wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 07:38 PM EDT

PDB ID	:	1NFV
Title	:	X-ray structure of Desulfovibrio desulfuricans bacterioferritin: the diiron centre in different catalytic states (as-isolated structure)
Authors	:	Macedo, S.; Romao, C.V.; Mitchell, E.; Matias, P.M.; Liu, M.Y.; Xavier, A.V.; LeGall, J.; Teixeira, M.; Lindley, P.; Carrondo, M.A.
Deposited on	:	2002-12-16
Resolution	:	1.95 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:

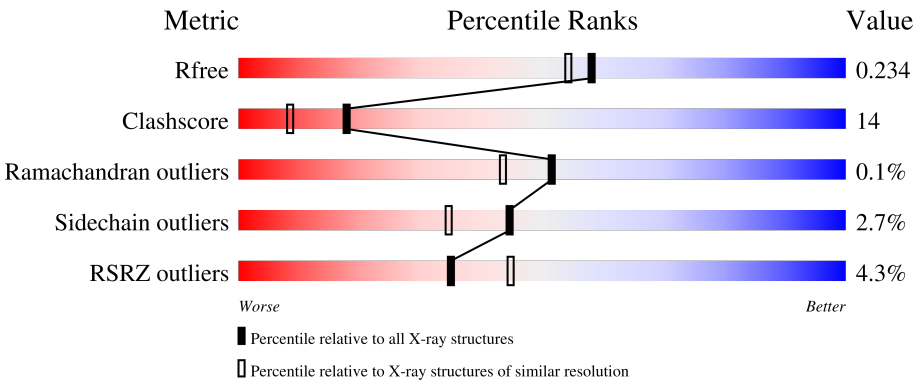
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	179	6% 75% 17% • 6%
1	B	179	5% 78% 15% • 5%
1	C	179	4% 72% 20% • 5%
1	D	179	5% 75% 17% • • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	179	5% 78% 17% 5%
1	F	179	4% 77% 17% 5%
1	G	179	2% 81% 13% 6%
1	H	179	7% 78% 16% 5%
1	I	179	3% 78% 16% 5%
1	J	179	5% 82% 12% 5%
1	K	179	2% 83% 11% 5%
1	L	179	2% 77% 17% 5%
1	M	179	4% 82% 13% 5%
1	N	179	3% 79% 15% 5%
1	O	179	3% 78% 16% 6%
1	P	179	4% 74% 20% 5%

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
3	SO4	A	1004	-	-	-	X
3	SO4	A	1105	-	-	X	-
3	SO4	F	1502	-	-	X	-
3	SO4	G	1603	-	-	-	X
3	SO4	H	1703	-	-	-	X
3	SO4	I	1802	-	-	X	-
3	SO4	J	1906	-	-	X	-
3	SO4	L	2102	-	-	X	-
3	SO4	M	2206	-	-	X	-
3	SO4	O	2409	-	-	-	X
4	GOL	A	1010	-	X	-	-
4	GOL	B	1011	-	X	-	-
4	GOL	B	1110	-	X	-	-
4	GOL	C	1210	-	X	-	-
4	GOL	D	1211	-	X	X	-
4	GOL	E	1410	-	X	X	-
4	GOL	E	1411	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	F	1510	-	X	-	-
4	GOL	F	1512	-	X	-	-
4	GOL	G	1610	-	X	-	-
4	GOL	G	1611	-	X	-	-
4	GOL	H	1710	-	X	-	-
4	GOL	H	1814	-	X	-	-
4	GOL	I	1713	-	X	-	-
4	GOL	I	1810	-	X	X	-
4	GOL	J	1811	-	X	-	-
4	GOL	J	1910	-	X	X	-
4	GOL	K	2011	-	X	-	-
4	GOL	M	2210	-	X	X	-
4	GOL	M	2211	-	X	-	-
4	GOL	N	2310	-	X	-	-
4	GOL	O	2410	-	X	-	-
4	GOL	O	2411	-	X	-	-
4	GOL	P	2510	-	X	-	-
6	3PY	D	1310	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25080 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.

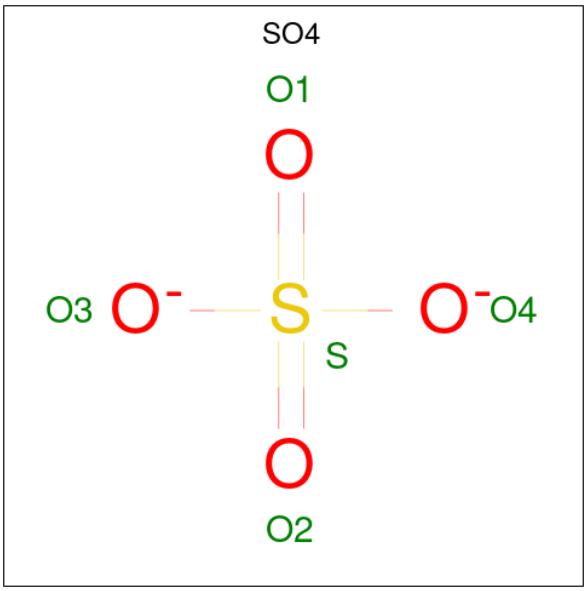
- Molecule 1 is a protein called bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	169	1365	848	239	272	6	0	4	0
1	B	170	1378	856	242	274	6	0	5	0
1	C	170	1361	845	236	274	6	0	4	0
1	D	170	1383	858	243	276	6	0	6	0
1	E	170	1374	852	240	276	6	0	5	0
1	F	170	1365	848	240	271	6	0	4	0
1	G	169	1380	856	243	275	6	0	6	0
1	H	170	1374	853	241	274	6	0	5	0
1	I	170	1382	858	242	276	6	0	5	0
1	J	170	1369	851	241	271	6	0	4	0
1	K	170	1378	855	241	276	6	0	5	0
1	L	170	1374	853	242	273	6	0	5	0
1	M	170	1373	853	241	273	6	0	4	0
1	N	170	1369	850	240	273	6	0	4	0
1	O	169	1366	847	239	274	6	0	5	0
1	P	170	1378	855	241	276	6	0	5	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	2	2	2	0	0
2	F	2	2	2	0	0
2	G	2	2	2	0	0
2	H	2	2	2	0	0
2	I	2	2	2	0	0
2	J	2	2	2	0	0
2	K	2	2	2	0	0
2	L	2	2	2	0	0
2	M	2	2	2	0	0
2	N	2	2	2	0	0
2	O	2	2	2	0	0
2	P	2	2	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0

Continued on next page...

Continued from previous page...

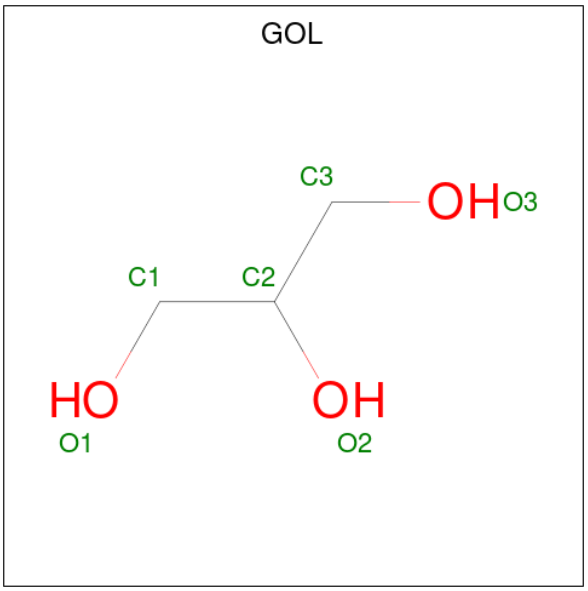
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	E	1	5	4	1		0	0
			Total	O	S			
3	E	1	5	4	1		0	0
			Total	O	S			
3	E	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	G	1	5	4	1		0	0
			Total	O	S			
3	G	1	5	4	1		0	0
			Total	O	S			
3	G	1	5	4	1		0	0
			Total	O	S			
3	H	1	5	4	1		0	0
			Total	O	S			
3	H	1	5	4	1		0	0
			Total	O	S			
3	H	1	5	4	1		0	0
			Total	O	S			
3	I	1	5	4	1		0	0
			Total	O	S			
3	I	1	5	4	1		0	0
			Total	O	S			
3	I	1	5	4	1		0	0
			Total	O	S			
3	I	1	5	4	1		0	0
			Total	O	S			
3	J	1	5	4	1		0	0
			Total	O	S			
3	J	1	5	4	1		0	0
			Total	O	S			
3	J	1	5	4	1		0	0
			Total	O	S			
3	K	1	5	4	1		0	0
			Total	O	S			
3	K	1	5	4	1		0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	K	1	5	4	1	0	0
			Total	O	S		
3	K	1	5	4	1	0	0
			Total	O	S		
3	L	1	5	4	1	0	0
			Total	O	S		
3	L	1	5	4	1	0	0
			Total	O	S		
3	L	1	5	4	1	0	0
			Total	O	S		
3	L	1	5	4	1	0	0
			Total	O	S		
3	M	1	5	4	1	0	0
			Total	O	S		
3	M	1	5	4	1	0	0
			Total	O	S		
3	N	1	5	4	1	0	0
			Total	O	S		
3	N	1	5	4	1	0	0
			Total	O	S		
3	N	1	5	4	1	0	0
			Total	O	S		
3	O	1	5	4	1	0	0
			Total	O	S		
3	O	1	5	4	1	0	0
			Total	O	S		
3	P	1	5	4	1	0	0
			Total	O	S		
3	P	1	5	4	1	0	0
			Total	O	S		
3	P	1	5	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



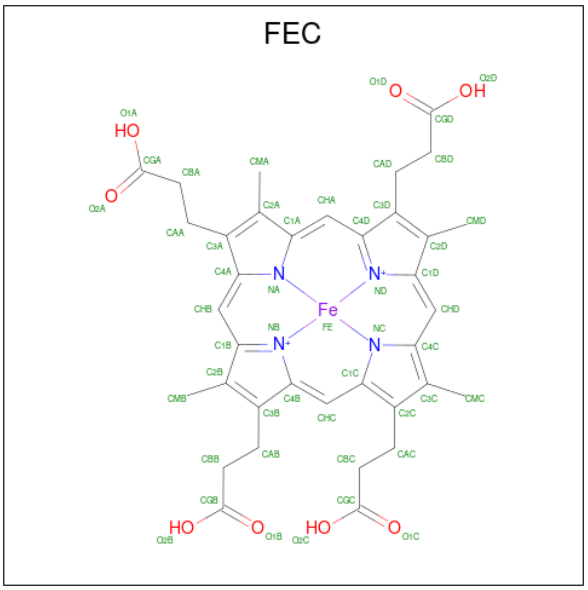
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	D	1	6	3	3	0	0
4	E	1	6	3	3	0	0
4	E	1	6	3	3	0	0
4	F	1	6	3	3	0	0
4	F	1	6	3	3	0	0
4	G	1	6	3	3	0	0
4	G	1	6	3	3	0	0
4	H	1	6	3	3	0	0
4	H	1	6	3	3	0	0
4	I	1	6	3	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	I	1	6	3	3		0	0
			Total	C	O			
4	J	1	6	3	3		0	0
			Total	C	O			
4	J	1	6	3	3		0	0
			Total	C	O			
4	K	1	6	3	3		0	0
			Total	C	O			
4	M	1	6	3	3		0	0
			Total	C	O			
4	M	1	6	3	3		0	0
			Total	C	O			
4	N	1	6	3	3		0	0
			Total	C	O			
4	O	1	6	3	3		0	0
			Total	C	O			
4	O	1	6	3	3		0	0
			Total	C	O			
4	P	1	6	3	3		0	0

- Molecule 5 is 1,3,5,8-TETRAMETHYL-PORPHINE-2,4,6,7-TETRAPROPIONIC ACID FERROUS COMPLEX (three-letter code: FEC) (formula: $C_{36}H_{36}FeN_4O_8$).



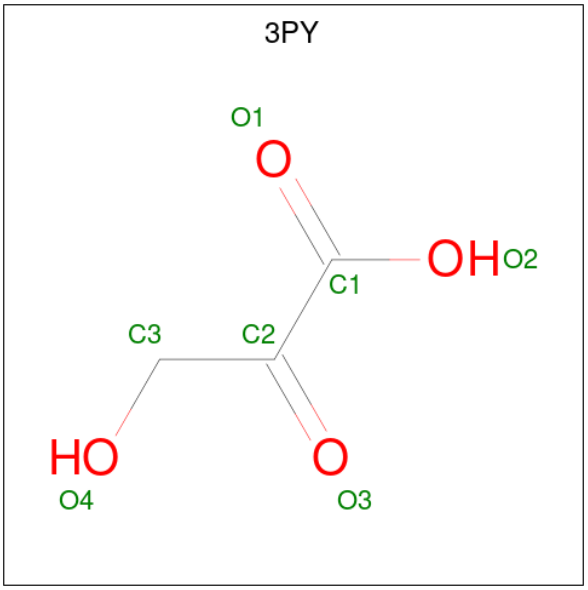
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	B	1	98	72	2	8	16	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	D	1	98	72	2	8	16	0	1
5	F	1	98	72	2	8	16	0	1
5	G	1	98	72	2	8	16	0	1
5	I	1	98	72	2	8	16	0	1
5	L	1	98	72	2	8	16	0	1
5	M	1	98	72	2	8	16	0	1
5	P	1	98	72	2	8	16	0	1

- Molecule 6 is 3-HYDROXYPYRUVIC ACID (three-letter code: 3PY) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	D	1	6	3	3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	131	131	131	0	0

Continued on next page...

Continued from previous page...

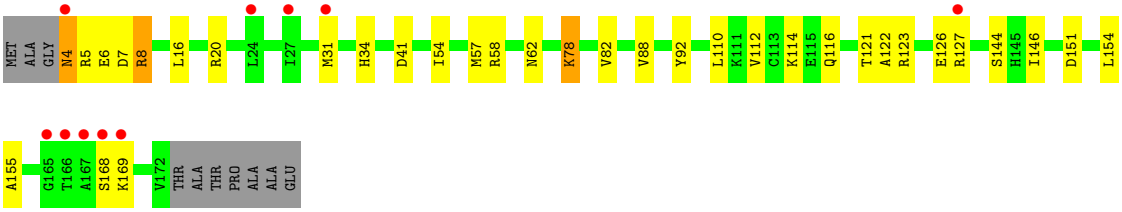
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	142	142	142	0	0
			Total	O		
7	C	117	117	117	0	0
			Total	O		
7	D	99	99	99	0	0
			Total	O		
7	E	101	101	101	0	0
			Total	O		
7	F	103	103	103	0	0
			Total	O		
7	G	146	146	146	0	0
			Total	O		
7	H	91	91	91	0	0
			Total	O		
7	I	131	131	131	0	0
			Total	O		
7	J	99	99	99	0	0
			Total	O		
7	K	130	130	130	0	0
			Total	O		
7	L	134	134	134	0	0
			Total	O		
7	M	122	122	122	0	0
			Total	O		
7	N	124	124	124	0	0
			Total	O		
7	O	105	105	105	0	0
			Total	O		
7	P	115	115	115	0	0

3 Residue-property plots (i)

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

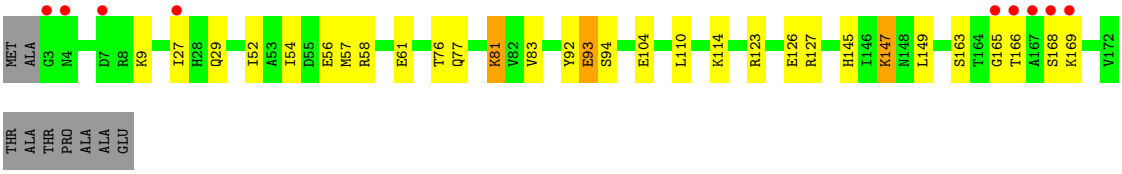
- Molecule 1: bacterioferritin

Chain A:



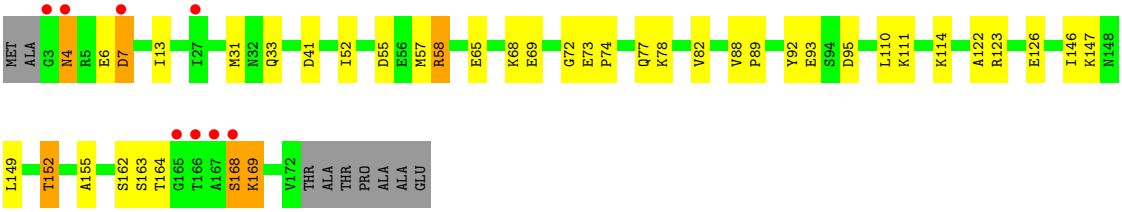
- Molecule 1: bacterioferritin

Chain B:



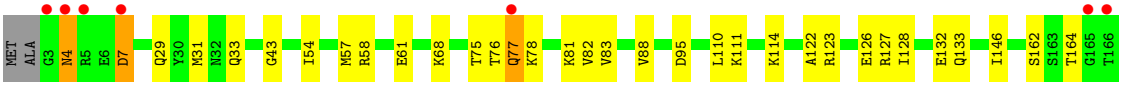
- Molecule 1: bacterioferritin

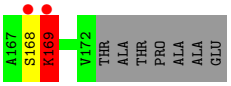
Chain C:



