wwPDB X-ray Structure Validation Summary Report (i)

Nov 8, 2023 – 06:36 AM EST

PDB ID	:	7SSF
Title	:	Light harvesting phycobiliprotein HaPE560 from the cryptophyte Hemiselmis andersenii CCMP644
Authors	:	Rathbone, H.W.; Michie, K.A.; Laos, A.L.; Curmi, P.M.G.
Deposited on	:	2021-11-10
Resolution	:	1.45 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

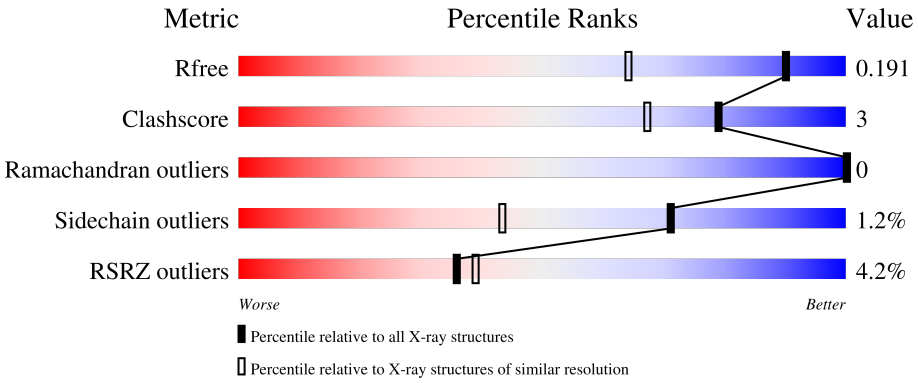
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	72	6% 97% .
1	C	72	% 96% .
1	E	72	% 99% .
1	G	72	3% 99% .
2	B	177	% 98% ..

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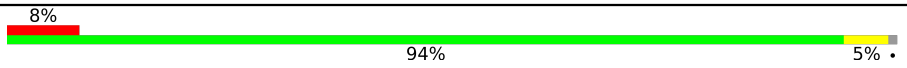
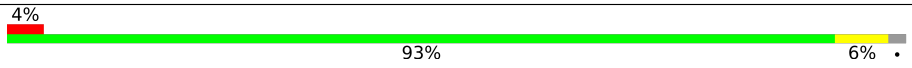
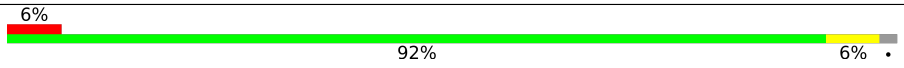
Mol	Chain	Length	Quality of chain
2	D	177	
2	F	177	
2	H	177	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17882 atoms, of which 8487 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 HaPE560 alpha subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	72	Total	C	H	N	O	S	0	5	0
			1149	352	572	106	113	6			
1	C	72	Total	C	H	N	O	S	0	3	0
			1133	345	568	107	107	6			
1	E	72	Total	C	H	N	O	S	0	4	0
			1136	348	568	104	109	7			
1	G	72	Total	C	H	N	O	S	0	3	0
			1125	344	564	104	107	6			

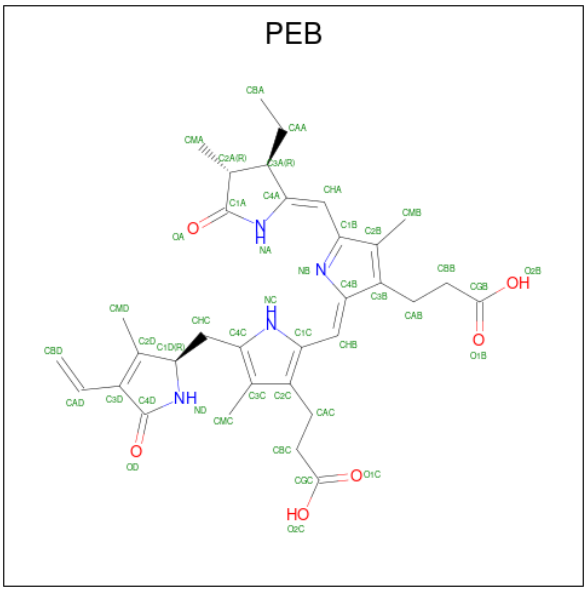
- Molecule 2 is a protein called Phycoerythrin550 beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	175	Total	C	H	N	O	S	0	19	0
			2818	862	1410	242	294	10			
2	D	175	Total	C	H	N	O	S	0	6	0
			2617	806	1314	222	264	11			
2	F	174	Total	C	H	N	O	S	0	22	0
			2824	862	1414	247	291	10			
2	H	173	Total	C	H	N	O	S	0	14	0
			2693	825	1348	232	278	10			

There are 4 discrepancies between the modelled and reference sequences:

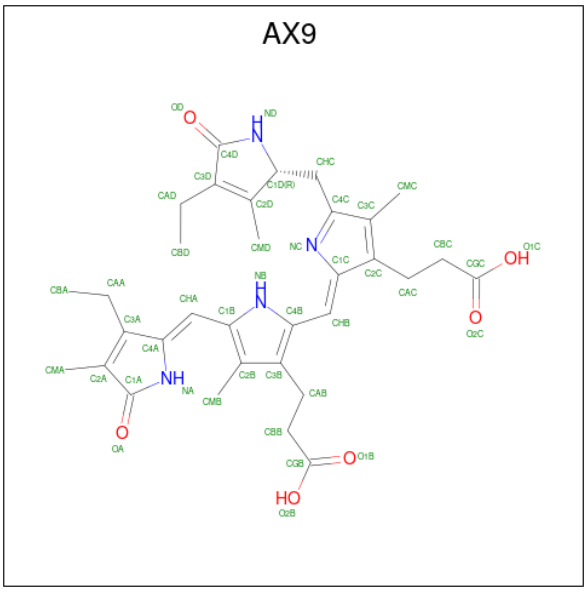
Chain	Residue	Modelled	Actual	Comment	Reference
B	172	VAL	GLU	conflict	UNP U5T8W0
D	172	VAL	GLU	conflict	UNP U5T8W0
F	172	VAL	GLU	conflict	UNP U5T8W0
H	172	VAL	GLU	conflict	UNP U5T8W0

- Molecule 3 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



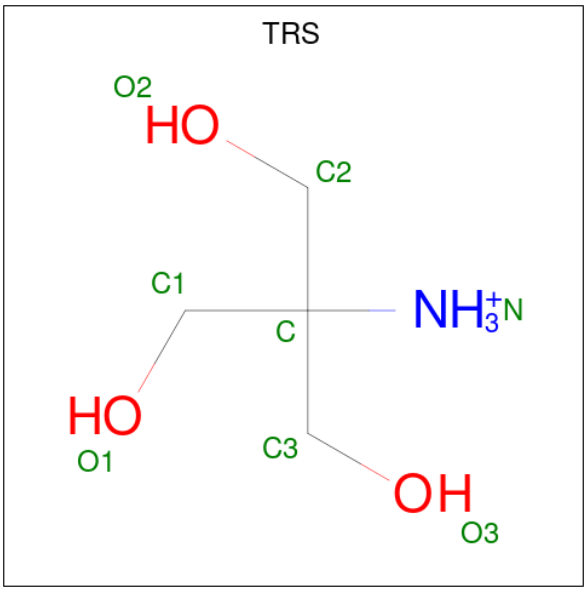
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	C	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	D	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	D	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	E	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	F	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	F	1	Total	C	H	N	O	0	1
			160	66	74	8	12		
3	G	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	H	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
3	H	1	Total	C	H	N	O	0	0
			80	33	37	4	6		

- Molecule 4 is DiCys-(15,16)-Dihydrobiliverdin (three-letter code: AX9) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	1
			158	66	72	8	12		
4	D	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
4	F	1	Total	C	H	N	O	0	1
			158	66	72	8	12		
4	H	1	Total	C	H	N	O	0	0
			79	33	36	4	6		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H N O 20 4 12 1 3	0	0
5	F	1	Total C H N O 16 4 8 1 3	0	1
5	H	1	Total C H N O 20 4 12 1 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Cl 1 1	0	0

- Molecule 7 is water.

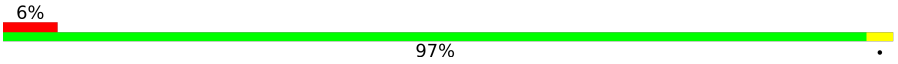
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	94	Total O 95 95	0	2
7	B	194	Total O 195 195	0	3
7	C	70	Total O 70 70	0	1
7	D	94	Total O 94 94	0	0
7	E	54	Total O 54 54	0	0
7	F	161	Total O 161 161	0	2
7	G	53	Total O 53 53	0	0
7	H	93	Total O 94 94	0	1

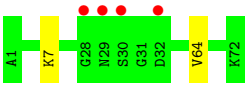
3 Residue-property plots (i)

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

- Molecule 1: HaPE560 alpha subunit

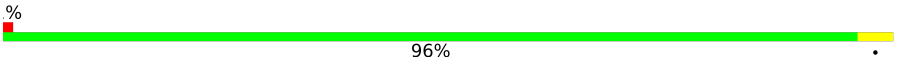
Chain A:

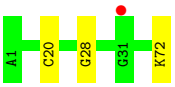




- Molecule 1: HaPE560 alpha subunit

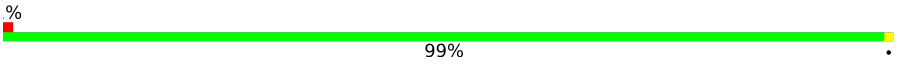
Chain C:

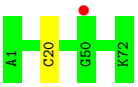




- Molecule 1: HaPE560 alpha subunit

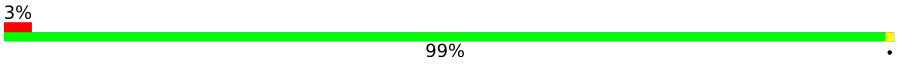
Chain E:

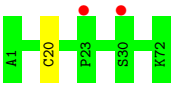




- Molecule 1: HaPE560 alpha subunit

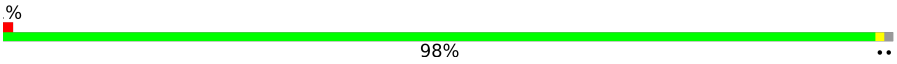
Chain G:

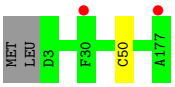




- Molecule 2: Phycoerythrin550 beta subunit

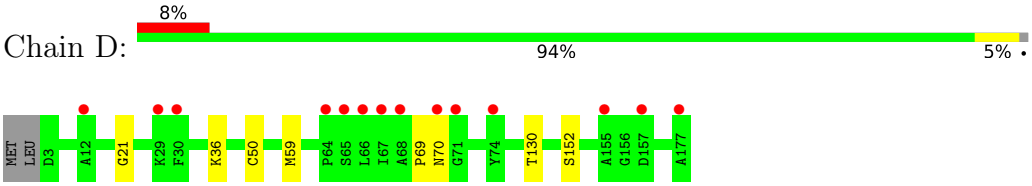
Chain B:





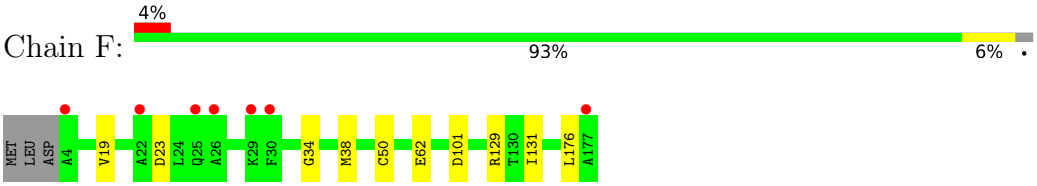
- Molecule 2: Phycoerythrin550 beta subunit

Chain D:



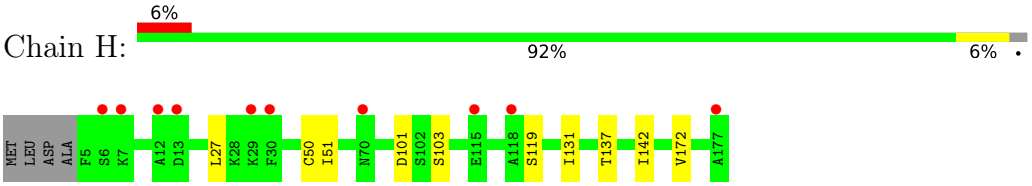
• Molecule 2: Phycoerythrin550 beta subunit

Chain F:



• Molecule 2: Phycoerythrin550 beta subunit

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.32Å 67.97Å 184.49Å 90.00° 99.33° 90.00°	Depositor
Resolution (Å)	28.94 – 1.45 28.94 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.94-1.45) 99.8 (28.94-1.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.154 , 0.192 0.153 , 0.191	Depositor DCC
R_{free} test set	9097 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17882	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PEB, AX9, LYZ, TRS

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	0.58	0/572	0.81	0/758
1	C	0.47	0/560	0.73	0/740
1	E	0.52	0/566	0.73	0/748
1	G	0.44	0/556	0.73	0/736
2	B	0.51	0/1433	0.68	0/1927
2	D	0.42	0/1325	0.63	0/1785
2	F	0.46	0/1430	0.67	0/1925
2	H	0.41	0/1373	0.61	0/1849
All	All	0.47	0/7815	0.68	0/10468

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	577	572	567	2	0
1	C	565	568	565	2	0
1	E	568	568	568	1	0
1	G	561	564	561	1	0
2	B	1408	1410	1380	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1303	1314	1294	9	0
2	F	1410	1414	1395	4	0
2	H	1345	1348	1317	5	0
3	A	43	37	37	2	0
3	B	86	74	74	3	0
3	C	43	37	37	3	0
3	D	86	74	74	8	0
3	E	43	37	37	3	0
3	F	129	111	111	5	0
3	G	43	37	37	3	0
3	H	86	74	74	5	0
4	B	86	72	0	0	0
4	D	43	36	0	1	0
4	F	86	72	0	0	0
4	H	43	36	0	0	0
5	B	8	12	12	0	0
5	F	8	8	12	0	0
5	H	8	12	12	0	0
6	F	1	0	0	0	0
7	A	95	0	0	1	0
7	B	195	0	0	0	0
7	C	70	0	0	0	0
7	D	94	0	0	1	0
7	E	54	0	0	0	0
7	F	161	0	0	0	0
7	G	53	0	0	0	0
7	H	94	0	0	0	0
All	All	9395	8487	8164	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 47 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)
3:B:202:PEB:HNA	3:B:202:PEB:HMB2	1.57	0.70
3:D:202:PEB:HMB2	3:D:202:PEB:HNA	1.57	0.69
3:H:202:PEB:HMB2	3:H:202:PEB:HNA	1.58	0.68
3:A:101:PEB:HMB2	3:A:101:PEB:HNA	1.63	0.64
3:F:202:PEB:HNA	3:F:202:PEB:HMB2	1.63	0.63

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	74/72 (103%)	70 (95%)	4 (5%)	0	100	100
1	C	72/72 (100%)	71 (99%)	1 (1%)	0	100	100
1	E	73/72 (101%)	73 (100%)	0	0	100	100
1	G	72/72 (100%)	71 (99%)	1 (1%)	0	100	100
2	B	194/177 (110%)	193 (100%)	1 (0%)	0	100	100
2	D	179/177 (101%)	177 (99%)	2 (1%)	0	100	100
2	F	194/177 (110%)	191 (98%)	3 (2%)	0	100	100
2	H	186/177 (105%)	183 (98%)	3 (2%)	0	100	100
All	All	1044/996 (105%)	1029 (99%)	15 (1%)	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	57/52 (110%)	57 (100%)	0	100	100
1	C	55/52 (106%)	54 (98%)	1 (2%)	59	26
1	E	56/52 (108%)	56 (100%)	0	100	100
1	G	55/52 (106%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	159/140 (114%)	158 (99%)	1 (1%)	86	69
2	D	144/140 (103%)	143 (99%)	1 (1%)	84	65
2	F	158/140 (113%)	156 (99%)	2 (1%)	69	40
2	H	152/140 (109%)	147 (97%)	5 (3%)	38	7
All	All	836/768 (109%)	826 (99%)	10 (1%)	71	43

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	101[B]	ASP
2	H	103	SER
2	H	119	SER
2	F	50	CYS
2	F	101	ASP

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LYZ	G	4	1	7,9,10	0.87	0	4,10,12	0.89	0
1	LYZ	E	4	1	7,9,10	0.80	0	4,10,12	0.70	0
1	LYZ	A	4	1	7,9,10	0.61	0	4,10,12	0.85	0
1	LYZ	C	4	1	7,9,10	0.78	0	4,10,12	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYZ	G	4	1	-	0/8/9/11	-
1	LYZ	E	4	1	-	1/8/9/11	-
1	LYZ	A	4	1	-	1/8/9/11	-
1	LYZ	C	4	1	-	0/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	4	LYZ	O-C-CA-CB
1	E	4	LYZ	O-C-CA-CB

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 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	E	101	1	43,46,46	3.60	28 (65%)	45,67,67	2.35	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	TRS	B	204	-	7,7,7	0.57	0	9,9,9	1.05	0
3	PEB	F	202	2	43,46,46	3.51	27 (62%)	45,67,67	2.24	16 (35%)
3	PEB	B	202	2	43,46,46	3.23	26 (60%)	45,67,67	2.19	13 (28%)
4	AX9	D	201	2	41,46,46	1.32	4 (9%)	41,67,67	1.58	6 (14%)
3	PEB	B	203	2	43,46,46	3.76	22 (51%)	45,67,67	1.89	13 (28%)
3	PEB	C	101	1	43,46,46	3.59	27 (62%)	45,67,67	2.20	14 (31%)
3	PEB	D	202	2	43,46,46	4.41	29 (67%)	45,67,67	2.62	17 (37%)
3	PEB	F	203[A]	2	43,46,46	4.62	32 (74%)	45,67,67	1.64	7 (15%)
4	AX9	B	201[A]	2	41,46,46	1.52	8 (19%)	41,67,67	1.44	9 (21%)
3	PEB	A	101	1	43,46,46	3.39	25 (58%)	45,67,67	2.19	15 (33%)
4	AX9	F	201[B]	2	41,46,46	1.53	9 (21%)	41,67,67	1.27	4 (9%)
4	AX9	H	201	2	41,46,46	1.41	8 (19%)	41,67,67	1.41	5 (12%)
3	PEB	D	203	2	43,46,46	4.74	33 (76%)	45,67,67	2.06	9 (20%)
3	PEB	H	203	2	43,46,46	4.84	32 (74%)	45,67,67	1.77	10 (22%)
5	TRS	F	204[A]	-	7,7,7	0.53	0	9,9,9	0.69	0
5	TRS	H	204	-	7,7,7	0.51	0	9,9,9	0.67	0
3	PEB	H	202	2	43,46,46	4.09	31 (72%)	45,67,67	2.49	19 (42%)
3	PEB	F	203[B]	2	43,46,46	3.89	26 (60%)	45,67,67	1.73	9 (20%)
4	AX9	B	201[B]	2	41,46,46	1.47	7 (17%)	41,67,67	1.24	4 (9%)
4	AX9	F	201[A]	2	41,46,46	1.49	8 (19%)	41,67,67	1.05	4 (9%)
3	PEB	G	101	1	43,46,46	4.11	31 (72%)	45,67,67	2.48	17 (37%)

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	E	101	1	-	3/24/74/74	0/4/4/4
5	TRS	B	204	-	-	0/9/9/9	-
3	PEB	F	202	2	-	6/24/74/74	0/4/4/4
3	PEB	B	202	2	-	6/24/74/74	0/4/4/4
4	AX9	D	201	2	-	11/26/74/74	0/4/4/4
3	PEB	B	203	2	-	9/24/74/74	0/4/4/4
3	PEB	C	101	1	-	6/24/74/74	0/4/4/4
3	PEB	D	202	2	-	4/24/74/74	0/4/4/4
3	PEB	F	203[A]	2	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AX9	B	201[A]	2	-	6/26/74/74	0/4/4/4
3	PEB	A	101	1	-	2/24/74/74	0/4/4/4
4	AX9	F	201[B]	2	-	8/26/74/74	0/4/4/4
4	AX9	H	201	2	-	9/26/74/74	0/4/4/4
3	PEB	D	203	2	-	9/24/74/74	0/4/4/4
3	PEB	H	203	2	-	11/24/74/74	0/4/4/4
5	TRS	F	204[A]	-	-	0/9/9/9	-
5	TRS	H	204	-	-	0/9/9/9	-
3	PEB	H	202	2	-	5/24/74/74	0/4/4/4
3	PEB	F	203[B]	2	-	8/24/74/74	0/4/4/4
4	AX9	B	201[B]	2	-	11/26/74/74	0/4/4/4
4	AX9	F	201[A]	2	-	7/26/74/74	0/4/4/4
3	PEB	G	101	1	-	3/24/74/74	0/4/4/4

The worst 5 of 413 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	203	PEB	CHB-C4B	13.56	1.46	1.35
3	D	202	PEB	CHB-C4B	12.96	1.45	1.35
3	D	203	PEB	CHB-C4B	11.94	1.45	1.35
3	F	203[A]	PEB	CHB-C4B	11.57	1.44	1.35
3	F	203[A]	PEB	C2A-C1A	9.90	1.60	1.52

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	202	PEB	C1C-CHB-C4B	-9.45	117.52	128.81
3	G	101	PEB	C1C-CHB-C4B	-8.62	118.52	128.81
3	H	202	PEB	C1C-CHB-C4B	-8.43	118.74	128.81
3	C	101	PEB	C1C-CHB-C4B	-7.09	120.34	128.81
3	D	203	PEB	C1C-CHB-C4B	-6.45	121.10	128.81

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	101	PEB	NB-C1B-CHA-C4A
3	A	101	PEB	C2B-C1B-CHA-C4A
3	B	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
3	B	203	PEB	NB-C1B-CHA-C4A
3	B	203	PEB	C2B-C1B-CHA-C4A

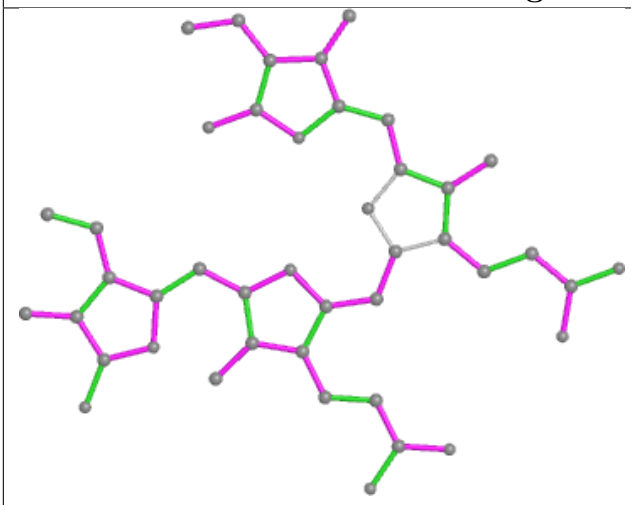
There are no ring outliers.

