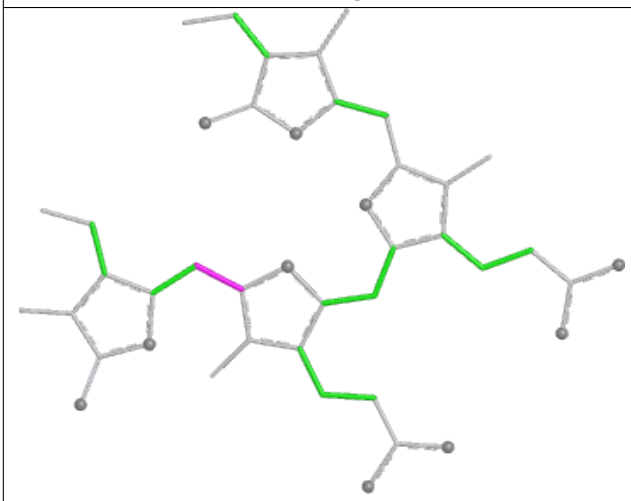
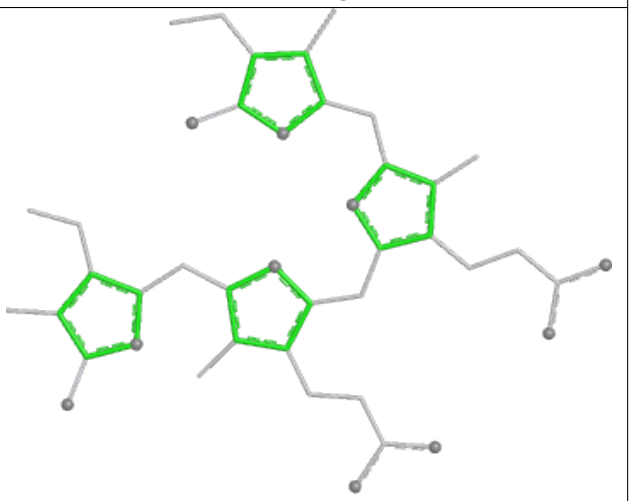