- Molecule 1: bacterioferritin

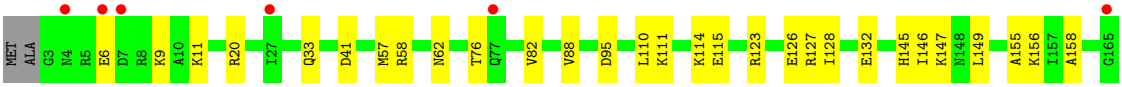
Chain D:

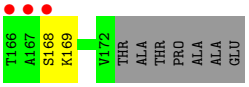




- Molecule 1: bacterioferritin

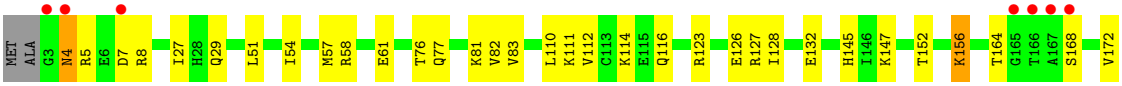
Chain E:





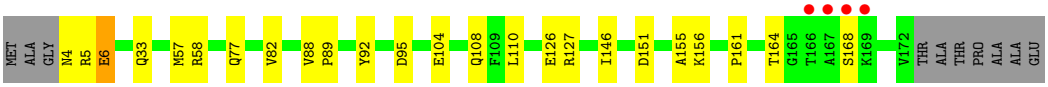
- Molecule 1: bacterioferritin

Chain F:



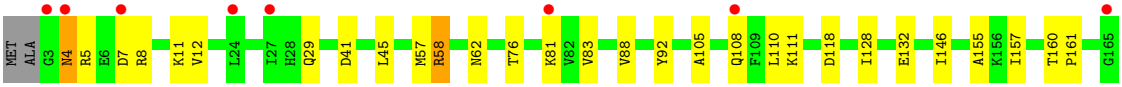
- Molecule 1: bacterioferritin

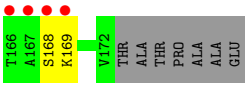
Chain G:



- Molecule 1: bacterioferritin

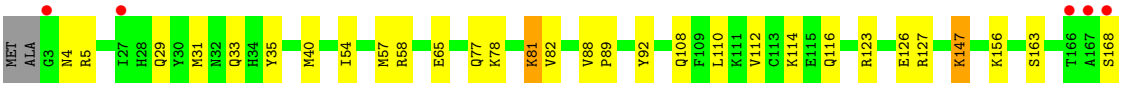
Chain H:

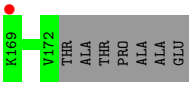




- Molecule 1: bacterioferritin

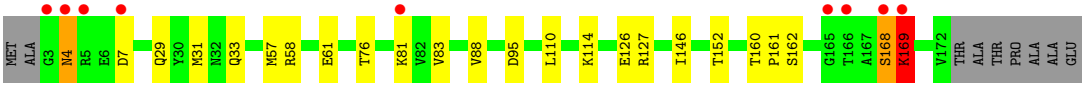
Chain I:





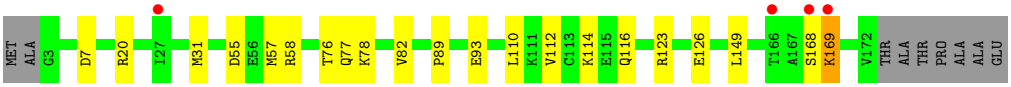
• Molecule 1: bacterioferritin

Chain J:



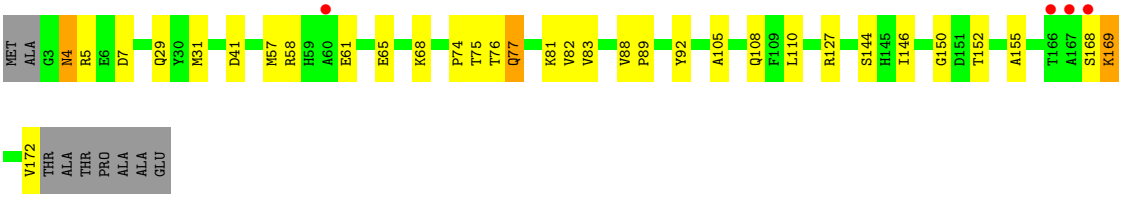
• Molecule 1: bacterioferritin

Chain K:



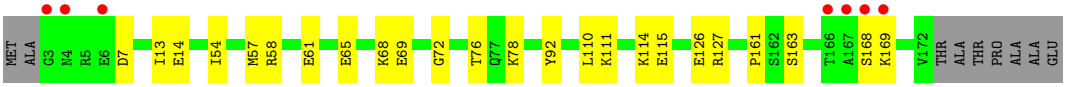
• Molecule 1: bacterioferritin

Chain L:



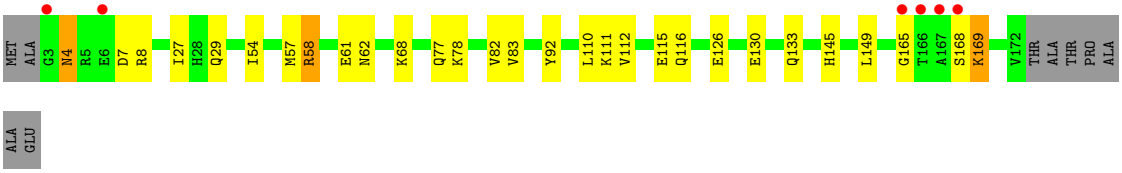
• Molecule 1: bacterioferritin

Chain M:



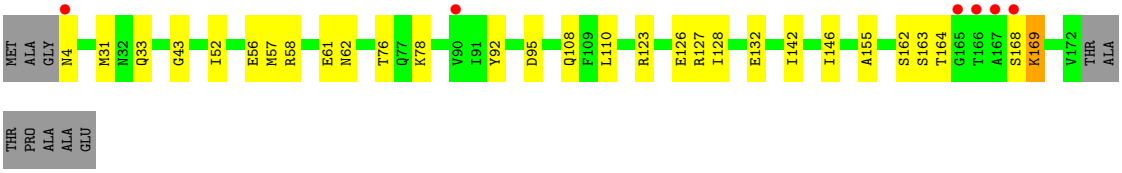
• Molecule 1: bacterioferritin

Chain N:



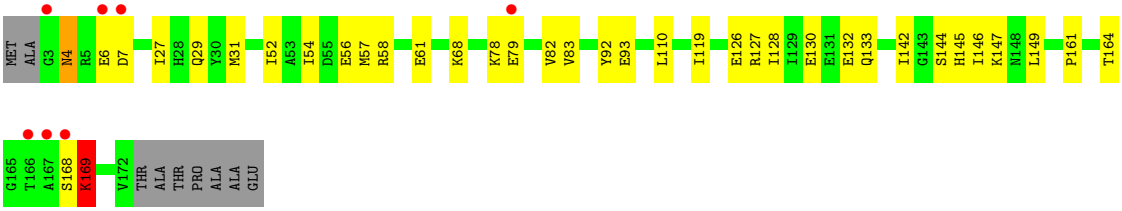
• Molecule 1: bacterioferritin

Chain O:



- Molecule 1: bacterioferritin

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	225.30Å 225.30Å 225.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.84 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-1.95) 99.2 (29.84-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.95Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.214 , 0.254 0.185 , 0.234	Depositor DCC
R_{free} test set	5260 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25080	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% 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: FEC, 3PY, GOL, FE, SO4

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	0.31	0/1385	0.93	3/1864 (0.2%)
1	B	0.31	0/1398	0.84	1/1880 (0.1%)
1	C	0.32	0/1381	0.89	3/1861 (0.2%)
1	D	0.51	2/1407 (0.1%)	0.86	0/1892
1	E	0.31	0/1398	0.84	1/1881 (0.1%)
1	F	0.31	0/1389	0.83	0/1868
1	G	0.44	2/1405 (0.1%)	0.91	1/1890 (0.1%)
1	H	0.32	0/1394	0.85	1/1876 (0.1%)
1	I	0.31	0/1402	0.86	1/1885 (0.1%)
1	J	0.34	0/1389	0.86	2/1868 (0.1%)
1	K	0.32	0/1398	0.88	3/1881 (0.2%)
1	L	1.07	2/1398 (0.1%)	0.90	3/1880 (0.2%)
1	M	0.31	0/1393	0.84	1/1873 (0.1%)
1	N	0.30	0/1389	0.80	1/1869 (0.1%)
1	O	0.77	2/1390 (0.1%)	0.92	3/1872 (0.2%)
1	P	0.60	2/1402 (0.1%)	0.85	3/1885 (0.2%)
All	All	0.48	10/22318 (0.0%)	0.87	27/30025 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	169[A]	LYS	CB-CG	27.00	2.25	1.52
1	L	169[B]	LYS	CB-CG	27.00	2.25	1.52
1	O	169[A]	LYS	CB-CG	18.20	2.01	1.52
1	O	169[B]	LYS	CB-CG	18.20	2.01	1.52
1	P	169[A]	LYS	CB-CG	13.45	1.88	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	169[A]	LYS	CA-CB-CG	-9.37	92.78	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	169[B]	LYS	CA-CB-CG	-9.37	92.78	113.40
1	O	169[A]	LYS	CA-CB-CG	-7.31	97.32	113.40
1	O	169[B]	LYS	CA-CB-CG	-7.31	97.32	113.40
1	C	58[A]	ARG	NE-CZ-NH2	-6.23	117.18	120.30

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	1365	0	1325	44	0
1	B	1378	0	1343	43	0
1	C	1361	0	1312	51	0
1	D	1383	0	1341	55	0
1	E	1374	0	1326	37	0
1	F	1365	0	1328	37	0
1	G	1380	0	1340	43	0
1	H	1374	0	1332	35	0
1	I	1382	0	1348	53	0
1	J	1369	0	1335	34	0
1	K	1378	0	1335	32	0
1	L	1374	0	1335	35	0
1	M	1373	0	1341	54	0
1	N	1369	0	1329	56	0
1	O	1366	0	1312	46	0
1	P	1378	0	1338	47	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	25	0	0	3	0
3	B	20	0	0	3	0
3	C	15	0	0	2	0
3	D	10	0	0	0	0
3	E	15	0	0	1	0
3	F	15	0	0	3	0
3	G	15	0	0	1	0
3	H	15	0	0	0	0
3	I	20	0	0	2	7
3	J	15	0	0	4	0
3	K	20	0	0	1	0
3	L	20	0	0	3	7
3	M	10	0	0	2	0
3	N	15	0	0	0	0
3	O	10	0	0	2	0
3	P	15	0	0	2	0
4	A	6	0	4	1	0
4	B	12	0	8	3	0
4	C	6	0	5	0	0
4	D	6	0	4	5	0
4	E	12	0	8	6	0
4	F	12	0	8	3	0
4	G	12	0	9	3	0
4	H	12	0	8	1	0
4	I	12	0	8	16	0
4	J	12	0	8	5	0
4	K	6	0	4	1	0
4	M	12	0	8	8	0
4	N	6	0	4	1	0
4	O	12	0	8	4	0
4	P	6	0	4	2	0
5	B	98	0	64	17	0
5	D	98	0	64	22	0
5	F	98	0	64	17	0
5	G	98	0	64	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	98	0	64	18	0
5	L	98	0	64	23	0
5	M	98	0	64	18	0
5	P	98	0	64	21	0
6	D	6	0	1	1	0
7	A	131	0	0	6	0
7	B	142	0	0	5	0
7	C	117	0	0	0	0
7	D	99	0	0	9	0
7	E	101	0	0	2	0
7	F	103	0	0	2	0
7	G	146	0	0	5	0
7	H	91	0	0	0	0
7	I	131	0	0	5	0
7	J	99	0	0	5	0
7	K	130	0	0	4	0
7	L	134	0	0	5	0
7	M	122	0	0	3	0
7	N	124	0	0	1	0
7	O	105	0	0	5	0
7	P	115	0	0	5	0
All	All	25080	0	21931	603	7

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 14.

The worst 5 of 603 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:168[A]:SER:CB	1:N:58[A]:ARG:HH22	1.00	1.53
1:G:168[A]:SER:CB	1:H:58[A]:ARG:HH22	1.23	1.49
1:O:58[B]:ARG:NH2	1:P:168[B]:SER:H	1.15	1.44
1:M:168[A]:SER:HB2	1:N:58[A]:ARG:NH2	1.32	1.44
1:G:168[A]:SER:HB2	1:H:58[A]:ARG:NH2	1.12	1.41

The worst 5 of 7 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)
3:I:1802:SO4:S	3:L:2102:SO4:S[9_465]	0.16	2.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1802:SO4:O1	3:L:2102:SO4:O3[9_465]	0.22	1.98
3:I:1802:SO4:O4	3:L:2102:SO4:O2[9_465]	0.35	1.85
3:I:1802:SO4:O2	3:L:2102:SO4:O4[9_465]	0.37	1.83
3:I:1802:SO4:O3	3:L:2102:SO4:O1[9_465]	0.49	1.71

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	171/179 (96%)	170 (99%)	1 (1%)	0	100	100
1	B	173/179 (97%)	170 (98%)	3 (2%)	0	100	100
1	C	172/179 (96%)	169 (98%)	3 (2%)	0	100	100
1	D	174/179 (97%)	173 (99%)	1 (1%)	0	100	100
1	E	173/179 (97%)	170 (98%)	3 (2%)	0	100	100
1	F	172/179 (96%)	170 (99%)	2 (1%)	0	100	100
1	G	173/179 (97%)	171 (99%)	2 (1%)	0	100	100
1	H	173/179 (97%)	171 (99%)	0	2 (1%)	13	4
1	I	173/179 (97%)	168 (97%)	5 (3%)	0	100	100
1	J	172/179 (96%)	169 (98%)	1 (1%)	2 (1%)	13	4
1	K	173/179 (97%)	169 (98%)	4 (2%)	0	100	100
1	L	173/179 (97%)	168 (97%)	5 (3%)	0	100	100
1	M	172/179 (96%)	170 (99%)	2 (1%)	0	100	100
1	N	172/179 (96%)	169 (98%)	1 (1%)	2 (1%)	13	4
1	O	172/179 (96%)	170 (99%)	2 (1%)	0	100	100
1	P	173/179 (97%)	168 (97%)	3 (2%)	2 (1%)	13	4
All	All	2761/2864 (96%)	2715 (98%)	38 (1%)	8 (0%)	51	30

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	169[A]	LYS
1	H	169[B]	LYS
1	J	168[A]	SER
1	J	168[B]	SER
1	N	169[A]	LYS

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	143/145 (99%)	140 (98%)	3 (2%)	53	46
1	B	144/145 (99%)	138 (96%)	6 (4%)	30	17
1	C	142/145 (98%)	130 (92%)	12 (8%)	10	3
1	D	145/145 (100%)	138 (95%)	7 (5%)	25	12
1	E	144/145 (99%)	143 (99%)	1 (1%)	84	82
1	F	143/145 (99%)	137 (96%)	6 (4%)	30	17
1	G	145/145 (100%)	144 (99%)	1 (1%)	84	82
1	H	143/145 (99%)	136 (95%)	7 (5%)	25	12
1	I	145/145 (100%)	141 (97%)	4 (3%)	43	33
1	J	143/145 (99%)	137 (96%)	6 (4%)	30	17
1	K	144/145 (99%)	140 (97%)	4 (3%)	43	33
1	L	144/145 (99%)	139 (96%)	5 (4%)	36	24
1	M	144/145 (99%)	143 (99%)	1 (1%)	84	82
1	N	143/145 (99%)	139 (97%)	4 (3%)	43	33
1	O	143/145 (99%)	142 (99%)	1 (1%)	84	82
1	P	145/145 (100%)	140 (97%)	5 (3%)	37	25
All	All	2300/2320 (99%)	2227 (97%)	73 (3%)	44	27