14 monomers are involved in 33 short contacts:

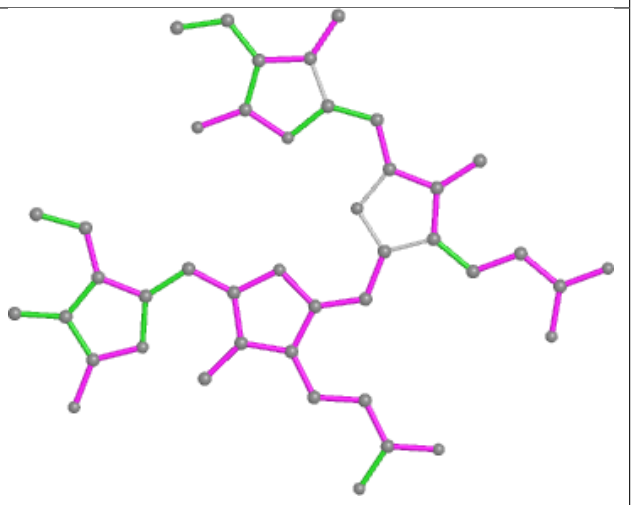
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	101	PEB	3	0
3	F	202	PEB	1	0
3	B	202	PEB	1	0
4	D	201	AX9	1	0
3	B	203	PEB	2	0
3	C	101	PEB	3	0
3	D	202	PEB	5	0
3	F	203[A]	PEB	3	0
3	A	101	PEB	2	0
3	D	203	PEB	3	0
3	H	203	PEB	4	0
3	H	202	PEB	1	0
3	F	203[B]	PEB	1	0
3	G	101	PEB	3	0

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.

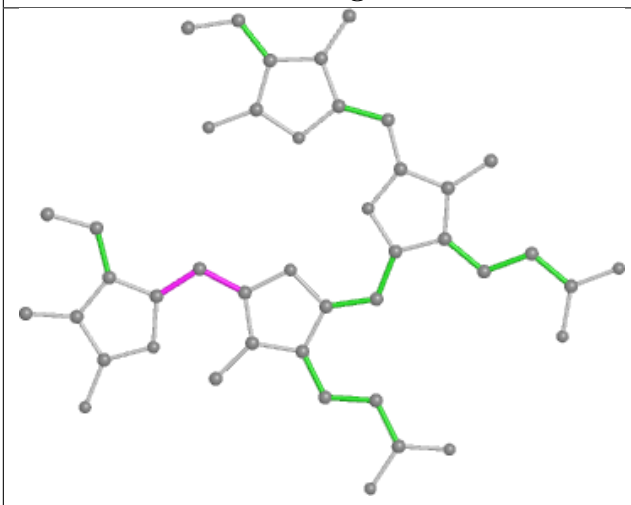
Ligand PEB E 101



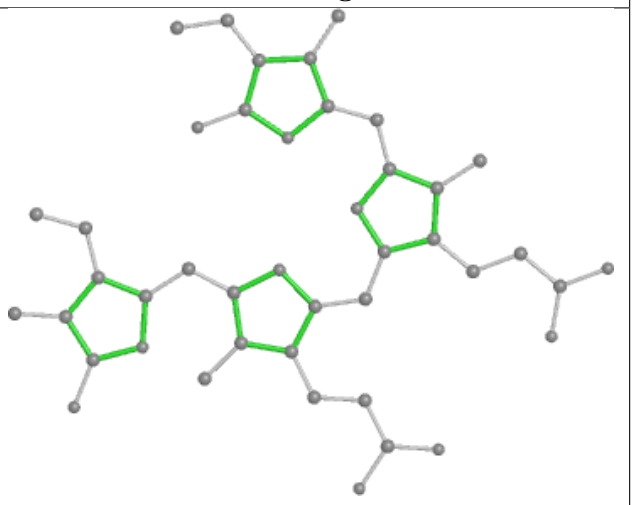
Bond lengths



Bond angles

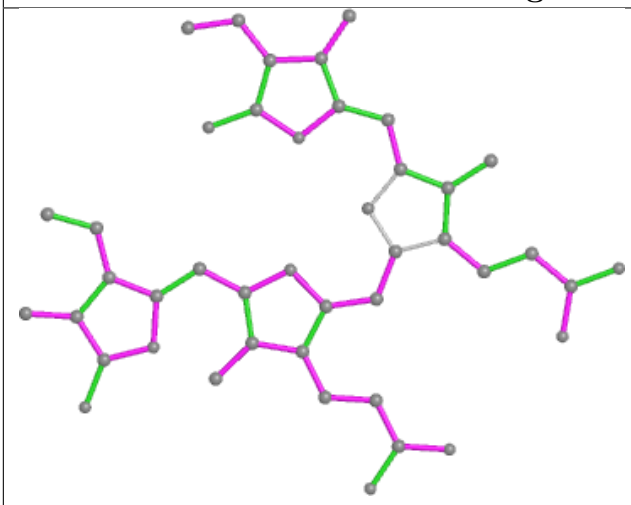


Torsions



Rings

Ligand PEB F 202



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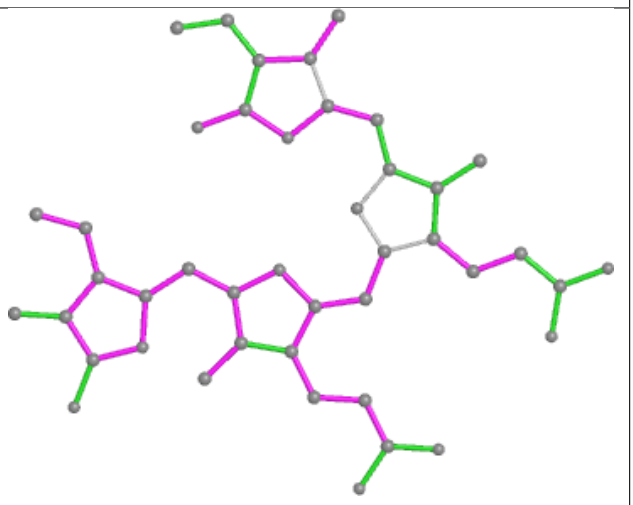

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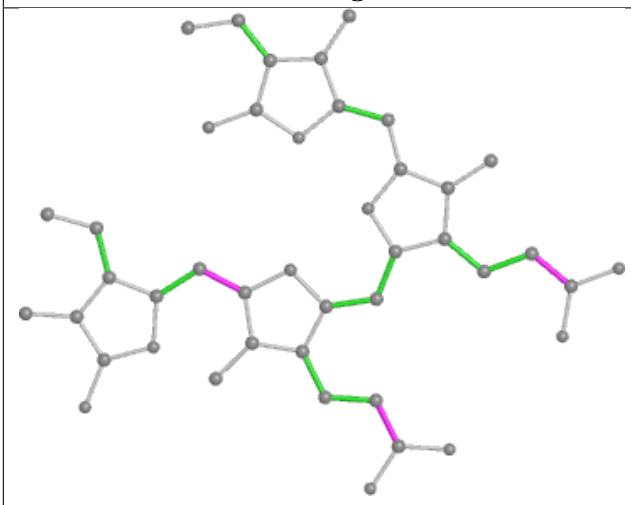

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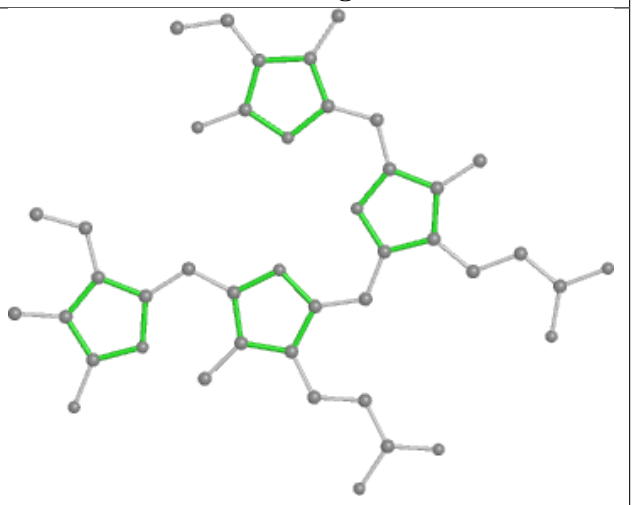

Rings

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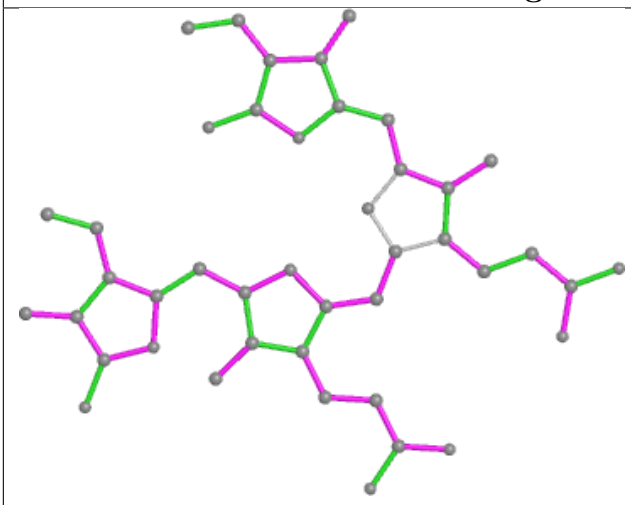

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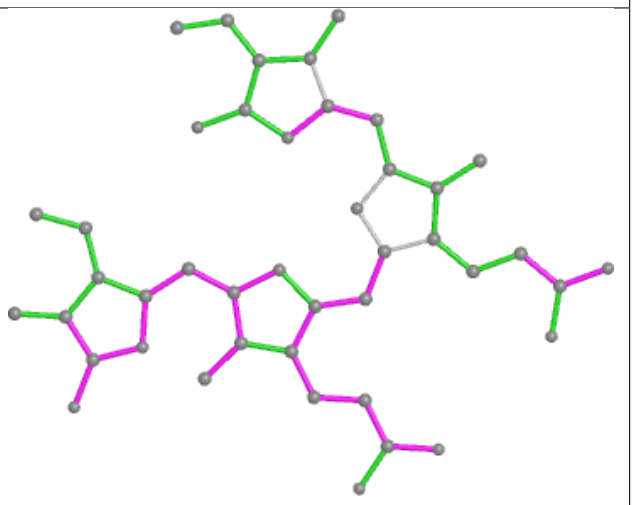

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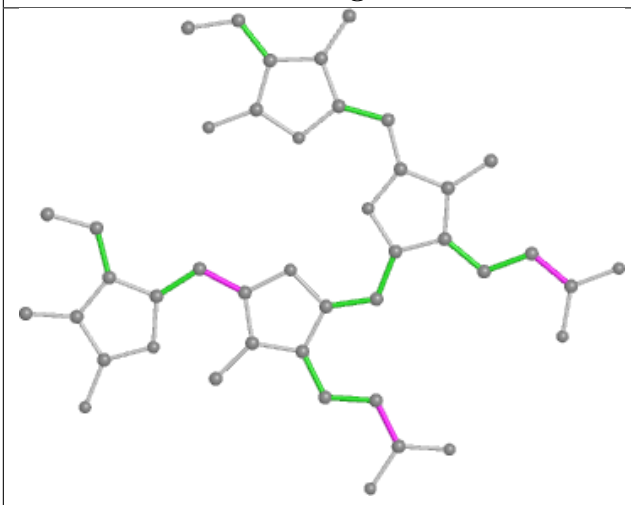

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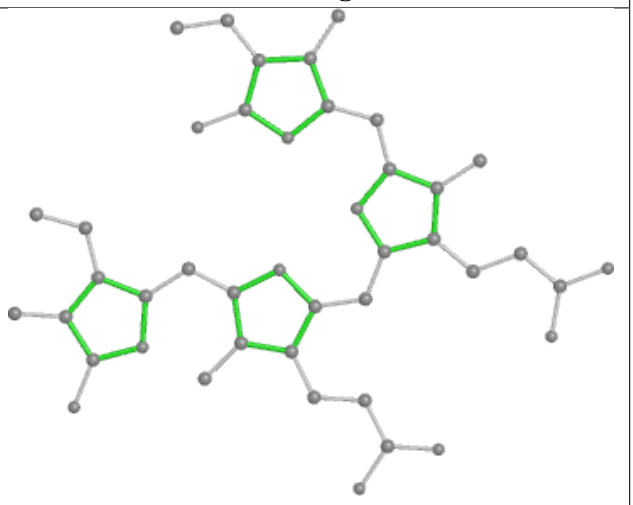
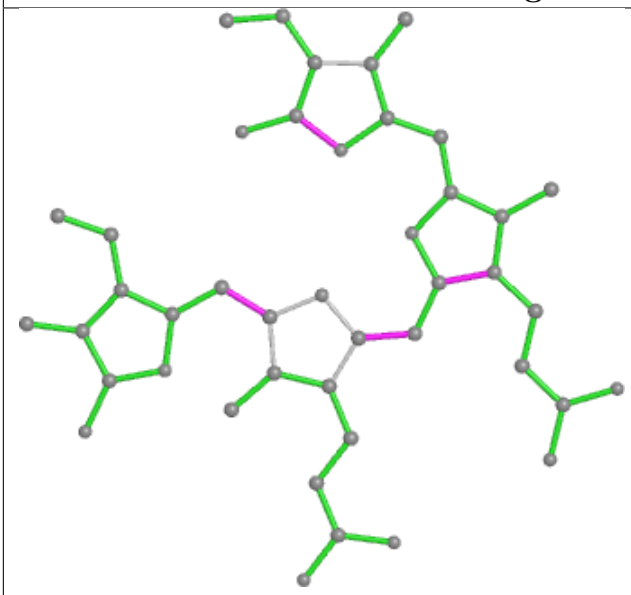


Rings

Ligand AX9 D 201



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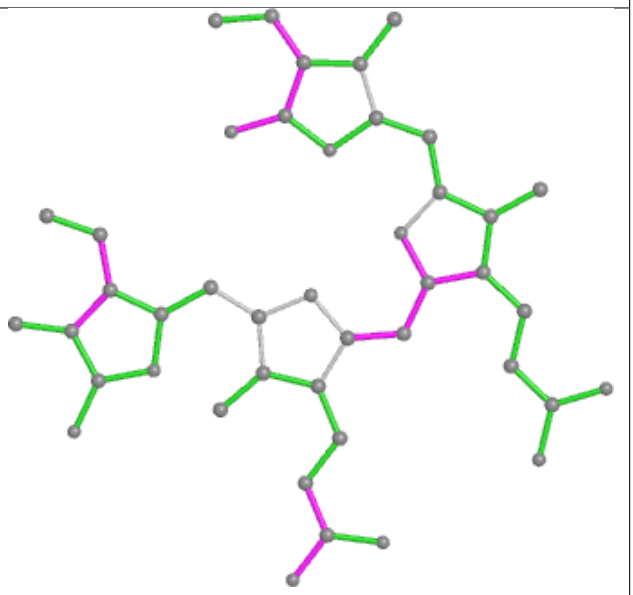

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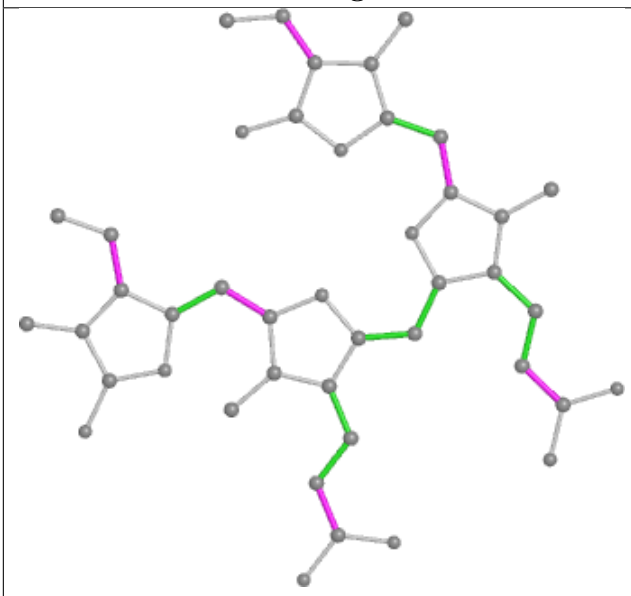

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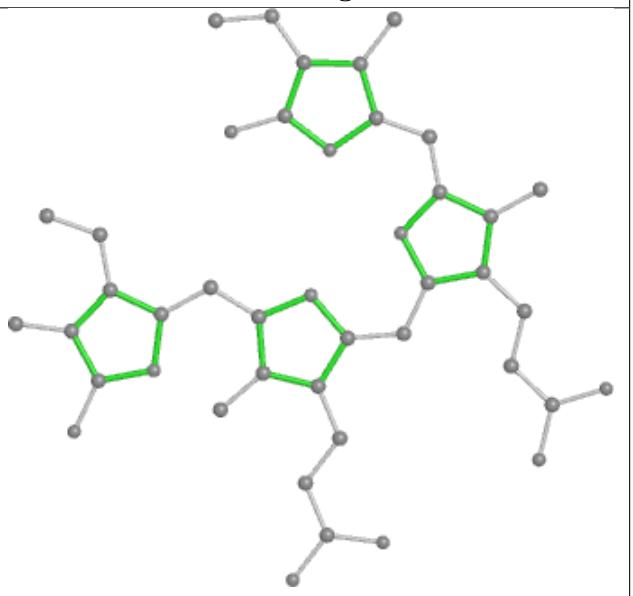
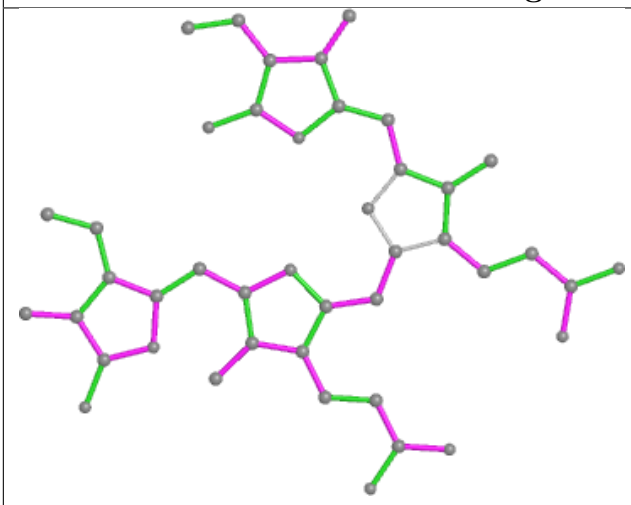