Bond angles

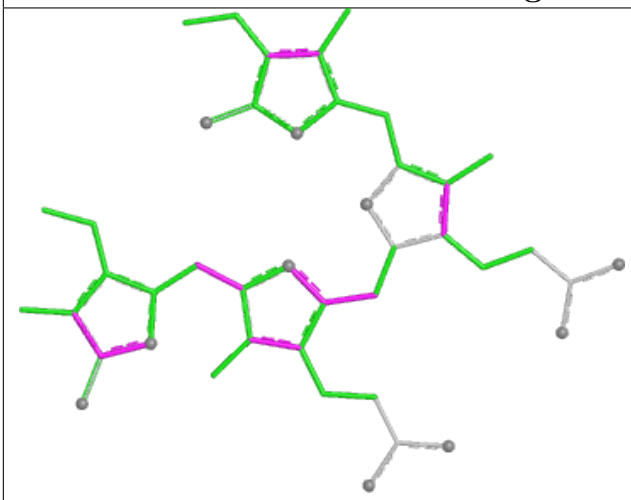


Torsions

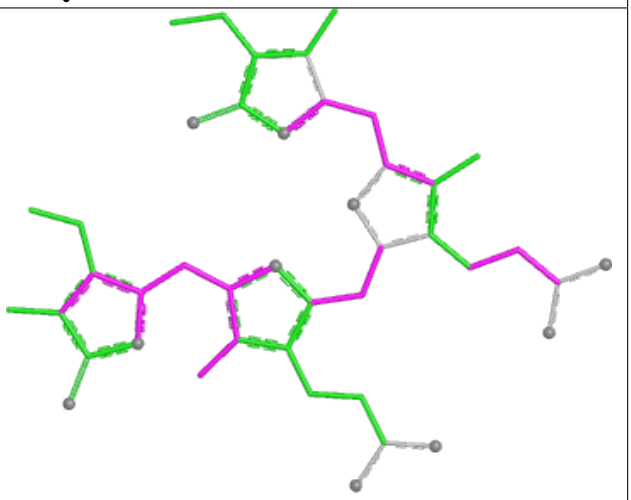


Rings

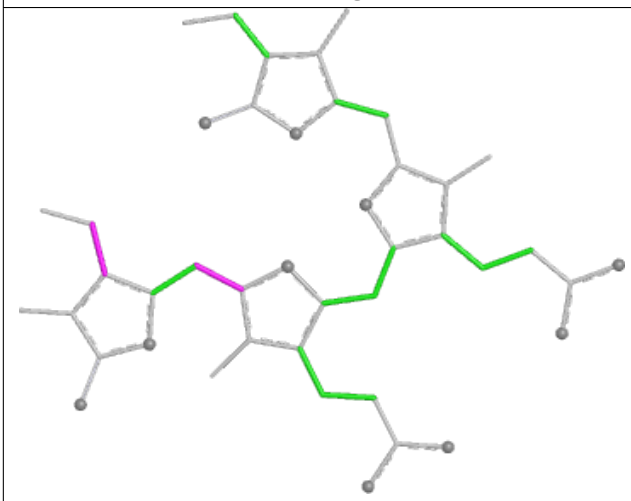
Ligand PEB Q 187



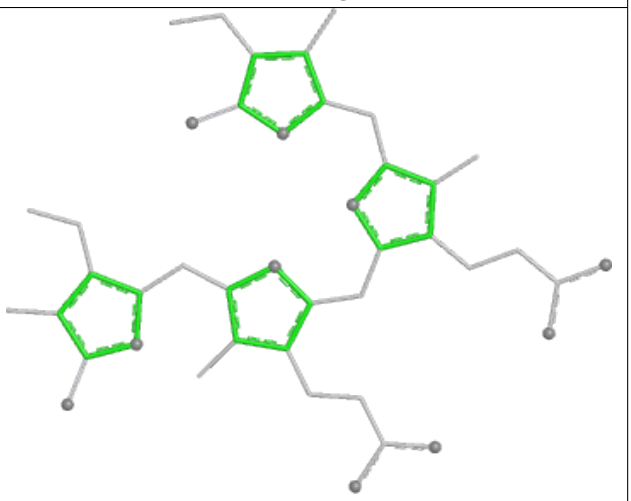
Bond lengths



Bond angles

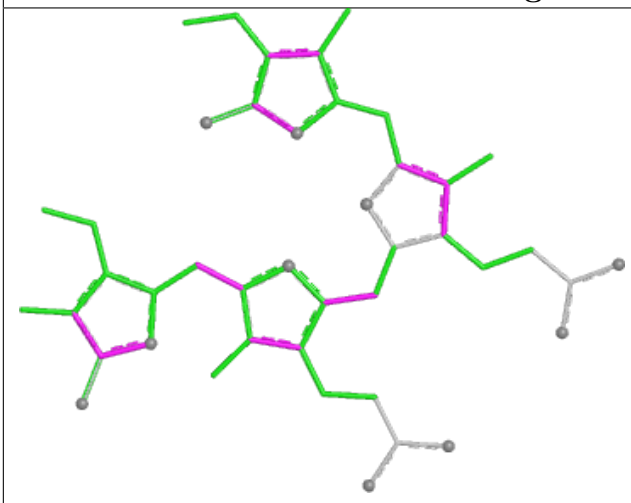


Torsions

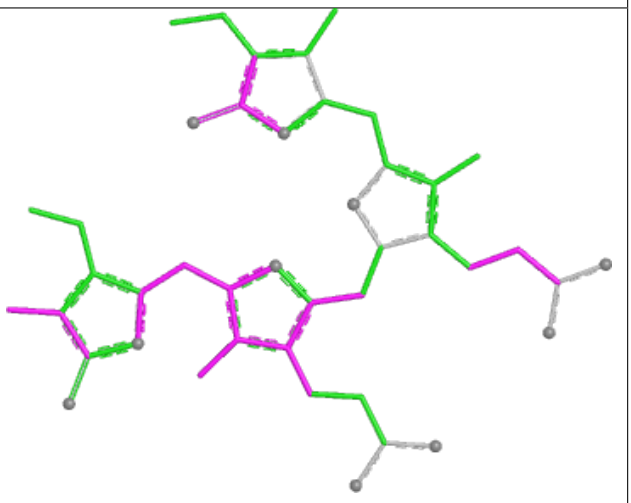


Rings

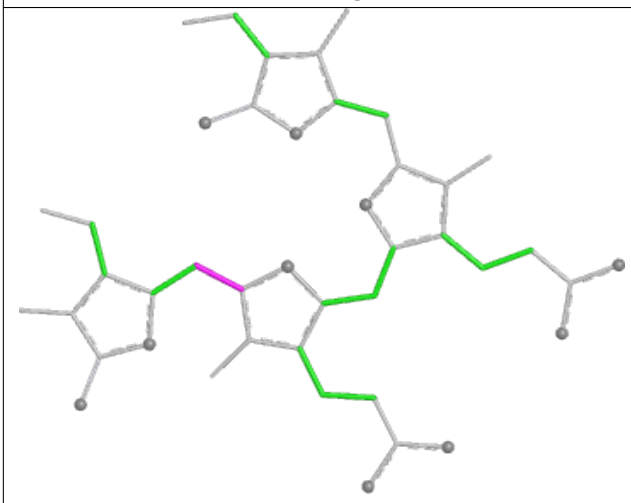
Ligand PEB C 166



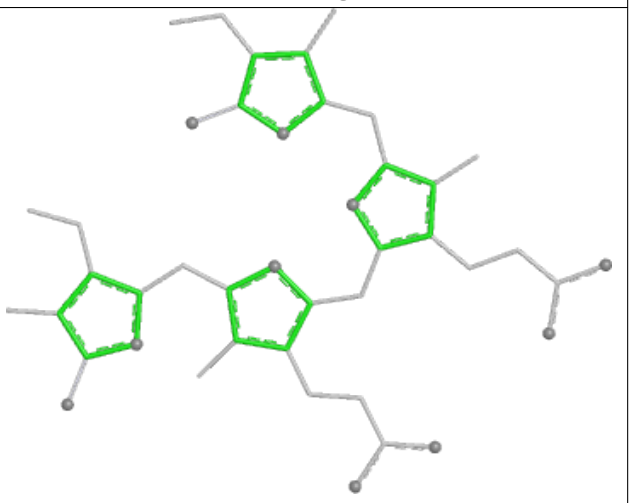
Bond lengths



Bond angles

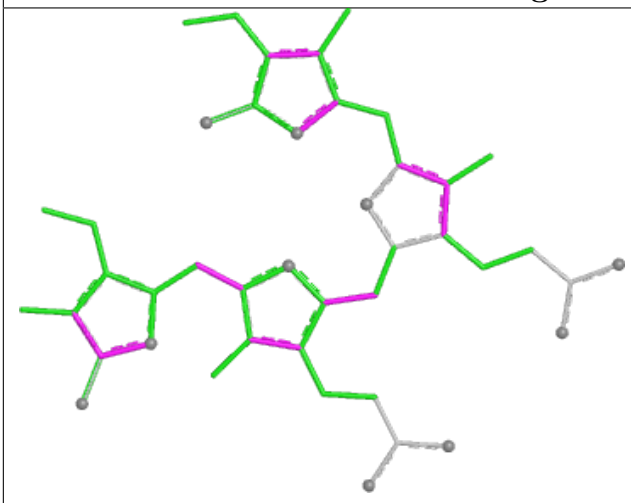


Torsions

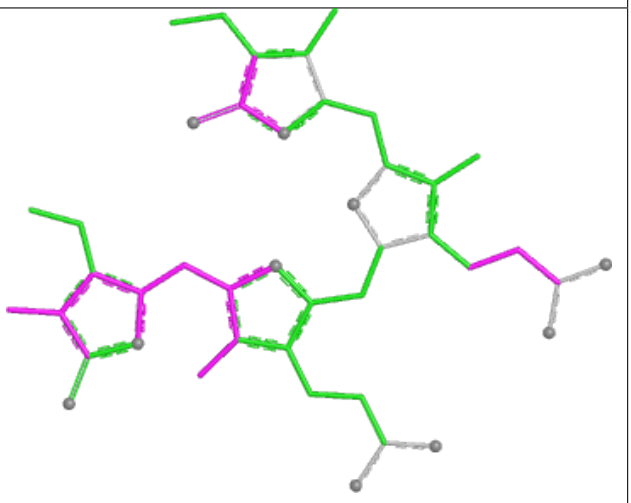


Rings

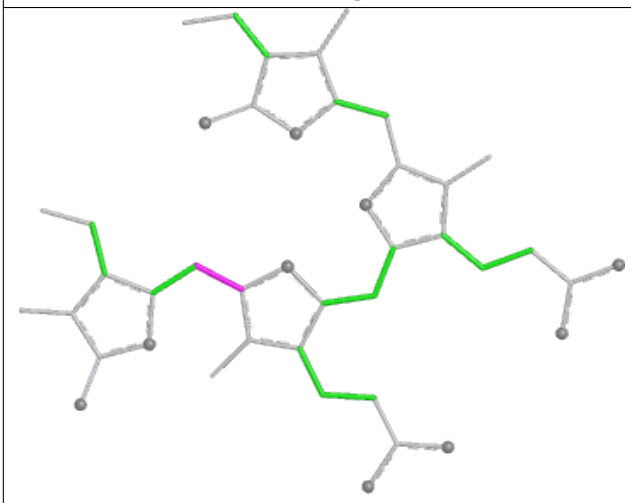
Ligand PEB I 166



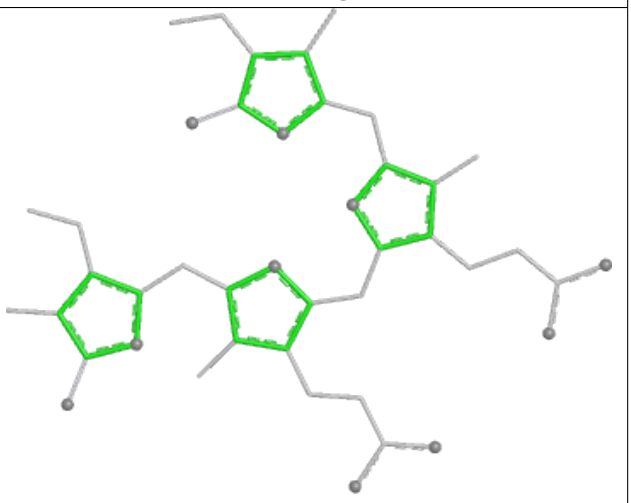
Bond lengths



Bond angles

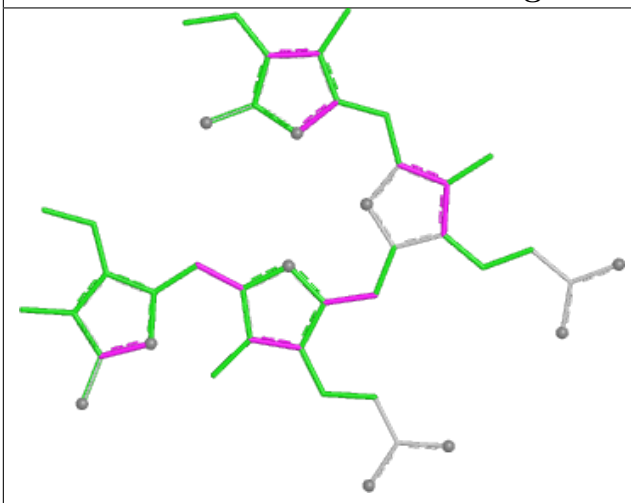


Torsions

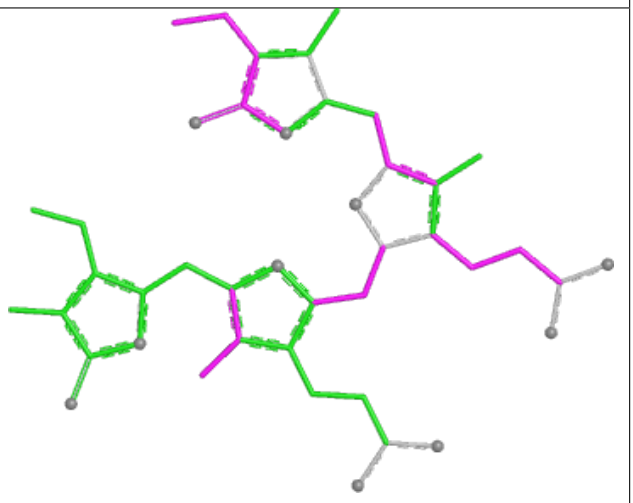


Rings

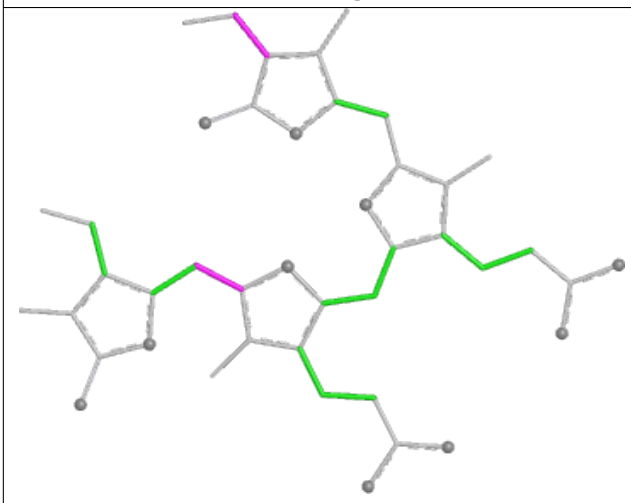
Ligand PEB U 188



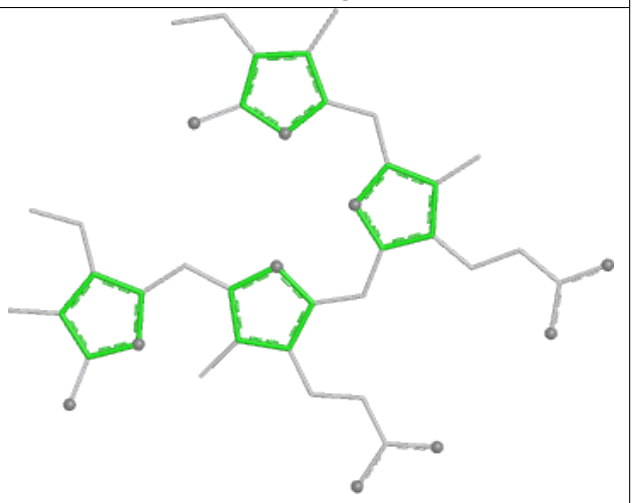
Bond lengths



Bond angles

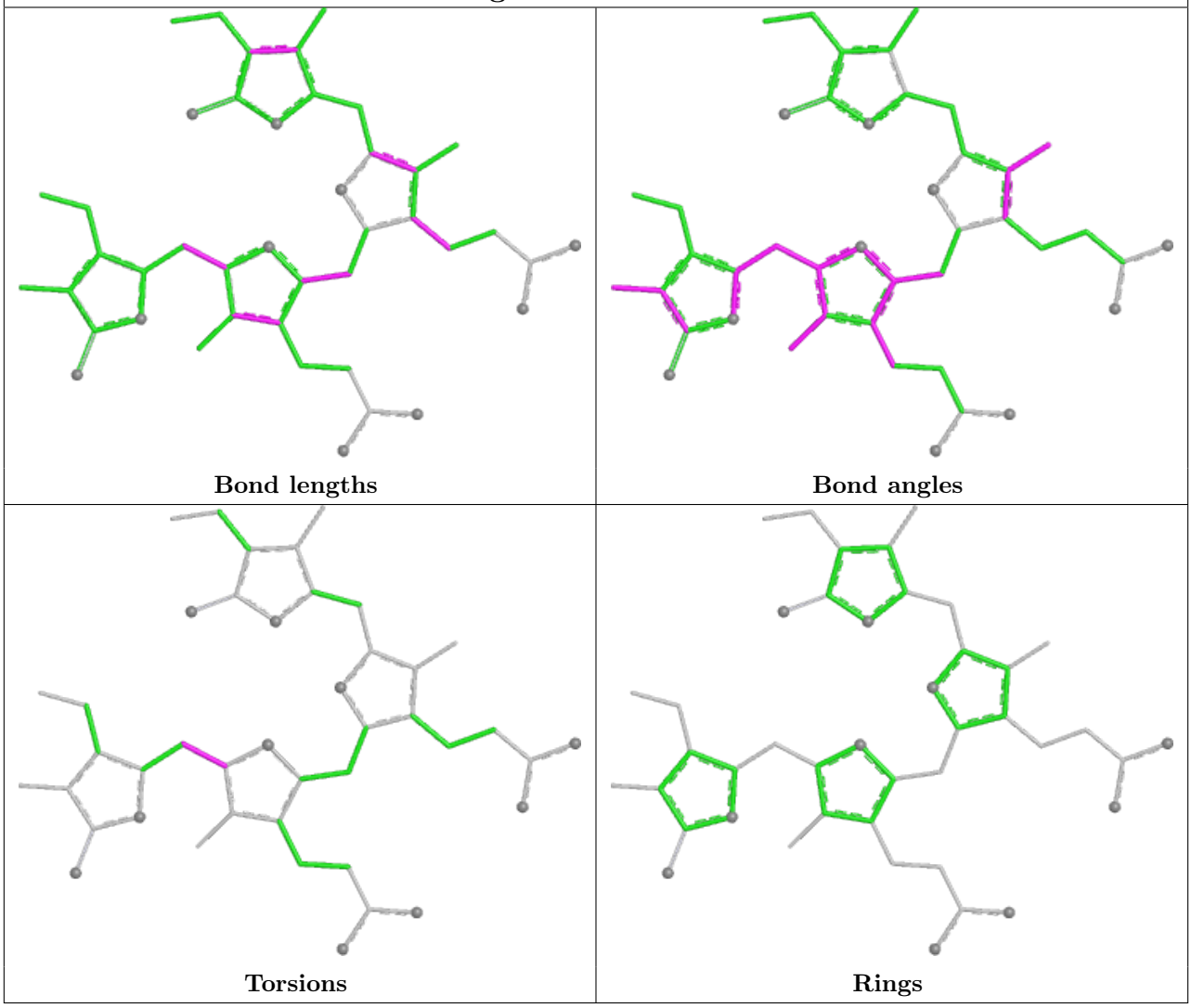


Torsions



Rings

Ligand PEB F 166



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

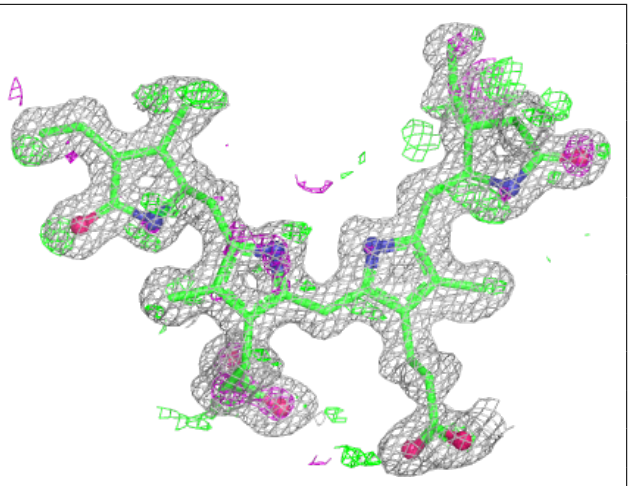
6.4 Ligands

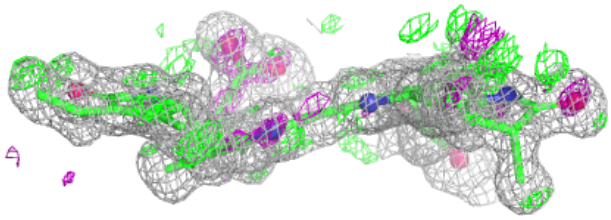
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PEB A 166:

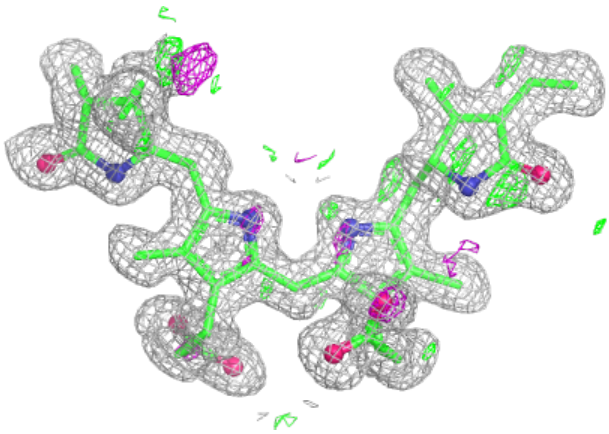
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

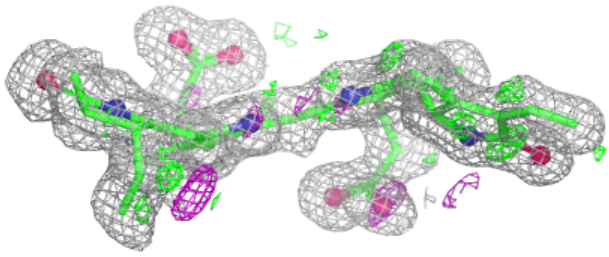


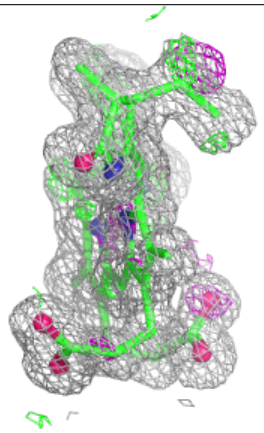


Electron density around PEB A 167:

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

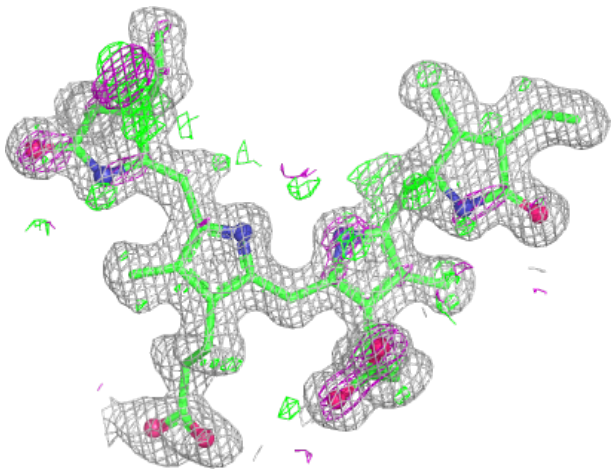


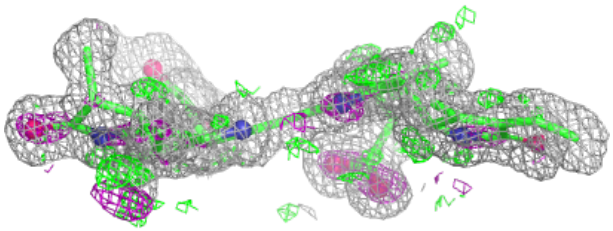


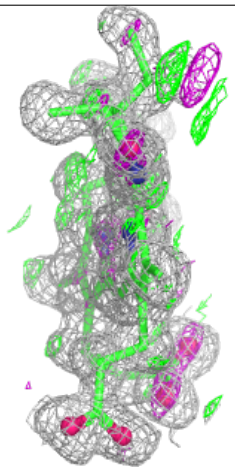


Electron density around PEB B 166:

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

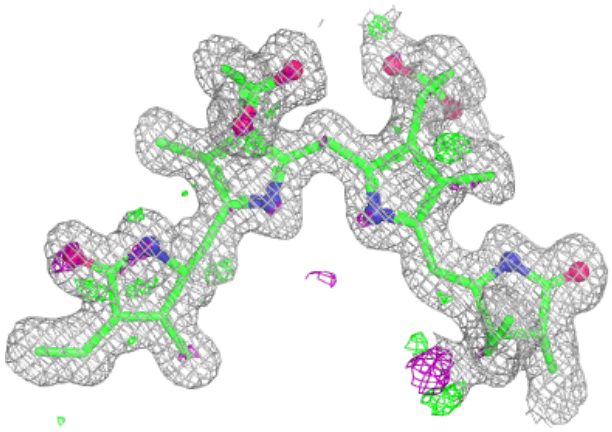


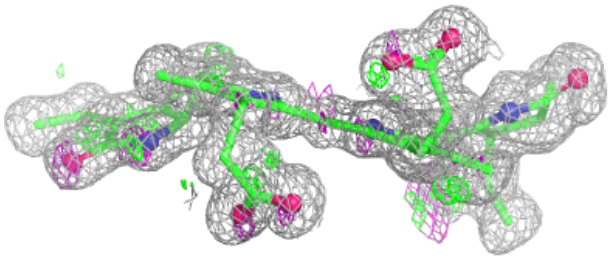


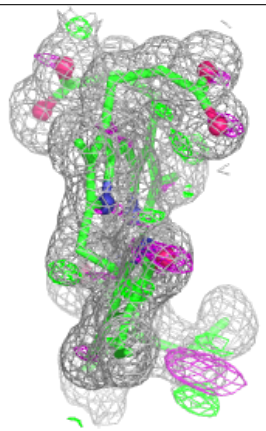


Electron density around PEB B 167:

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

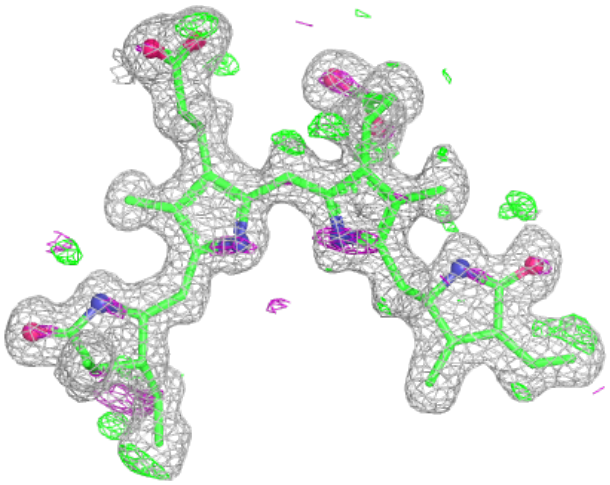


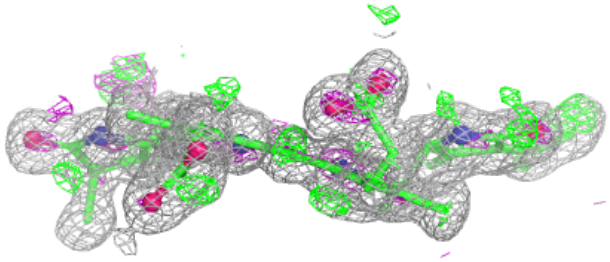


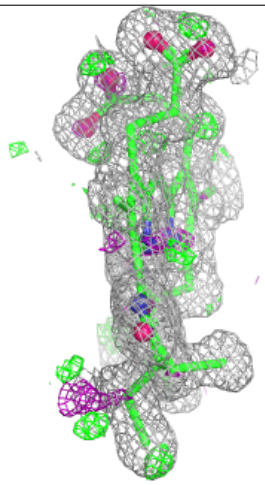


Electron density around PEB C 166:

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

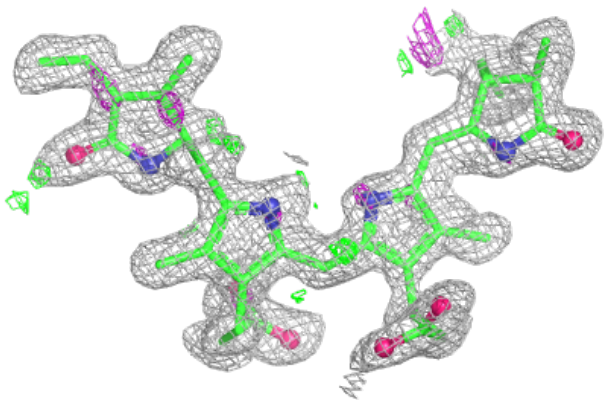


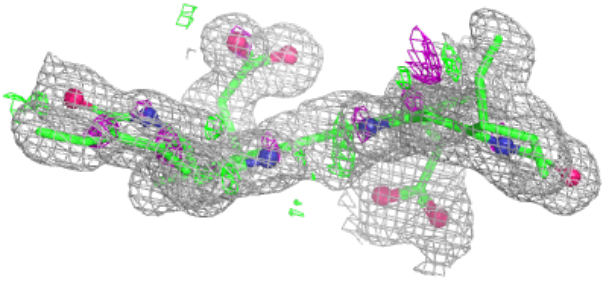


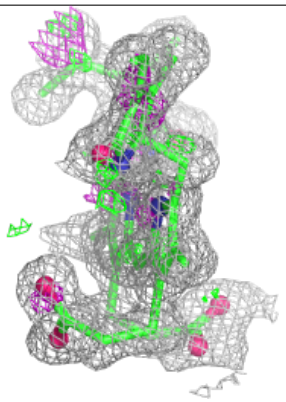


Electron density around PEB C 167:

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

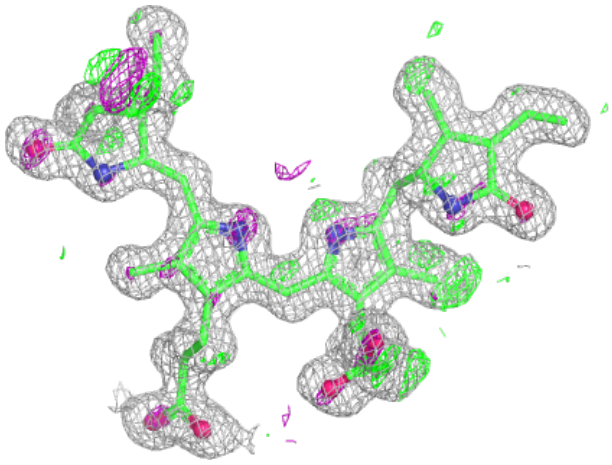


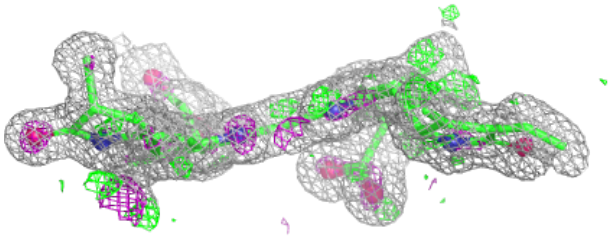


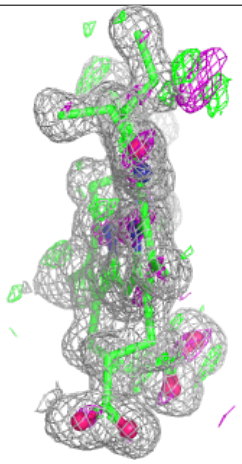


Electron density around PEB D 166:

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

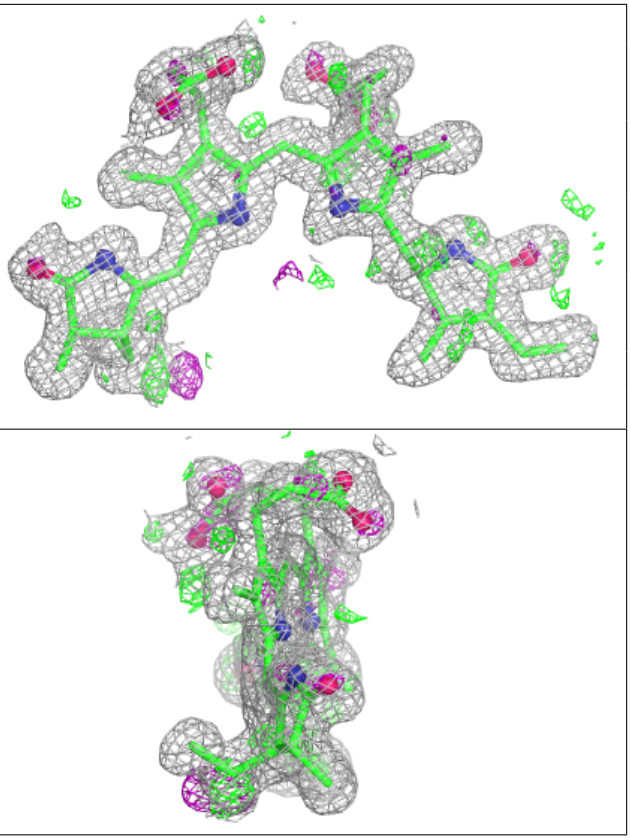


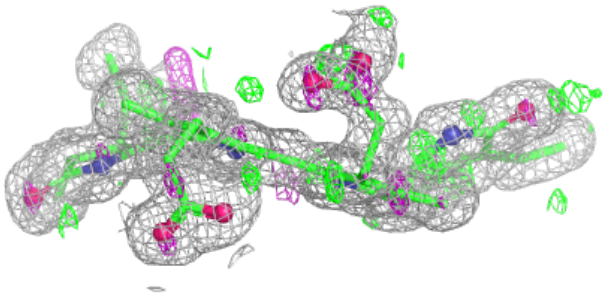




Electron density around PEB D 167:

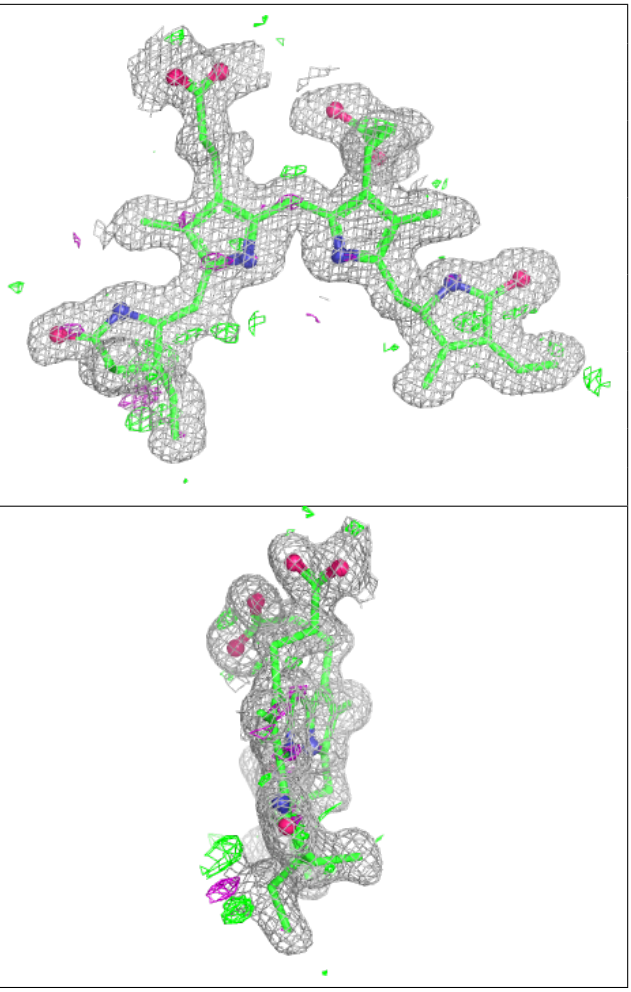
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