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	93[B]	GLU
1	L	77[B]	GLN
1	N	58[B]	ARG
1	D	77[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	29	GLN
1	L	29	GLN
1	P	148	ASN
1	P	29	GLN
1	J	62	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 124 ligands modelled in this entry, 32 are monoatomic - leaving 92 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	SO4	H	1706	-	4,4,4	0.46	0	6,6,6	0.87	0
4	GOL	K	2011	-	5,5,5	4.44	5 (100%)	5,5,5	4.81	3 (60%)
3	SO4	P	2506	-	4,4,4	0.46	0	6,6,6	0.56	0
4	GOL	G	1611	-	5,5,5	4.39	5 (100%)	5,5,5	4.39	3 (60%)
3	SO4	P	2501	-	4,4,4	1.91	1 (25%)	6,6,6	0.91	0
3	SO4	G	1603	-	4,4,4	2.02	1 (25%)	6,6,6	0.89	0
4	GOL	I	1810	1	5,5,5	4.38	5 (100%)	5,5,5	3.88	3 (60%)
3	SO4	I	1806	-	4,4,4	0.39	0	6,6,6	0.60	0
4	GOL	E	1411	-	5,5,5	4.45	5 (100%)	5,5,5	4.19	3 (60%)
4	GOL	F	1512	-	5,5,5	4.54	5 (100%)	5,5,5	3.72	3 (60%)
3	SO4	M	2206	-	4,4,4	0.23	0	6,6,6	0.40	0
3	SO4	A	1004	-	4,4,4	1.88	1 (25%)	6,6,6	0.92	0
3	SO4	A	1008	-	4,4,4	0.53	0	6,6,6	2.46	2 (33%)
5	FEC	I	1807[B]	1	40,56,56	1.21	4 (10%)	42,90,90	2.03	12 (28%)
3	SO4	L	2102	3	4,4,4	1.95	1 (25%)	6,6,6	0.86	0
4	GOL	J	1811	-	5,5,5	4.52	5 (100%)	5,5,5	5.39	3 (60%)
5	FEC	L	2108[B]	1	40,56,56	1.26	4 (10%)	42,90,90	1.78	9 (21%)
3	SO4	K	2001	-	4,4,4	1.93	1 (25%)	6,6,6	0.95	0
5	FEC	P	2507[A]	1	40,56,56	1.21	4 (10%)	42,90,90	1.97	12 (28%)
3	SO4	K	1504	-	4,4,4	1.94	1 (25%)	6,6,6	0.86	0
4	GOL	B	1110	-	5,5,5	4.51	5 (100%)	5,5,5	4.49	3 (60%)
4	GOL	M	2211	-	5,5,5	4.52	5 (100%)	5,5,5	4.58	3 (60%)
4	GOL	P	2510	-	5,5,5	4.46	5 (100%)	5,5,5	4.69	3 (60%)
5	FEC	D	1311[A]	1	40,56,56	1.25	4 (10%)	42,90,90	2.01	13 (30%)
5	FEC	M	2207[B]	1	40,56,56	1.28	4 (10%)	42,90,90	1.69	14 (33%)
3	SO4	B	1005	-	4,4,4	0.53	0	6,6,6	2.46	2 (33%)
4	GOL	D	1211	-	5,5,5	4.50	5 (100%)	5,5,5	4.66	3 (60%)
4	GOL	I	1713	-	5,5,5	4.48	5 (100%)	5,5,5	5.59	3 (60%)
3	SO4	B	1106	-	4,4,4	0.13	0	6,6,6	1.50	0
4	GOL	M	2210	1	5,5,5	4.51	5 (100%)	5,5,5	4.39	2 (40%)
4	GOL	H	1710	-	5,5,5	4.53	5 (100%)	5,5,5	5.65	3 (60%)
3	SO4	L	2107	-	4,4,4	1.94	1 (25%)	6,6,6	0.86	0
3	SO4	O	2406	-	4,4,4	0.30	0	6,6,6	1.07	0
4	GOL	E	1410	-	5,5,5	4.53	5 (100%)	5,5,5	4.34	3 (60%)
3	SO4	D	1303	-	4,4,4	0.17	0	6,6,6	0.60	0
4	GOL	J	1910	-	5,5,5	4.56	5 (100%)	5,5,5	4.88	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FEC	L	2108[A]	1	40,56,56	1.25	3 (7%)	42,90,90	1.84	11 (26%)
4	GOL	O	2411	-	5,5,5	4.42	5 (100%)	5,5,5	3.91	3 (60%)
3	SO4	F	1502	-	4,4,4	1.91	1 (25%)	6,6,6	0.92	0
5	FEC	F	1507[B]	1	40,56,56	1.25	4 (10%)	42,90,90	1.91	10 (23%)
3	SO4	A	1105	-	4,4,4	0.53	0	6,6,6	2.46	2 (33%)
3	SO4	C	1201	-	4,4,4	1.93	1 (25%)	6,6,6	0.93	0
3	SO4	H	1703	-	4,4,4	0.28	0	6,6,6	0.58	0
6	3PY	D	1310	1	5,5,6	12.83	5 (100%)	5,5,7	7.82	5 (100%)
3	SO4	N	2303	-	4,4,4	0.18	0	6,6,6	0.81	0
3	SO4	F	1501	-	4,4,4	2.02	1 (25%)	6,6,6	0.84	0
3	SO4	N	2306	-	4,4,4	0.18	0	6,6,6	0.76	0
3	SO4	B	1104	-	4,4,4	2.02	1 (25%)	6,6,6	0.89	0
3	SO4	D	1301	-	4,4,4	1.99	1 (25%)	6,6,6	0.88	0
3	SO4	O	2409	-	4,4,4	0.46	0	6,6,6	0.56	0
3	SO4	P	2503	-	4,4,4	0.20	0	6,6,6	0.92	0
3	SO4	F	1506	-	4,4,4	0.26	0	6,6,6	1.31	1 (16%)
3	SO4	A	1001	-	4,4,4	1.80	1 (25%)	6,6,6	0.94	0
3	SO4	I	1801	-	4,4,4	1.93	1 (25%)	6,6,6	0.92	0
3	SO4	L	2101	-	4,4,4	1.91	1 (25%)	6,6,6	0.92	0
5	FEC	G	1608[B]	1	40,56,56	1.23	4 (10%)	42,90,90	1.92	14 (33%)
4	GOL	F	1510	-	5,5,5	4.45	5 (100%)	5,5,5	4.78	3 (60%)
3	SO4	C	1206	-	4,4,4	0.34	0	6,6,6	0.63	0
3	SO4	B	1101	-	4,4,4	1.88	1 (25%)	6,6,6	0.92	0
3	SO4	J	1904	-	4,4,4	1.93	1 (25%)	6,6,6	0.91	0
5	FEC	F	1507[A]	1	40,56,56	1.28	4 (10%)	42,90,90	1.69	13 (30%)
5	FEC	I	1807[A]	1	40,56,56	1.22	4 (10%)	42,90,90	1.93	13 (30%)
3	SO4	G	1606	-	4,4,4	0.24	0	6,6,6	0.71	0
3	SO4	E	1304	1	4,4,4	1.92	1 (25%)	6,6,6	0.93	0
3	SO4	H	1701	-	4,4,4	1.84	1 (25%)	6,6,6	0.84	0
3	SO4	L	2103	1	4,4,4	1.94	1 (25%)	6,6,6	0.86	0
3	SO4	J	1906	-	4,4,4	0.16	0	6,6,6	0.95	0
5	FEC	B	1107[B]	1	40,56,56	1.21	3 (7%)	42,90,90	2.01	11 (26%)
3	SO4	E	1406	-	4,4,4	0.30	0	6,6,6	1.22	1 (16%)
3	SO4	M	2201	-	4,4,4	1.89	1 (25%)	6,6,6	0.93	0
3	SO4	I	1803	-	4,4,4	0.33	0	6,6,6	0.49	0
3	SO4	E	1401	-	4,4,4	1.92	1 (25%)	6,6,6	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FEC	M	2207[A]	1	40,56,56	1.26	4 (10%)	42,90,90	1.74	10 (23%)
4	GOL	C	1210	-	5,5,5	4.37	5 (100%)	5,5,5	4.98	3 (60%)
3	SO4	C	1203	-	4,4,4	0.40	0	6,6,6	0.98	0
5	FEC	G	1608[A]	1	40,56,56	1.22	4 (10%)	42,90,90	1.83	14 (33%)
4	GOL	G	1610	-	5,5,5	4.53	5 (100%)	5,5,5	5.68	3 (60%)
3	SO4	A	1006	-	4,4,4	0.24	0	6,6,6	1.10	0
4	GOL	N	2310	-	5,5,5	4.51	5 (100%)	5,5,5	5.50	3 (60%)
3	SO4	J	1901	-	4,4,4	1.89	1 (25%)	6,6,6	0.84	0
4	GOL	B	1011	-	5,5,5	4.62	5 (100%)	5,5,5	4.00	3 (60%)
3	SO4	K	2006	-	4,4,4	0.17	0	6,6,6	0.67	0
3	SO4	N	2301	-	4,4,4	1.94	1 (25%)	6,6,6	0.81	0
3	SO4	I	1802	3	4,4,4	1.96	2 (50%)	6,6,6	0.79	0
4	GOL	O	2410	-	5,5,5	4.40	5 (100%)	5,5,5	4.82	3 (60%)
4	GOL	H	1814	-	5,5,5	4.64	5 (100%)	5,5,5	4.75	3 (60%)
5	FEC	P	2507[B]	1	40,56,56	1.19	4 (10%)	42,90,90	2.08	13 (30%)
3	SO4	K	2003	-	4,4,4	1.91	1 (25%)	6,6,6	0.92	0
5	FEC	B	1107[A]	1	40,56,56	1.21	3 (7%)	42,90,90	1.93	12 (28%)
3	SO4	G	1607	-	4,4,4	0.34	0	6,6,6	0.49	0
4	GOL	A	1010	-	5,5,5	4.64	5 (100%)	5,5,5	5.84	3 (60%)
5	FEC	D	1311[B]	1	40,56,56	1.23	4 (10%)	42,90,90	1.69	9 (21%)

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
4	GOL	K	2011	-	-	2/4/4/4	-
5	FEC	G	1608[A]	1	-	10/20/120/120	-
4	GOL	D	1211	-	-	3/4/4/4	-
4	GOL	G	1611	-	-	2/4/4/4	-
4	GOL	G	1610	-	-	3/4/4/4	-
4	GOL	I	1713	-	-	3/4/4/4	-
4	GOL	I	1810	1	-	3/4/4/4	-
5	FEC	G	1608[B]	1	-	9/20/120/120	-
4	GOL	N	2310	-	-	4/4/4/4	-
4	GOL	F	1510	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	F	1512	-	-	2/4/4/4	-
4	GOL	E	1411	-	-	4/4/4/4	-
4	GOL	M	2210	1	-	2/4/4/4	-
4	GOL	H	1710	-	-	2/4/4/4	-
4	GOL	E	1410	-	-	2/4/4/4	-
4	GOL	B	1011	-	-	2/4/4/4	-
5	FEC	F	1507[A]	1	-	8/20/120/120	-
5	FEC	I	1807[A]	1	-	10/20/120/120	-
4	GOL	J	1910	-	-	2/4/4/4	-
5	FEC	I	1807[B]	1	-	13/20/120/120	-
5	FEC	L	2108[A]	1	-	9/20/120/120	-
4	GOL	O	2411	-	-	4/4/4/4	-
5	FEC	F	1507[B]	1	-	6/20/120/120	-
4	GOL	J	1811	-	-	3/4/4/4	-
5	FEC	L	2108[B]	1	-	9/20/120/120	-
5	FEC	P	2507[A]	1	-	8/20/120/120	-
4	GOL	O	2410	-	-	3/4/4/4	-
4	GOL	H	1814	-	-	3/4/4/4	-
5	FEC	P	2507[B]	1	-	10/20/120/120	-
5	FEC	B	1107[A]	1	-	9/20/120/120	-
4	GOL	B	1110	-	-	2/4/4/4	-
4	GOL	M	2211	-	-	2/4/4/4	-
4	GOL	P	2510	-	-	2/4/4/4	-
5	FEC	B	1107[B]	1	-	8/20/120/120	-
5	FEC	D	1311[A]	1	-	10/20/120/120	-
4	GOL	A	1010	-	-	2/4/4/4	-
6	3PY	D	1310	1	-	0/1/4/6	-
5	FEC	D	1311[B]	1	-	8/20/120/120	-
5	FEC	M	2207[A]	1	-	10/20/120/120	-
5	FEC	M	2207[B]	1	-	8/20/120/120	-
4	GOL	C	1210	-	-	2/4/4/4	-

The worst 5 of 213 bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1310	3PY	C3-C2	-20.42	1.21	1.51
6	D	1310	3PY	O1-C1	17.86	1.63	1.22
4	A	1010	GOL	C3-C2	-7.61	1.20	1.51
4	H	1710	GOL	C3-C2	-7.43	1.21	1.51
6	D	1310	3PY	O3-C2	7.39	1.35	1.23

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1310	3PY	O4-C3-C2	12.04	145.08	112.66
4	A	1010	GOL	O3-C3-C2	11.00	162.95	110.20
4	I	1713	GOL	O3-C3-C2	10.39	160.02	110.20
4	N	2310	GOL	O3-C3-C2	10.15	158.86	110.20
4	J	1811	GOL	O3-C3-C2	10.09	158.60	110.20

There are no chirality outliers.

5 of 206 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1010	GOL	O1-C1-C2-C3
4	C	1210	GOL	O1-C1-C2-C3
4	E	1410	GOL	O1-C1-C2-C3
4	E	1411	GOL	O1-C1-C2-C3
4	G	1611	GOL	O1-C1-C2-C3

There are no ring outliers.

59 monomers are involved in 247 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	2011	GOL	1	0
3	P	2506	SO4	1	0
4	G	1611	GOL	1	0
3	P	2501	SO4	1	0
4	I	1810	GOL	15	0
3	M	2206	SO4	2	0
5	I	1807[B]	FEC	9	0
3	L	2102	SO4	1	7
4	J	1811	GOL	1	0
5	L	2108[B]	FEC	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	2507[A]	FEC	8	0
3	K	1504	SO4	1	0
4	B	1110	GOL	3	0
4	M	2211	GOL	3	0
4	P	2510	GOL	2	0
5	D	1311[A]	FEC	8	0
5	M	2207[B]	FEC	8	0
3	B	1005	SO4	1	0
4	D	1211	GOL	5	0
4	I	1713	GOL	1	0
3	B	1106	SO4	1	0
4	M	2210	GOL	5	0
4	H	1710	GOL	1	0
3	L	2107	SO4	1	0
3	O	2406	SO4	1	0
4	E	1410	GOL	6	0
4	J	1910	GOL	4	0
5	L	2108[A]	FEC	11	0
4	O	2411	GOL	2	0
3	F	1502	SO4	2	0
5	F	1507[B]	FEC	13	0
3	A	1105	SO4	3	0
6	D	1310	3PY	1	0
3	F	1501	SO4	1	0
3	B	1104	SO4	1	0
3	O	2409	SO4	1	0
5	G	1608[B]	FEC	6	0
4	F	1510	GOL	3	0
3	C	1206	SO4	1	0
3	J	1904	SO4	1	0
5	F	1507[A]	FEC	4	0
5	I	1807[A]	FEC	9	0
3	G	1606	SO4	1	0
3	E	1304	SO4	1	0
3	L	2103	SO4	1	0
3	J	1906	SO4	3	0
5	B	1107[B]	FEC	7	0
3	I	1803	SO4	1	0
5	M	2207[A]	FEC	10	0
3	C	1203	SO4	1	0
5	G	1608[A]	FEC	9	0
4	G	1610	GOL	2	0

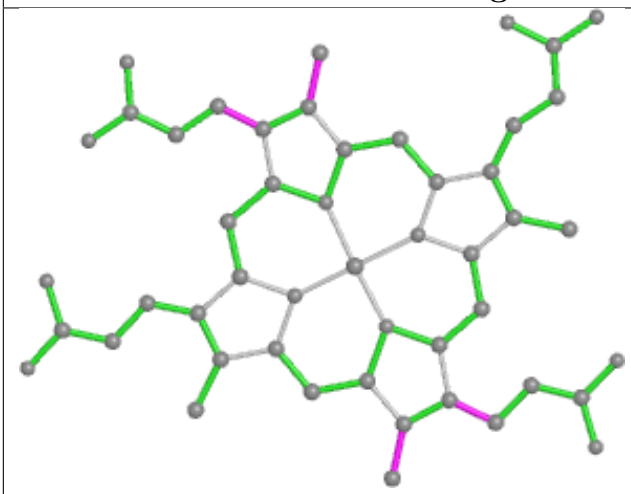
Continued on next page...

Continued from previous page...

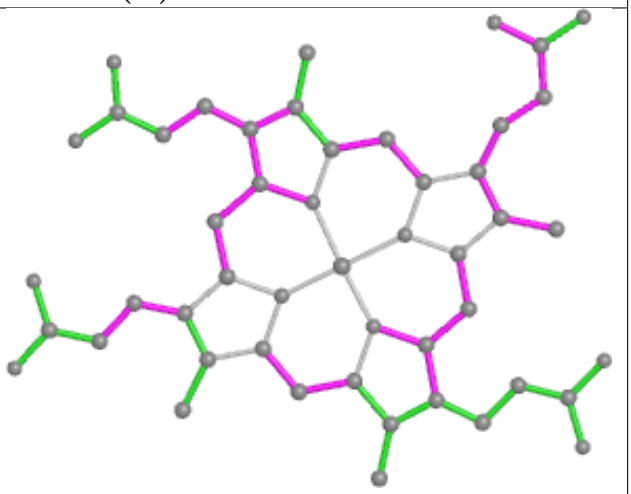
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	2310	GOL	1	0
3	I	1802	SO4	1	7
4	O	2410	GOL	2	0
5	P	2507[B]	FEC	13	0
5	B	1107[A]	FEC	10	0
4	A	1010	GOL	1	0
5	D	1311[B]	FEC	14	0

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.