Rings

Ligand PEB B 203



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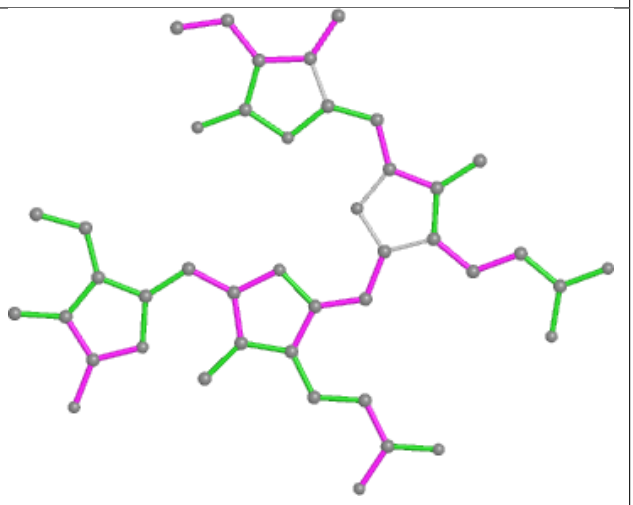
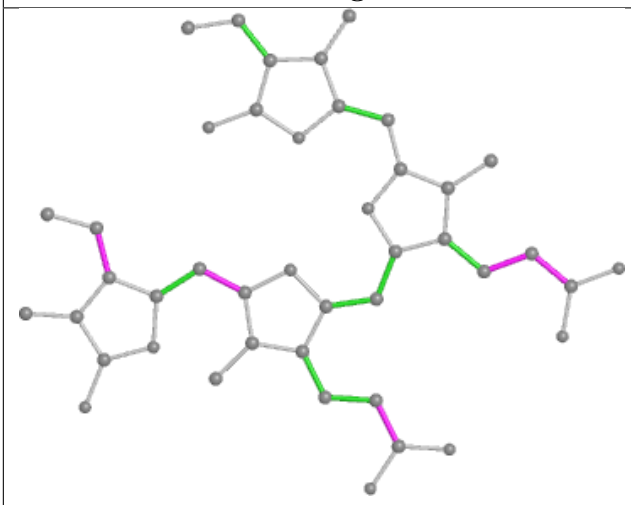


Bond angles



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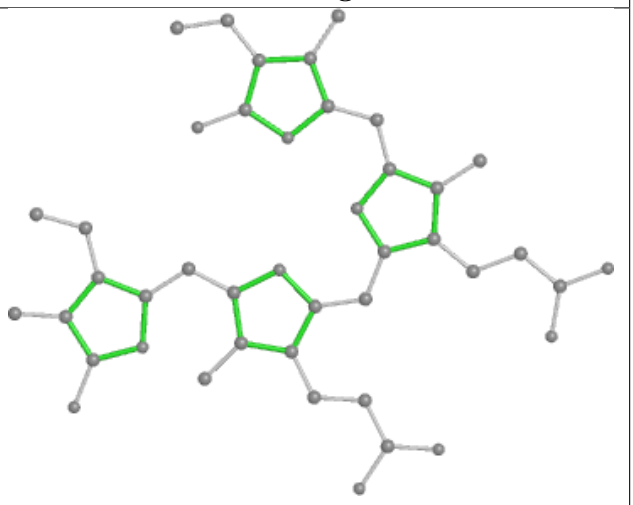
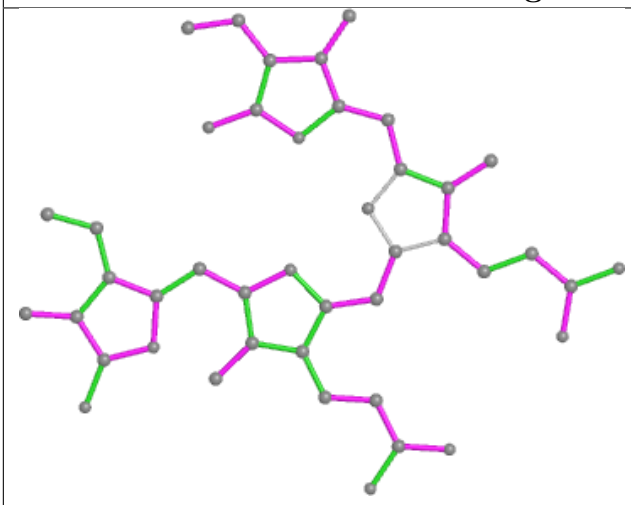


Rings

Ligand PEB C 101



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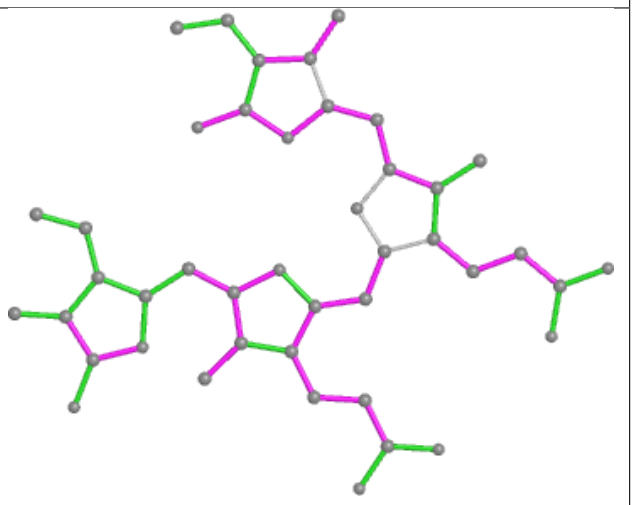

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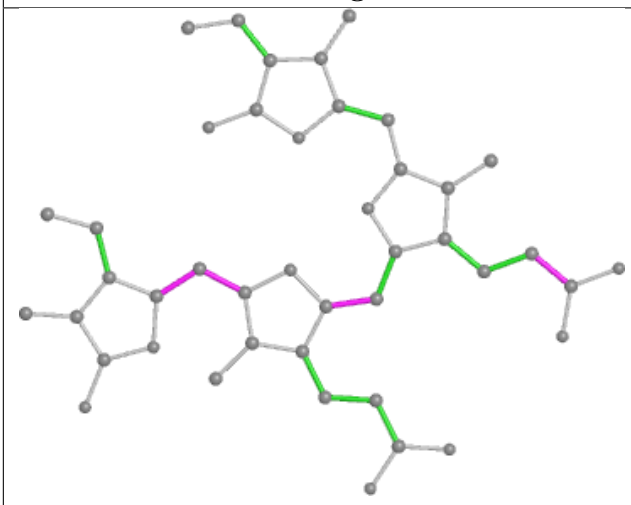

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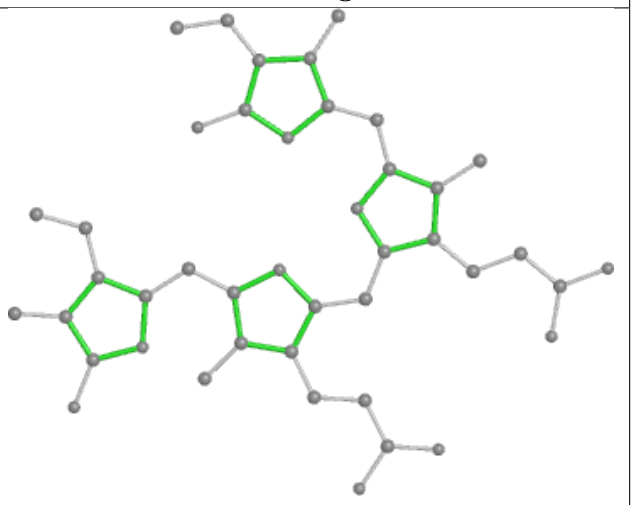
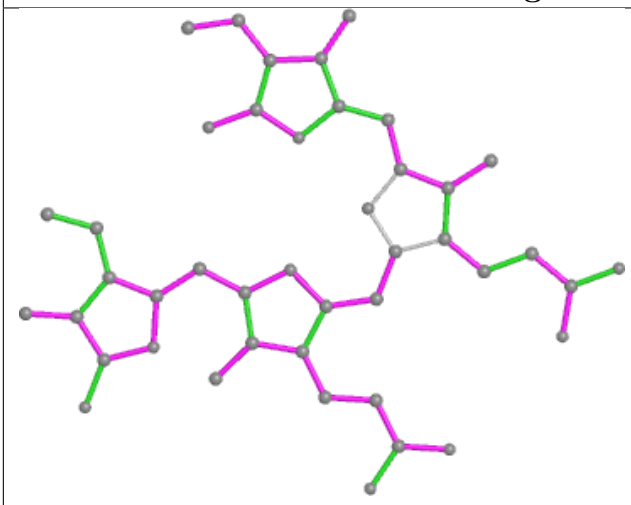
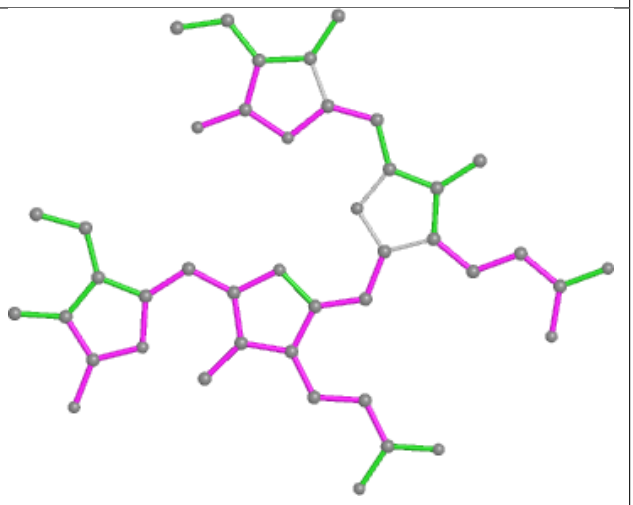


Rings

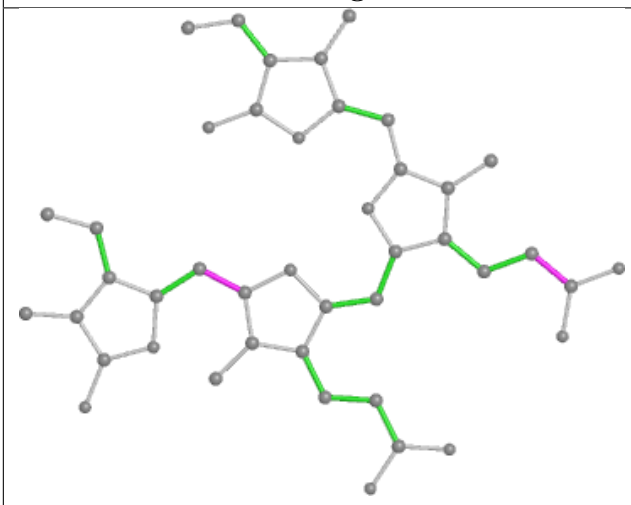
Ligand PEB D 202



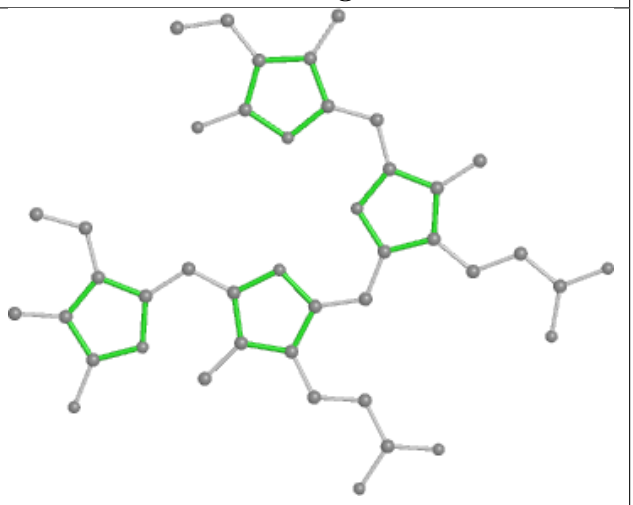
Bond lengths



Bond angles

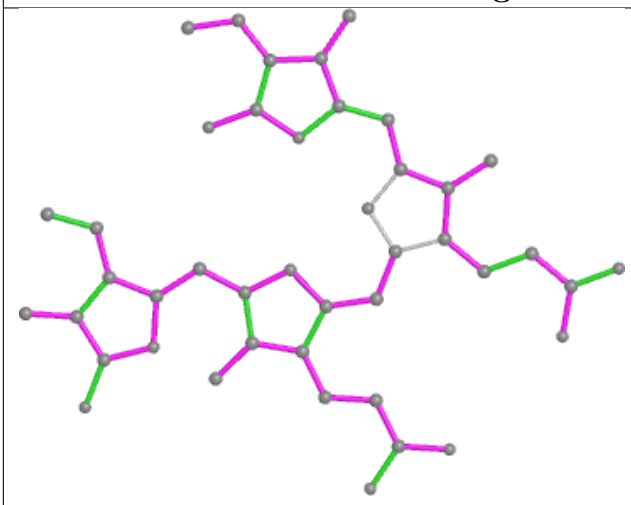


Torsions

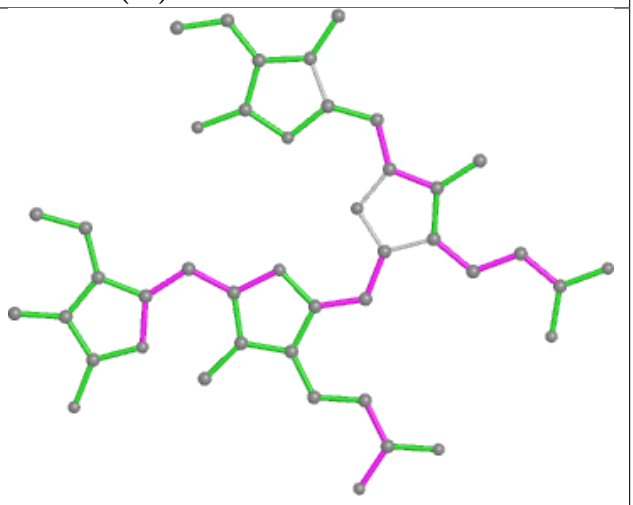


Rings

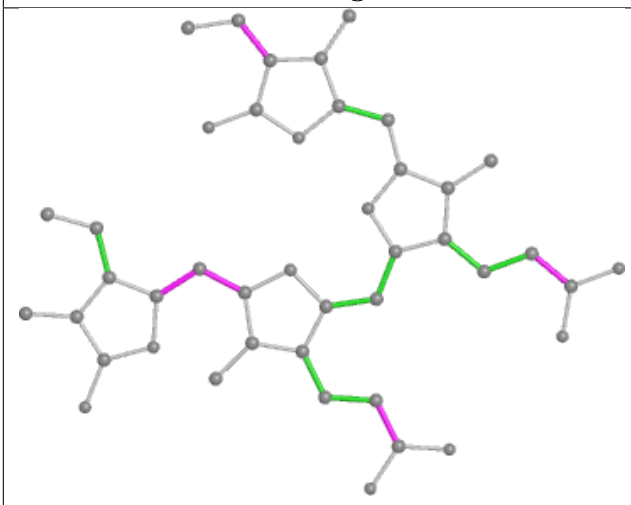
Ligand PEB F 203 (A)



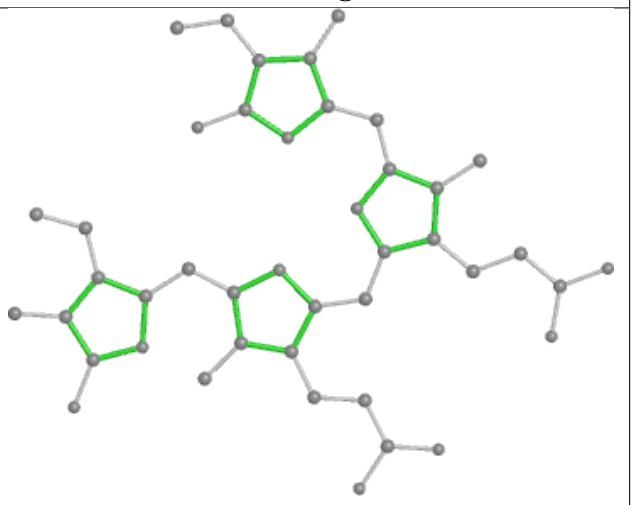
Bond lengths



Bond angles

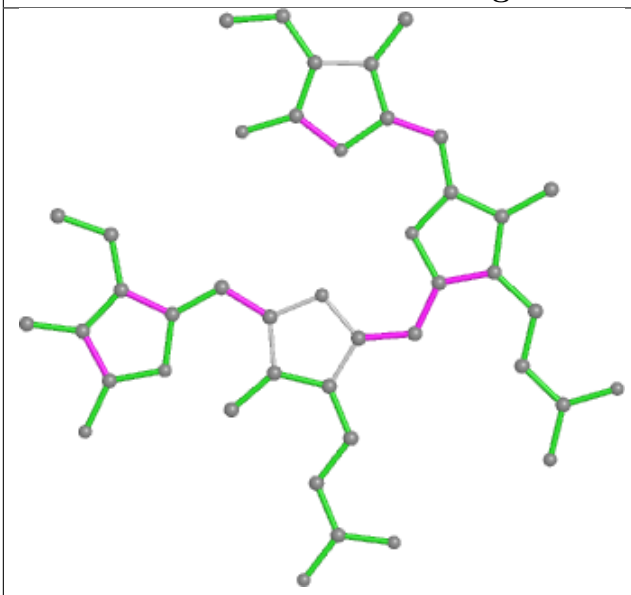


Torsions

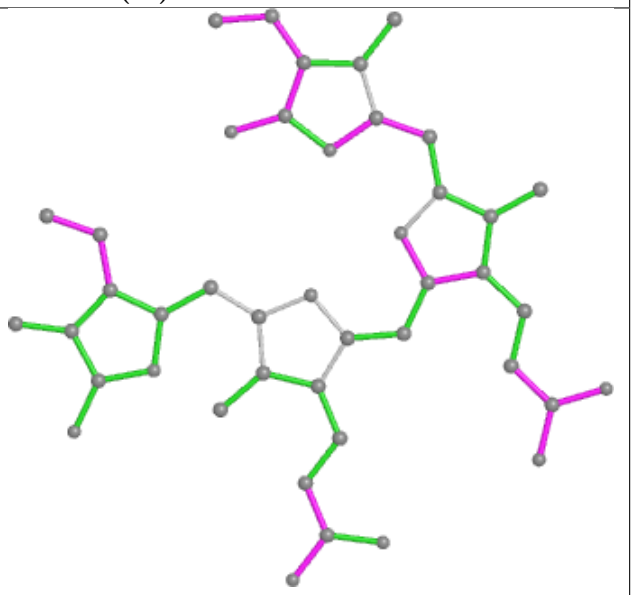


Rings

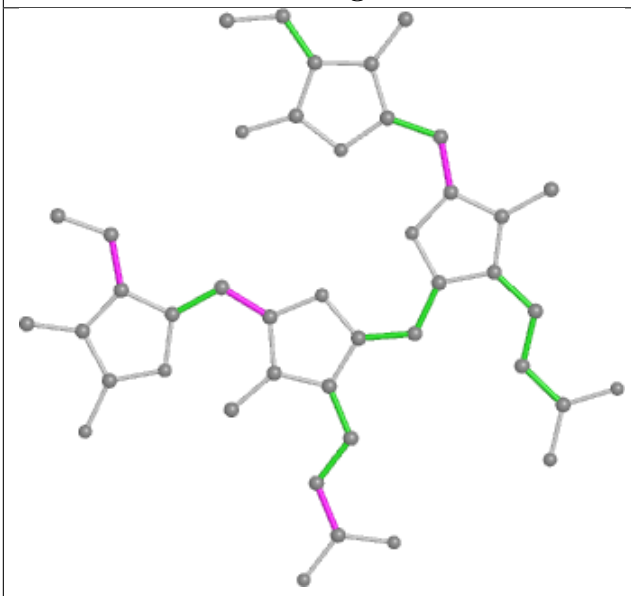
Ligand AX9 B 201 (A)