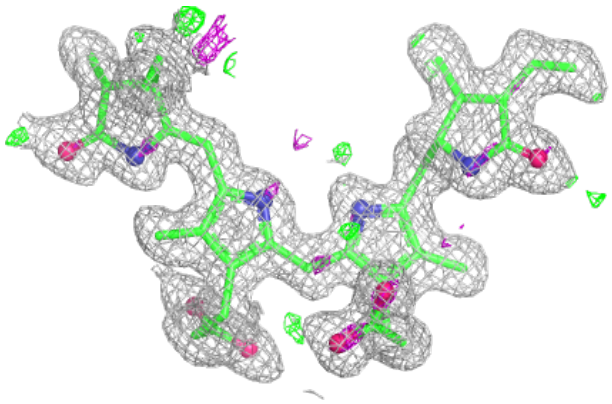
Electron density around PEB E 166:

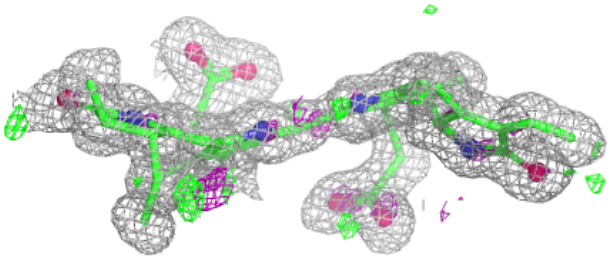
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

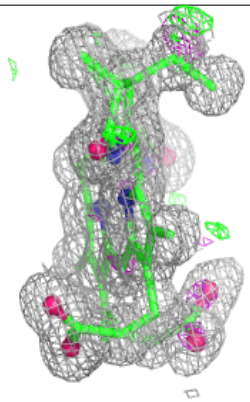


Electron density around PEB E 167:

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

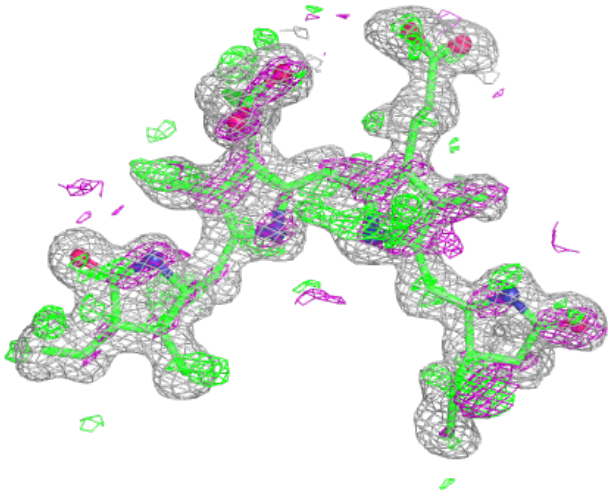


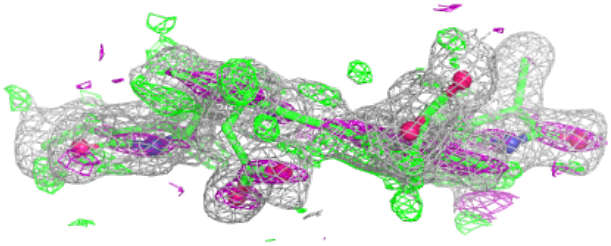




Electron density around PEB F 166:

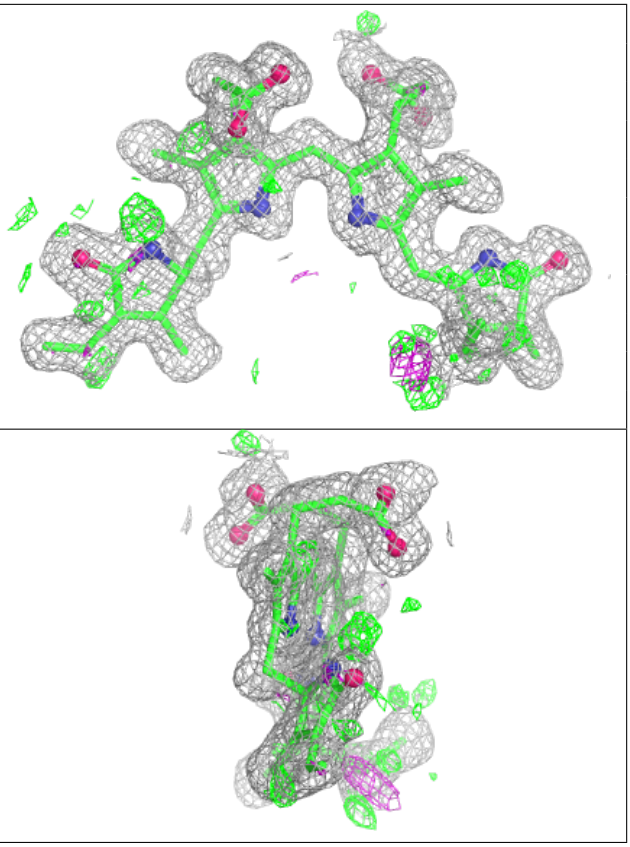
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

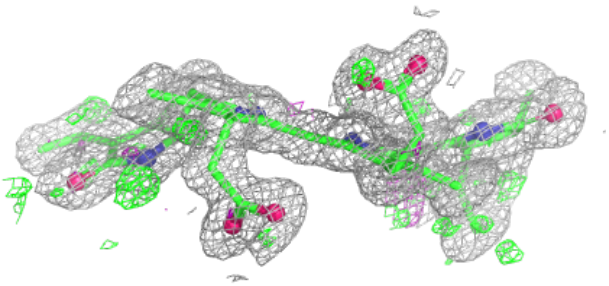




Electron density around PEB F 167:

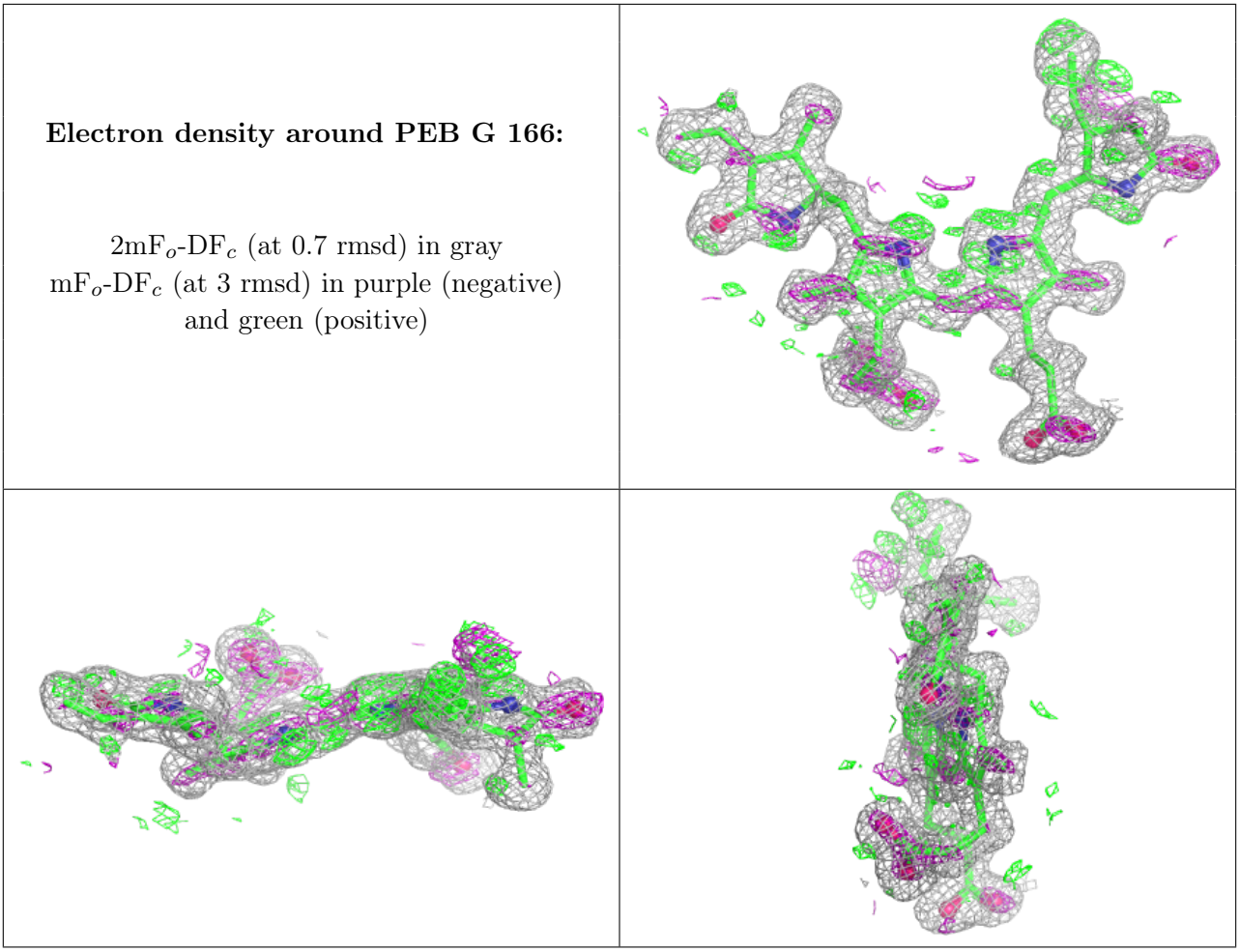
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





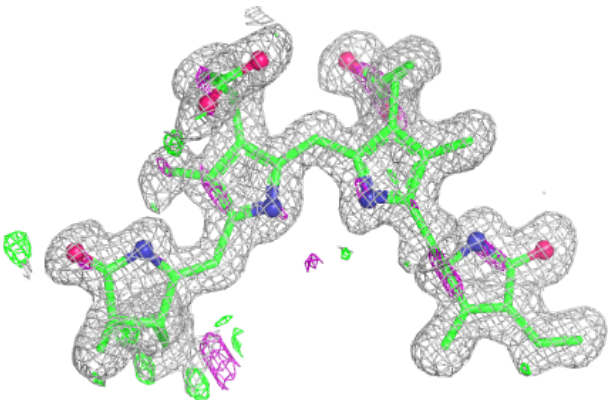
Electron density around PEB G 166:

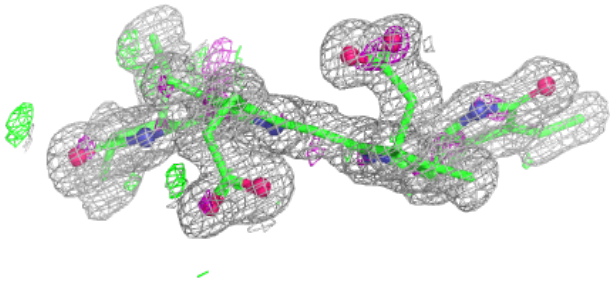
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

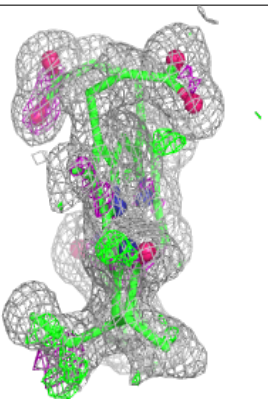


Electron density around PEB G 167:

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

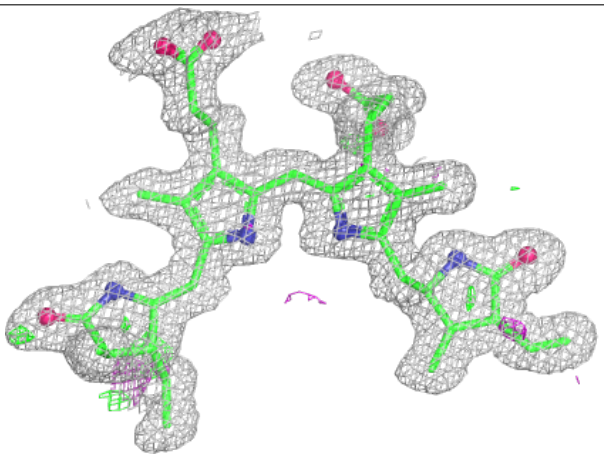


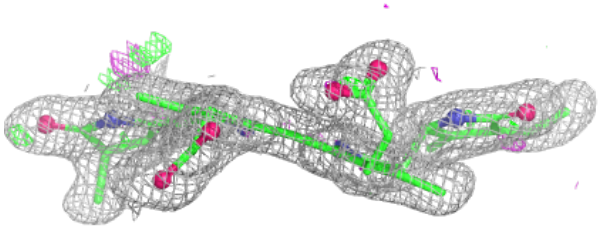


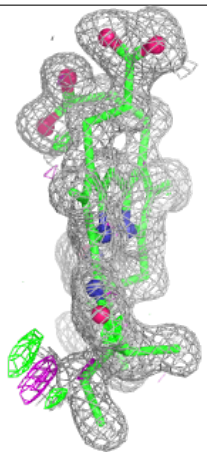


Electron density around PEB H 166:

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

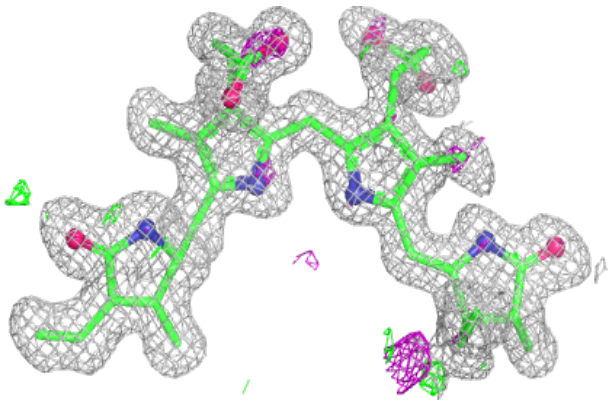


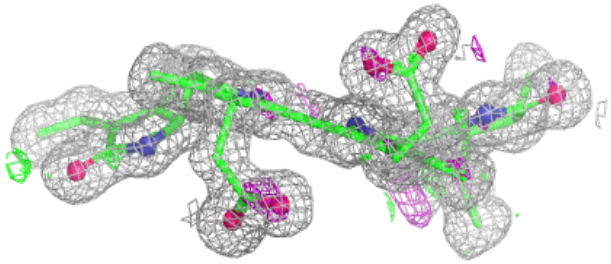


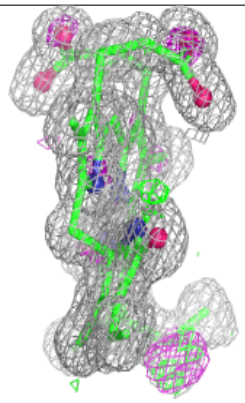


Electron density around PEB H 167:

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

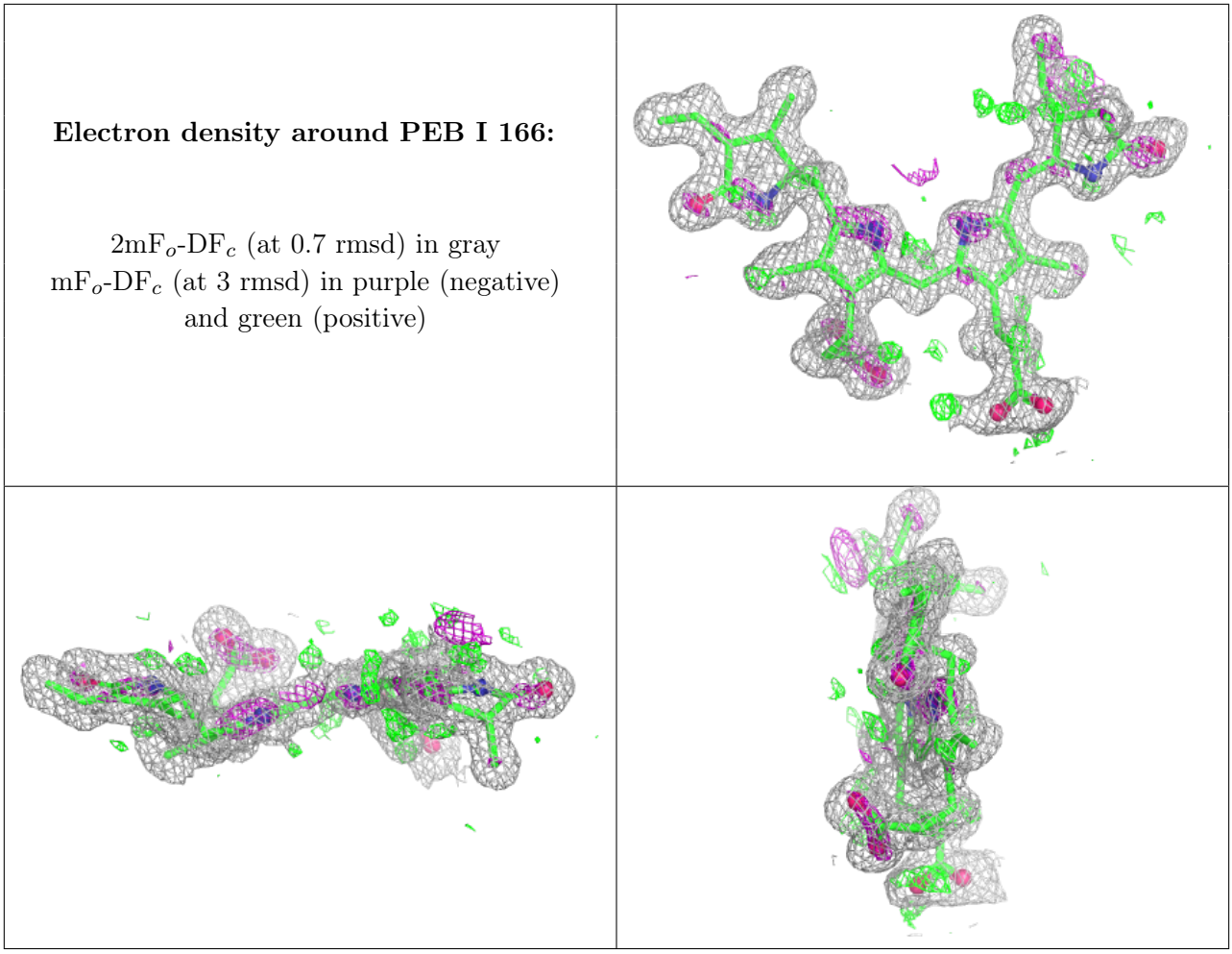






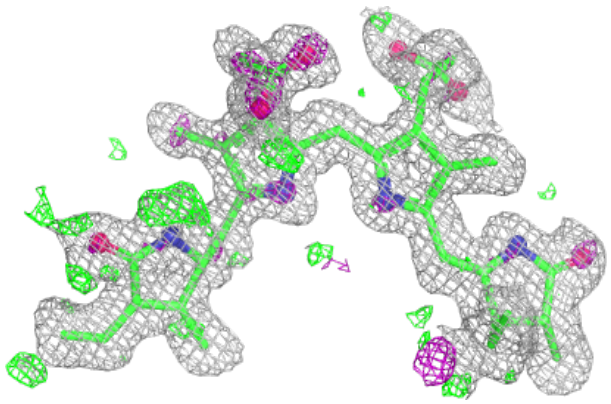
Electron density around PEB I 166:

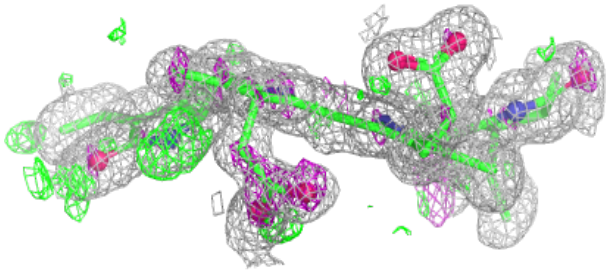
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