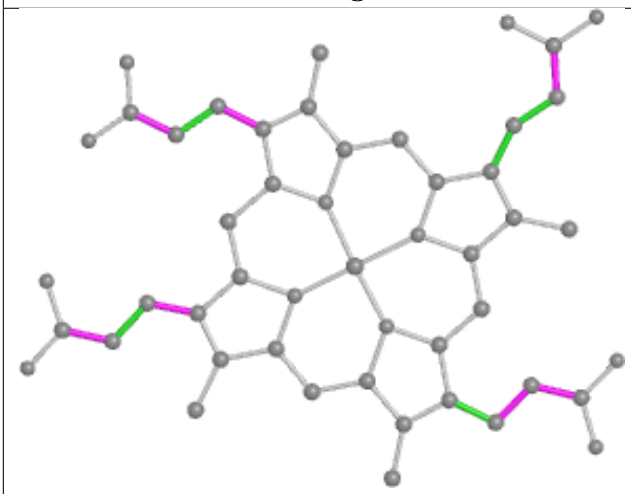
Ligand FEC I 1807 (B)



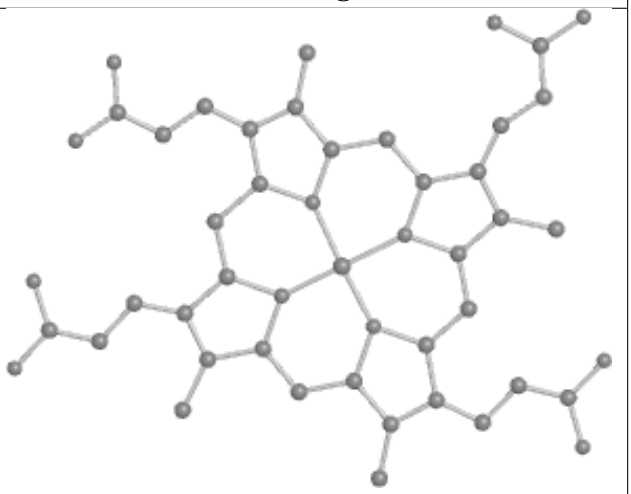
Bond lengths



Bond angles

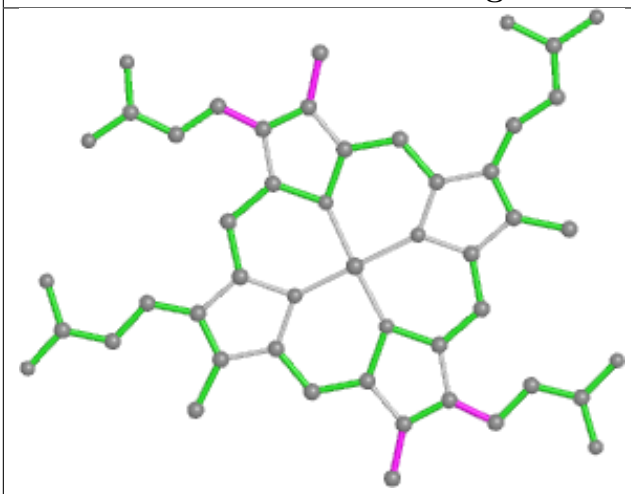


Torsions

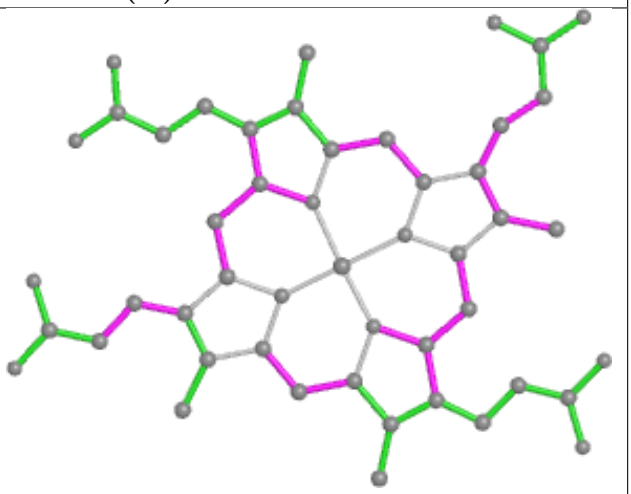


Rings

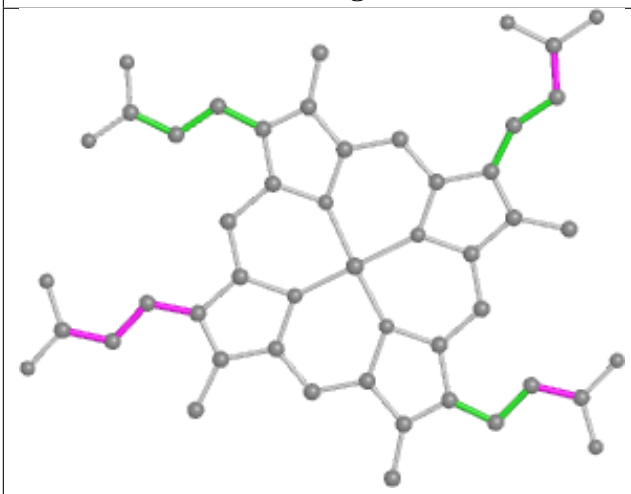
Ligand FEC L 2108 (B)



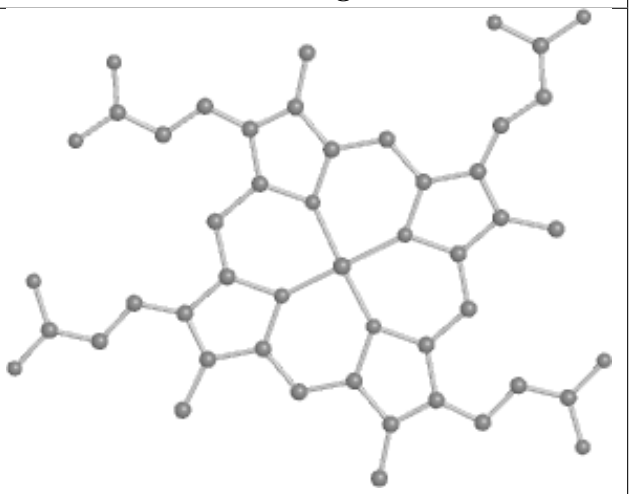
Bond lengths



Bond angles

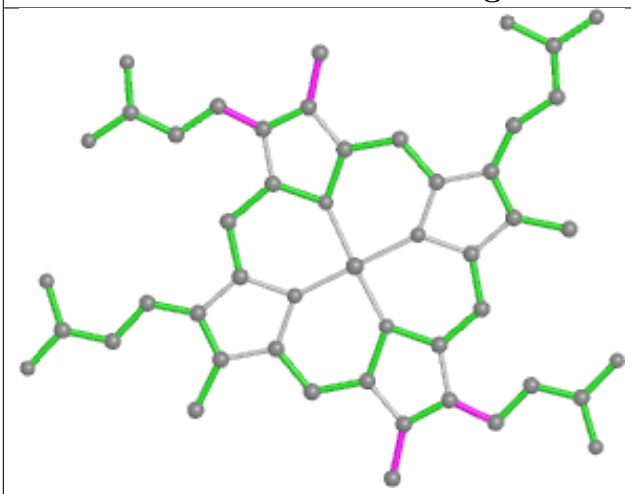


Torsions

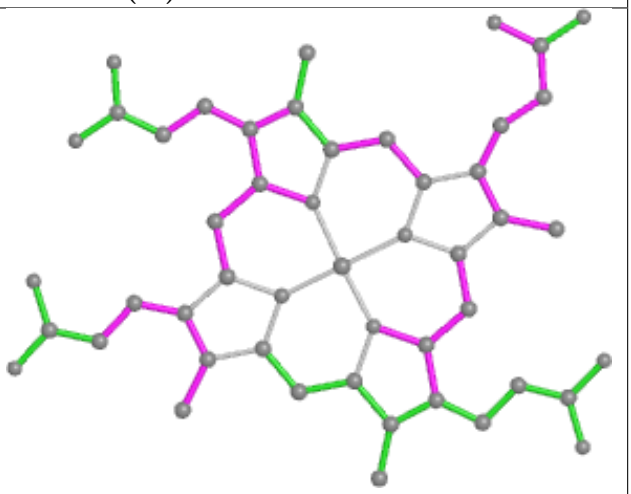


Rings

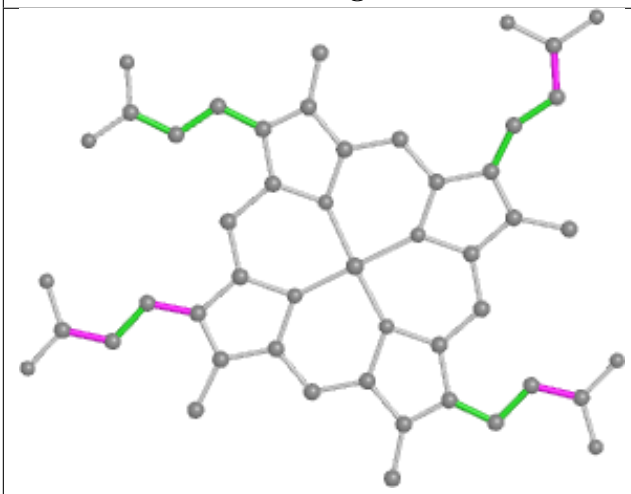
Ligand FEC P 2507 (A)



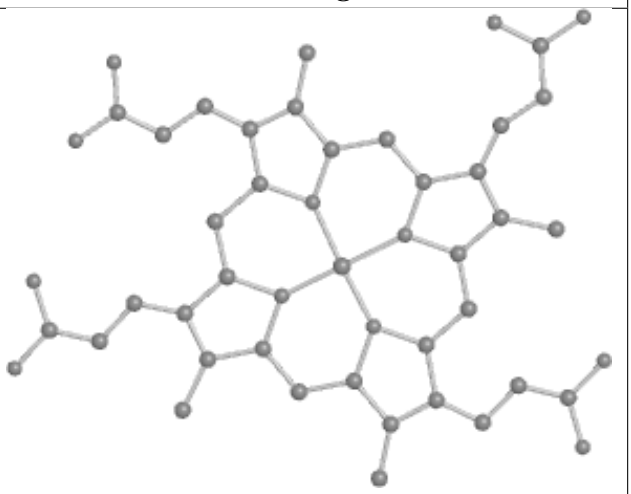
Bond lengths



Bond angles

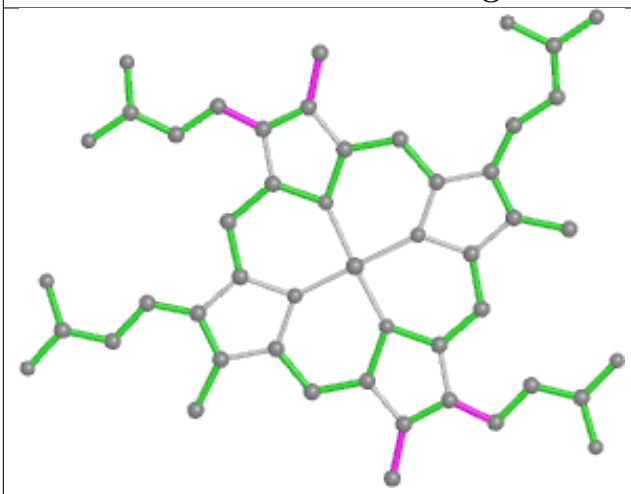


Torsions

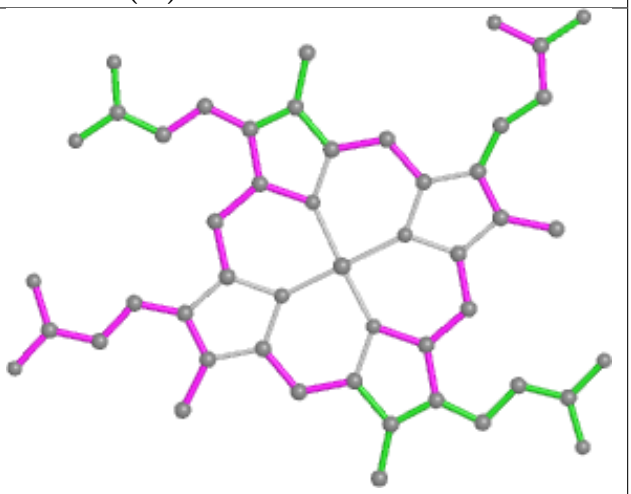


Rings

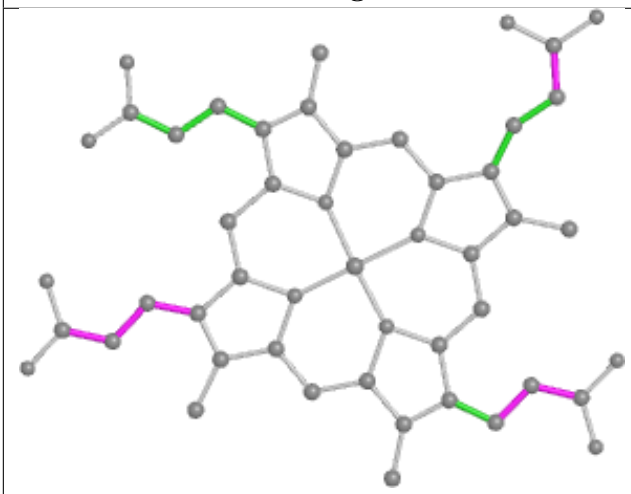
Ligand FEC D 1311 (A)



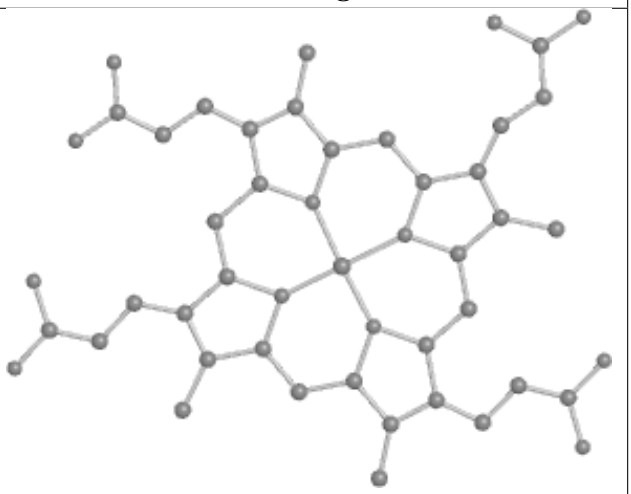
Bond lengths



Bond angles

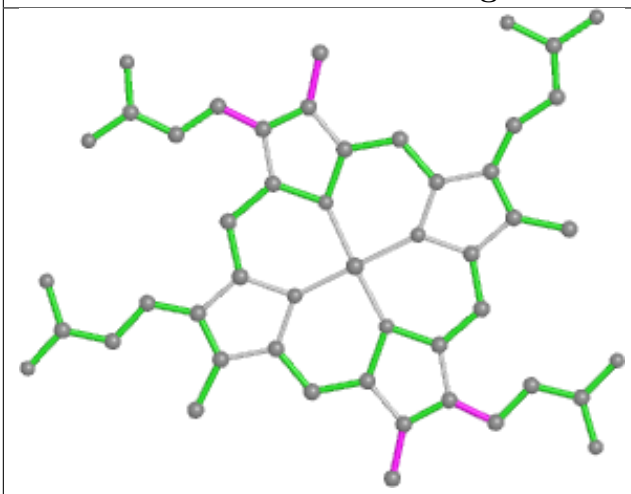


Torsions

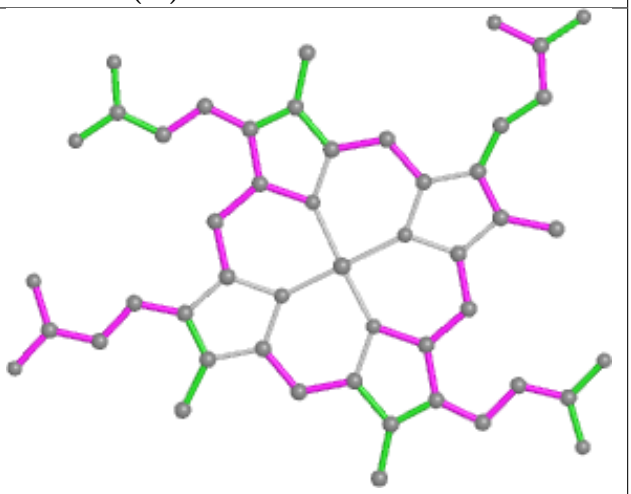


Rings

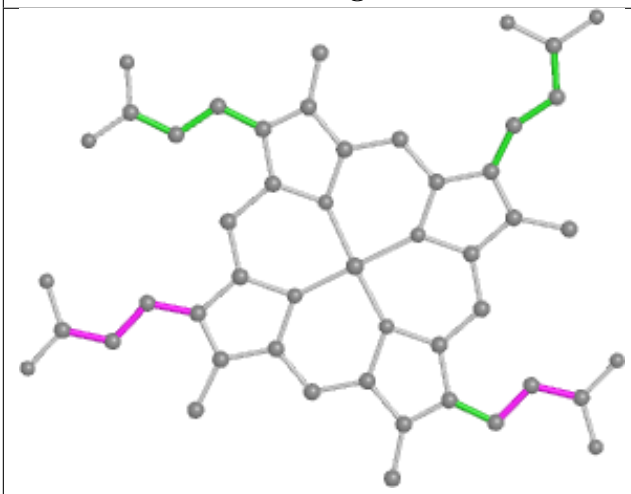
Ligand FEC M 2207 (B)