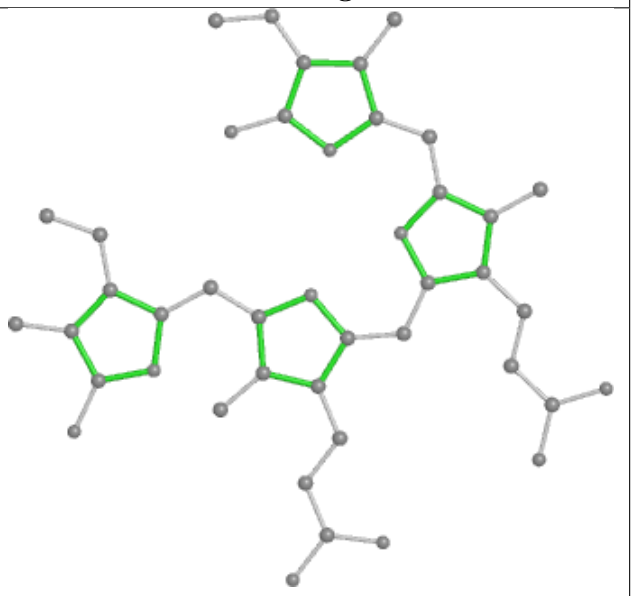
Bond lengths



Bond angles

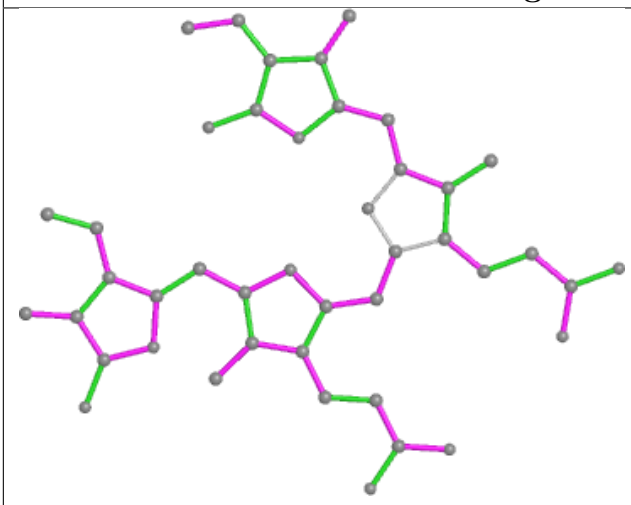


Torsions



Rings

Ligand PEB A 101



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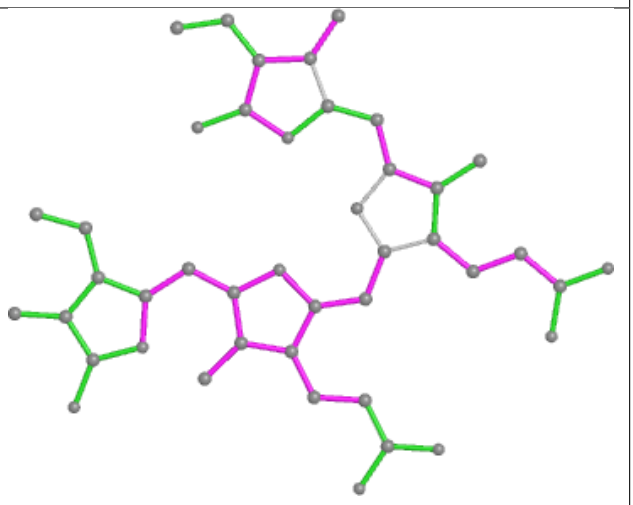
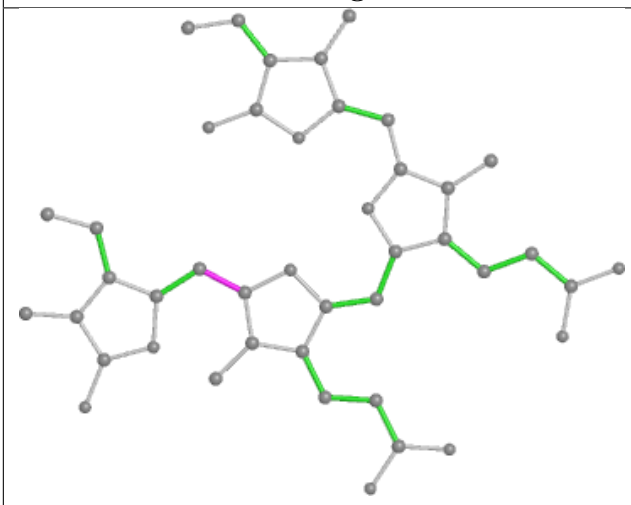
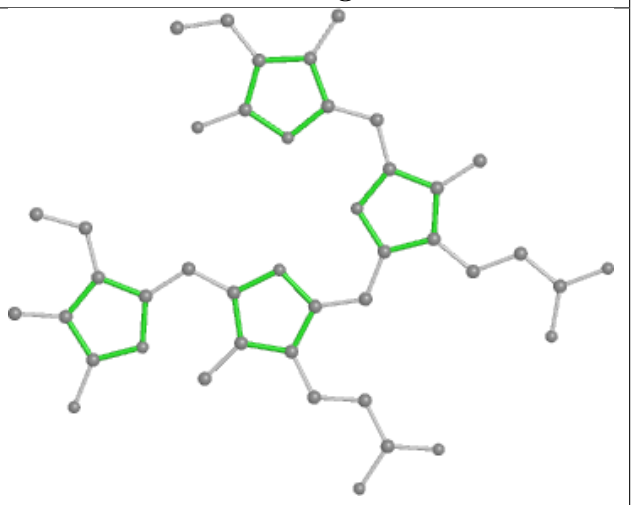


Bond angles

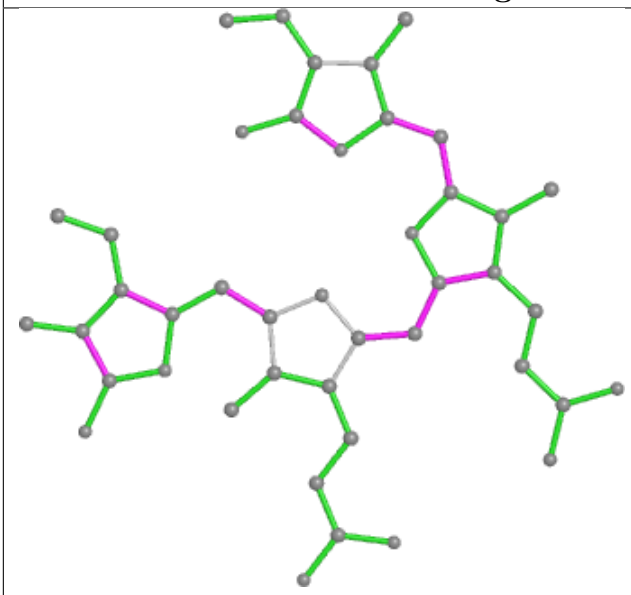


Torsions

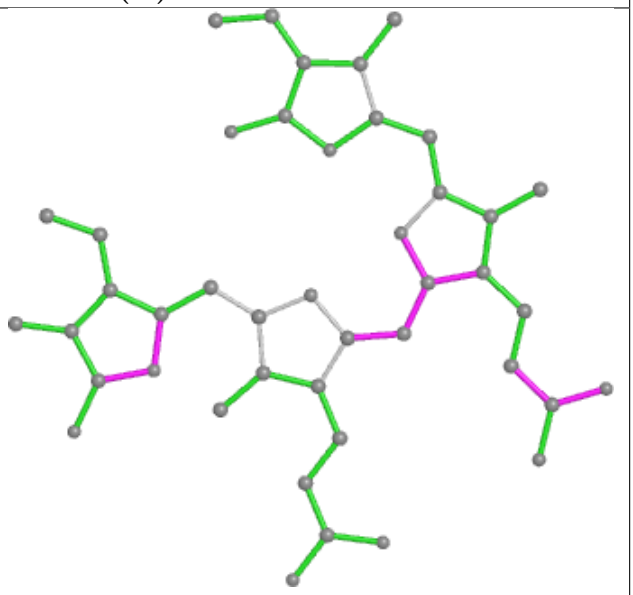


Rings

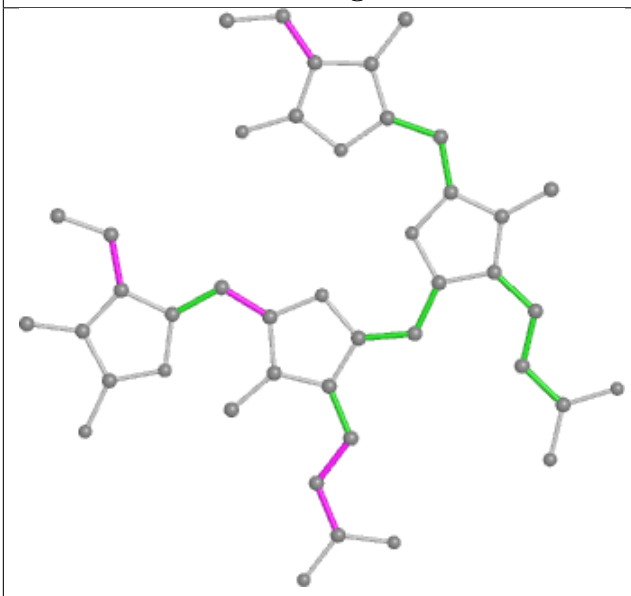
Ligand AX9 F 201 (B)



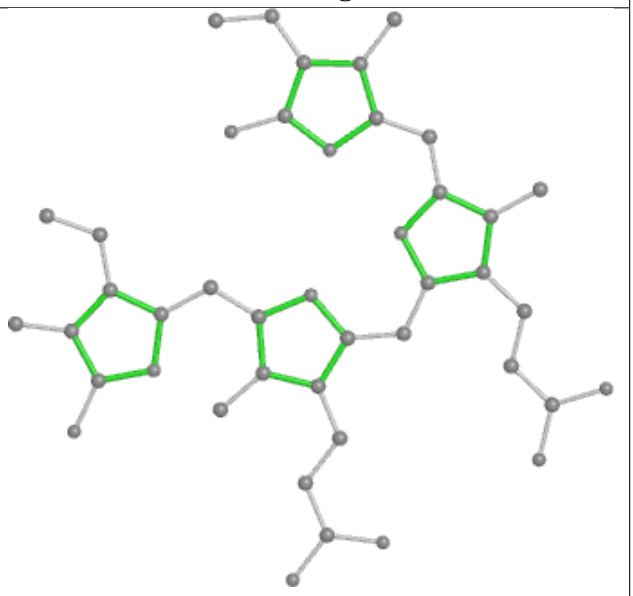
Bond lengths



Bond angles

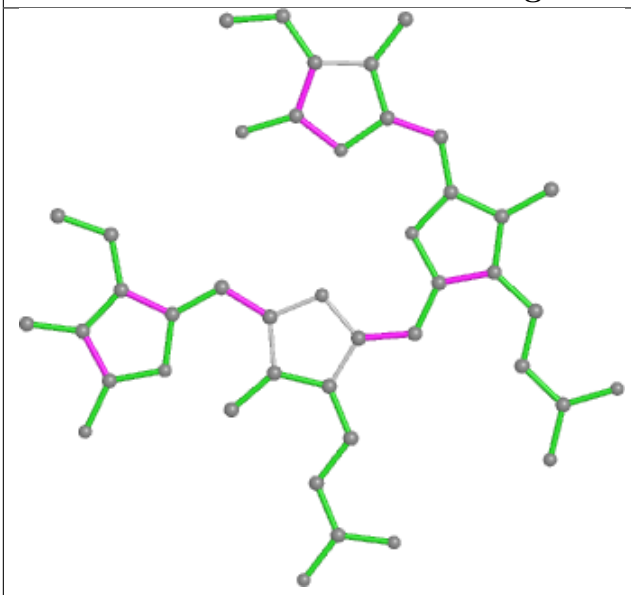


Torsions

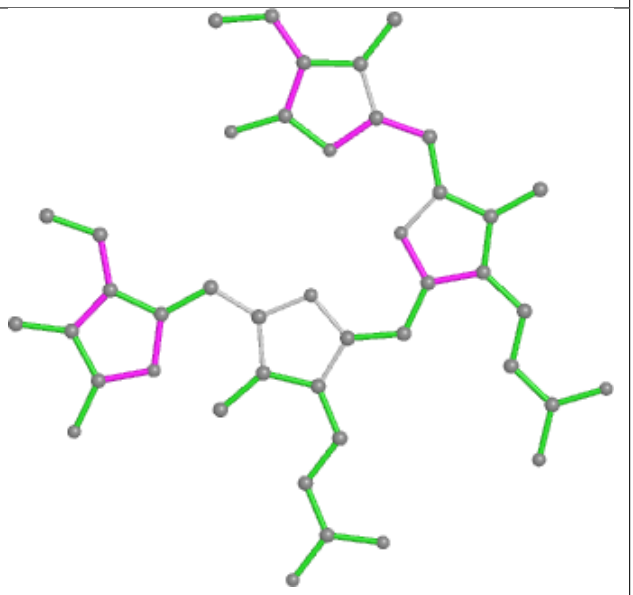


Rings

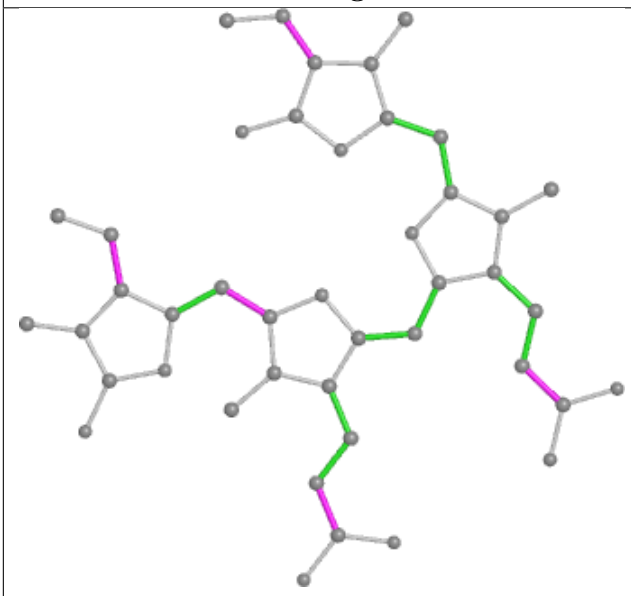
Ligand AX9 H 201



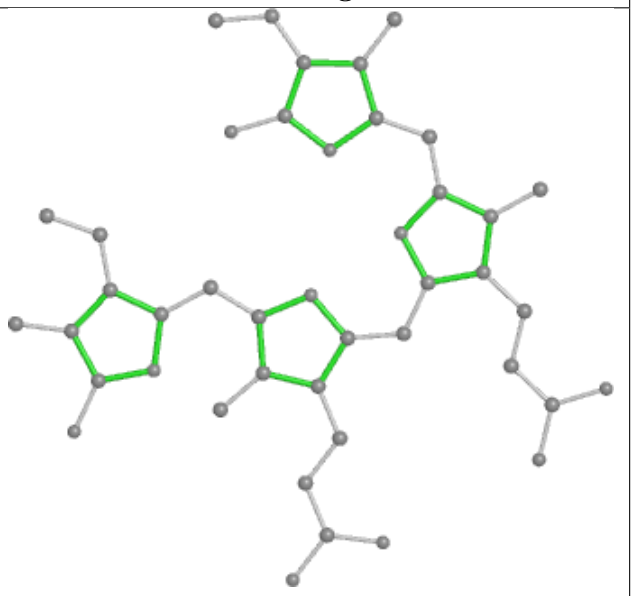
Bond lengths



Bond angles

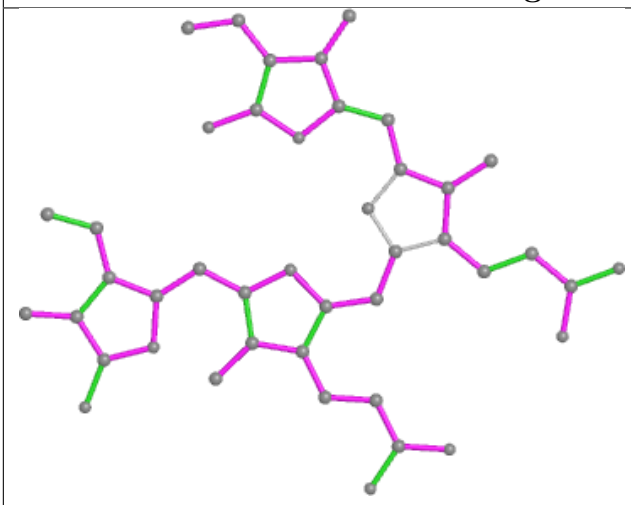


Torsions

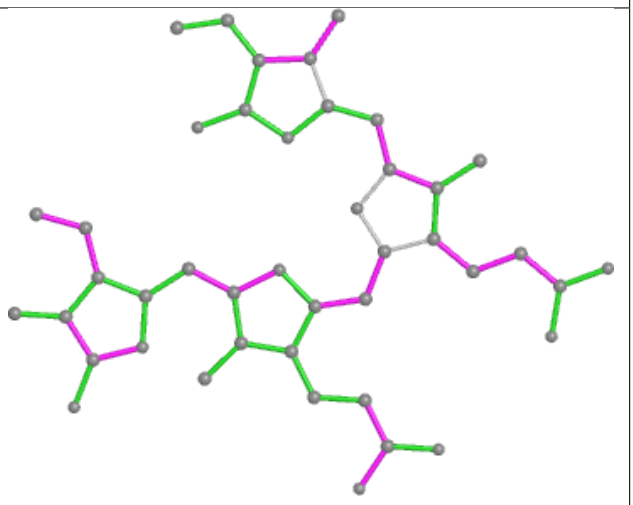


Rings

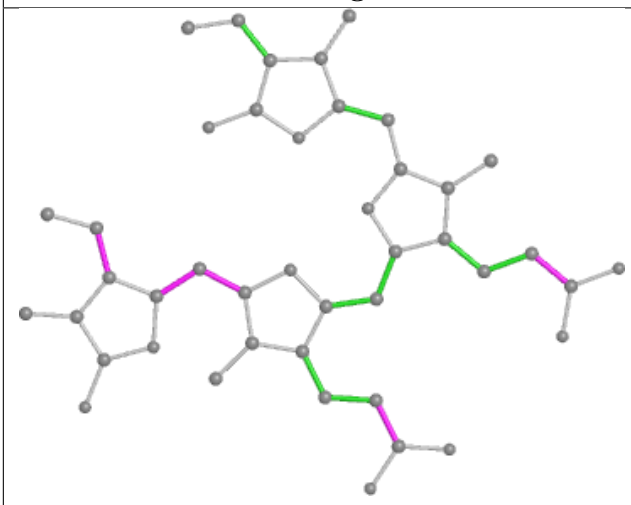
Ligand PEB D 203



Bond lengths



Bond angles



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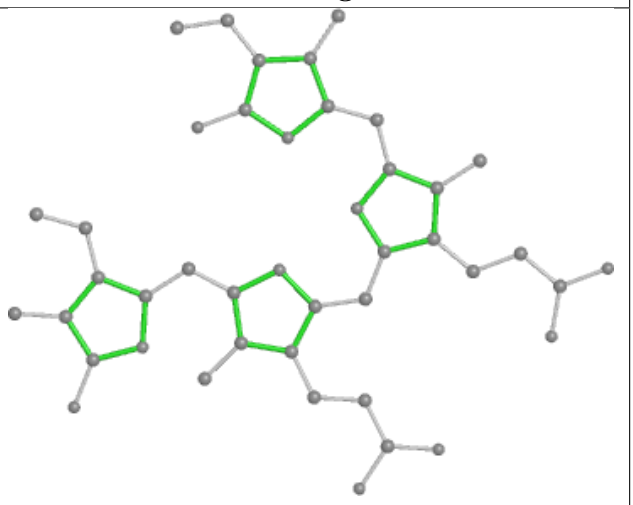
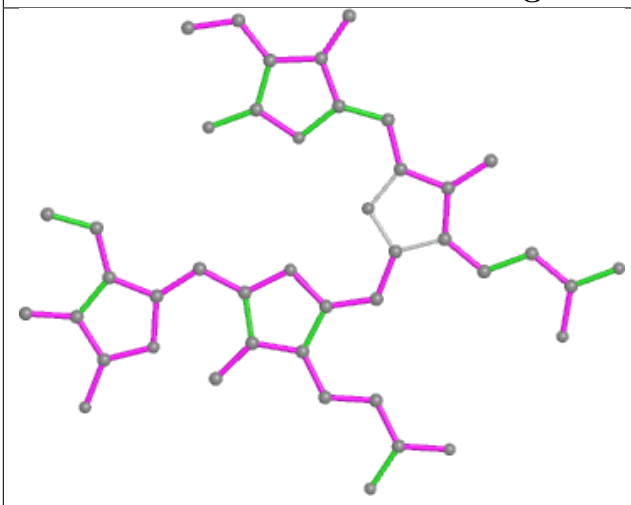
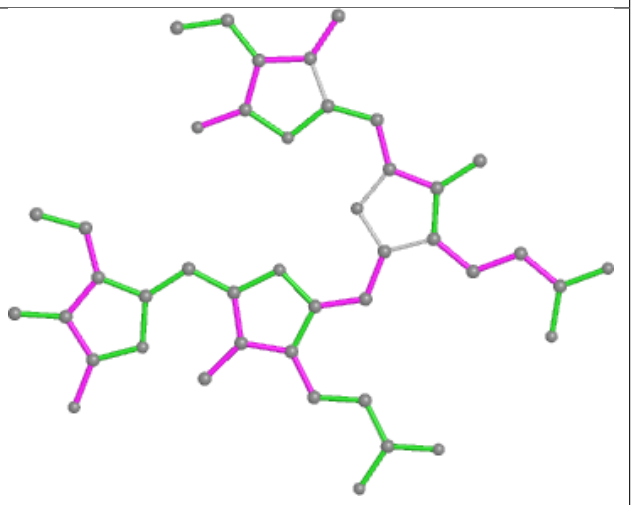