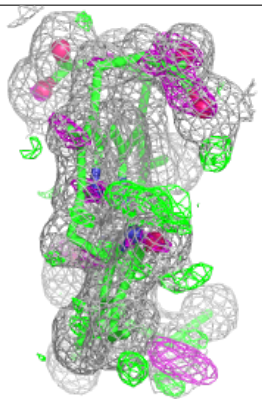


Electron density around PEB I 167:

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

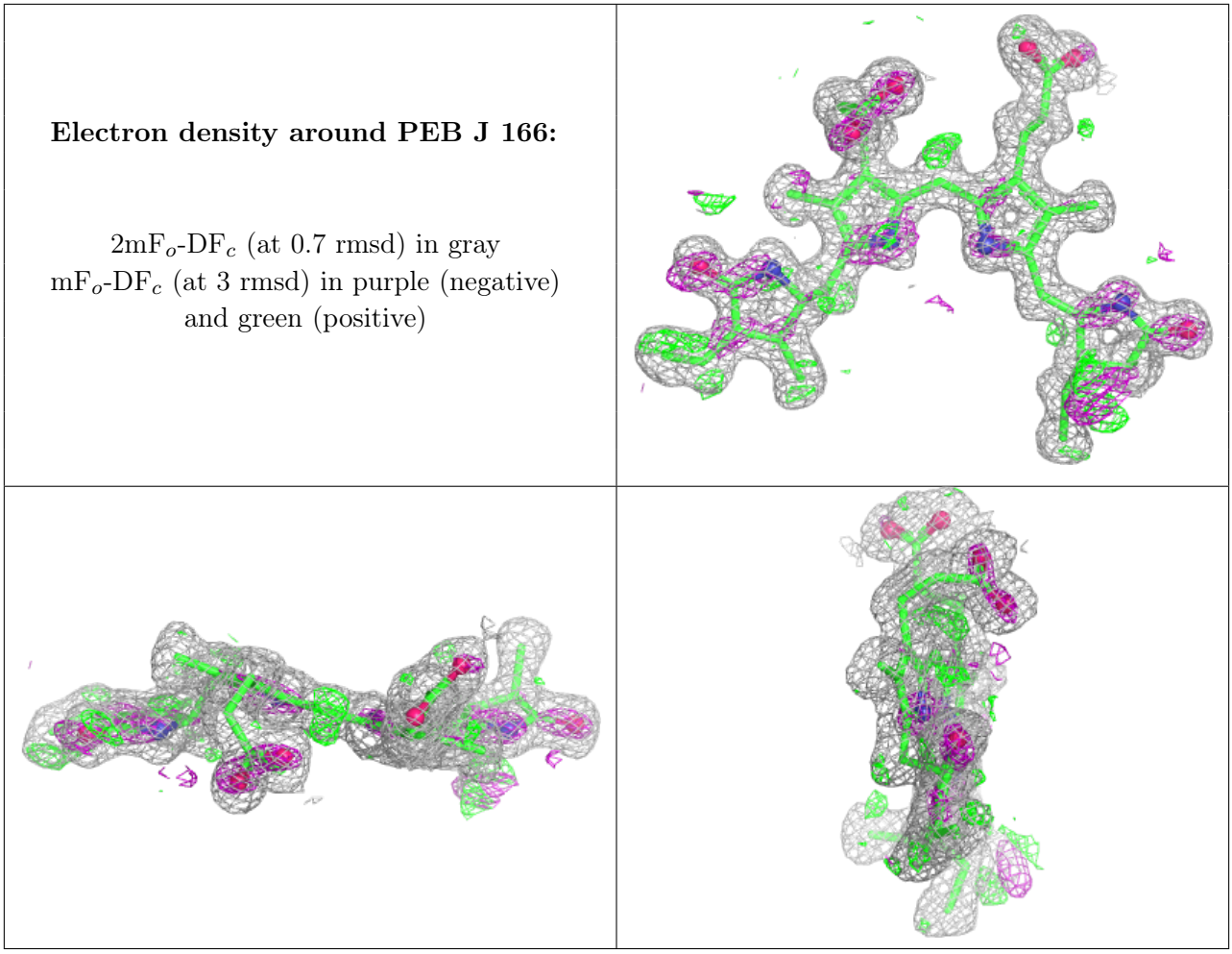






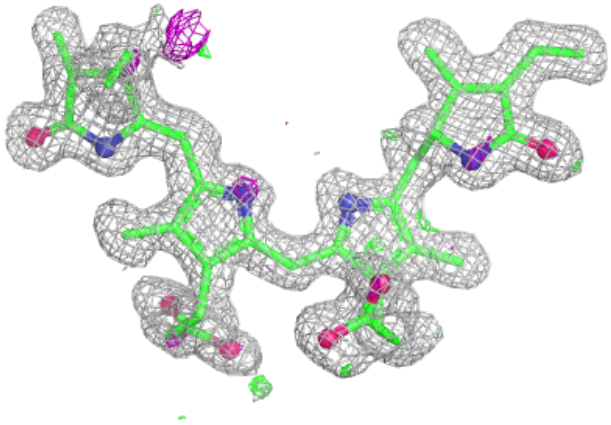
Electron density around PEB J 166:

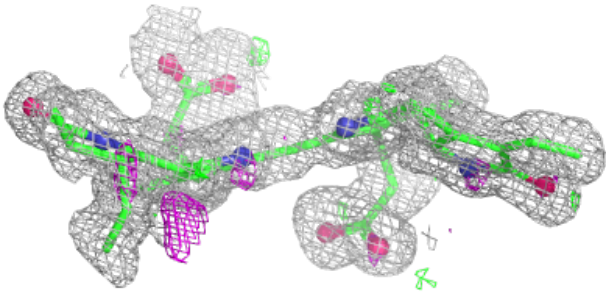
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

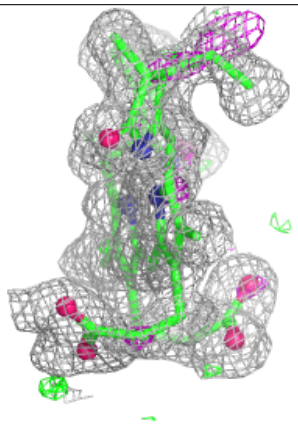


Electron density around PEB J 167:

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

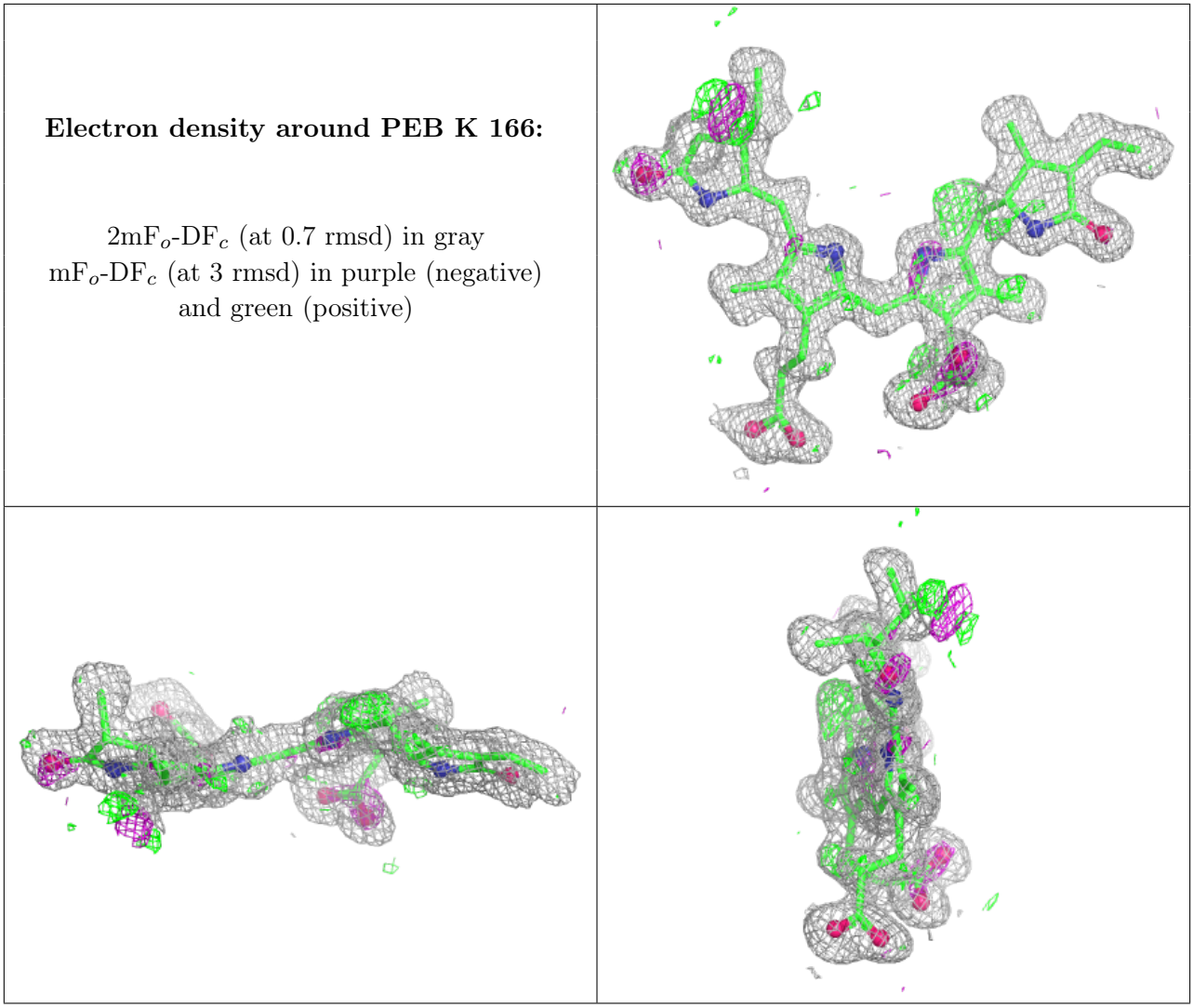






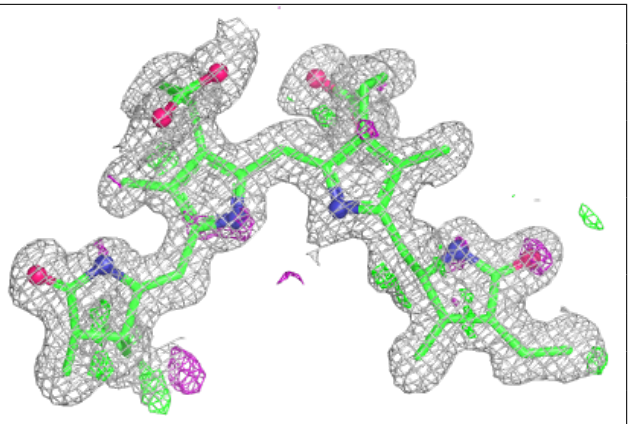
Electron density around PEB K 166:

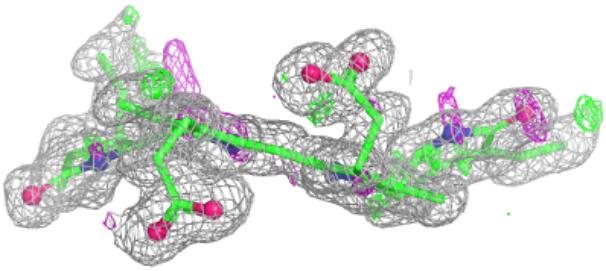
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

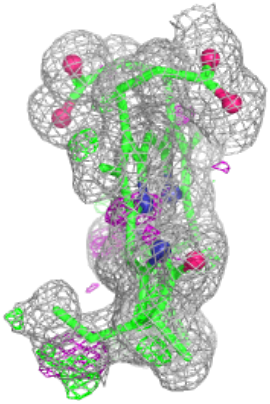


Electron density around PEB K 167:

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

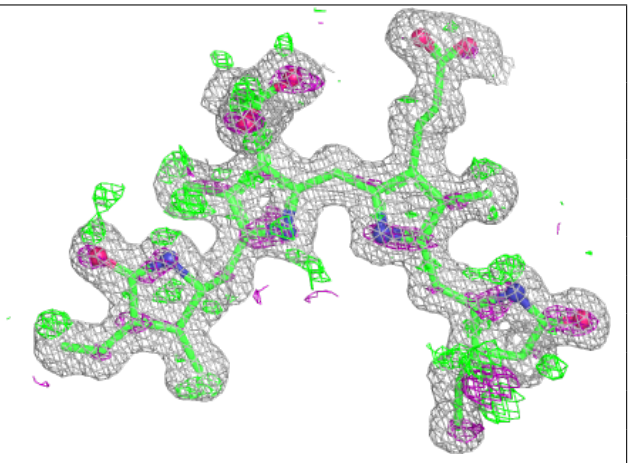


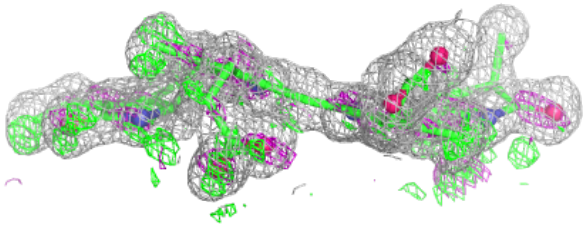


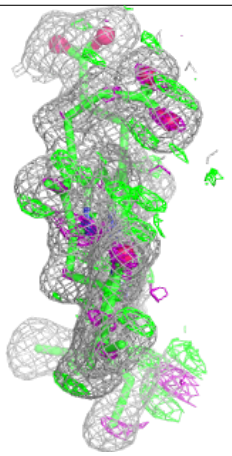


Electron density around PEB L 166:

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

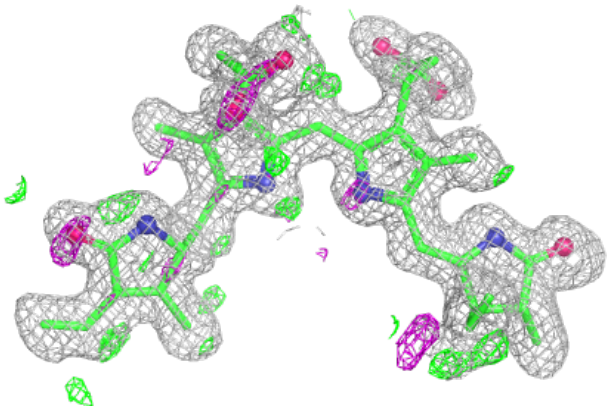


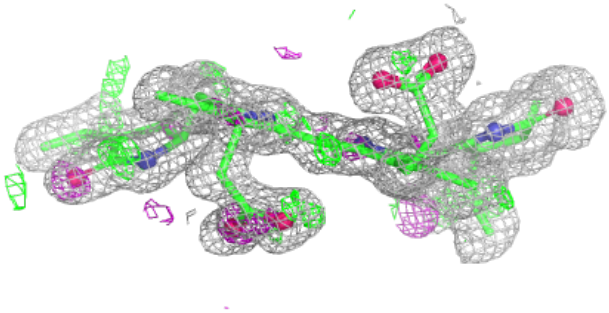


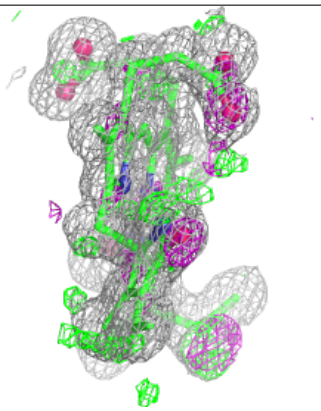


Electron density around PEB L 167:

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

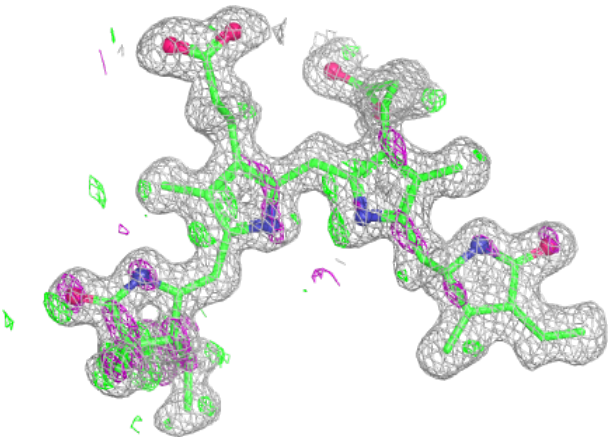


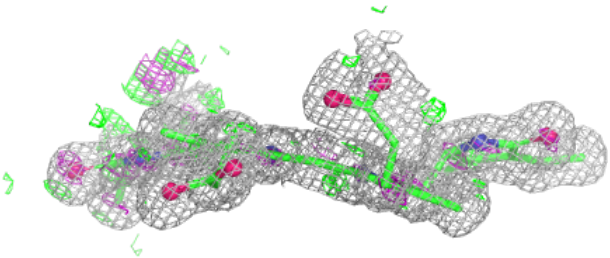


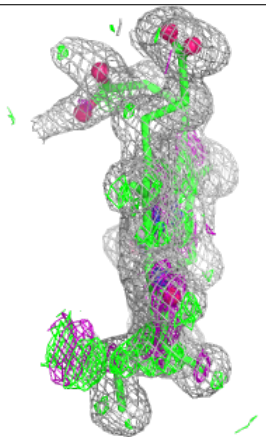


Electron density around PEB M 186:

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

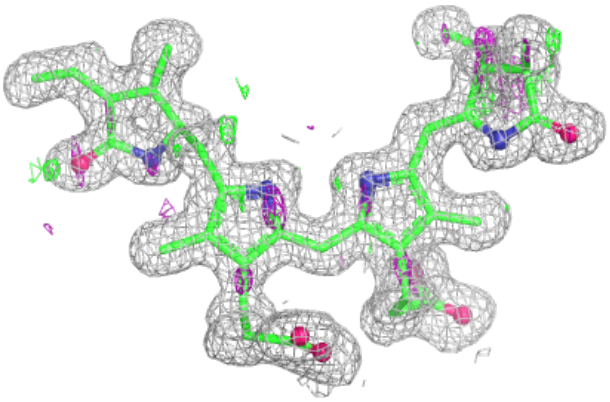


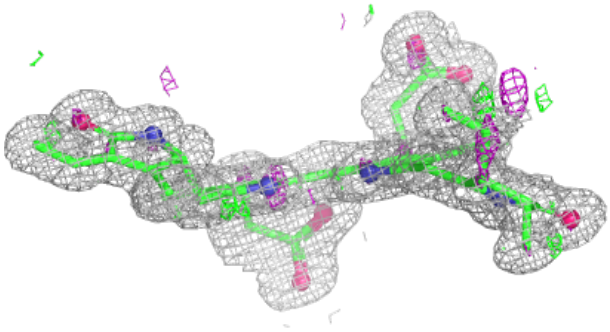


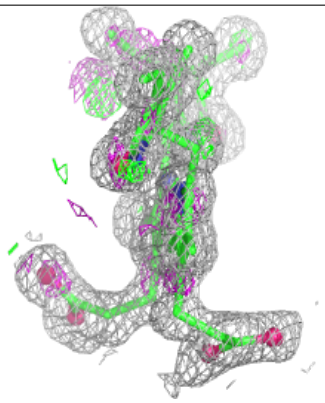


Electron density around PEB M 187:

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

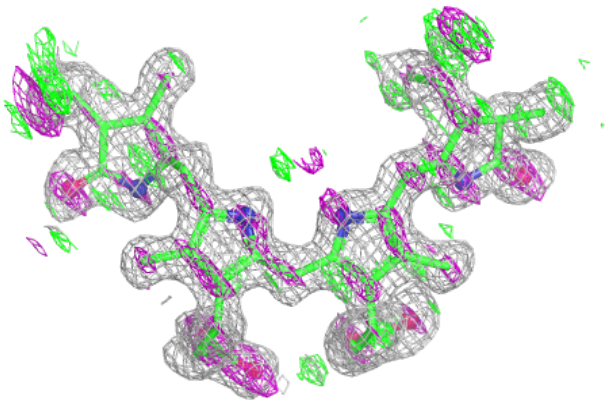


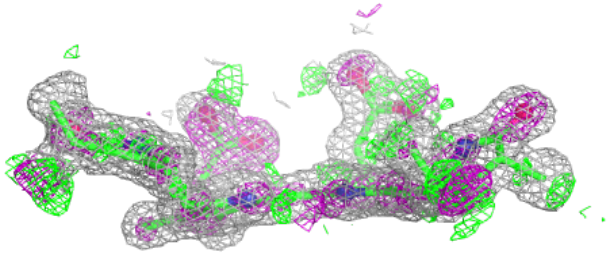


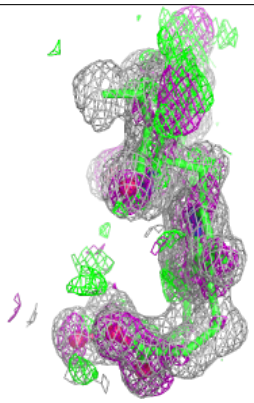


Electron density around PEB M 188:

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

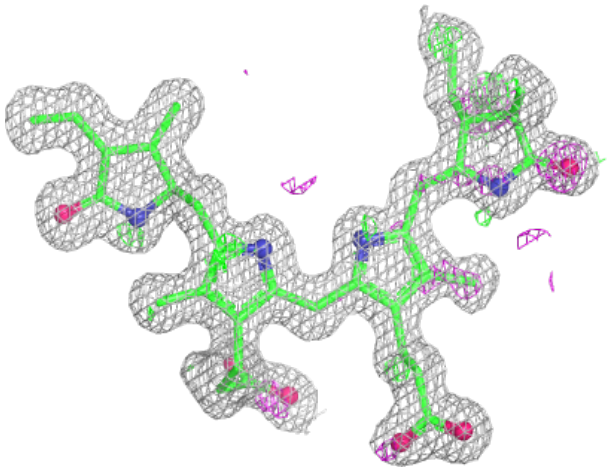


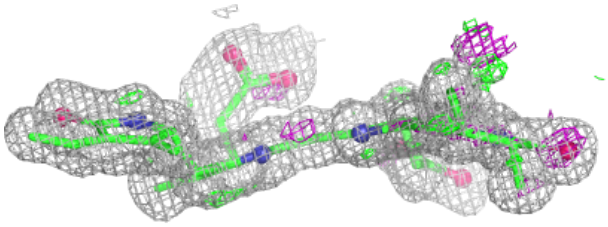


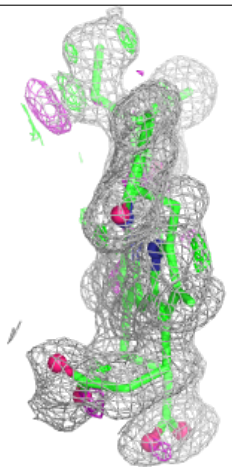


Electron density around PEB N 186:

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

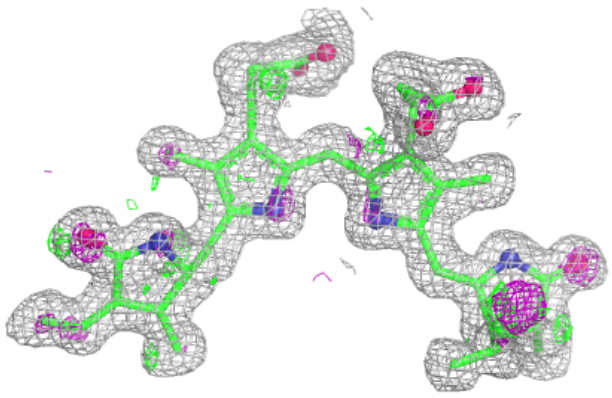


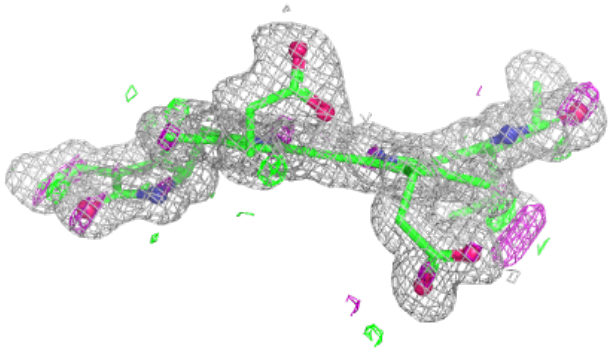


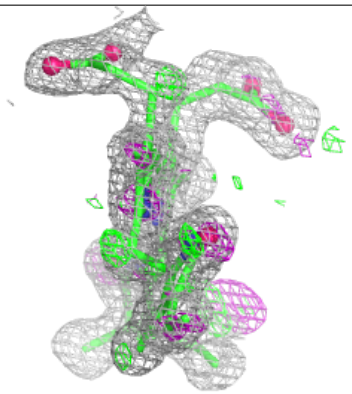


Electron density around PEB N 187:

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

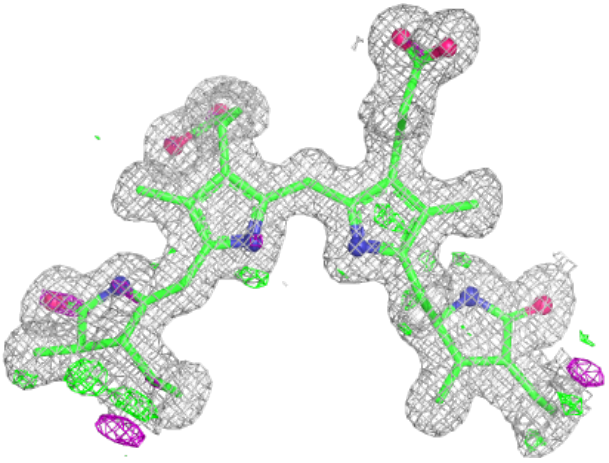


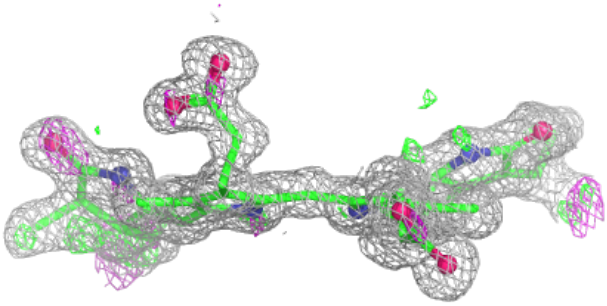


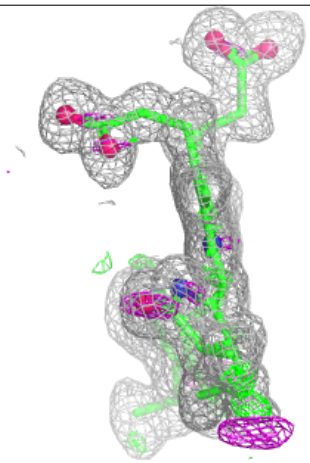


Electron density around PEB N 188:

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

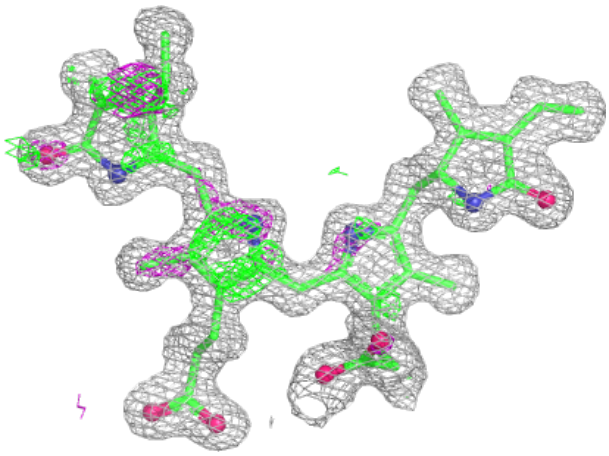


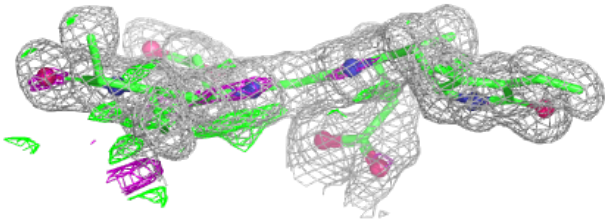


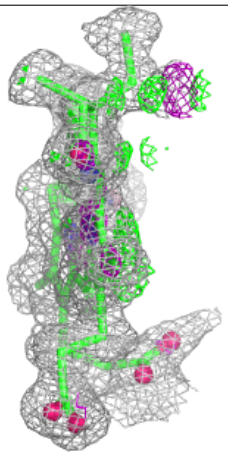


Electron density around PEB O 186:

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

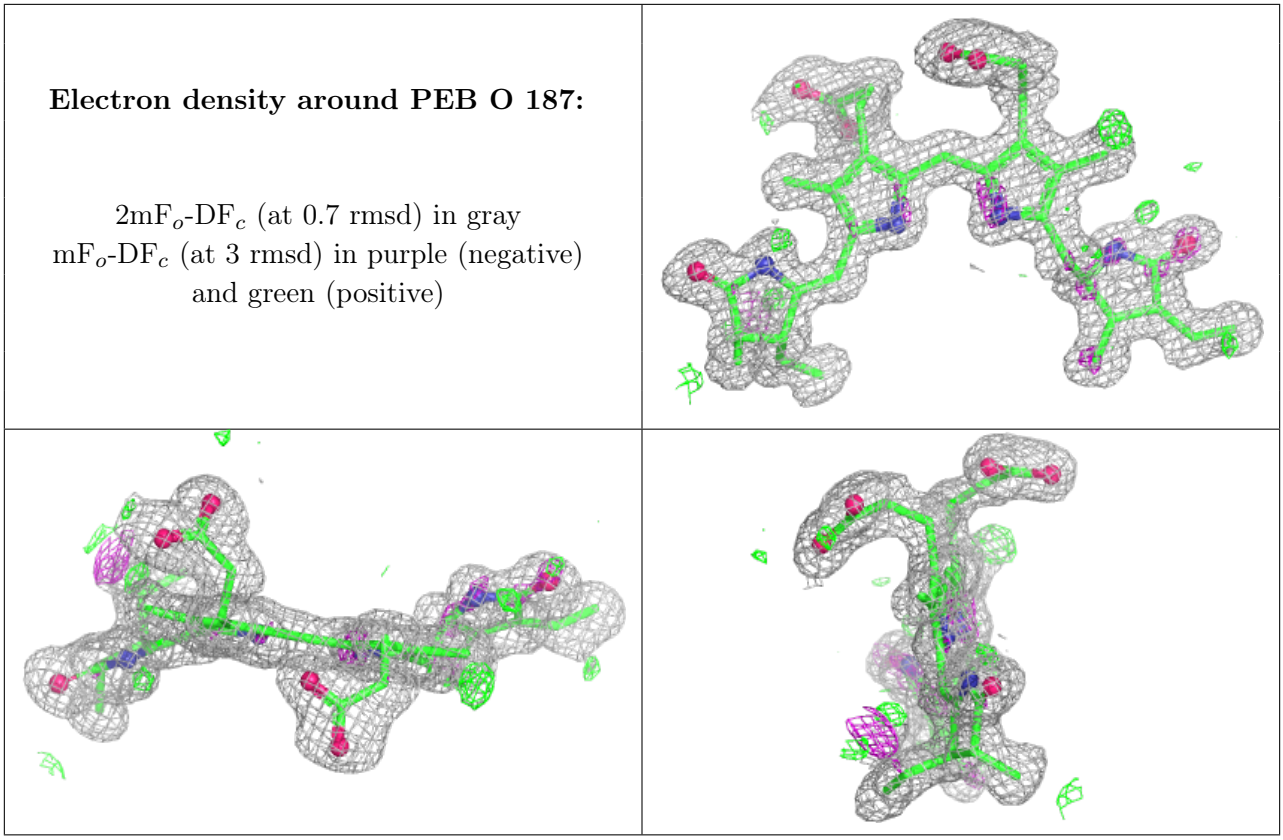






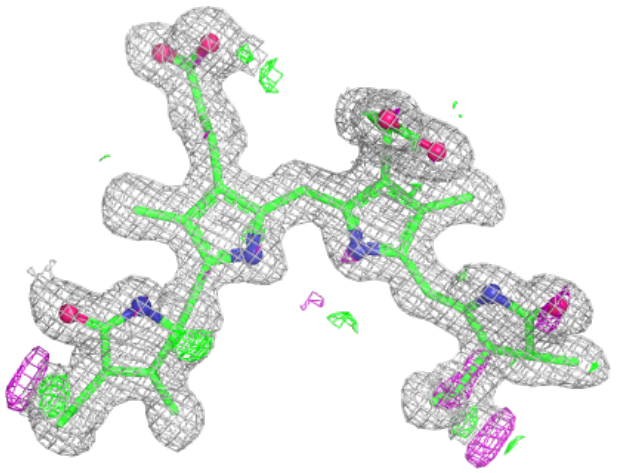
Electron density around PEB O 187:

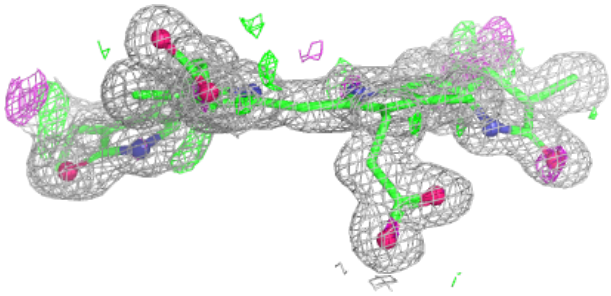
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

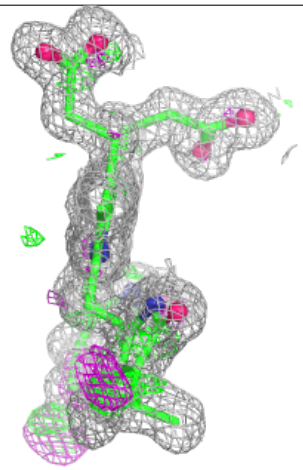


Electron density around PEB O 188:

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

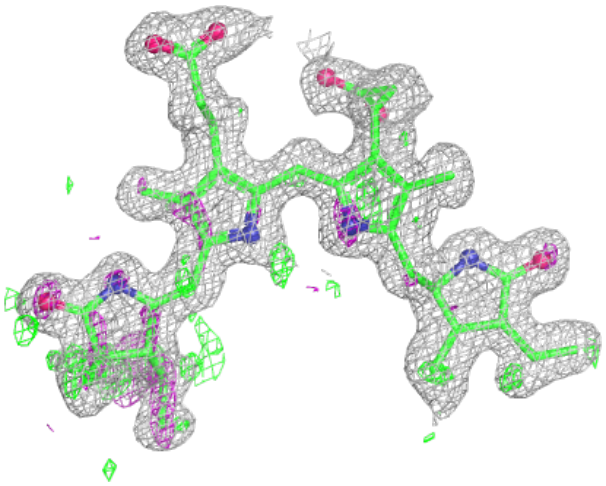


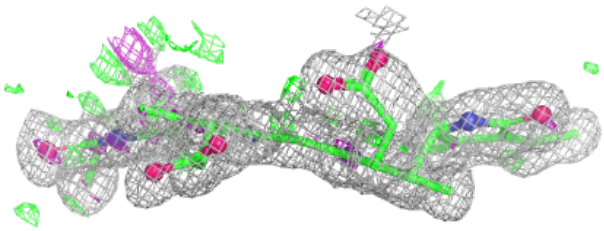


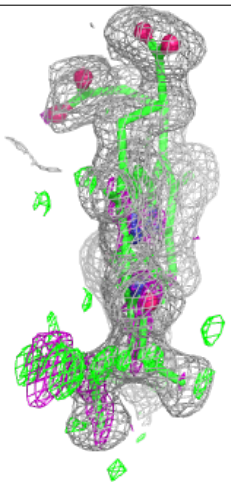


Electron density around PEB P 186:

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

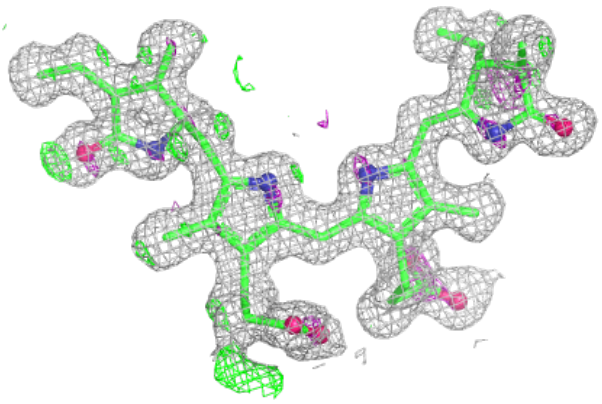


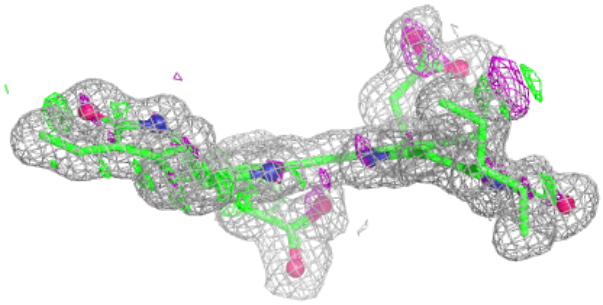


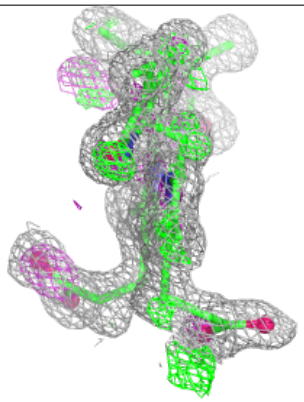


Electron density around PEB P 187:

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

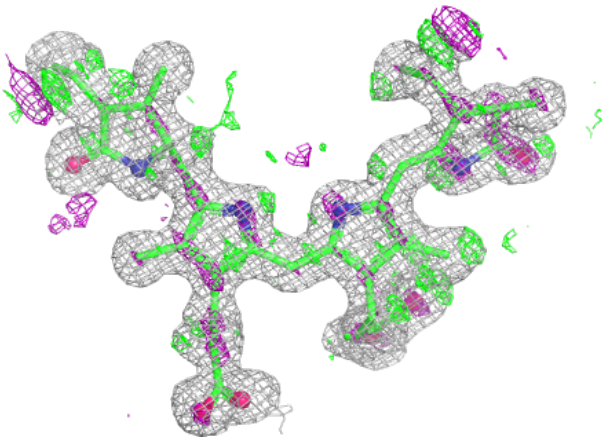


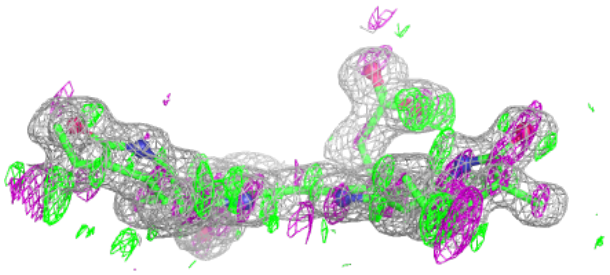


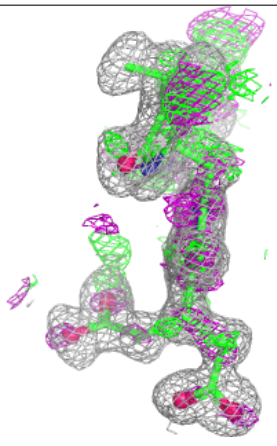


Electron density around PEB P 188:

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

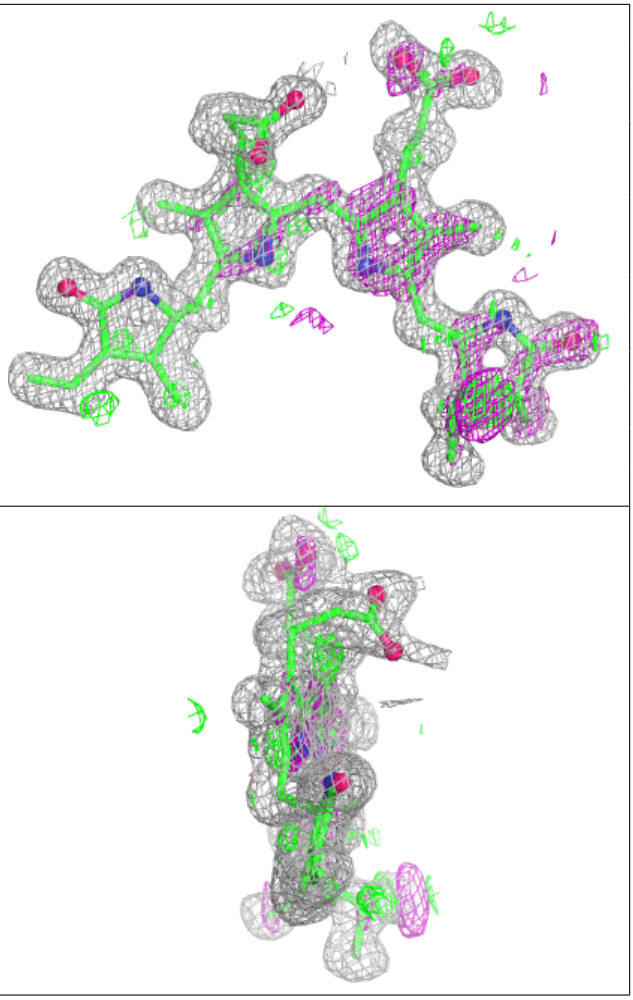






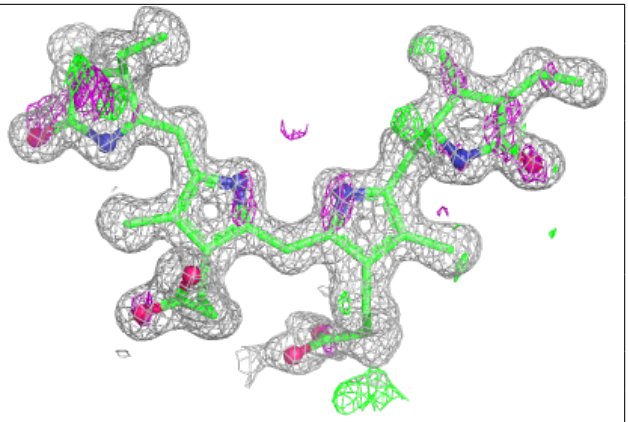
Electron density around PEB Q 186:

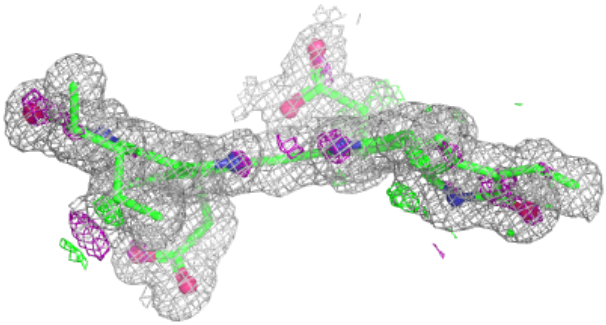
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

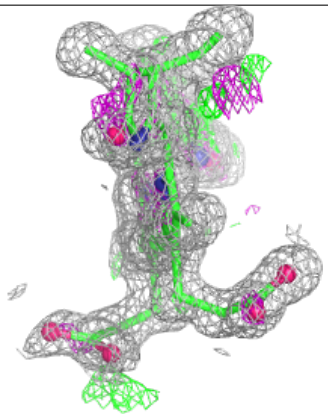


Electron density around PEB Q 187:

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

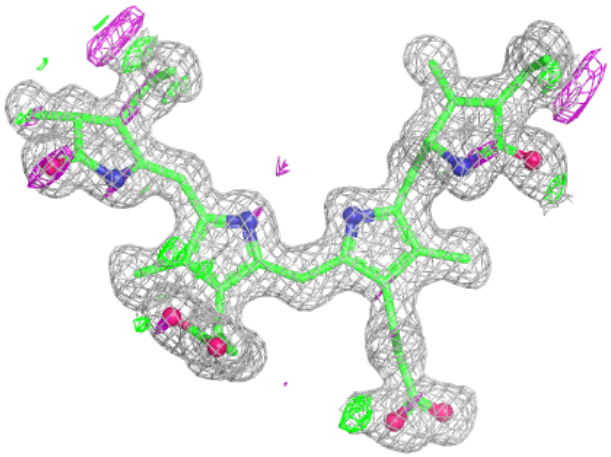


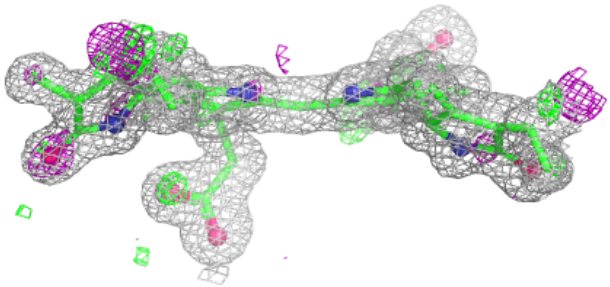


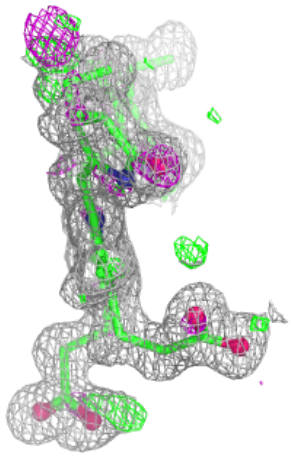


Electron density around PEB Q 188:

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

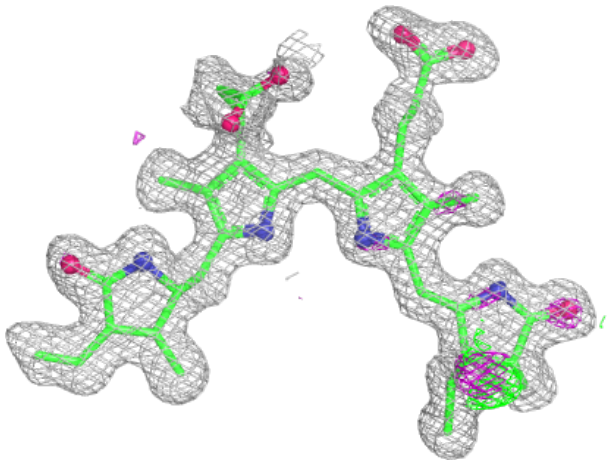


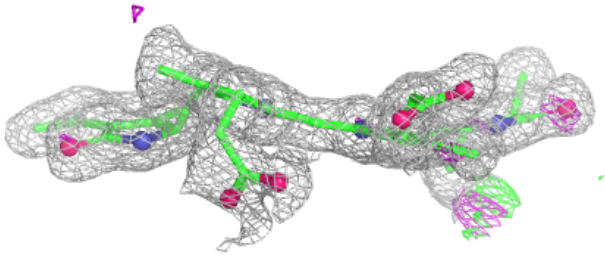


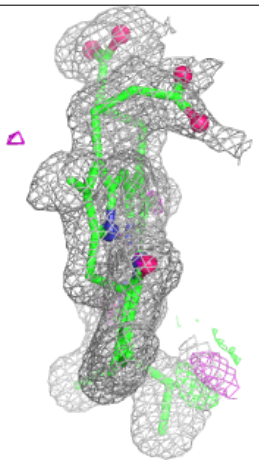


Electron density around PEB R 186:

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

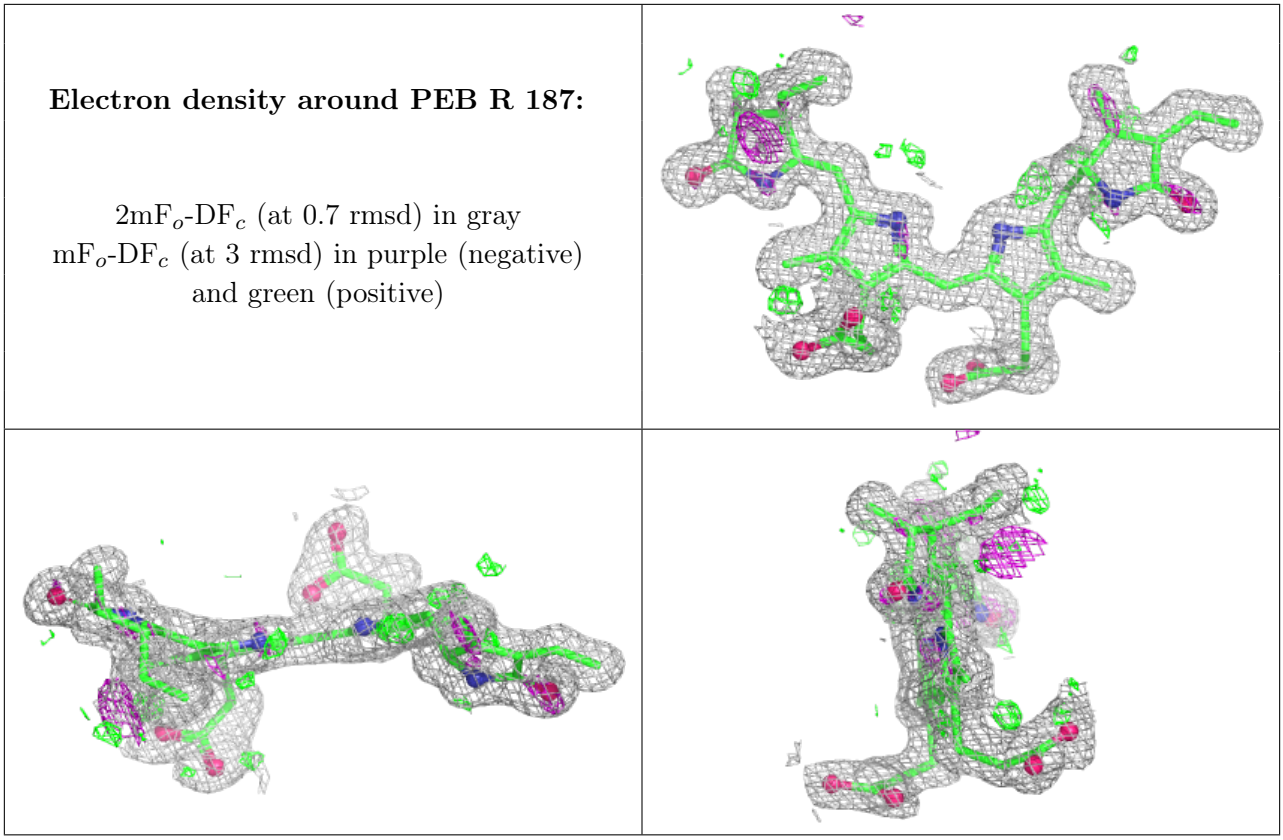






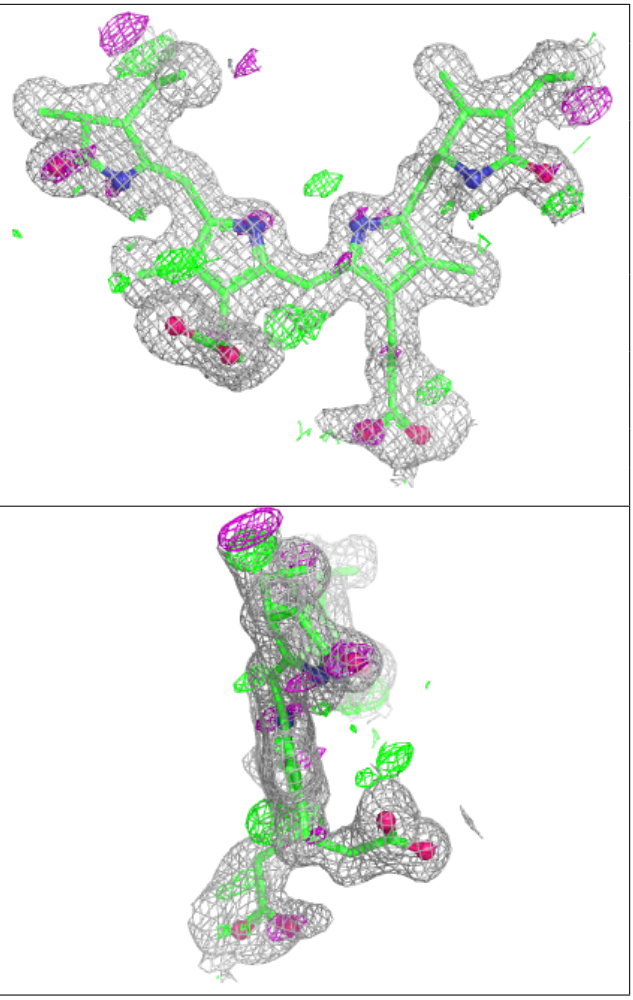
Electron density around PEB R 187:

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



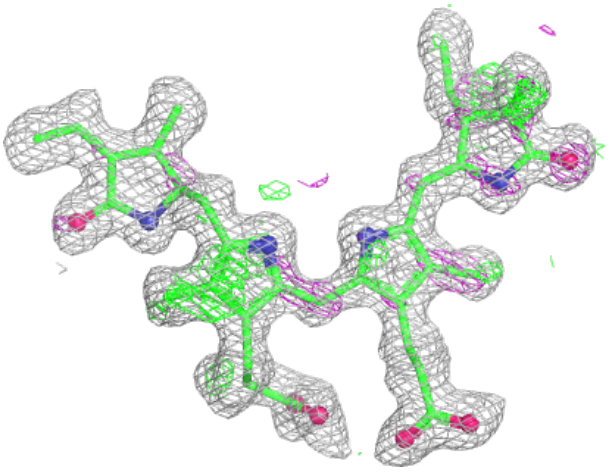
Electron density around PEB R 188:

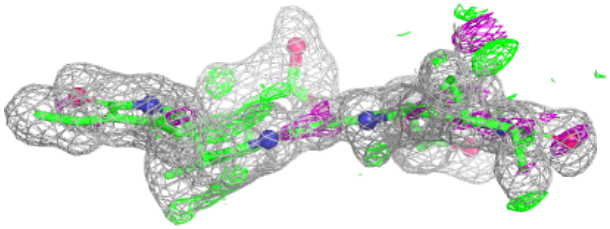
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

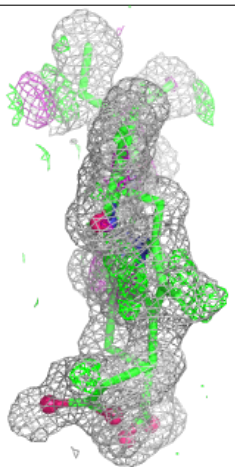


Electron density around PEB S 186 (A):

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

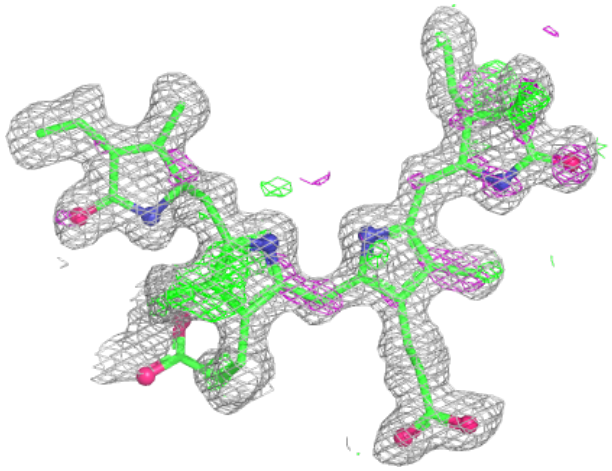


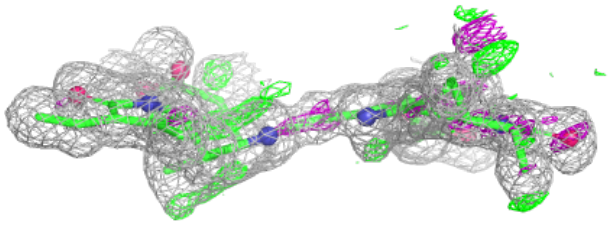


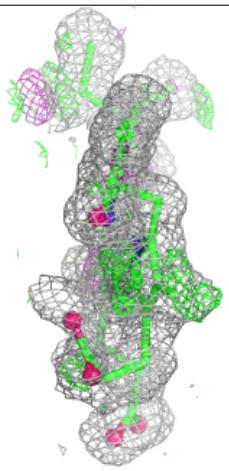


Electron density around PEB S 186 (B):

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

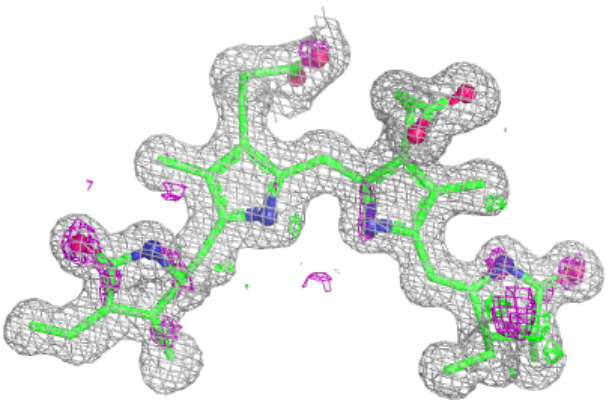


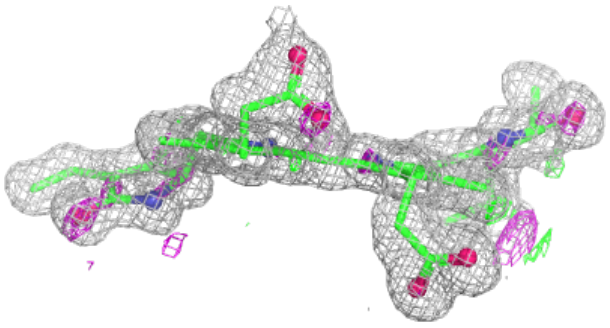


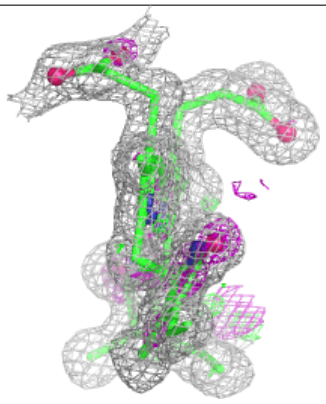


Electron density around PEB S 187:

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

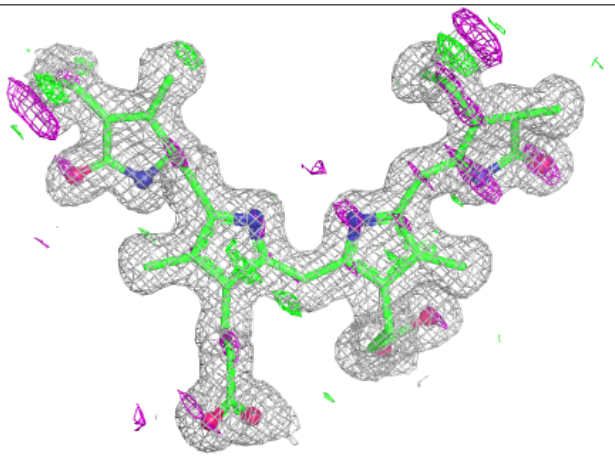


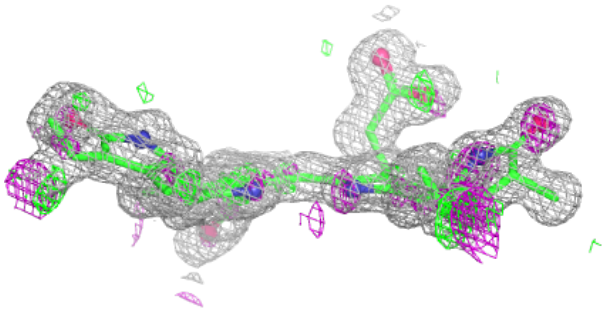


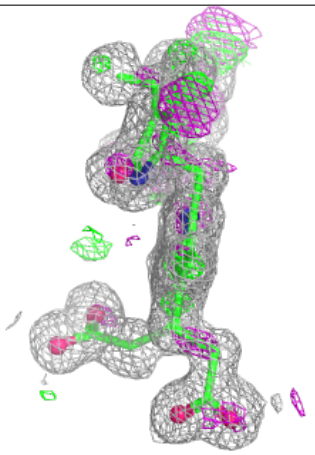


Electron density around PEB S 188:

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

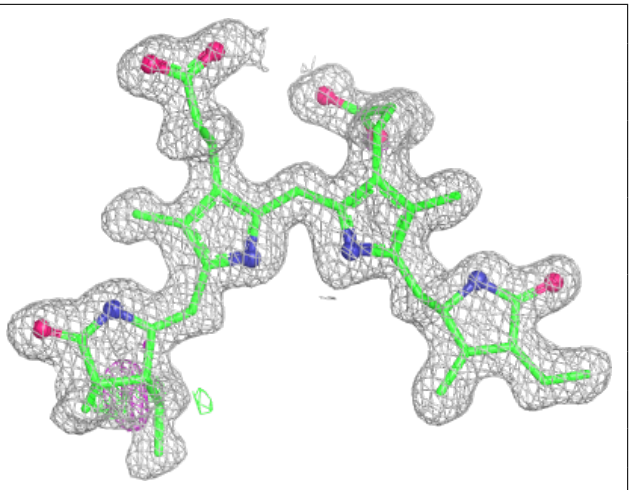


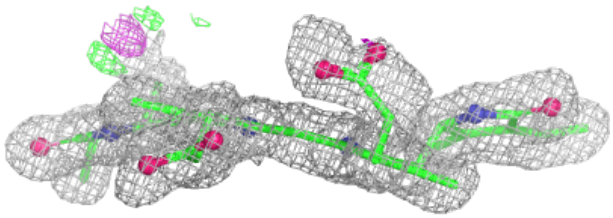


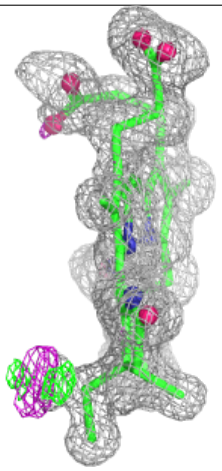


Electron density around PEB T 186:

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

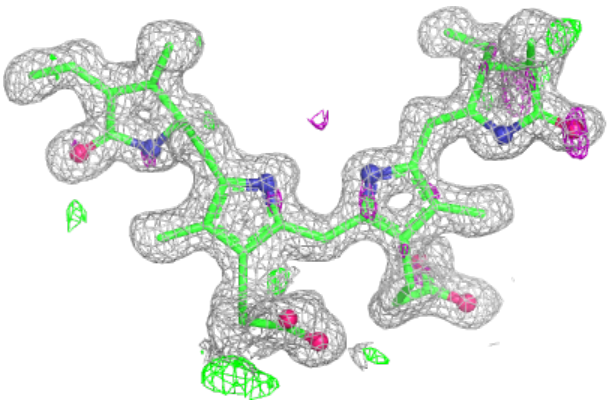


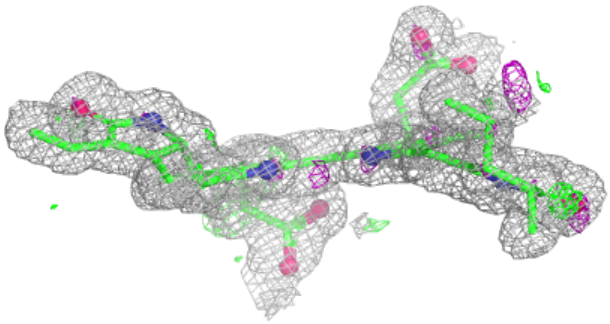


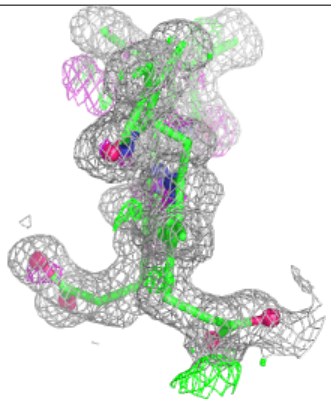


Electron density around PEB T 187:

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

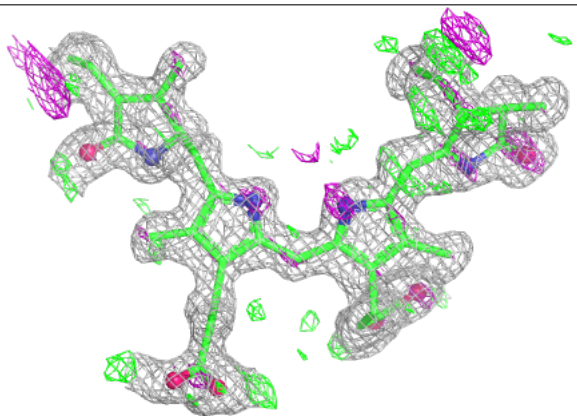


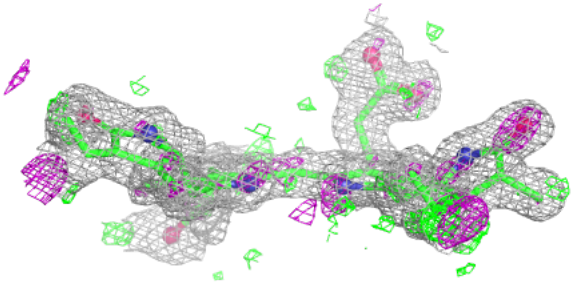


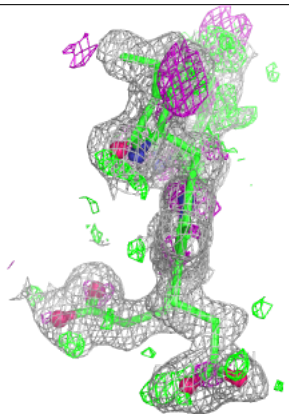


Electron density around PEB T 188:

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

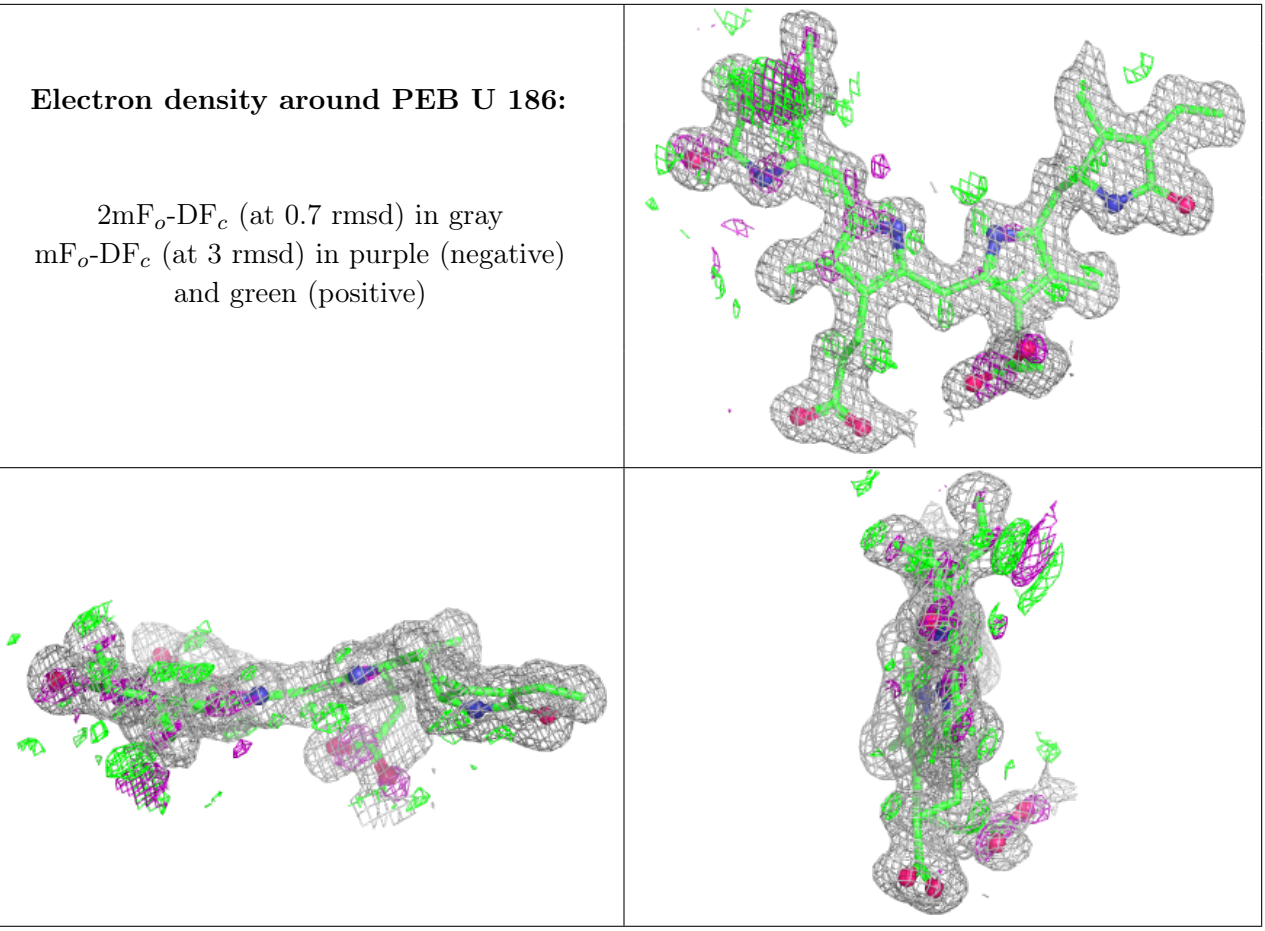






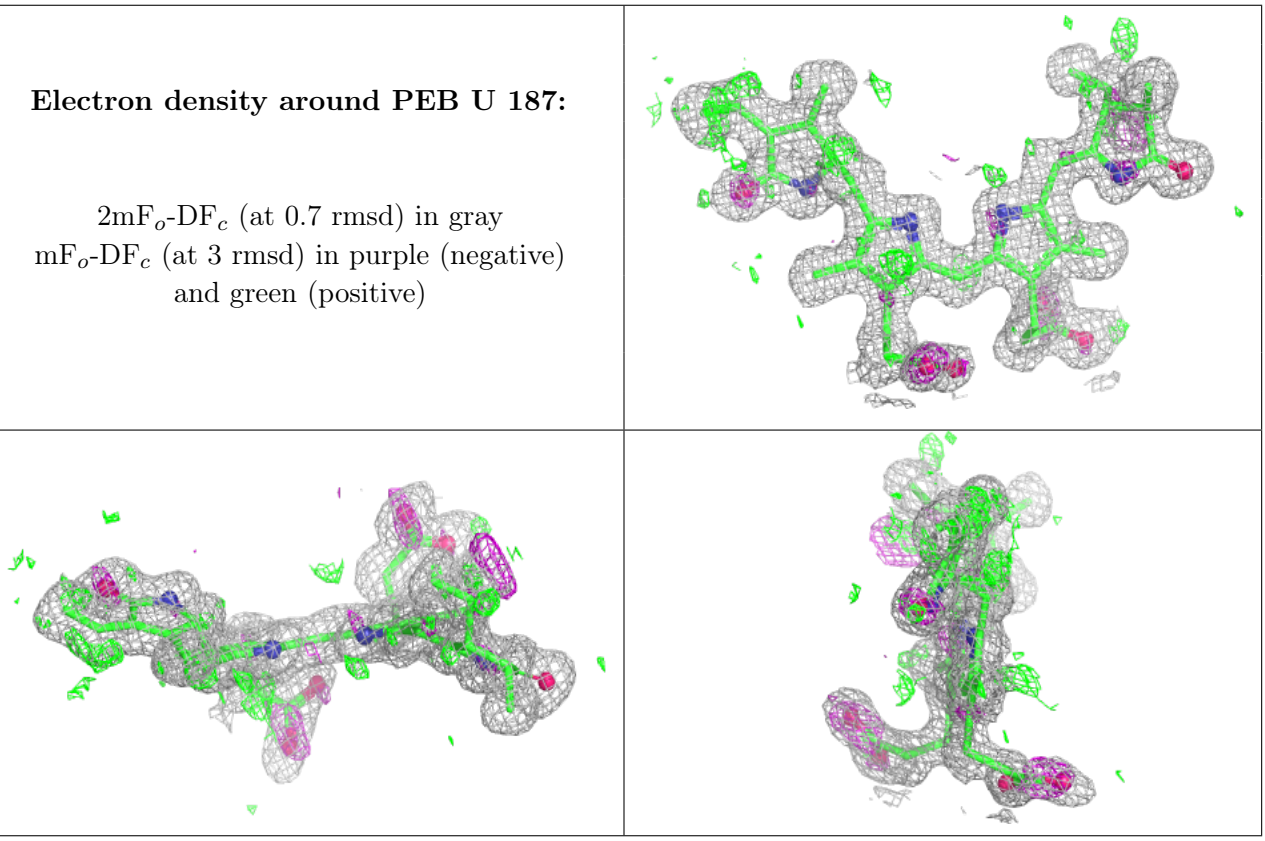
Electron density around PEB U 186:

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



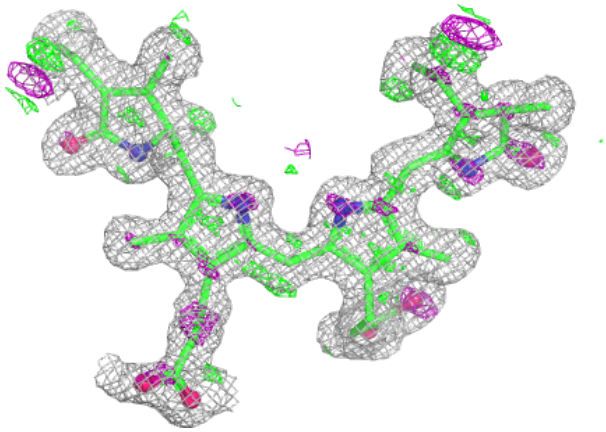
Electron density around PEB U 187:

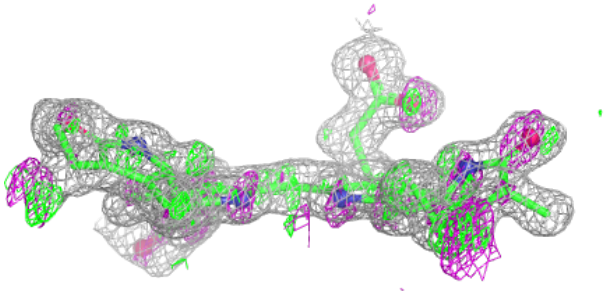
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

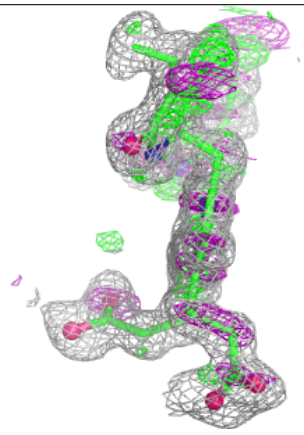


Electron density around PEB U 188:

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

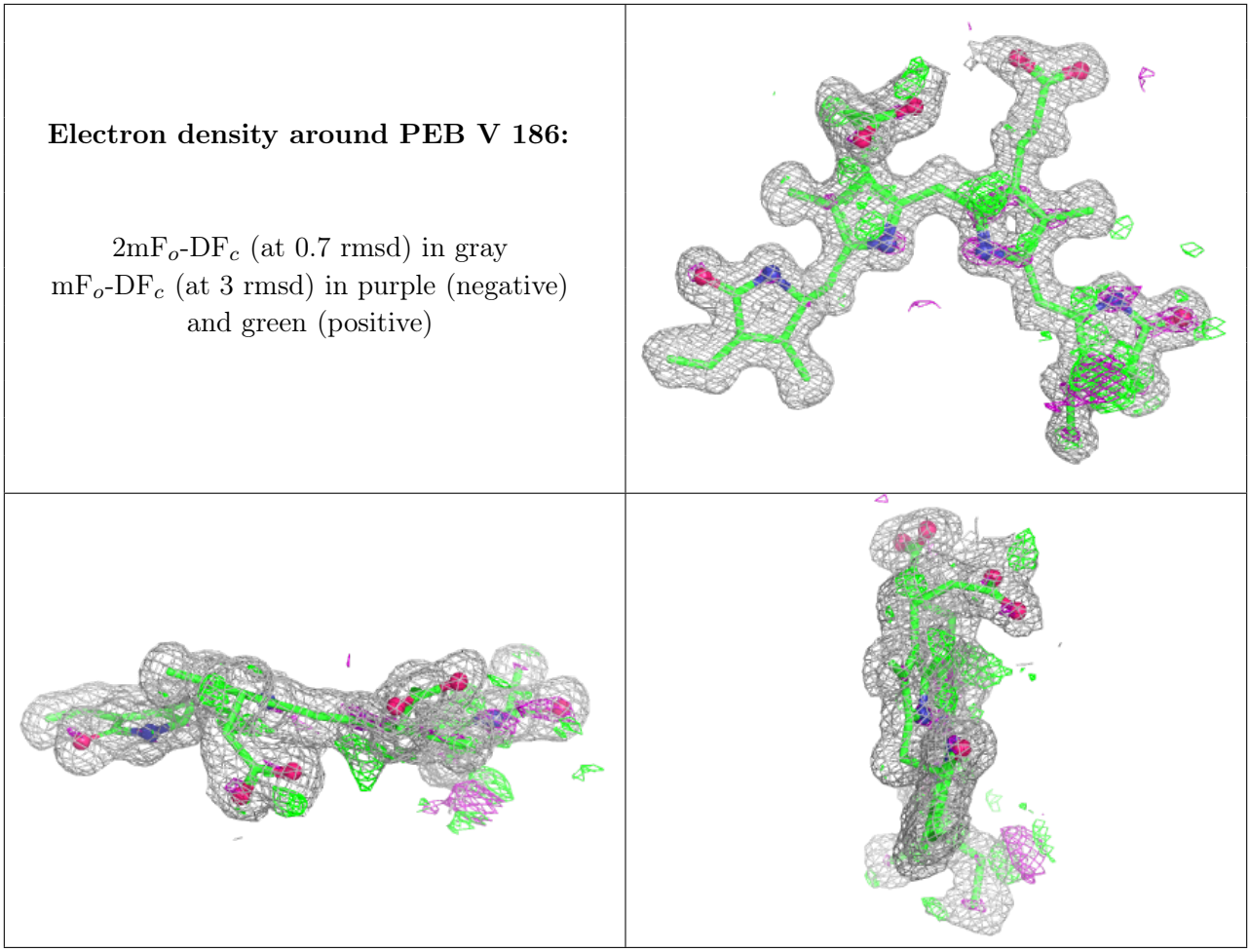






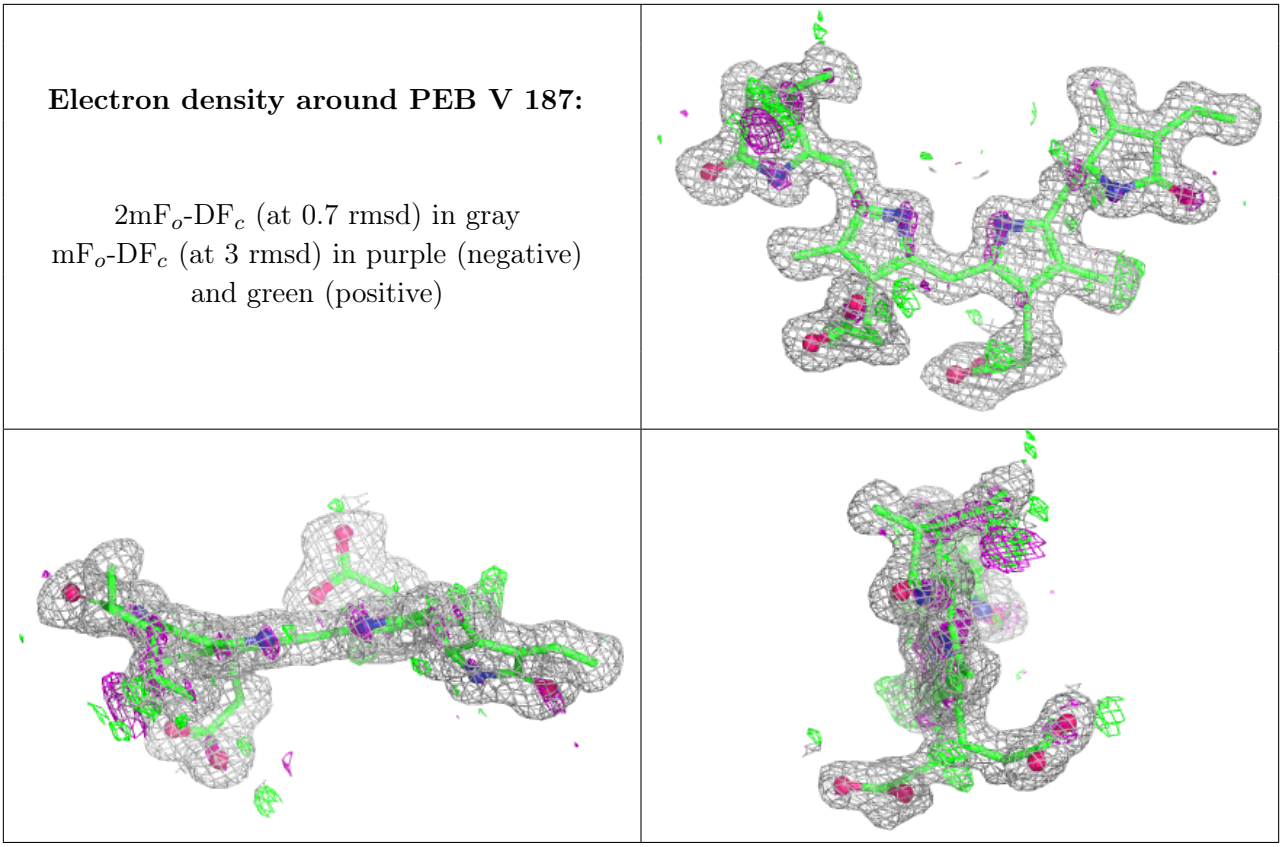
Electron density around PEB V 186:

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



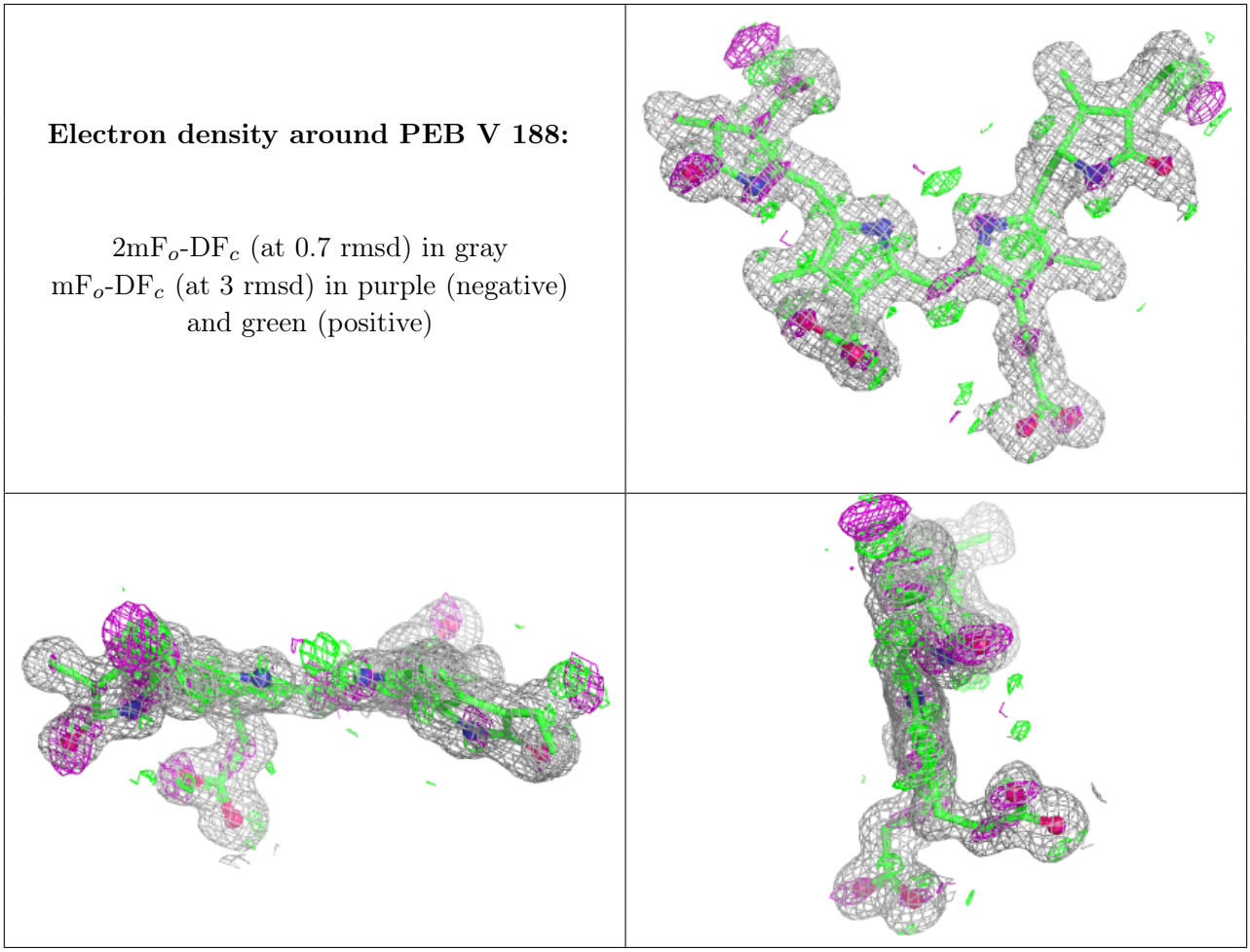
Electron density around PEB V 187:

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



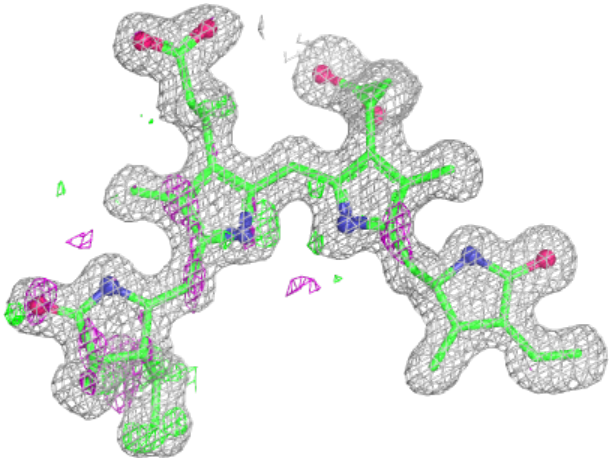
Electron density around PEB V 188:

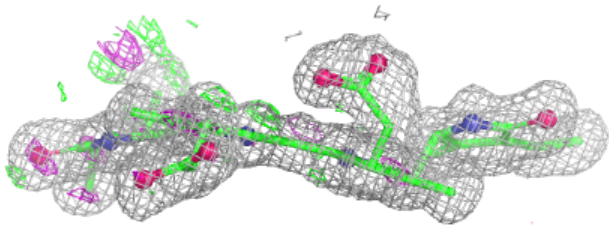
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

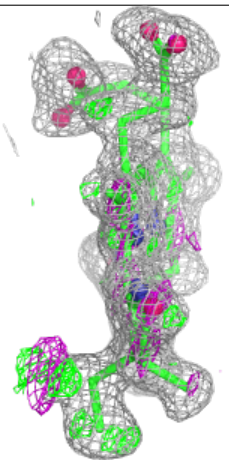


Electron density around PEB W 186:

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

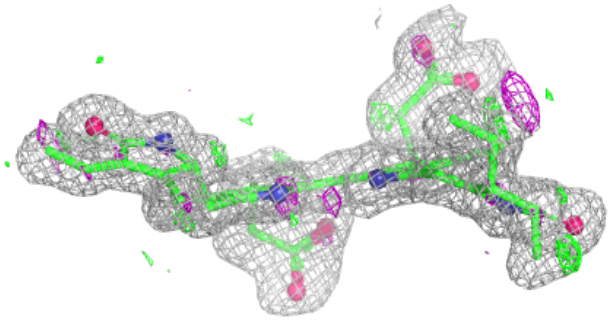


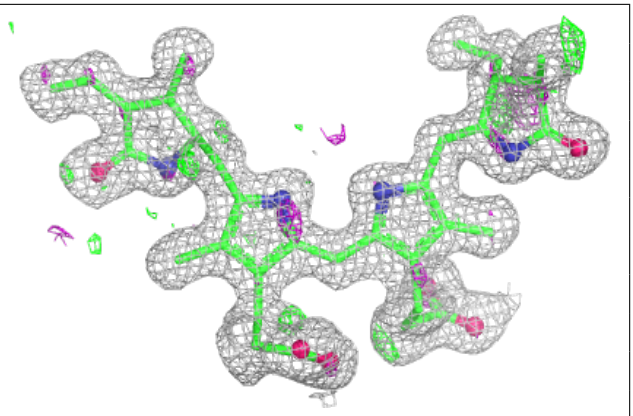


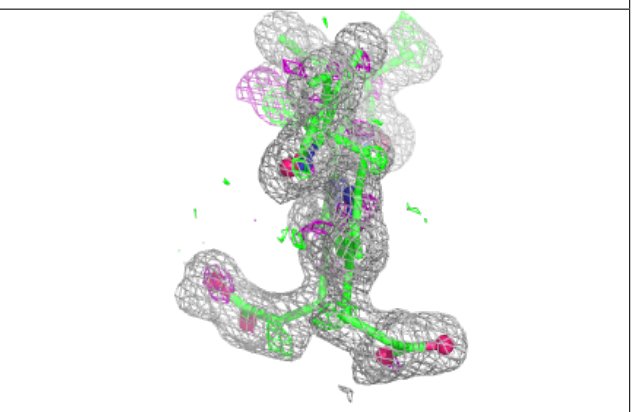


Electron density around PEB W 187:

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

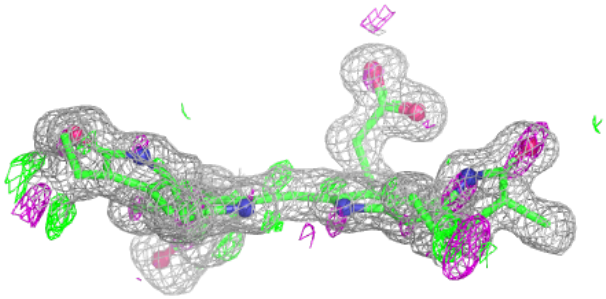


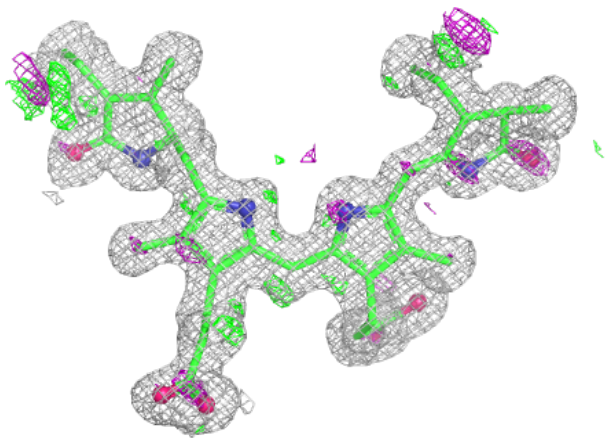


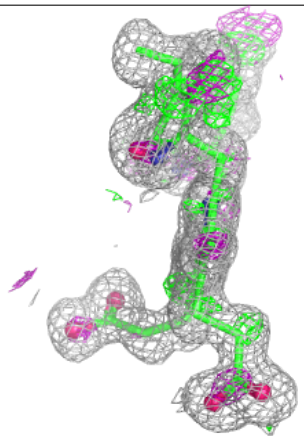


Electron density around PEB W 188:

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

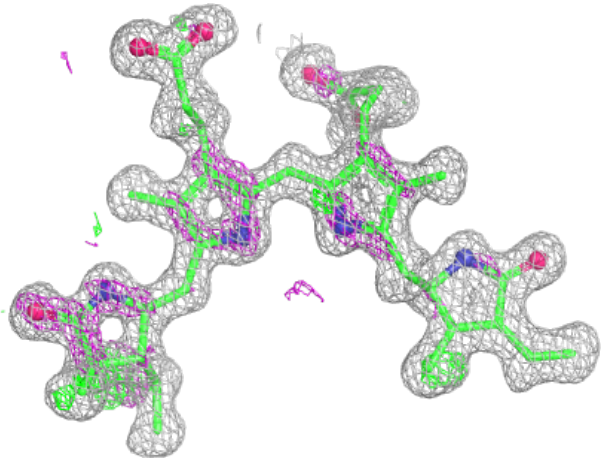


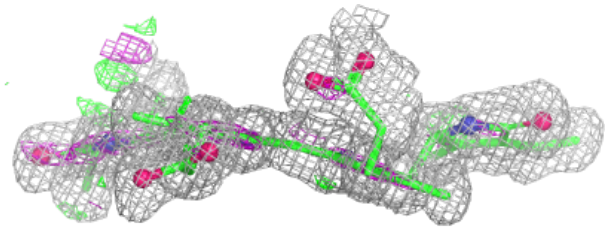


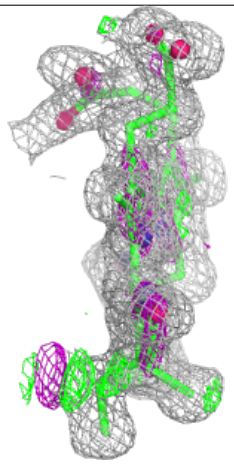


Electron density around PEB X 186:

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

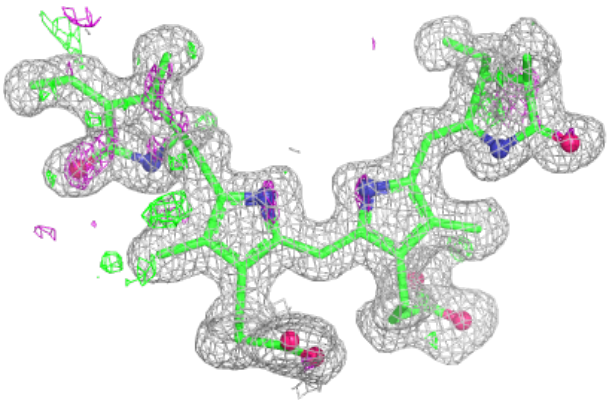


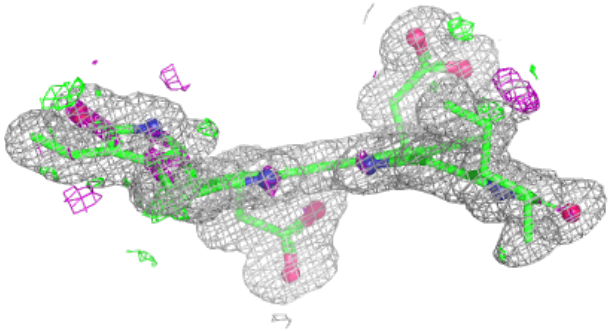


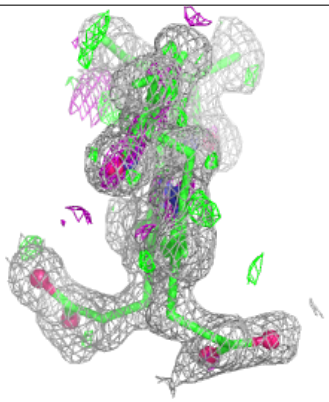


Electron density around PEB X 187:

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

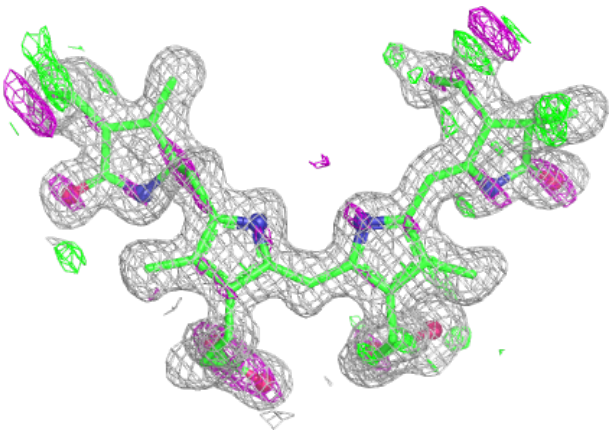


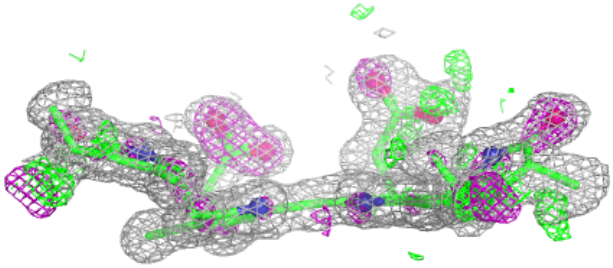


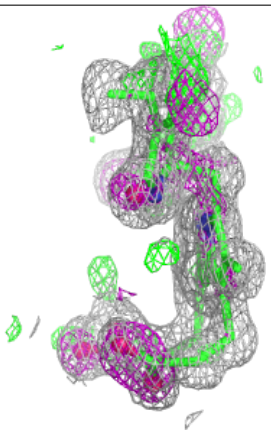


Electron density around PEB X 188:

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







6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.