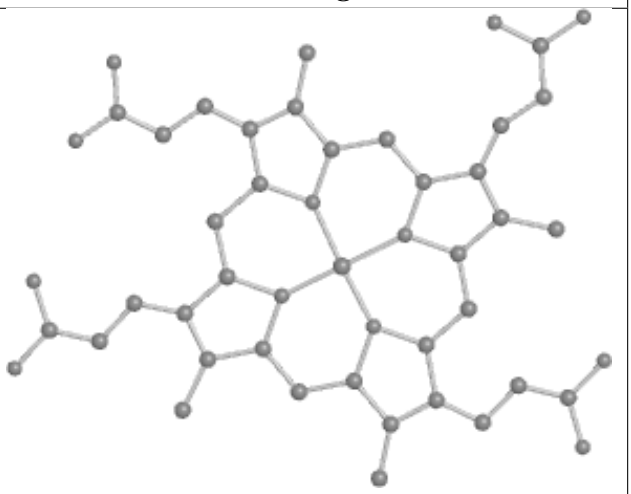
Bond lengths



Bond angles

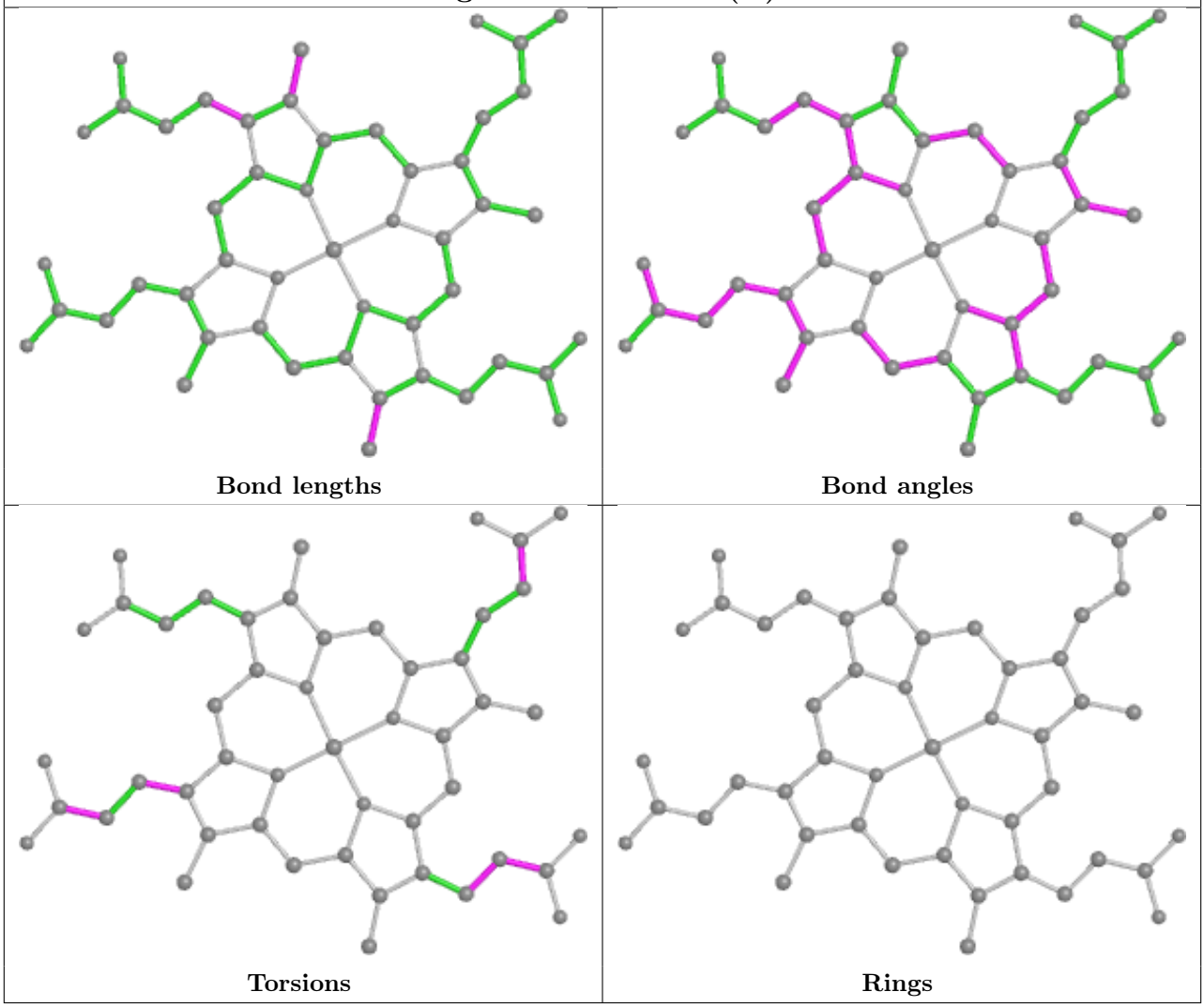


Torsions

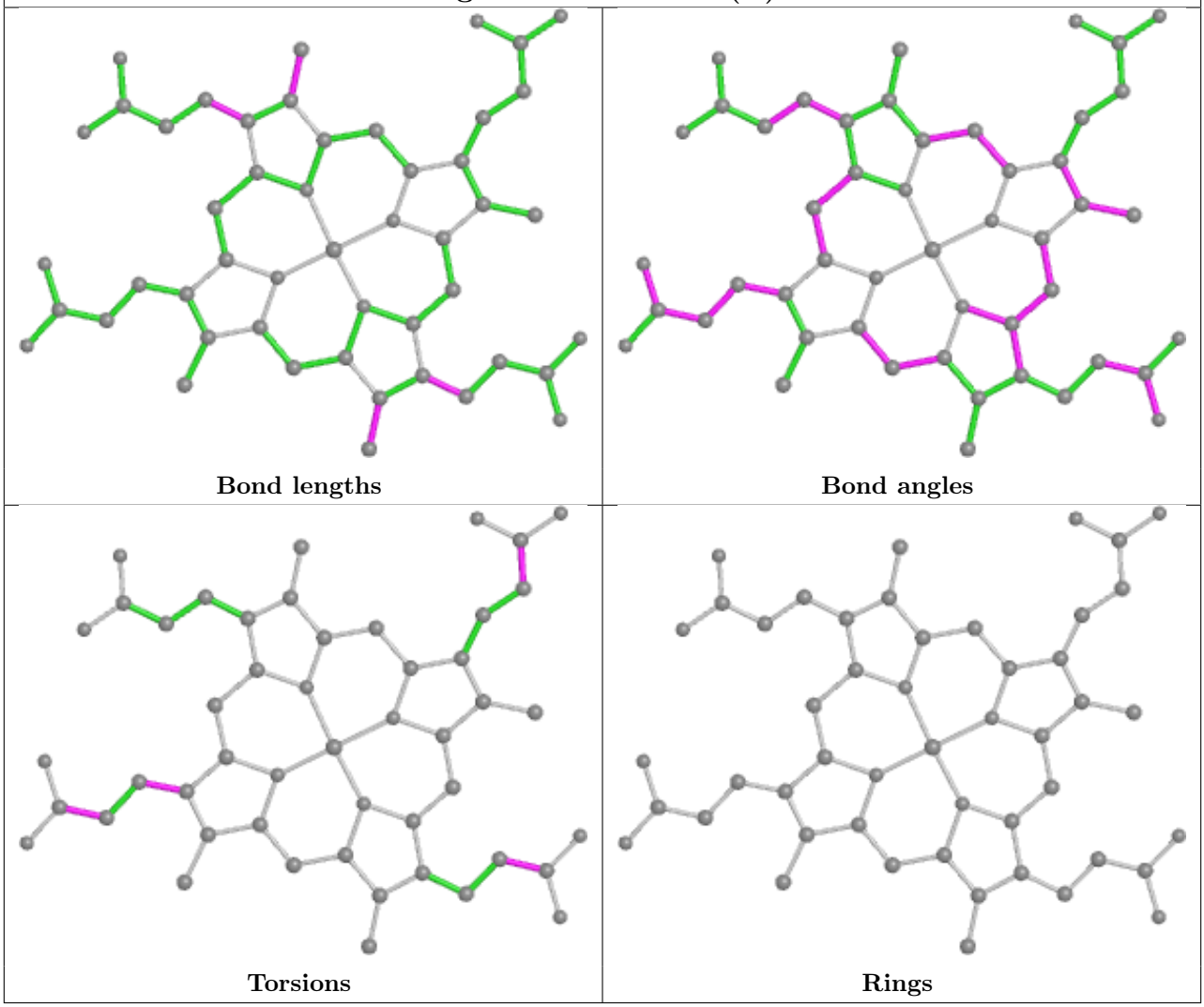


Rings

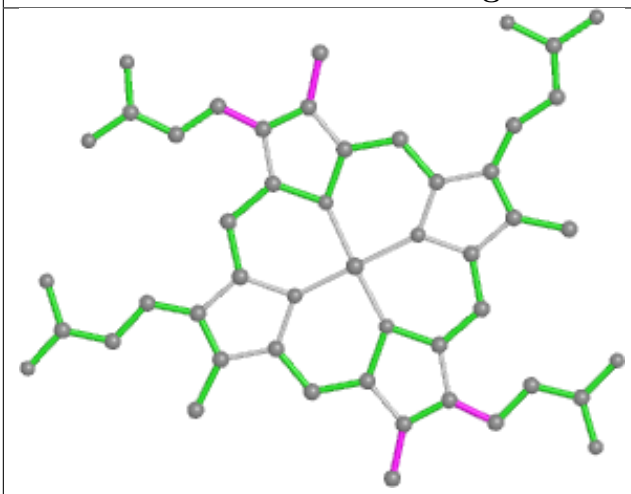
Ligand FEC L 2108 (A)



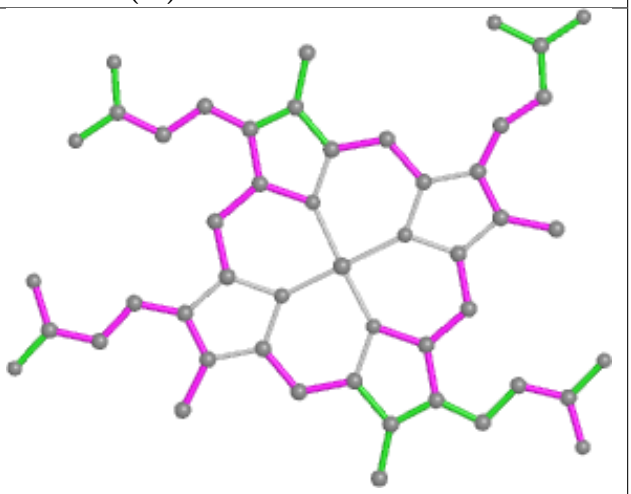
Ligand FEC F 1507 (B)



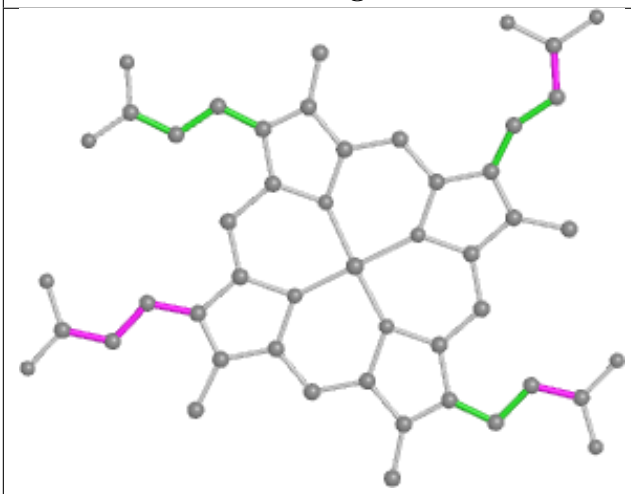
Ligand FEC G 1608 (B)