Rings

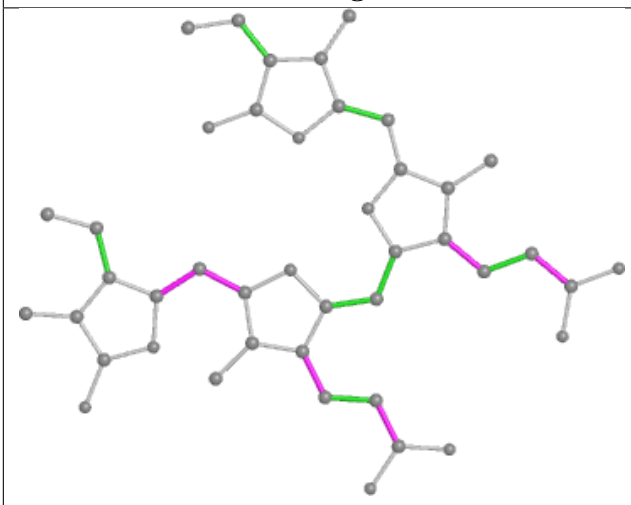
Ligand PEB H 203



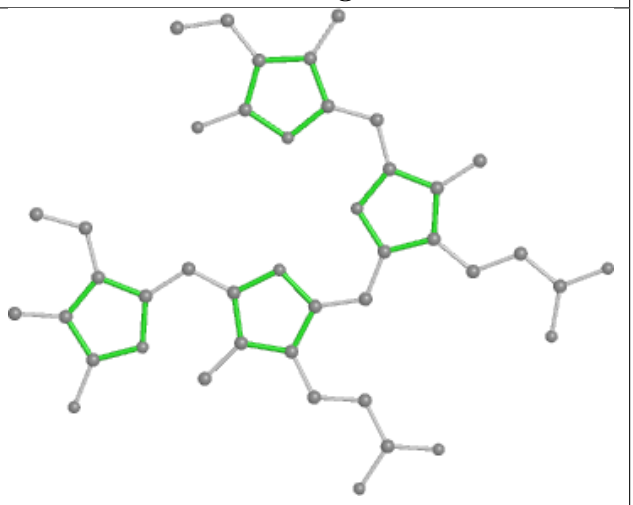
Bond lengths



Bond angles

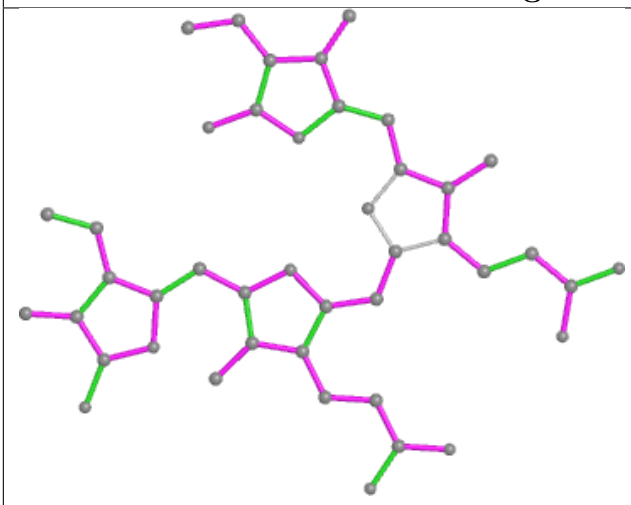


Torsions

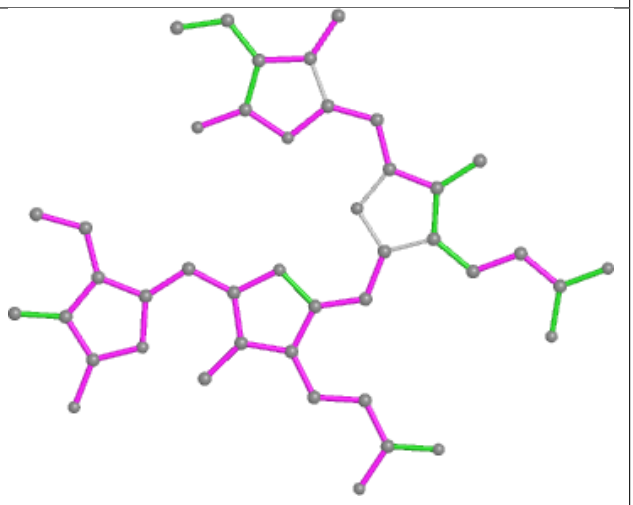


Rings

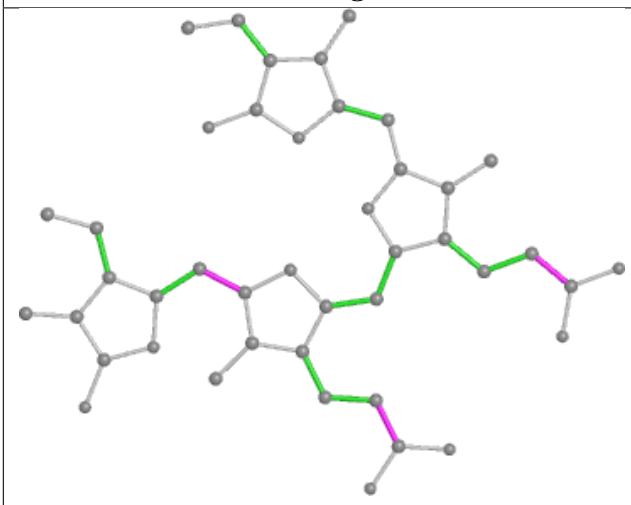
Ligand PEB H 202



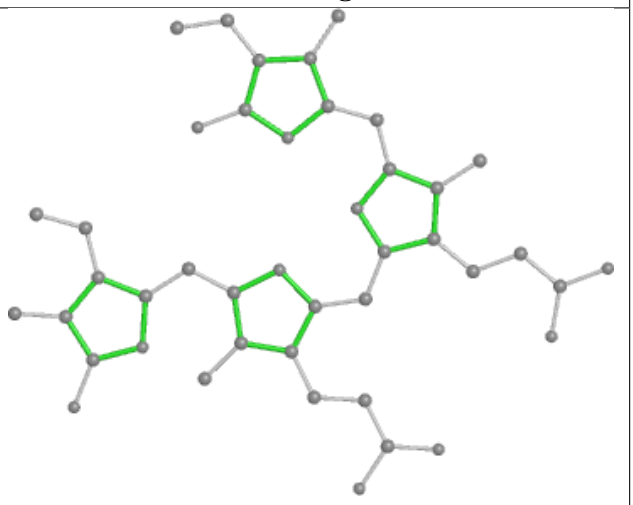
Bond lengths



Bond angles

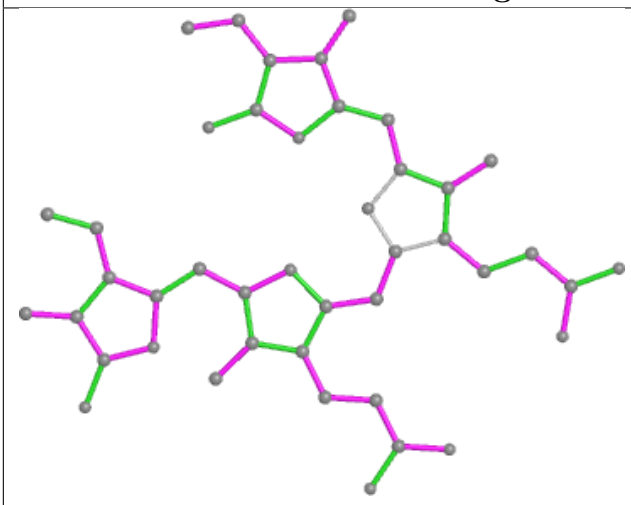


Torsions

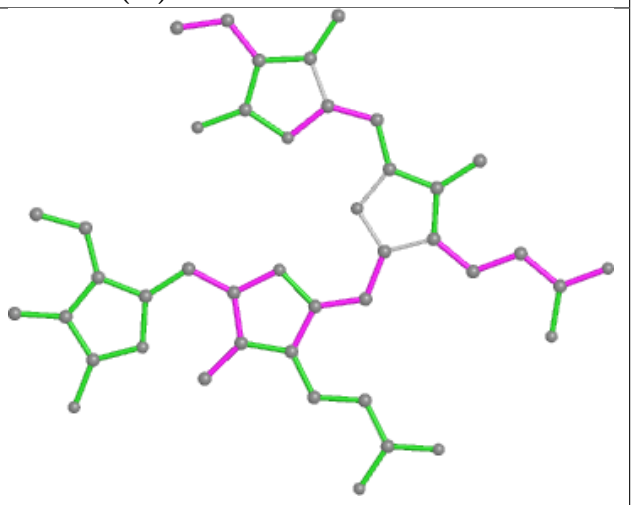


Rings

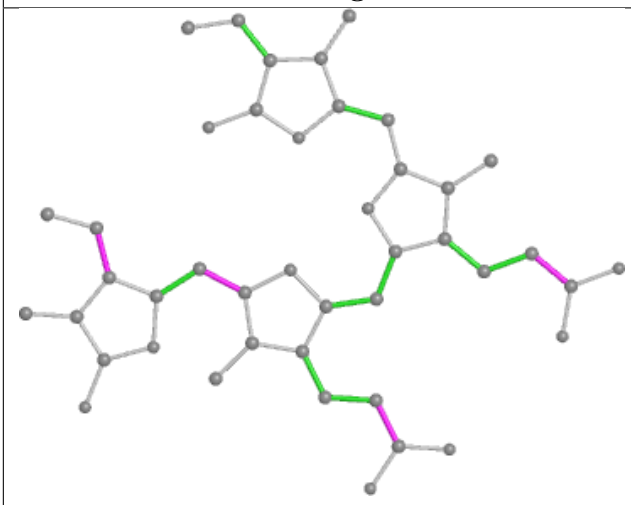
Ligand PEB F 203 (B)



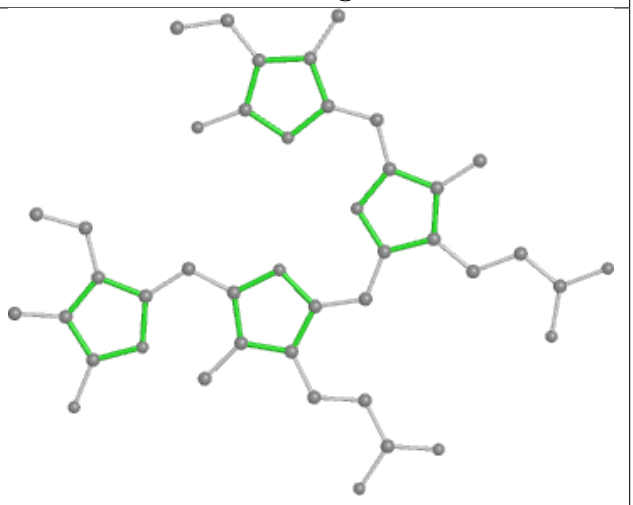
Bond lengths



Bond angles

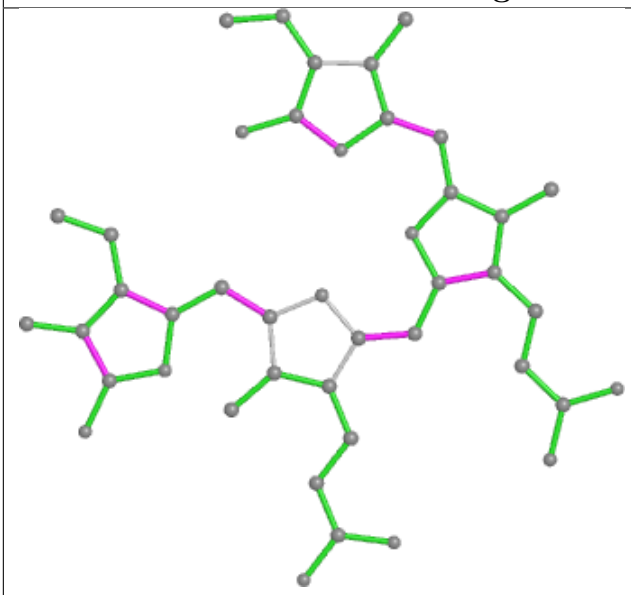


Torsions

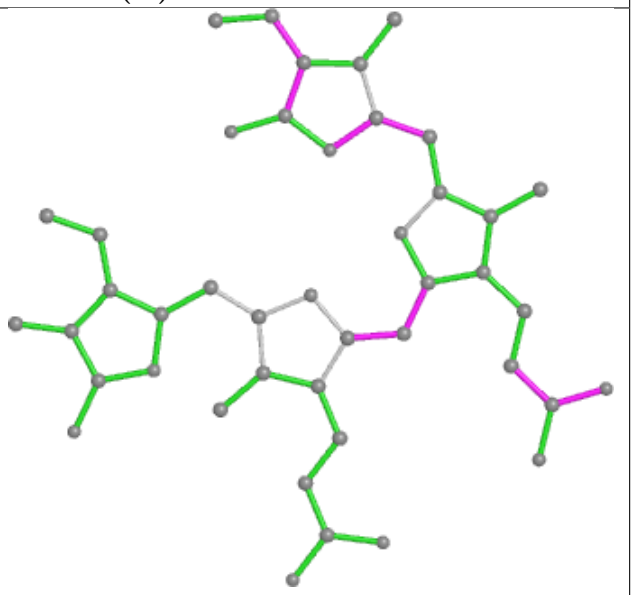


Rings

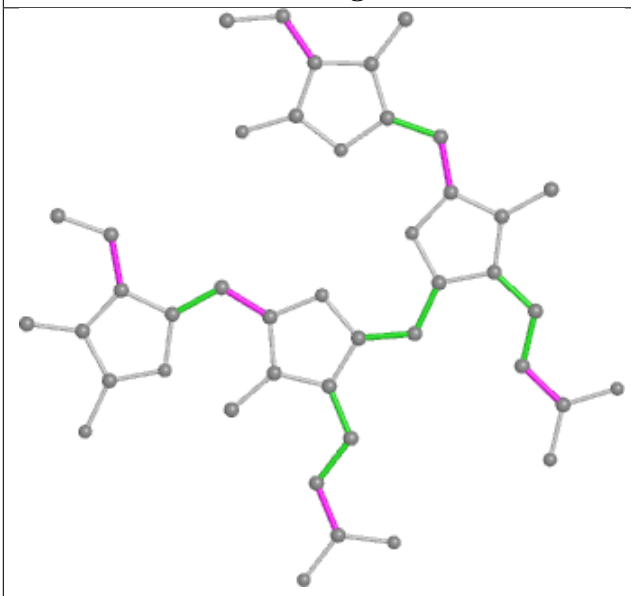
Ligand AX9 B 201 (B)



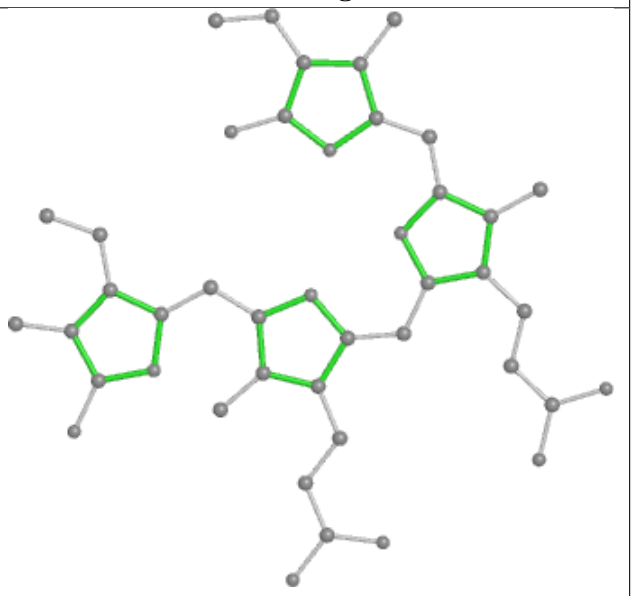
Bond lengths



Bond angles

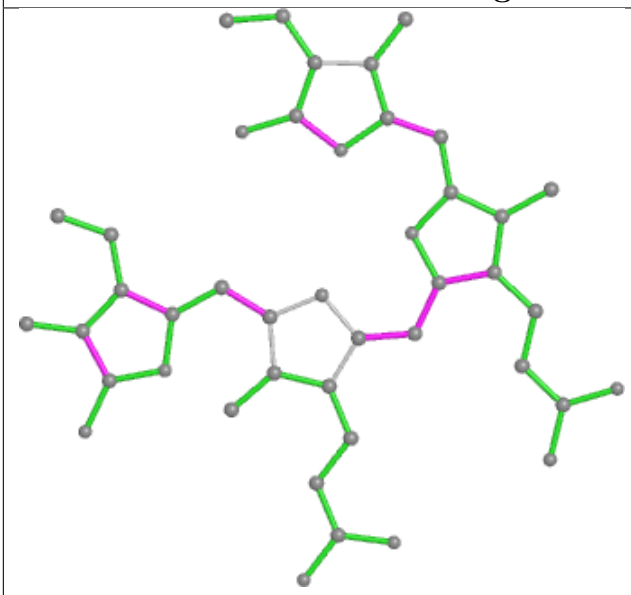


Torsions

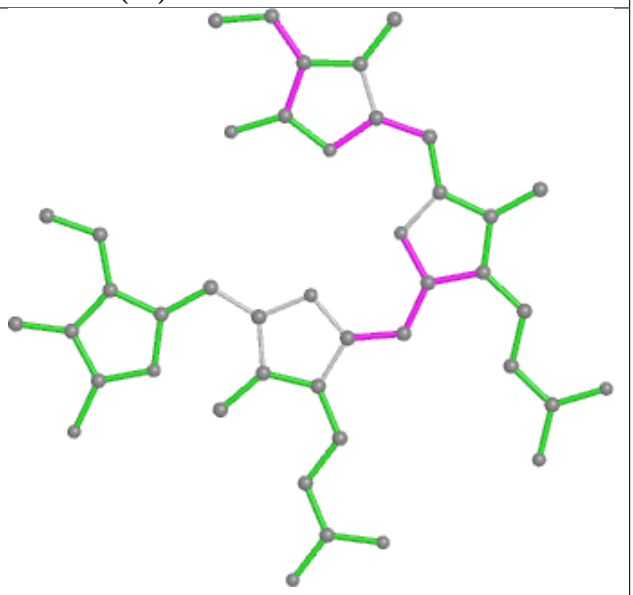


Rings

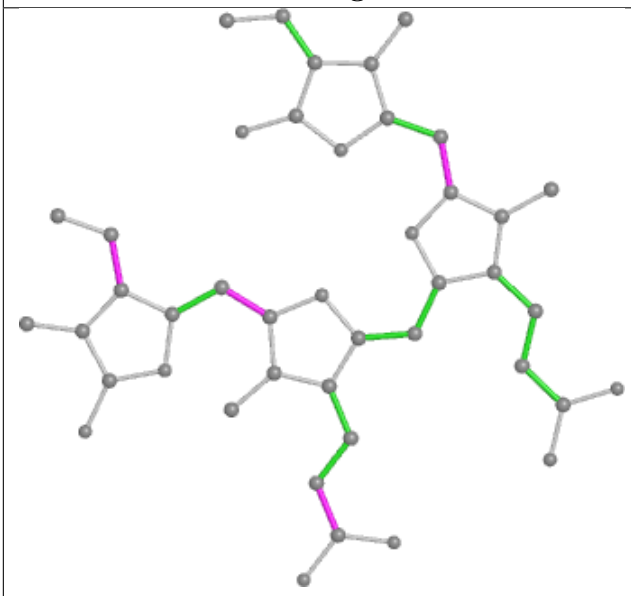
Ligand AX9 F 201 (A)



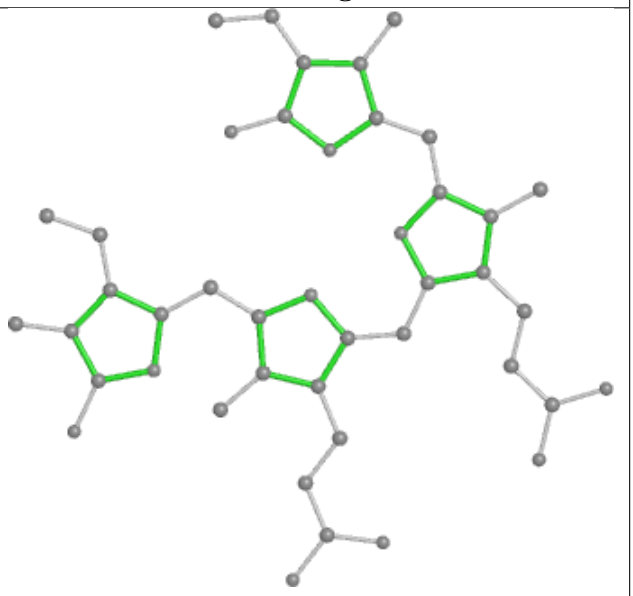
Bond lengths



Bond angles

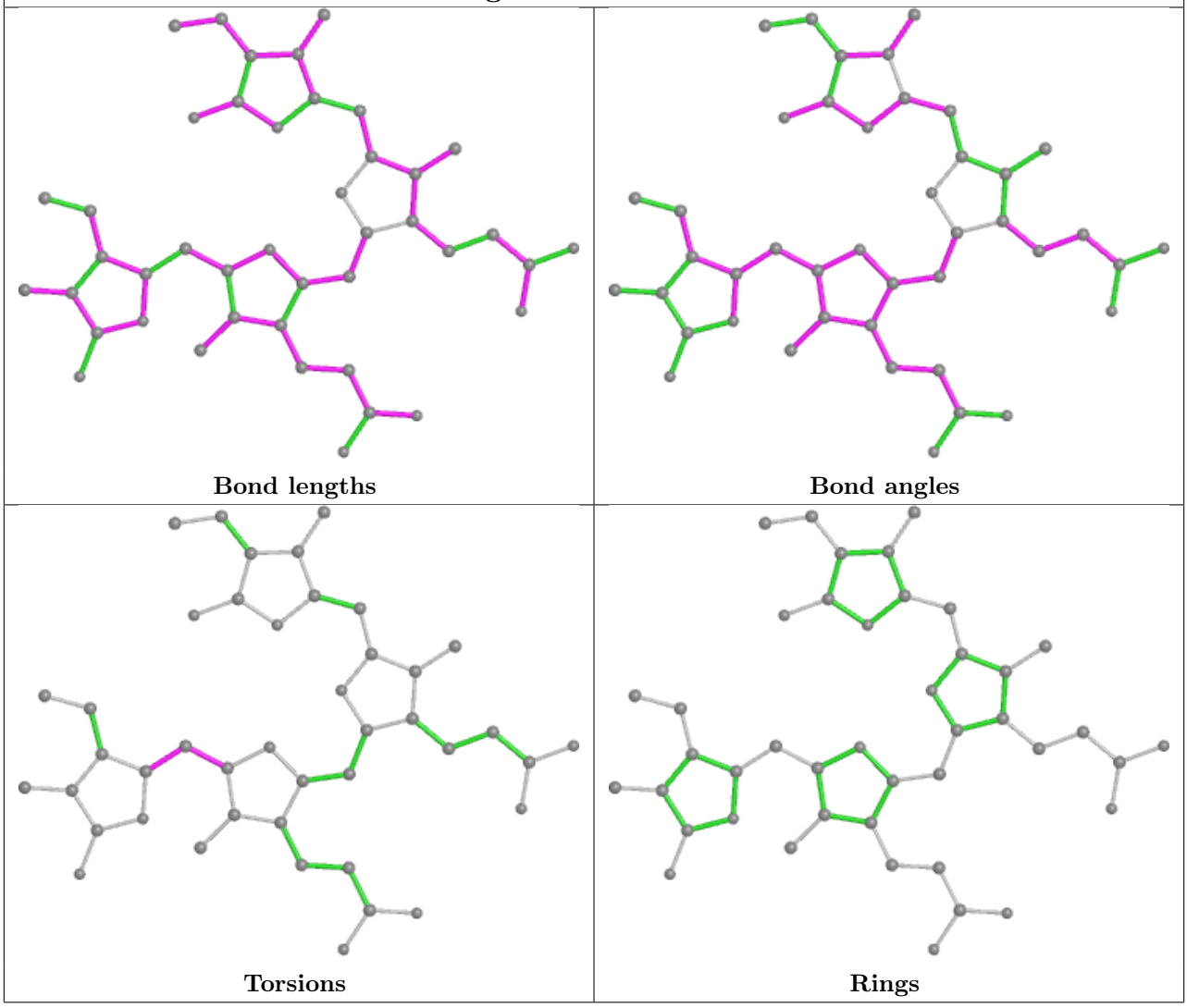


Torsions



Rings

Ligand PEB G 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	71/72 (98%)	-0.09	4 (5%)	24	26	10, 16, 50, 71	0
1	C	71/72 (98%)	-0.06	1 (1%)	75	76	13, 21, 44, 54	0
1	E	71/72 (98%)	-0.16	1 (1%)	75	76	14, 19, 38, 58	0
1	G	71/72 (98%)	0.01	2 (2%)	53	55	14, 25, 49, 56	0
2	B	175/177 (98%)	-0.09	2 (1%)	80	82	9, 15, 32, 58	0
2	D	175/177 (98%)	0.34	14 (8%)	12	14	14, 28, 46, 69	0
2	F	174/177 (98%)	0.01	7 (4%)	38	40	11, 17, 43, 61	0
2	H	173/177 (97%)	0.31	10 (5%)	23	25	14, 28, 48, 61	0
All	All	981/996 (98%)	0.08	41 (4%)	36	39	9, 21, 45, 71	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	30	PHE	7.5
2	D	30	PHE	7.3
2	D	70	ASN	5.7
2	H	30	PHE	5.4
1	A	30	SER	4.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LYZ	C	4	10/11	0.93	0.11	27,38,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LYZ	G	4	10/11	0.94	0.12	31,38,45,50	0
1	LYZ	E	4	10/11	0.95	0.07	22,31,42,42	0
1	LYZ	A	4	10/11	0.97	0.07	12,19,29,30	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

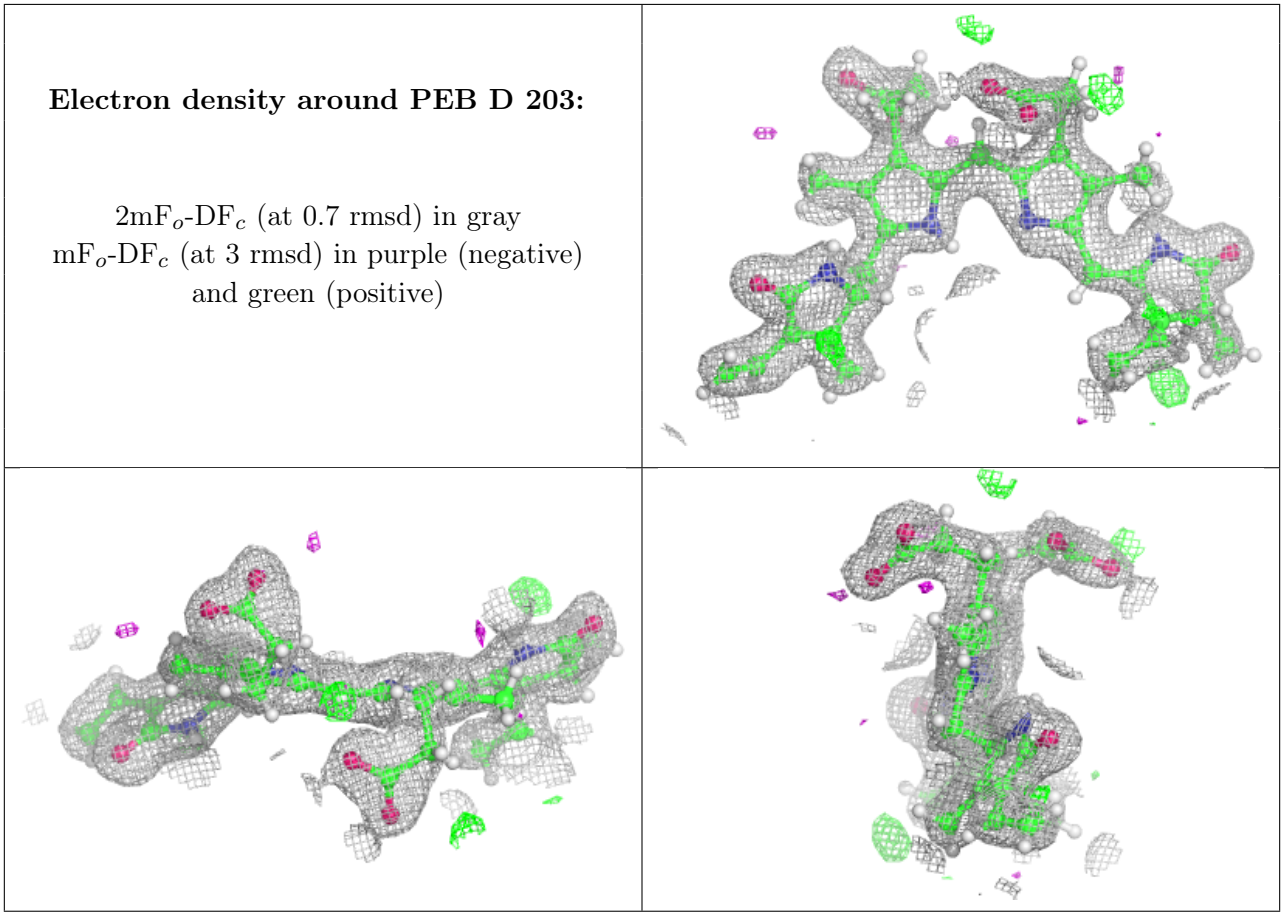
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEB	D	203	43/43	0.86	0.12	19,32,47,51	0
3	PEB	H	203	43/43	0.86	0.12	20,31,50,56	0
5	TRS	B	204	8/8	0.88	0.19	20,33,47,56	0
5	TRS	F	204[A]	8/8	0.90	0.15	21,27,29,33	16
5	TRS	H	204	8/8	0.90	0.15	27,40,48,58	0
4	AX9	D	201	43/43	0.91	0.09	14,22,36,40	0
3	PEB	G	101	43/43	0.91	0.10	15,24,36,47	0
3	PEB	D	202	43/43	0.92	0.10	15,22,31,52	0
3	PEB	H	202	43/43	0.92	0.10	16,22,31,42	0
4	AX9	H	201	43/43	0.92	0.10	13,22,39,43	0
3	PEB	B	203	43/43	0.94	0.09	11,16,26,39	0
3	PEB	E	101	43/43	0.95	0.08	12,16,23,31	0
3	PEB	F	202	43/43	0.95	0.09	11,17,25,38	0
4	AX9	F	201[A]	43/43	0.95	0.10	6,14,18,24	79
4	AX9	F	201[B]	43/43	0.95	0.10	7,17,24,35	79
3	PEB	B	202	43/43	0.96	0.08	11,14,25,38	0
3	PEB	C	101	43/43	0.96	0.08	12,18,25,32	0
3	PEB	F	203[A]	43/43	0.96	0.09	9,21,31,31	80
4	AX9	B	201[A]	43/43	0.96	0.09	7,14,23,28	79
4	AX9	B	201[B]	43/43	0.96	0.09	5,14,25,28	79
3	PEB	F	203[B]	43/43	0.96	0.09	8,15,23,34	80
3	PEB	A	101	43/43	0.97	0.07	9,14,19,33	0
6	CL	F	205	1/1	0.99	0.04	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

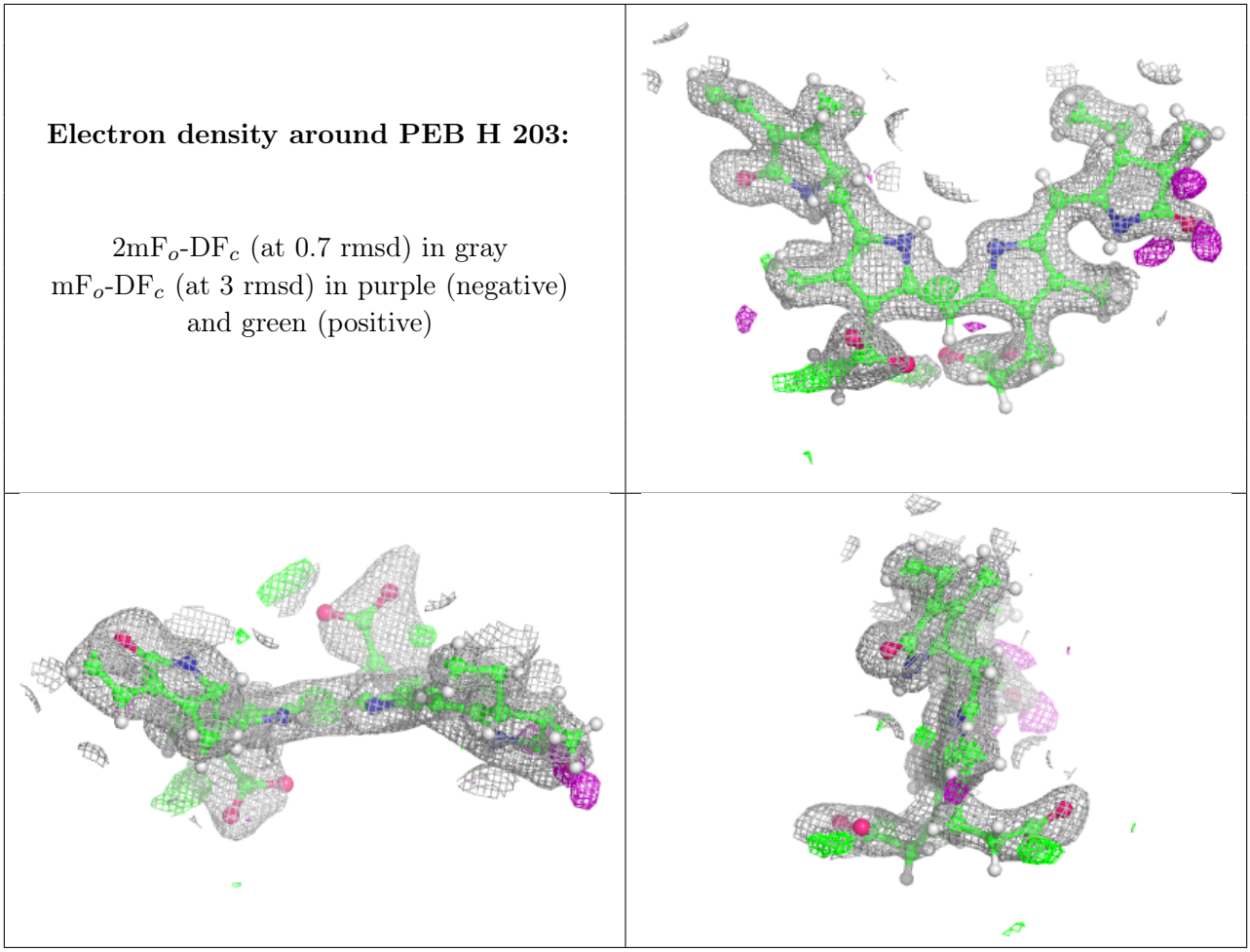
Electron density around PEB D 203:

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



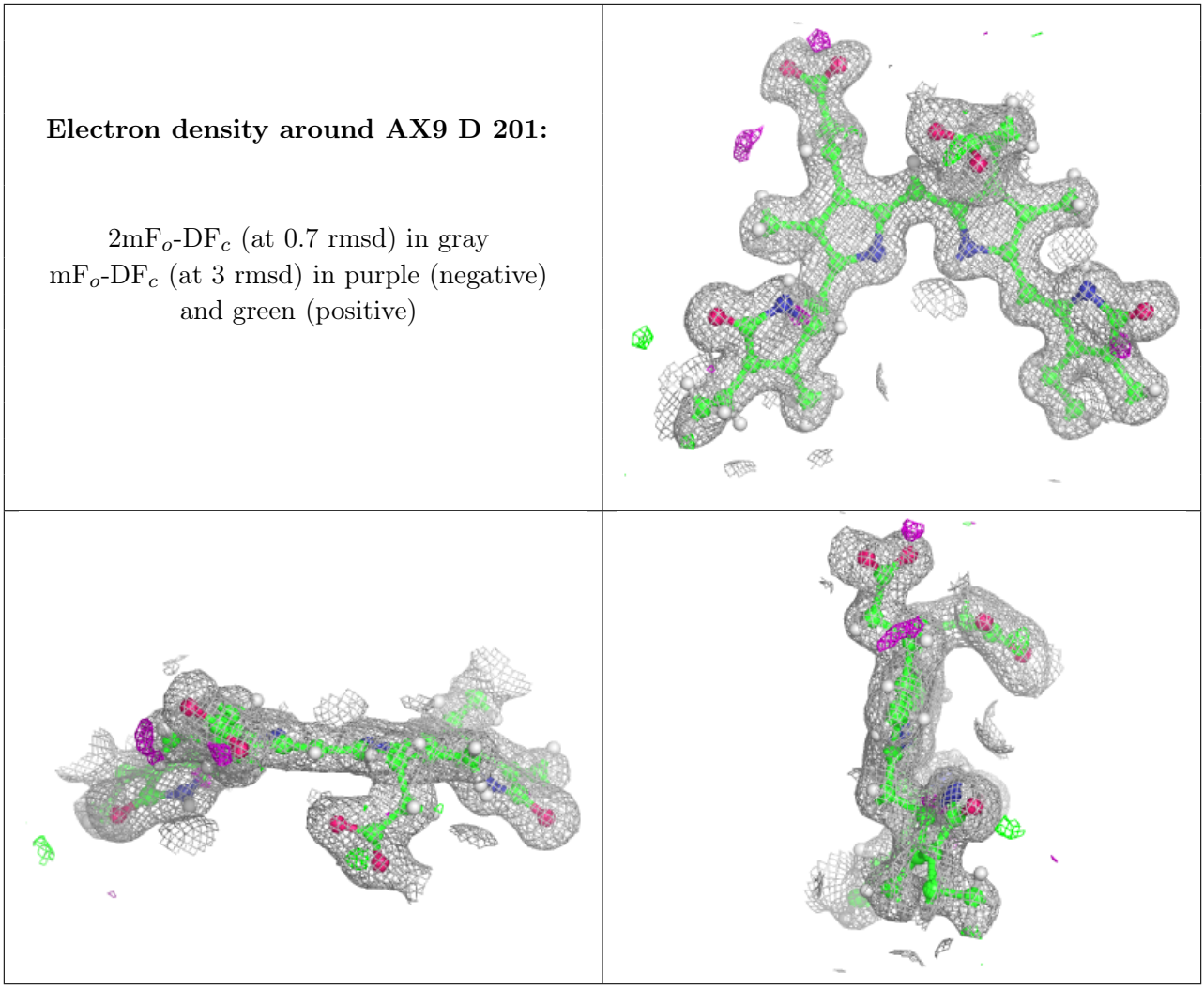
Electron density around PEB H 203:

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



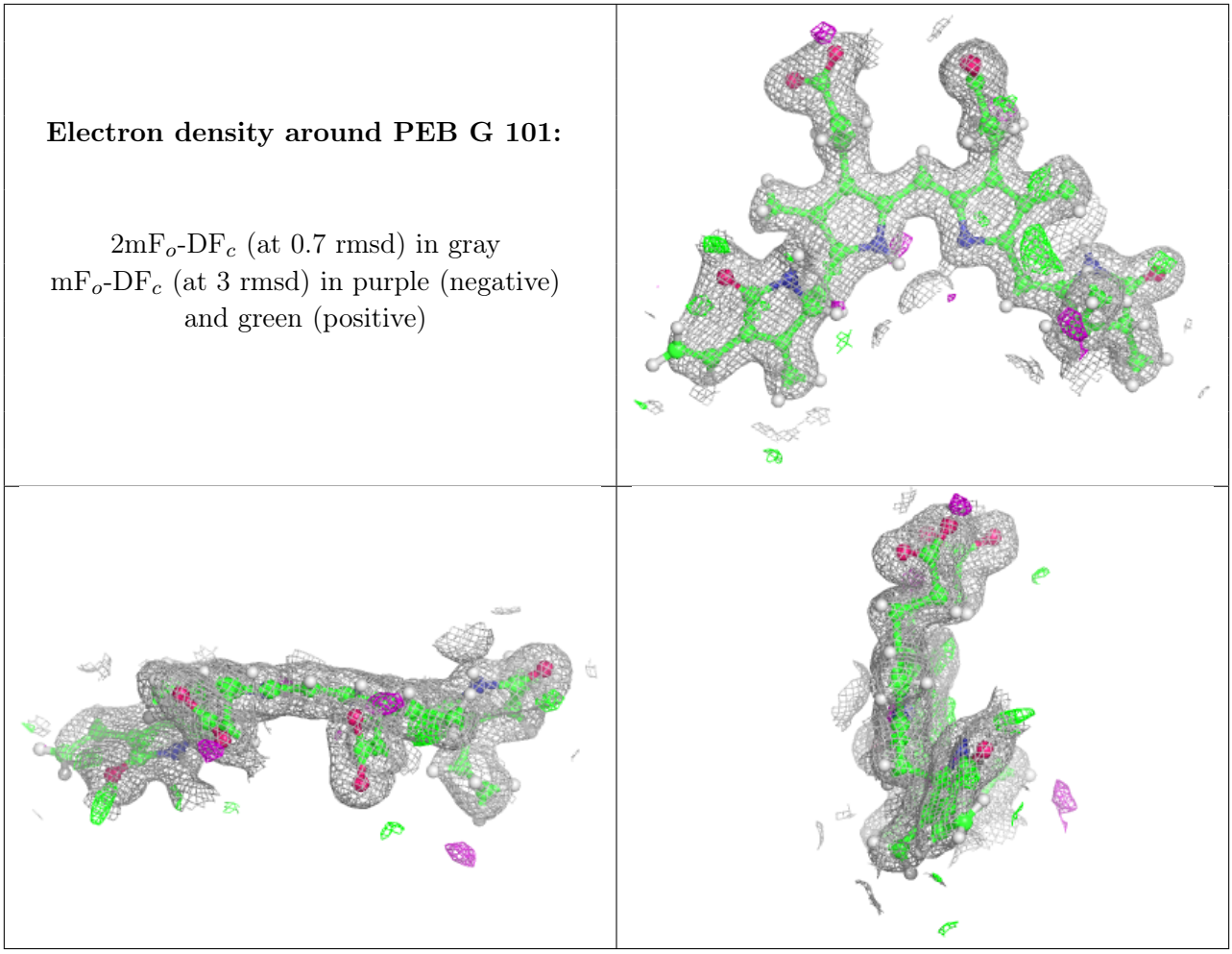
Electron density around AX9 D 201:

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



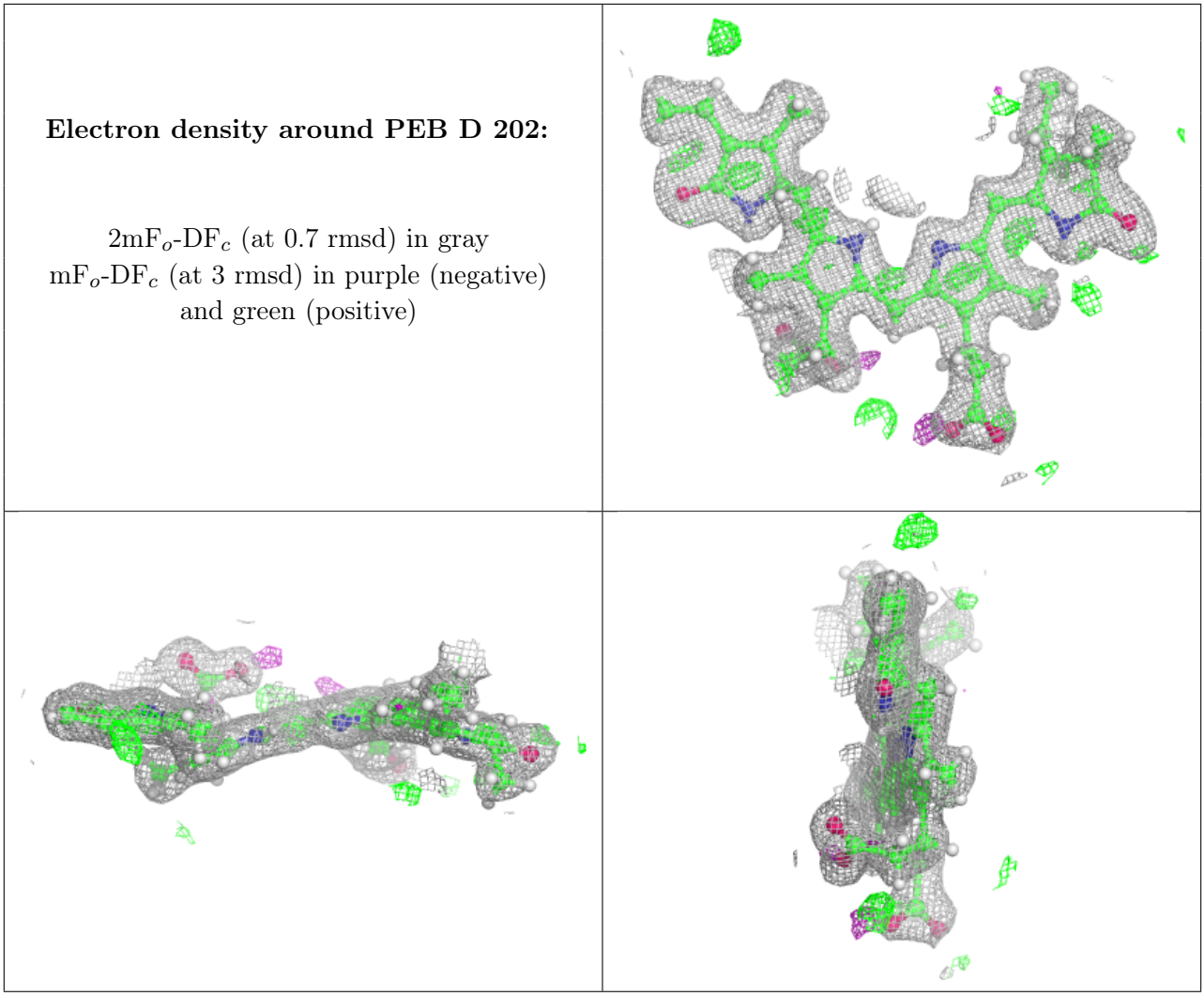
Electron density around PEB G 101:

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



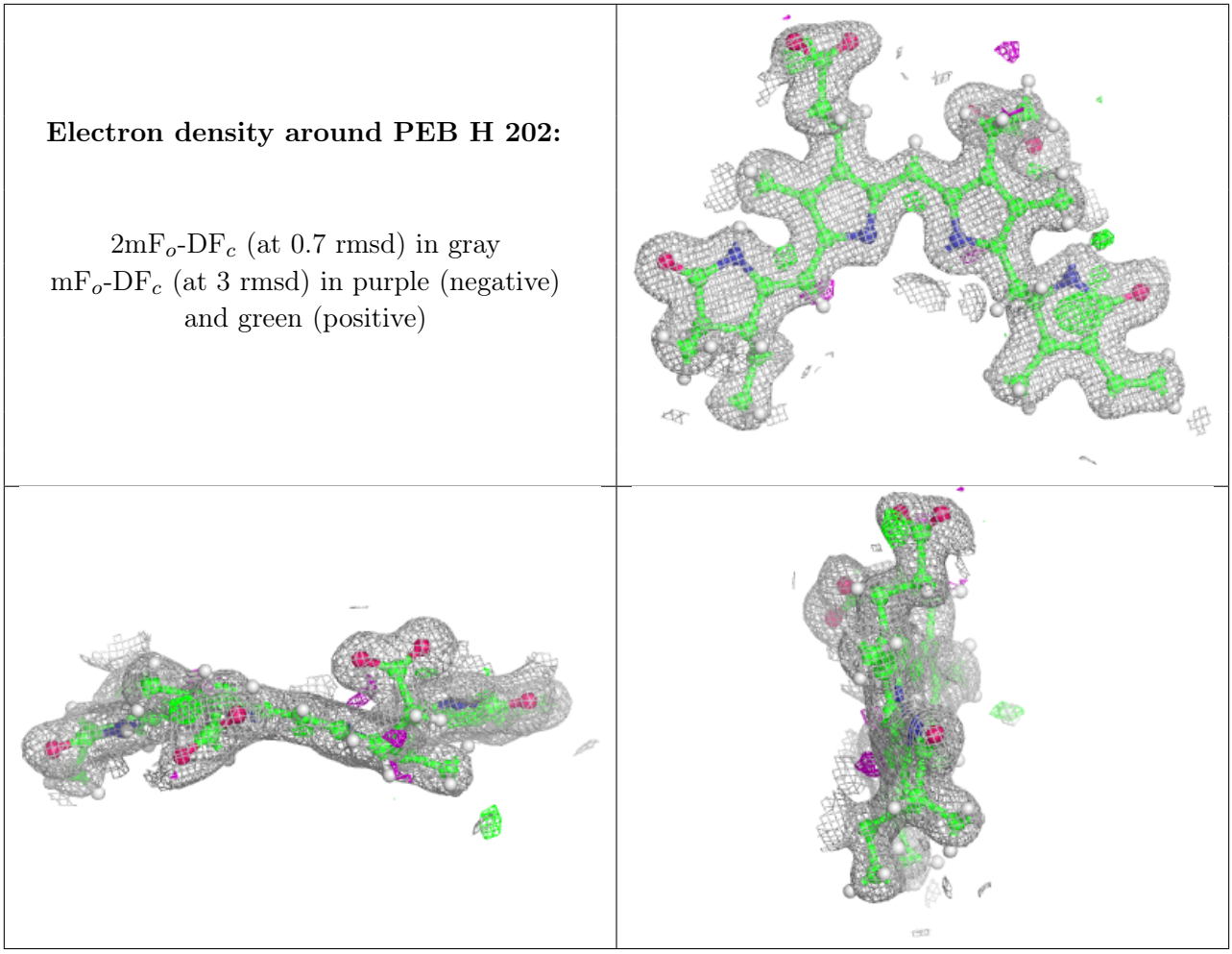
Electron density around PEB D 202:

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



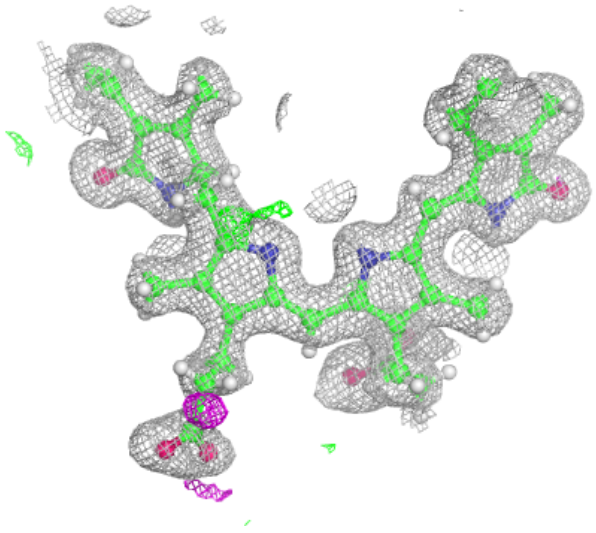
Electron density around PEB H 202:

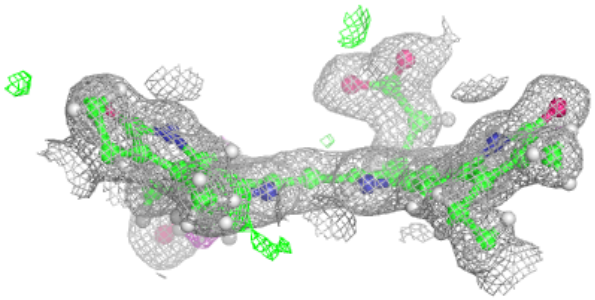
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

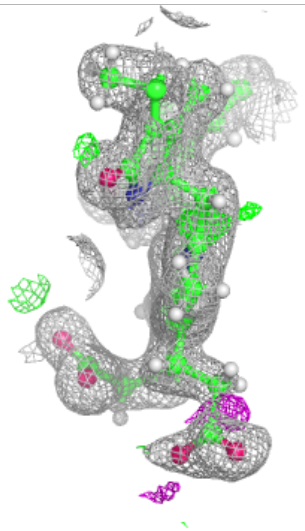


Electron density around AX9 H 201:

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

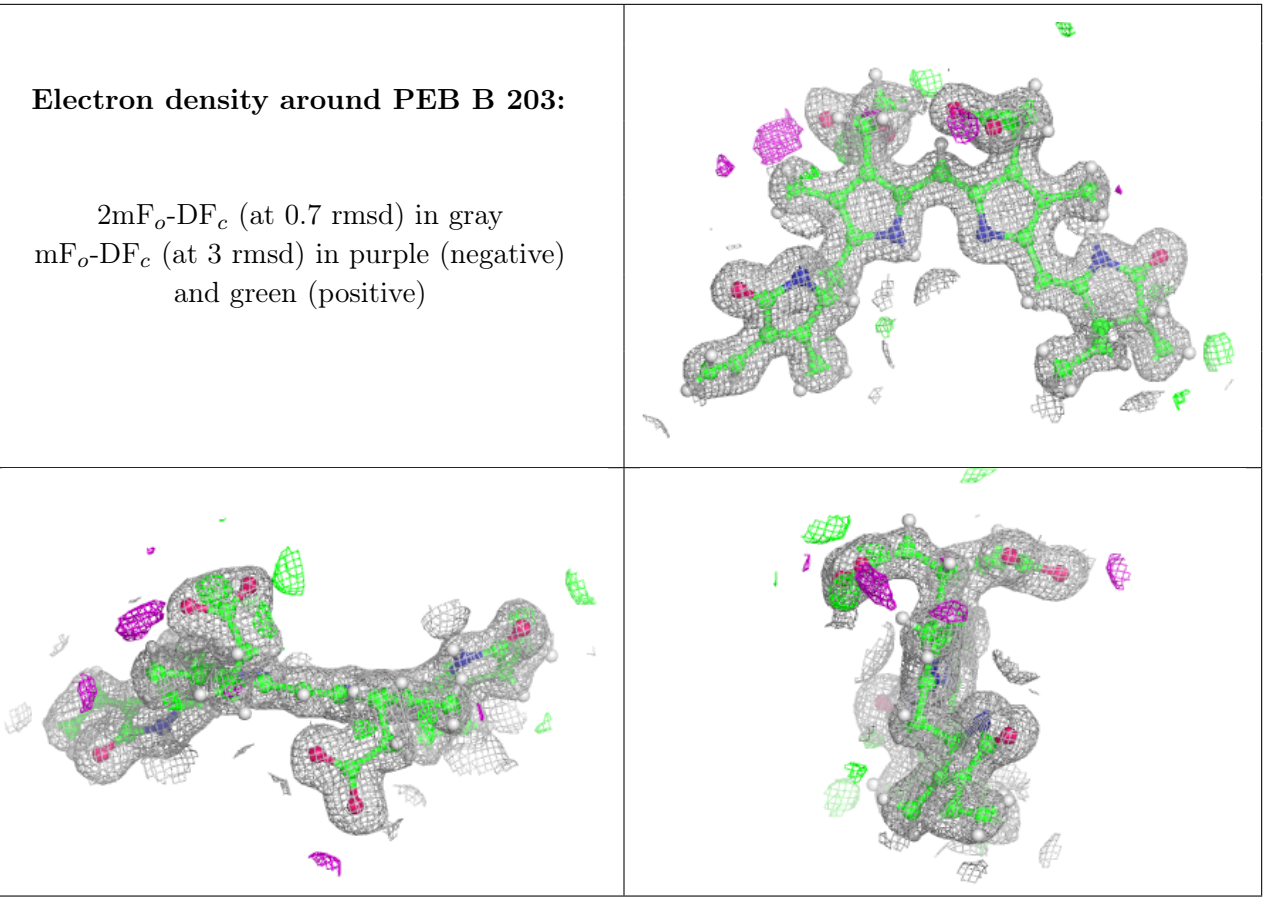






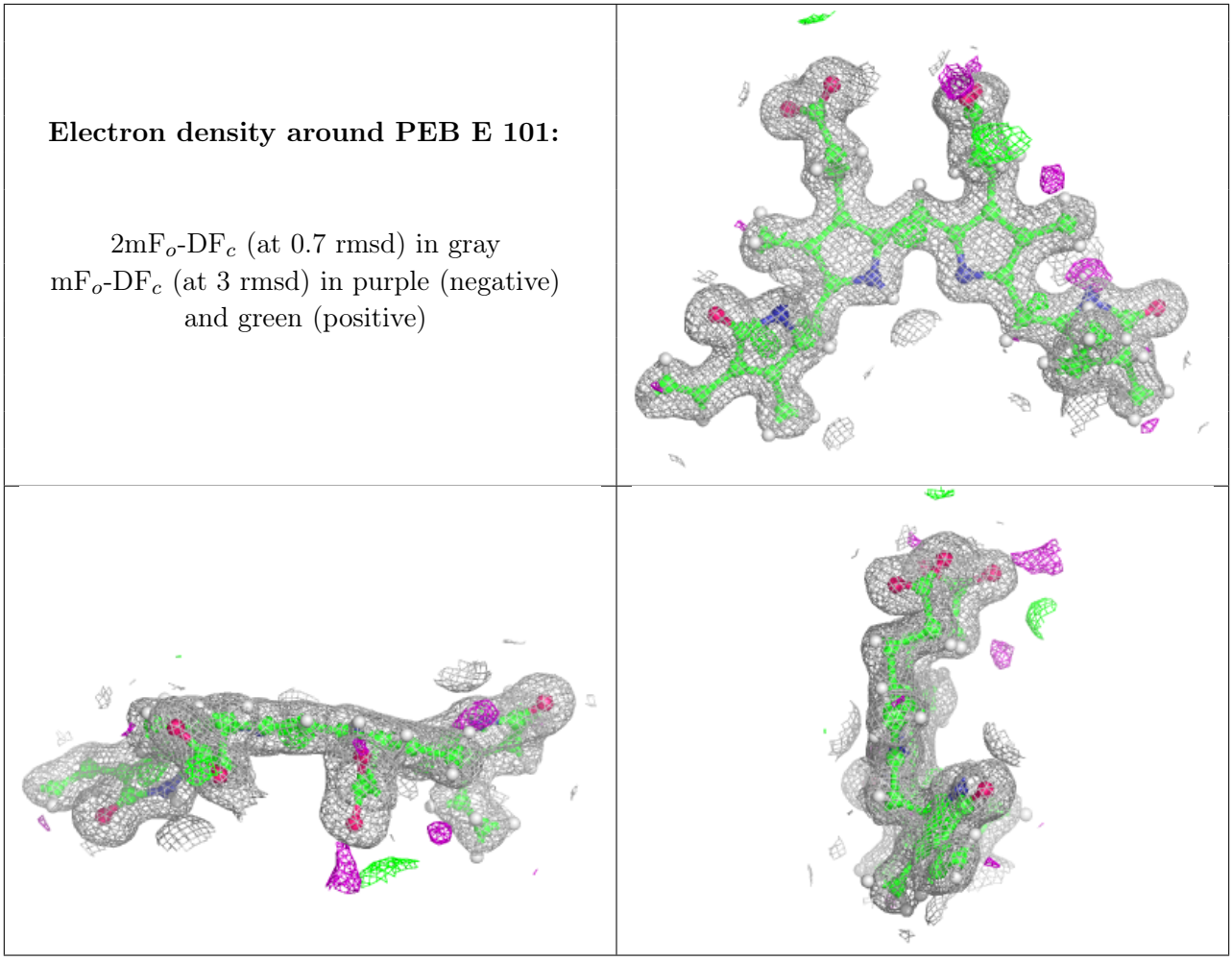
Electron density around PEB B 203:

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



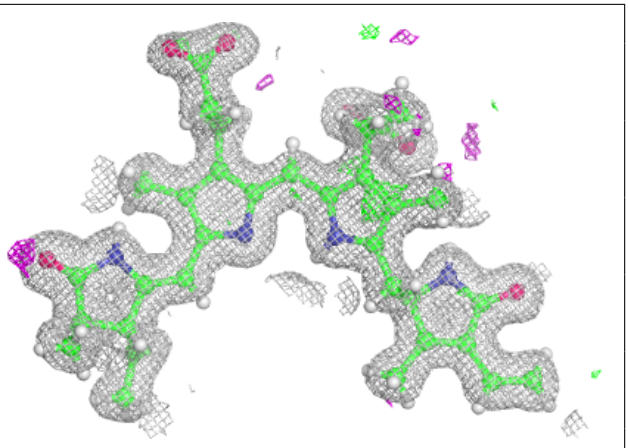
Electron density around PEB E 101:

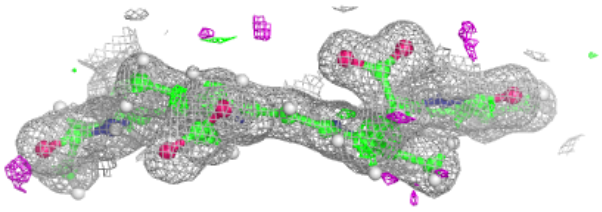
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

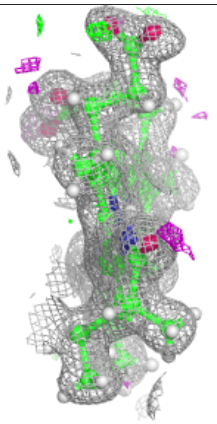


Electron density around PEB F 202:

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

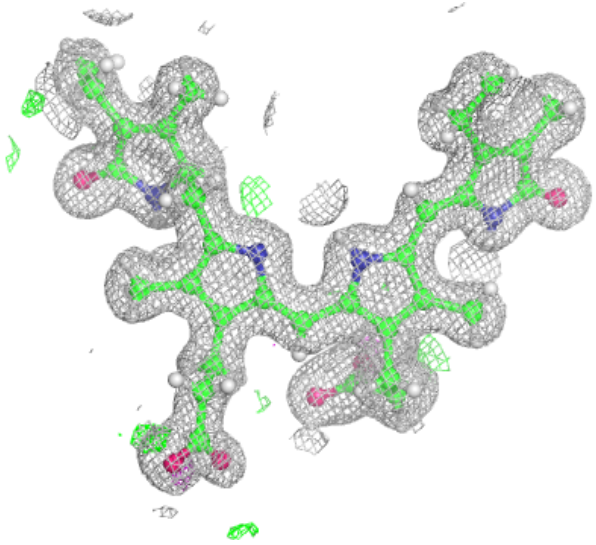


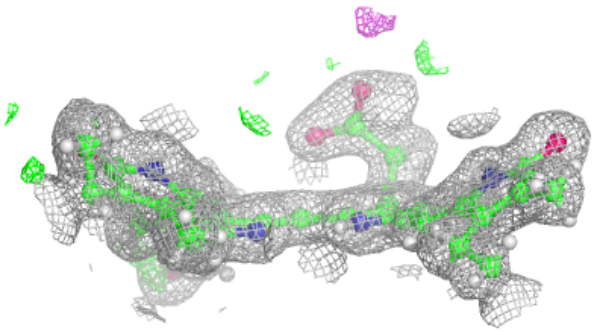


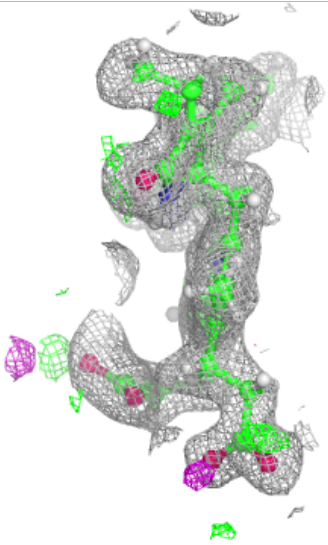


Electron density around AX9 F 201 (A):