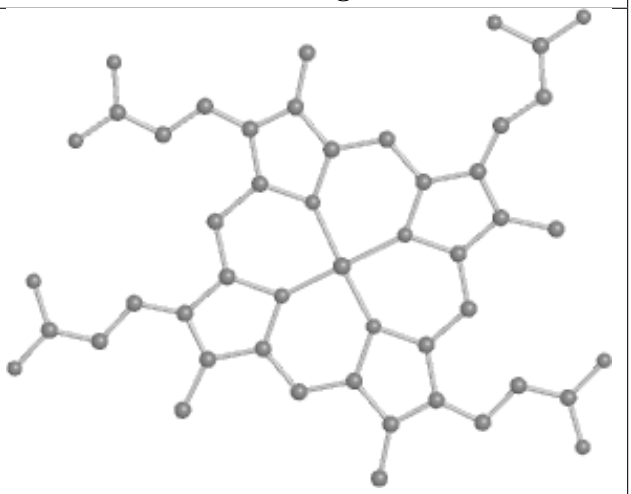
Bond lengths



Bond angles

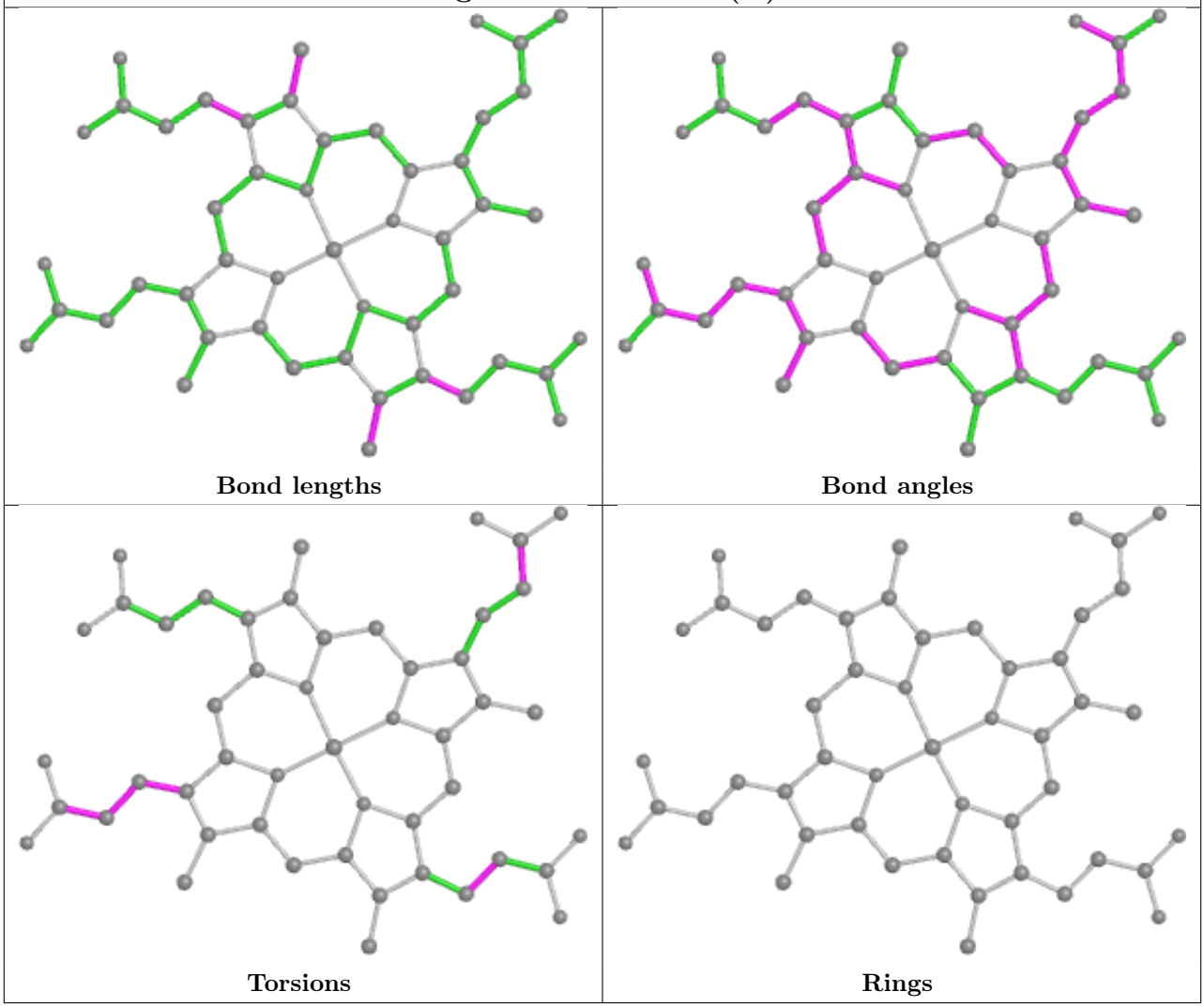


Torsions

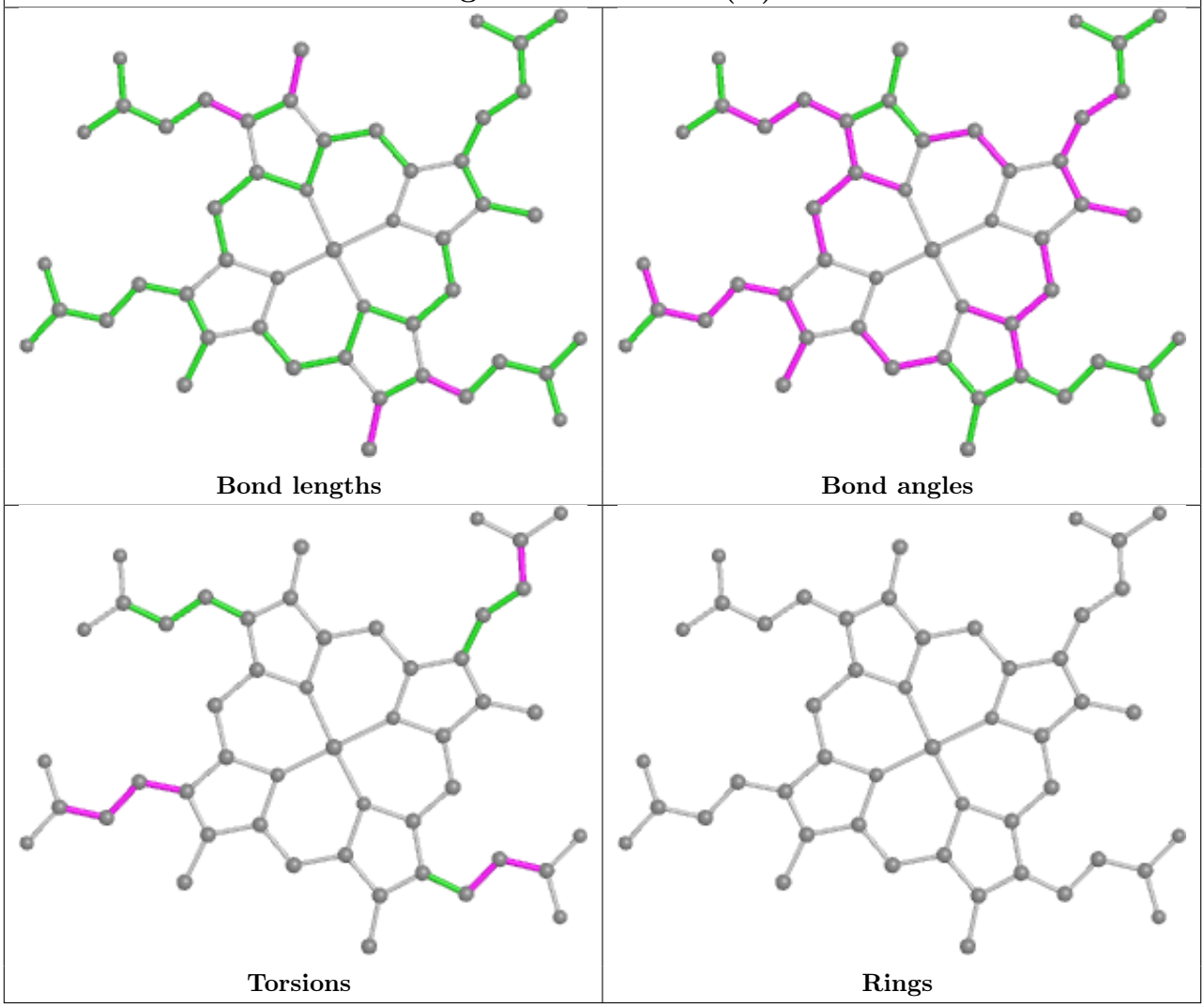


Rings

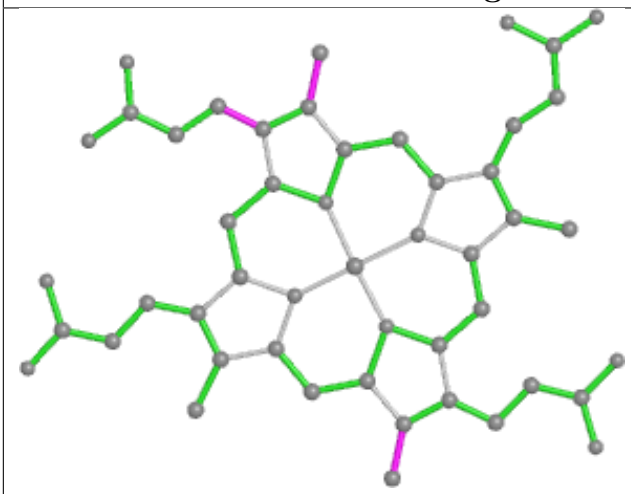
Ligand FEC F 1507 (A)



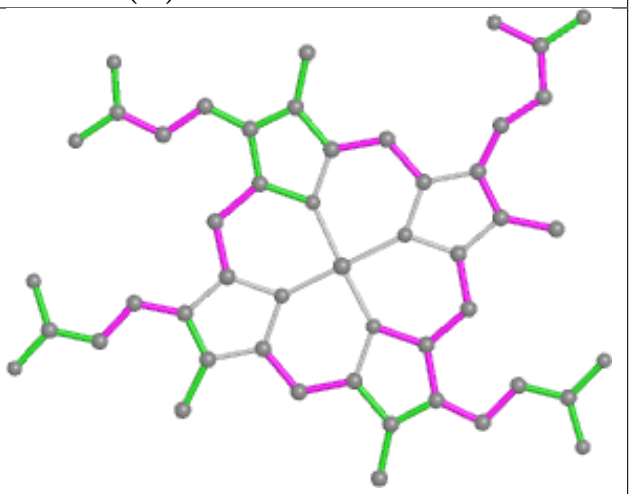
Ligand FEC I 1807 (A)



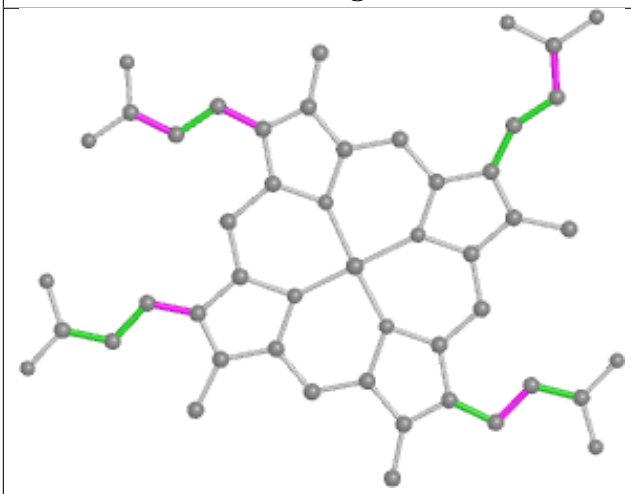
Ligand FEC B 1107 (B)



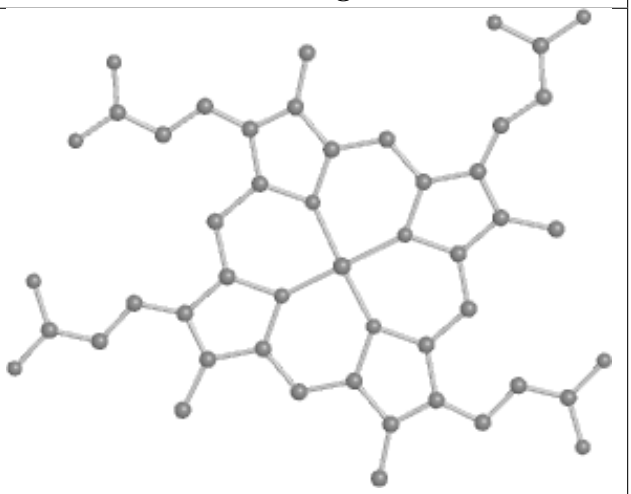
Bond lengths



Bond angles

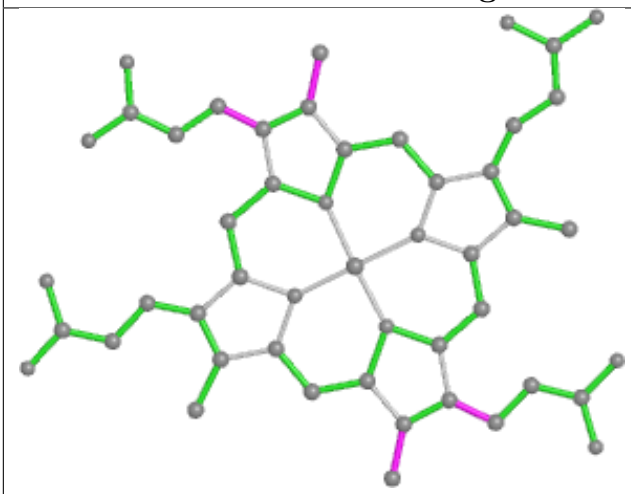


Torsions

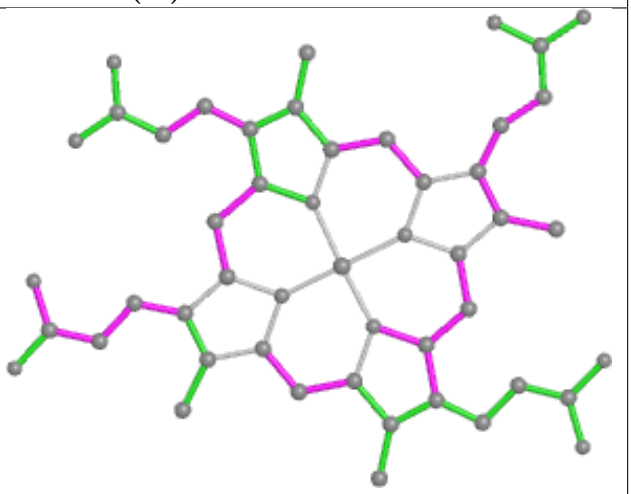


Rings

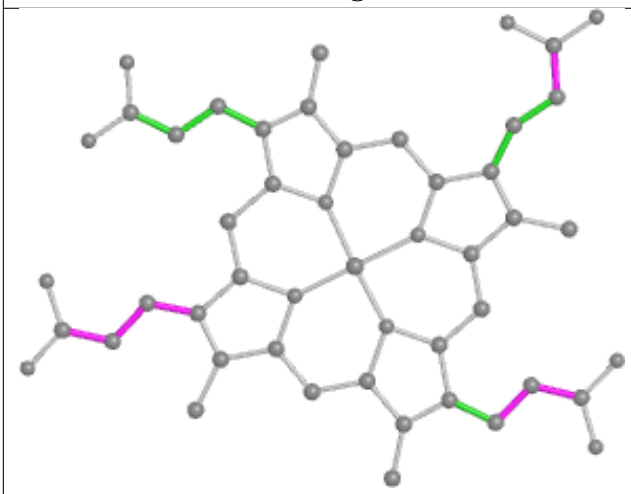
Ligand FEC M 2207 (A)



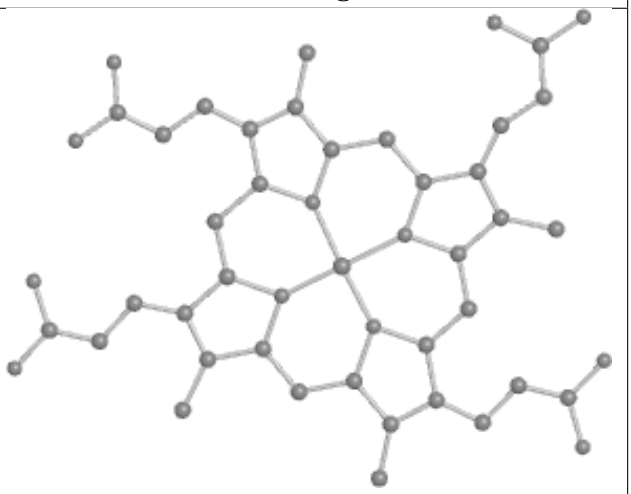
Bond lengths



Bond angles

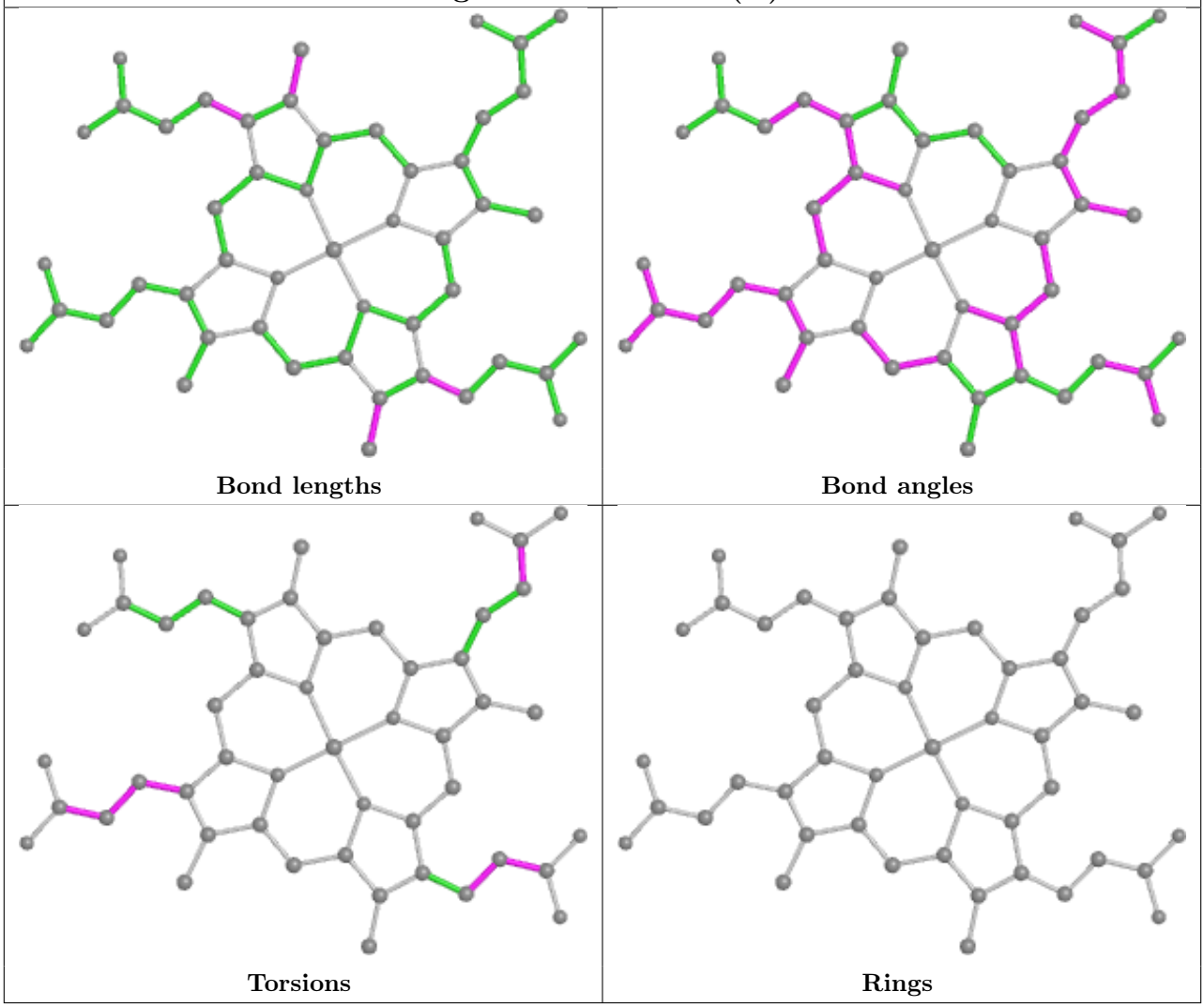


Torsions

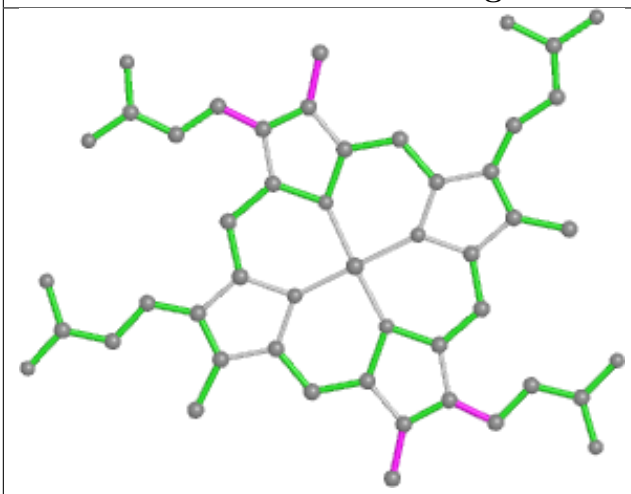


Rings

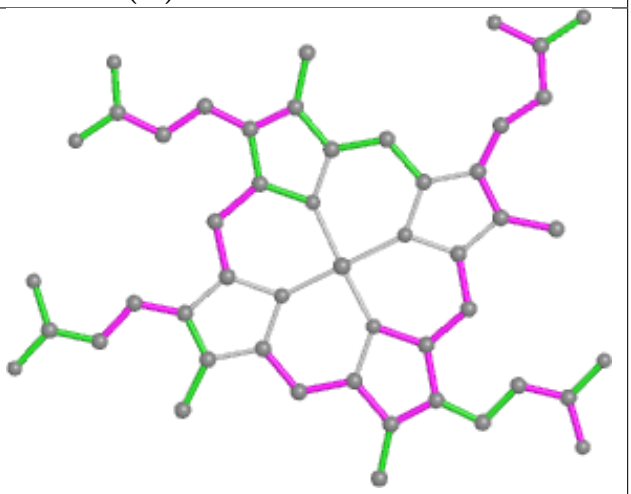
Ligand FEC G 1608 (A)