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

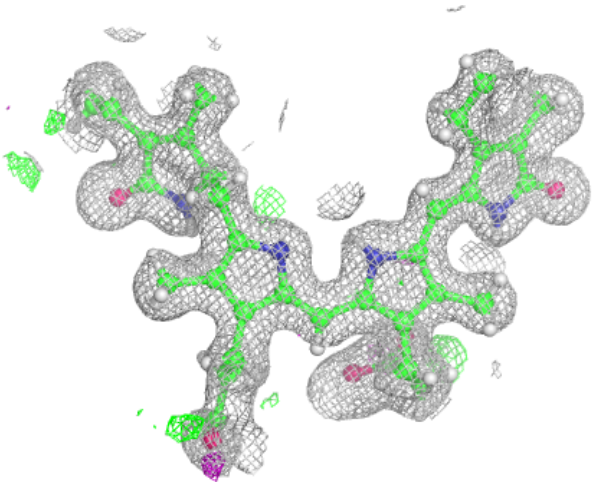


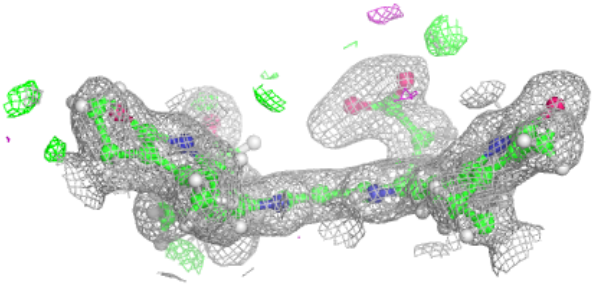


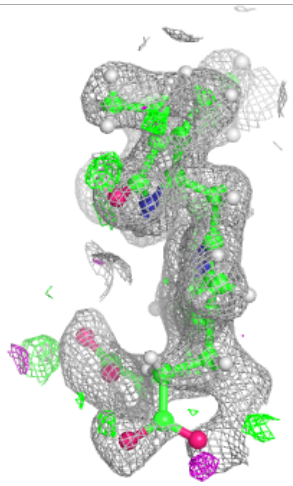


Electron density around AX9 F 201 (B):

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

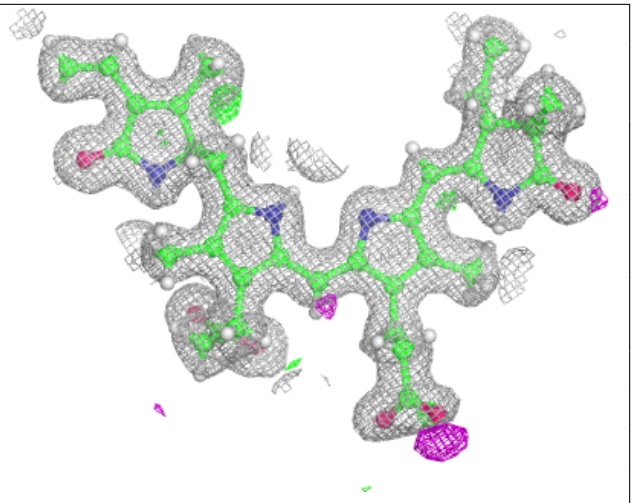


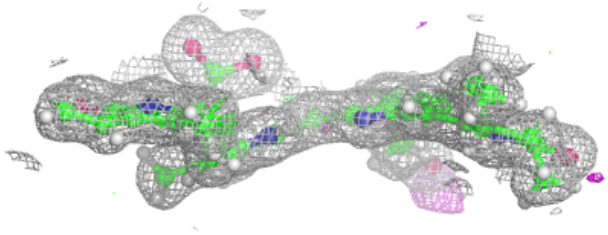


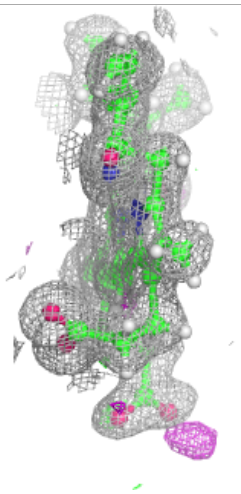


Electron density around PEB B 202:

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

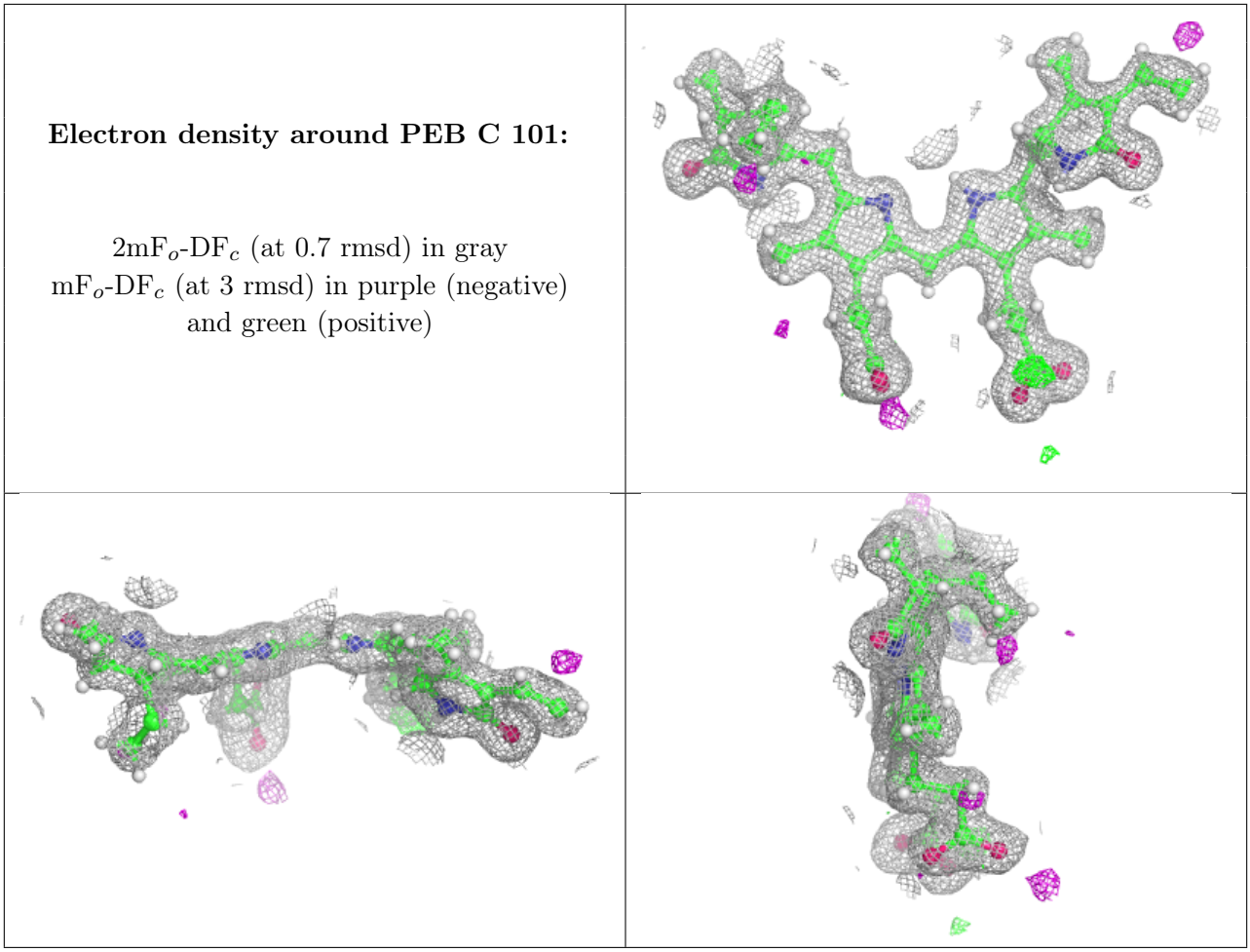






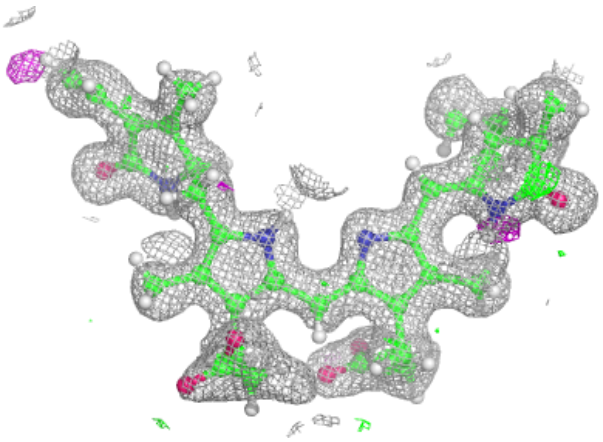
Electron density around PEB C 101:

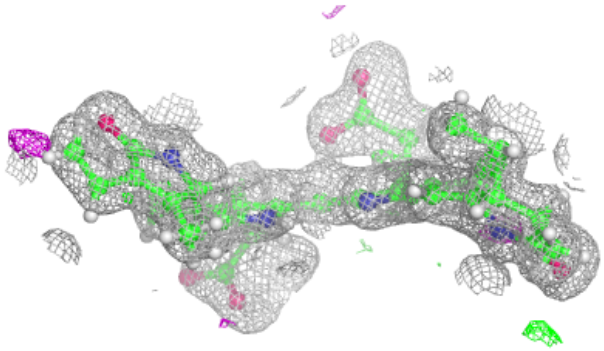
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

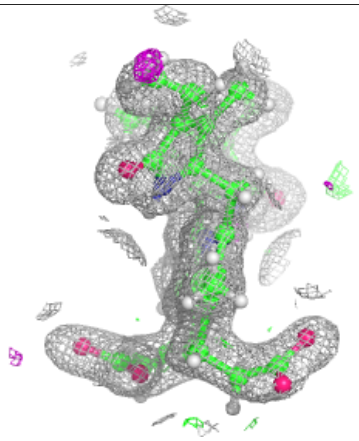


Electron density around PEB F 203 (A):

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

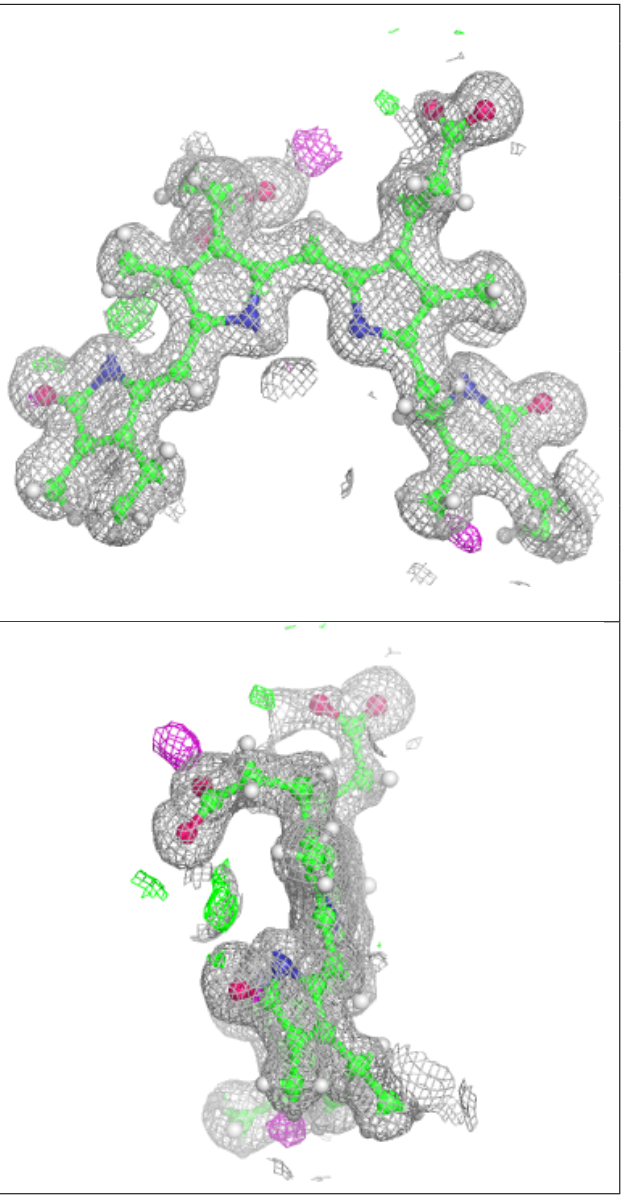






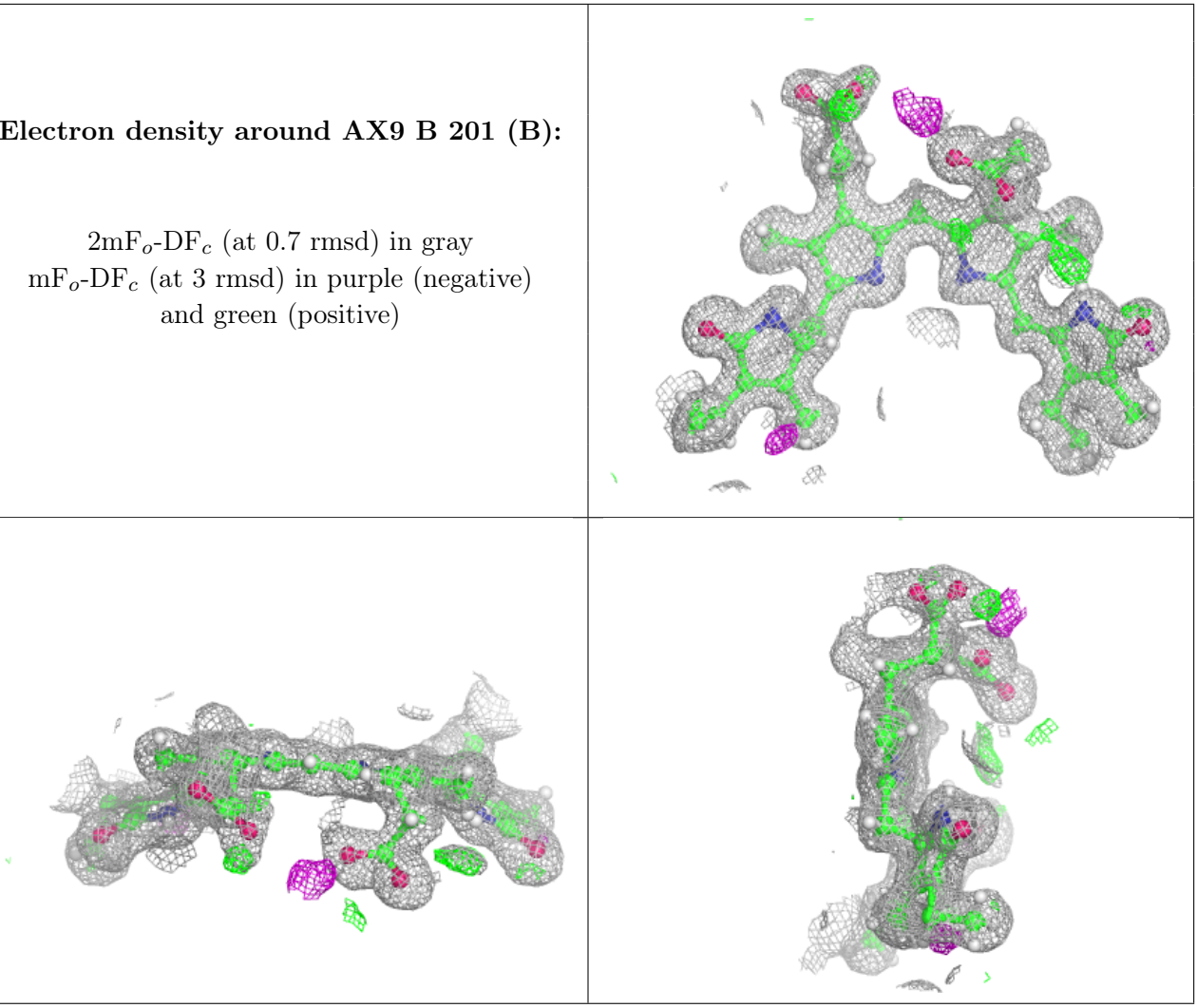
Electron density around AX9 B 201 (A):

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



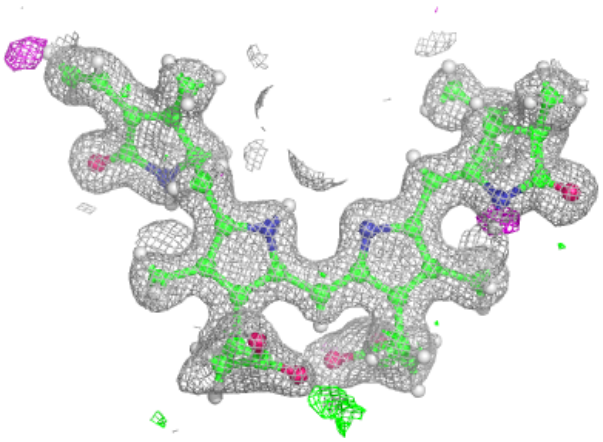
Electron density around AX9 B 201 (B):

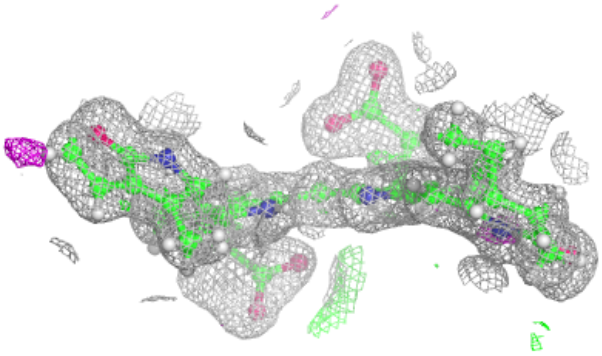
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

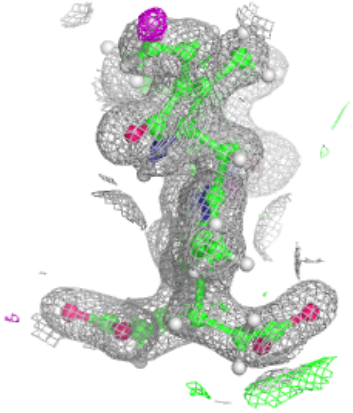


Electron density around PEB F 203 (B):

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

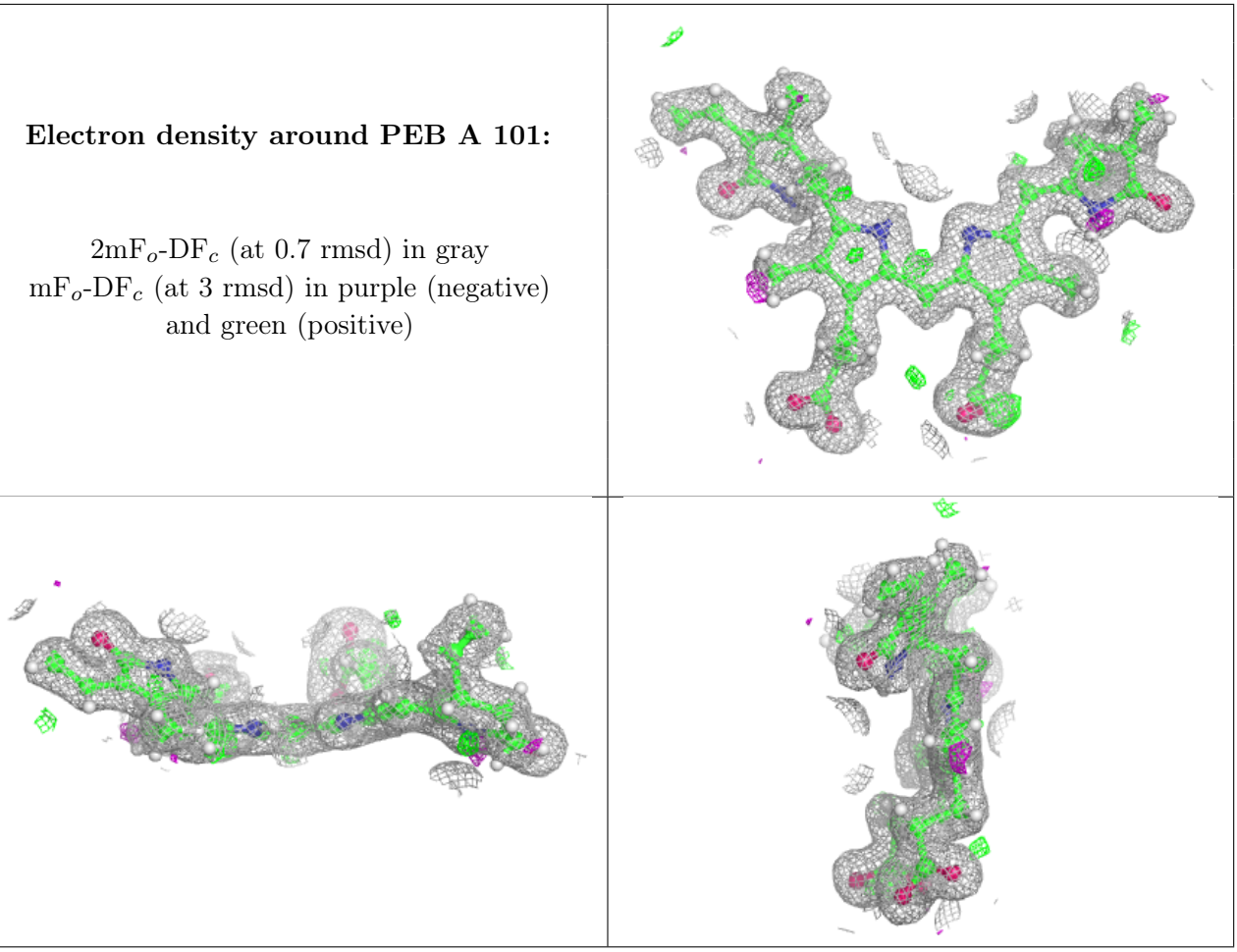






Electron density around PEB A 101:

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



6.5 Other polymers (i)

There are no such residues in this entry.