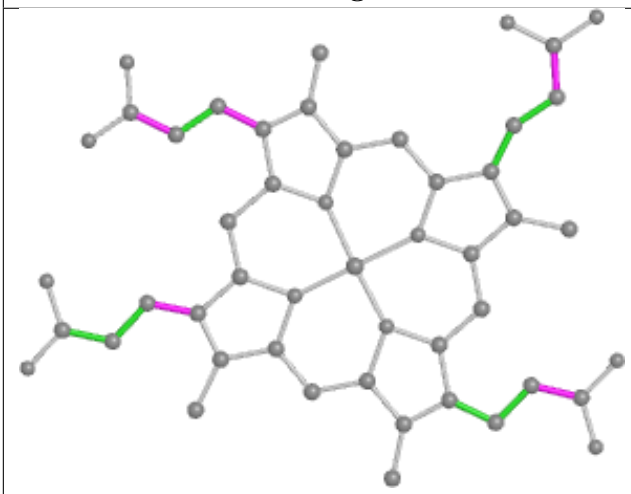
Ligand FEC P 2507 (B)



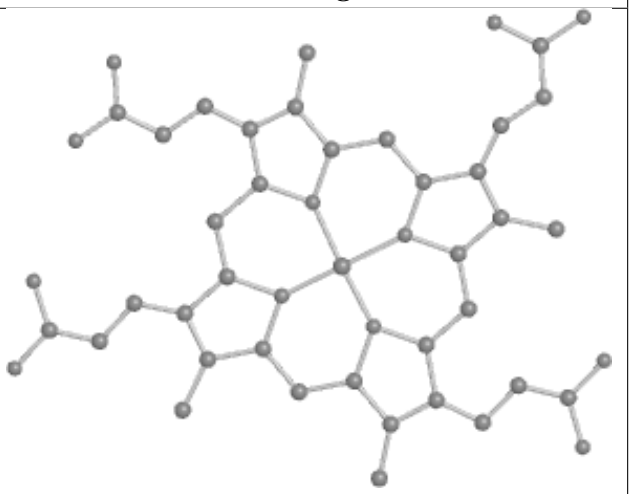
Bond lengths



Bond angles

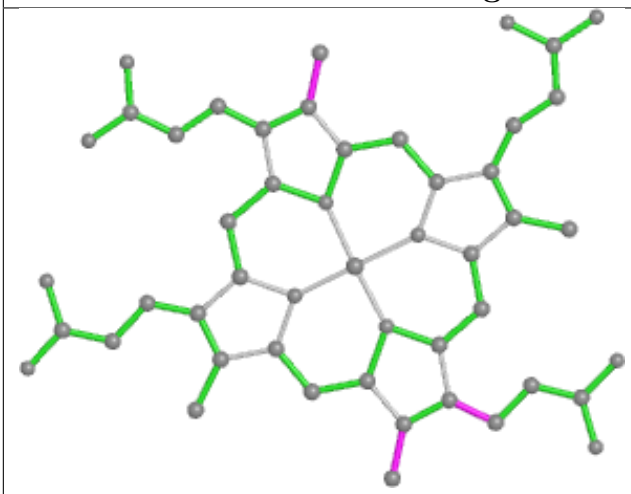


Torsions

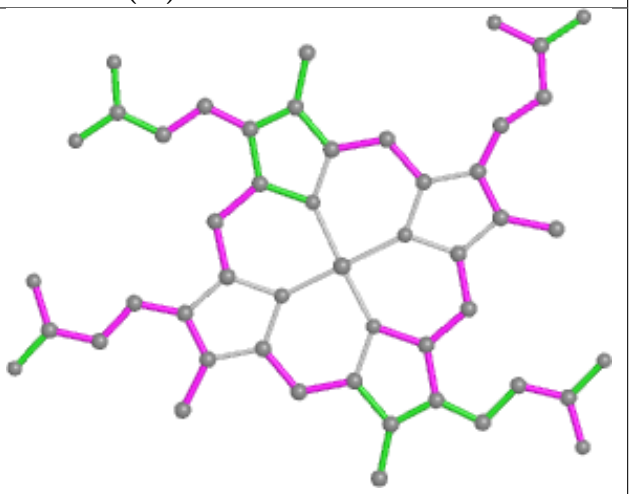


Rings

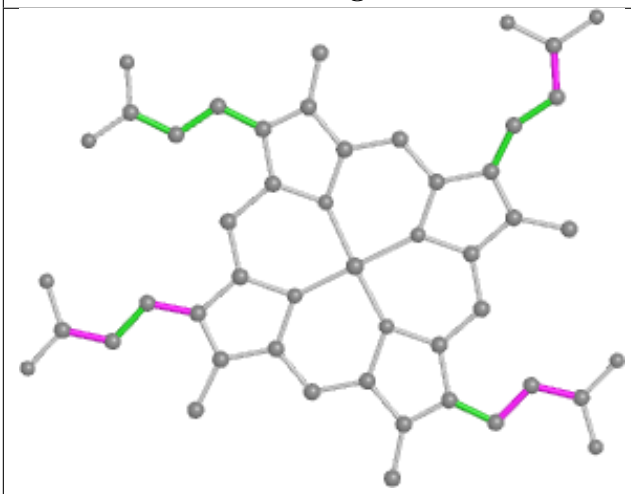
Ligand FEC B 1107 (A)



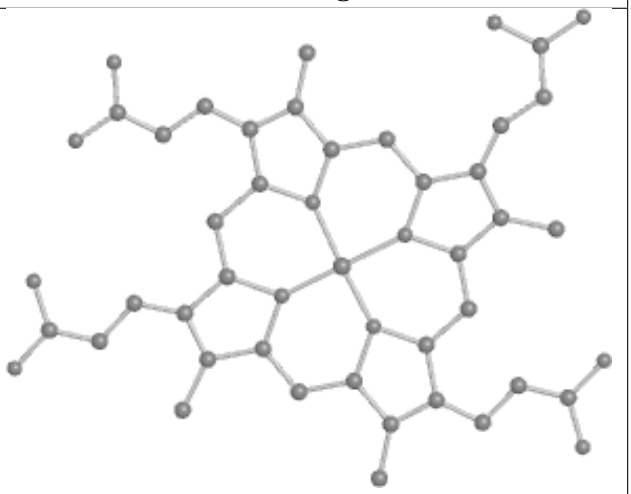
Bond lengths



Bond angles

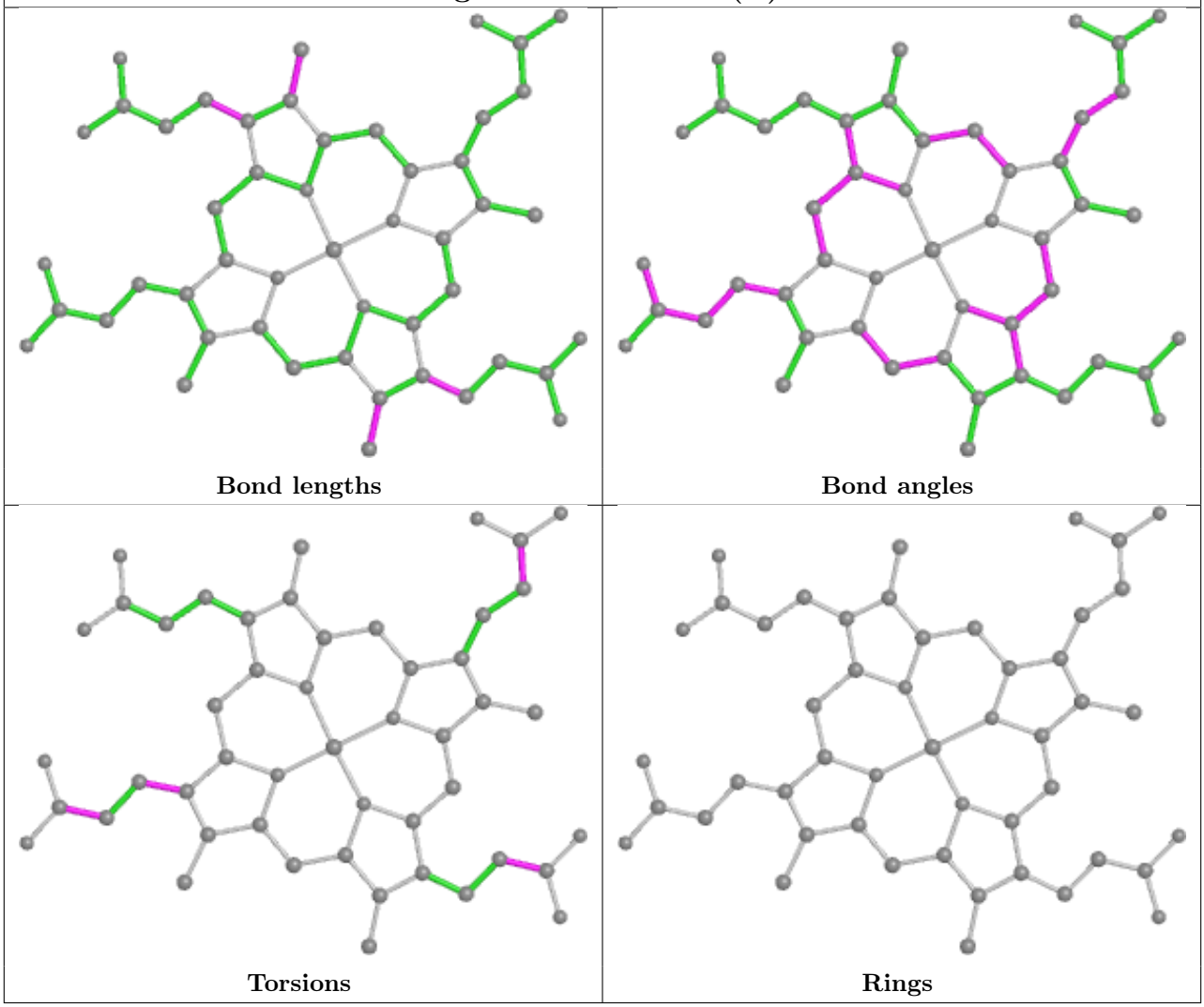


Torsions



Rings

Ligand FEC D 1311 (B)



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	169/179 (94%)	0.11	10 (5%)	22	30	16, 24, 43, 65	0
1	B	170/179 (94%)	-0.03	9 (5%)	26	35	15, 24, 45, 65	0
1	C	170/179 (94%)	-0.05	8 (4%)	31	41	16, 25, 45, 65	0
1	D	170/179 (94%)	0.02	9 (5%)	26	35	16, 25, 44, 65	1 (0%)
1	E	170/179 (94%)	0.05	9 (5%)	26	35	17, 25, 47, 65	1 (0%)
1	F	170/179 (94%)	-0.03	7 (4%)	37	46	16, 25, 46, 68	1 (0%)
1	G	169/179 (94%)	-0.08	4 (2%)	59	68	15, 24, 43, 65	0
1	H	170/179 (94%)	0.01	12 (7%)	16	24	16, 25, 44, 65	0
1	I	170/179 (94%)	-0.00	6 (3%)	44	53	16, 24, 43, 65	0
1	J	170/179 (94%)	-0.02	9 (5%)	26	35	17, 25, 47, 65	0
1	K	170/179 (94%)	-0.06	4 (2%)	59	68	16, 24, 46, 68	0
1	L	170/179 (94%)	-0.01	4 (2%)	59	68	16, 24, 43, 65	1 (0%)
1	M	170/179 (94%)	-0.04	7 (4%)	37	46	15, 24, 47, 65	0
1	N	170/179 (94%)	-0.03	6 (3%)	44	53	16, 24, 43, 65	0
1	O	169/179 (94%)	0.10	6 (3%)	42	52	16, 25, 44, 68	1 (0%)
1	P	170/179 (94%)	-0.09	7 (4%)	37	46	17, 25, 48, 65	0
All	All	2717/2864 (94%)	-0.01	117 (4%)	35	45	15, 25, 46, 68	5 (0%)

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	THR	7.2
1	A	166	THR	7.1
1	E	168[A]	SER	6.8
1	N	166	THR	6.6
1	I	166	THR	6.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	1004	5/5	0.45	0.48	66,66,67,67	5
3	SO4	G	1607	5/5	0.61	0.38	67,67,70,70	0
3	SO4	J	1901	5/5	0.73	0.29	66,67,67,69	0
3	SO4	K	1504	5/5	0.73	0.23	78,78,78,79	0
3	SO4	E	1304	5/5	0.75	0.39	65,65,67,67	0
3	SO4	O	2409	5/5	0.76	0.40	57,63,66,67	0
4	GOL	E	1411	6/6	0.77	0.19	34,56,92,108	0
2	FE	B	201	1/1	0.78	0.09	44,44,44,44	0
3	SO4	D	1303	5/5	0.78	0.23	39,44,45,50	5
4	GOL	J	1910	6/6	0.78	0.30	46,52,80,104	0
3	SO4	G	1603	5/5	0.79	0.41	73,73,74,75	0
3	SO4	P	2503	5/5	0.79	0.28	42,43,47,49	5
2	FE	L	201	1/1	0.79	0.11	42,42,42,42	0
4	GOL	I	1713	6/6	0.79	0.21	52,57,84,157	0
3	SO4	L	2103	5/5	0.79	0.36	78,78,78,79	0
3	SO4	H	1703	5/5	0.80	0.48	40,43,48,48	0
4	GOL	A	1010	6/6	0.81	0.29	42,68,89,111	0
4	GOL	I	1810	6/6	0.81	0.30	27,42,66,76	0
3	SO4	F	1502	5/5	0.81	0.44	69,69,69,71	0
3	SO4	K	2001	5/5	0.82	0.26	51,53,53,54	0
4	GOL	B	1110	6/6	0.82	0.20	40,46,69,84	0
4	GOL	H	1710	6/6	0.83	0.26	50,52,61,94	0
4	GOL	H	1814	6/6	0.83	0.16	38,49,55,61	0
3	SO4	E	1401	5/5	0.83	0.28	67,68,68,68	0
3	SO4	L	2101	5/5	0.83	0.20	64,64,65,65	0
4	GOL	G	1611	6/6	0.83	0.19	31,53,70,78	0
3	SO4	C	1201	5/5	0.84	0.19	65,65,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	P	2501	5/5	0.84	0.18	62,62,63,63	0
3	SO4	J	1906	5/5	0.85	0.35	50,51,59,59	0
3	SO4	M	2206	5/5	0.85	0.31	58,60,67,70	0
3	SO4	G	1606	5/5	0.86	0.26	58,65,67,73	0
4	GOL	G	1610	6/6	0.86	0.20	44,46,56,106	0
4	GOL	M	2211	6/6	0.86	0.16	40,61,98,143	0
4	GOL	P	2510	6/6	0.86	0.28	32,51,74,105	0
2	FE	M	201	1/1	0.87	0.10	40,40,40,40	0
4	GOL	C	1210	6/6	0.87	0.29	32,43,67,71	0
3	SO4	C	1206	5/5	0.87	0.36	46,46,47,49	0
3	SO4	D	1301	5/5	0.87	0.24	58,59,60,60	0
3	SO4	I	1803	5/5	0.87	0.36	67,67,70,70	0
4	GOL	N	2310	6/6	0.87	0.18	38,48,69,155	0
4	GOL	O	2410	6/6	0.87	0.21	47,53,59,61	0
2	FE	A	201	1/1	0.87	0.12	44,44,44,44	0
6	3PY	D	1310	6/7	0.87	0.19	50,63,70,78	0
3	SO4	A	1001	5/5	0.88	0.22	53,54,54,55	0
2	FE	D	201	1/1	0.88	0.09	46,46,46,46	0
4	GOL	J	1811	6/6	0.88	0.23	40,57,107,154	0
3	SO4	O	2406	5/5	0.88	0.20	41,44,46,47	5
4	GOL	F	1510	6/6	0.88	0.21	52,62,92,104	0
3	SO4	B	1101	5/5	0.88	0.17	66,66,67,67	0
3	SO4	B	1106	5/5	0.88	0.34	64,66,74,75	0
2	FE	F	201	1/1	0.88	0.06	46,46,46,46	0
3	SO4	H	1706	5/5	0.88	0.34	47,55,58,60	0
3	SO4	A	1105	5/5	0.89	0.47	51,53,55,61	0
3	SO4	N	2306	5/5	0.89	0.23	60,65,69,71	0
3	SO4	A	1006	5/5	0.89	0.36	56,67,69,74	0
3	SO4	C	1203	5/5	0.89	0.34	56,58,62,64	0
3	SO4	B	1104	5/5	0.90	0.15	73,73,74,75	0
3	SO4	H	1701	5/5	0.90	0.21	54,54,55,56	0
3	SO4	N	2303	5/5	0.90	0.50	64,68,70,72	0
4	GOL	B	1011	6/6	0.90	0.17	24,48,57,79	0
4	GOL	M	2210	6/6	0.90	0.25	34,50,95,99	0
3	SO4	A	1008	5/5	0.91	0.42	51,53,55,61	0
4	GOL	D	1211	6/6	0.91	0.12	45,49,55,68	0
3	SO4	I	1806	5/5	0.91	0.30	62,65,67,69	0
3	SO4	F	1506	5/5	0.91	0.25	65,67,68,69	0
3	SO4	L	2107	5/5	0.91	0.19	78,78,78,79	0
3	SO4	M	2201	5/5	0.91	0.18	51,51,52,53	0
2	FE	K	201	1/1	0.91	0.09	43,43,43,43	0
3	SO4	N	2301	5/5	0.91	0.21	62,63,63,63	0

Continued on next page...

Continued from previous page...

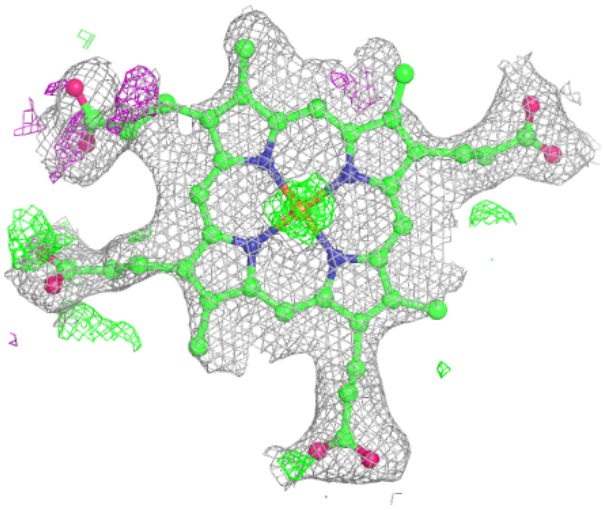
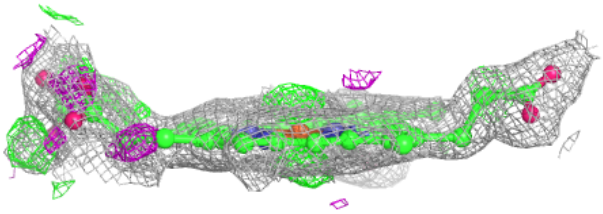
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	F	1501	5/5	0.91	0.15	66,66,67,67	0
2	FE	G	201	1/1	0.92	0.08	43,43,43,43	0
4	GOL	K	2011	6/6	0.92	0.14	46,57,59,146	0
4	GOL	O	2411	6/6	0.92	0.10	26,52,74,76	0
2	FE	H	201	1/1	0.92	0.09	43,43,43,43	0
4	GOL	E	1410	6/6	0.92	0.24	39,50,75,155	0
2	FE	J	201	1/1	0.93	0.07	46,46,46,46	0
3	SO4	J	1904	5/5	0.93	0.21	61,61,62,63	5
2	FE	N	201	1/1	0.93	0.09	43,43,43,43	0
2	FE	C	201	1/1	0.93	0.08	46,46,46,46	0
3	SO4	B	1005	5/5	0.93	0.28	51,53,55,61	0
3	SO4	K	2003	5/5	0.93	0.29	69,69,69,71	0
2	FE	I	201	1/1	0.93	0.09	43,43,43,43	0
3	SO4	E	1406	5/5	0.94	0.22	62,67,67,70	0
3	SO4	I	1801	5/5	0.94	0.17	61,61,62,63	0
2	FE	E	201	1/1	0.95	0.07	44,44,44,44	0
4	GOL	F	1512	6/6	0.95	0.14	22,37,47,49	0
3	SO4	K	2006	5/5	0.95	0.23	52,55,60,61	0
3	SO4	P	2506	5/5	0.95	0.24	57,63,66,67	0
3	SO4	I	1802	5/5	0.95	0.15	36,37,38,38	0
5	FEC	D	1311[A]	49/49	0.95	0.19	15,19,28,37	49
5	FEC	D	1311[B]	49/49	0.95	0.19	10,19,28,46	49
2	FE	P	201	1/1	0.95	0.05	45,45,45,45	0
5	FEC	B	1107[B]	49/49	0.96	0.20	15,18,27,38	49
2	FE	O	201	1/1	0.96	0.09	46,46,46,46	0
3	SO4	L	2102	5/5	0.96	0.16	78,78,78,79	5
5	FEC	F	1507[A]	49/49	0.96	0.17	15,19,29,36	49
5	FEC	F	1507[B]	49/49	0.96	0.17	16,19,31,38	49
5	FEC	G	1608[A]	49/49	0.96	0.19	15,18,28,37	49
5	FEC	G	1608[B]	49/49	0.96	0.19	10,17,29,38	49
5	FEC	P	2507[A]	49/49	0.96	0.17	15,18,28,37	49
5	FEC	P	2507[B]	49/49	0.96	0.17	16,18,28,33	49
5	FEC	B	1107[A]	49/49	0.96	0.20	15,18,28,37	49
5	FEC	L	2108[B]	49/49	0.97	0.19	13,18,28,39	49
5	FEC	M	2207[A]	49/49	0.97	0.18	14,18,28,37	49
5	FEC	M	2207[B]	49/49	0.97	0.18	13,18,27,39	49
5	FEC	I	1807[A]	49/49	0.97	0.18	15,19,28,37	49
5	FEC	I	1807[B]	49/49	0.97	0.18	14,19,27,38	49
5	FEC	L	2108[A]	49/49	0.97	0.19	15,18,28,37	49
2	FE	A	200	1/1	0.98	0.07	27,27,27,27	0
2	FE	K	200	1/1	0.99	0.06	28,28,28,28	0
2	FE	C	200	1/1	0.99	0.04	28,28,28,28	0

Continued on next page...

Continued from previous page...

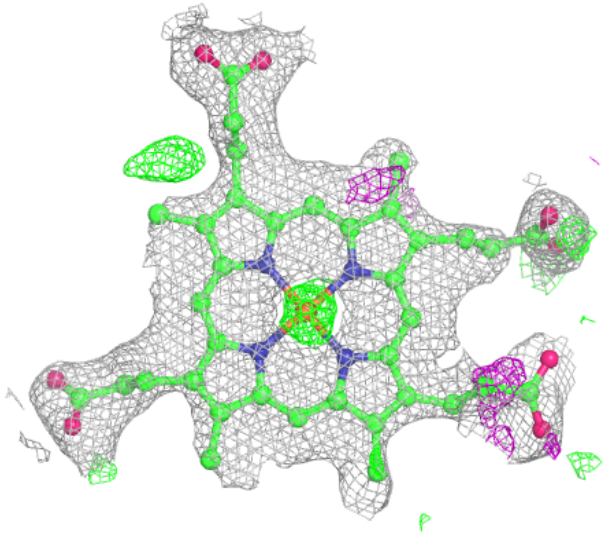
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	L	200	1/1	0.99	0.07	26,26,26,26	0
2	FE	H	200	1/1	0.99	0.04	26,26,26,26	0
2	FE	M	200	1/1	0.99	0.07	26,26,26,26	0
2	FE	F	200	1/1	0.99	0.06	29,29,29,29	0
2	FE	N	200	1/1	0.99	0.05	25,25,25,25	0
2	FE	I	200	1/1	0.99	0.06	27,27,27,27	0
2	FE	O	200	1/1	0.99	0.07	29,29,29,29	0
2	FE	E	200	1/1	0.99	0.08	29,29,29,29	0
2	FE	P	200	1/1	0.99	0.05	28,28,28,28	0
2	FE	J	200	1/1	0.99	0.05	30,30,30,30	0
2	FE	G	200	1/1	0.99	0.06	26,26,26,26	0
2	FE	D	200	1/1	1.00	0.06	29,29,29,29	0
2	FE	B	200	1/1	1.00	0.07	25,25,25,25	0

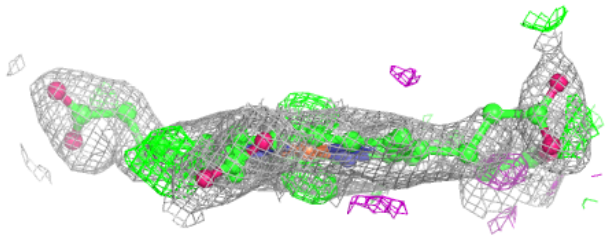
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

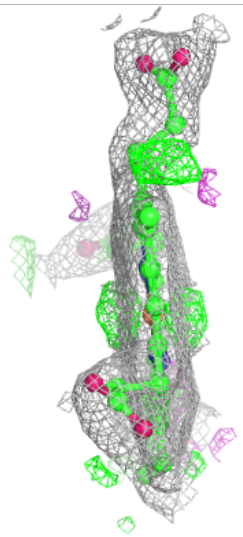
Electron density around FEC D 1311 (A): 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around FEC D 1311 (B):

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

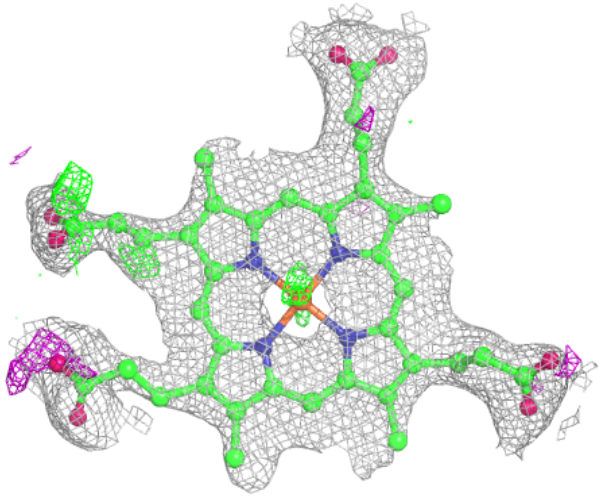


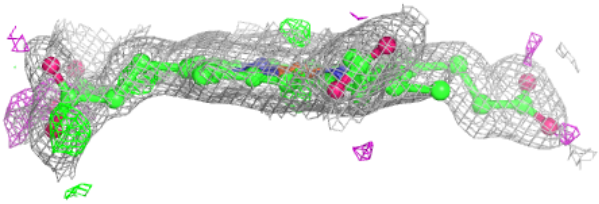


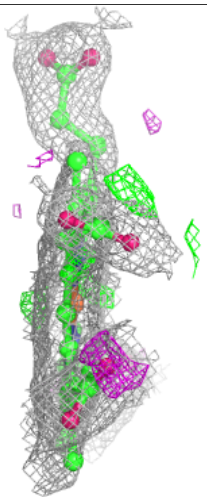


Electron density around FEC B 1107 (B):

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

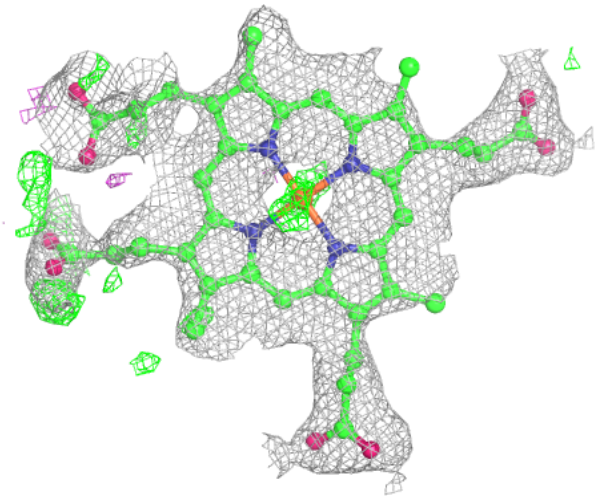


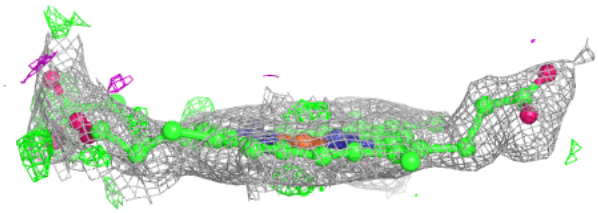


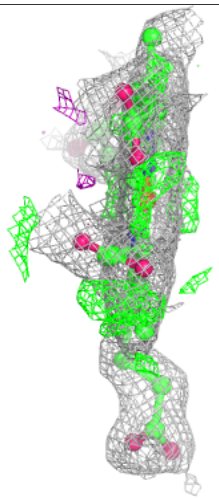


Electron density around FEC F 1507 (A):

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

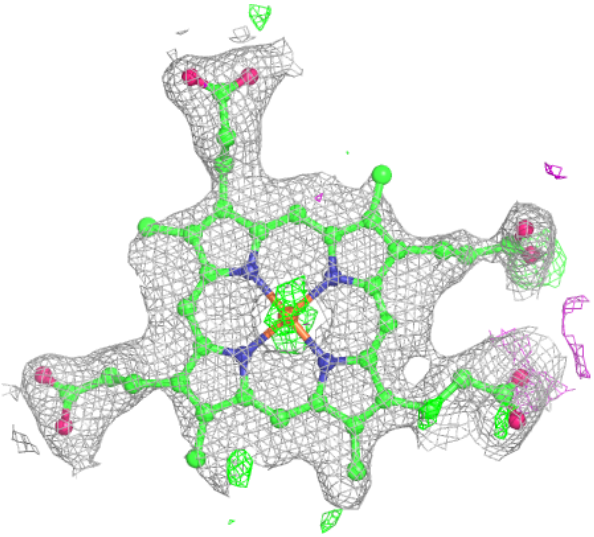


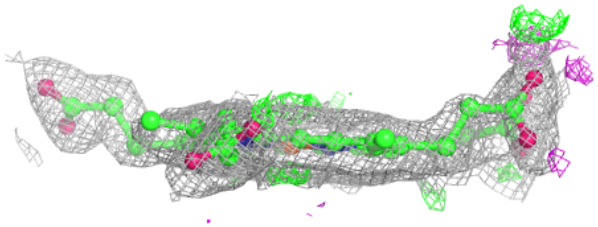


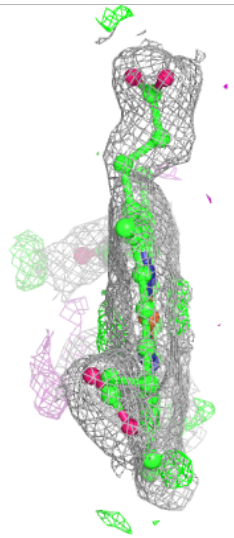


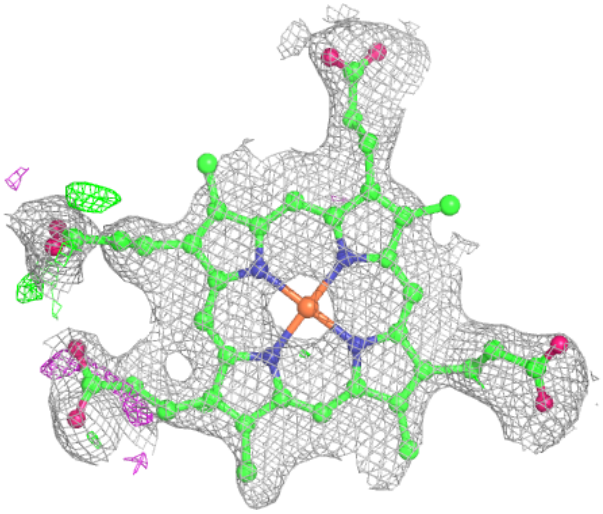
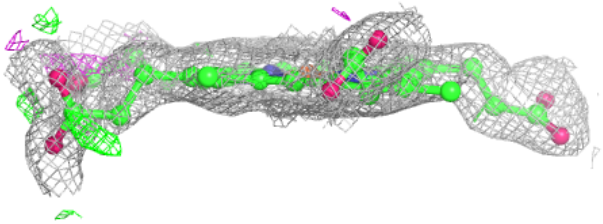
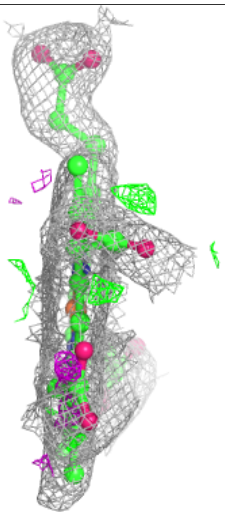
Electron density around FEC F 1507 (B):

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



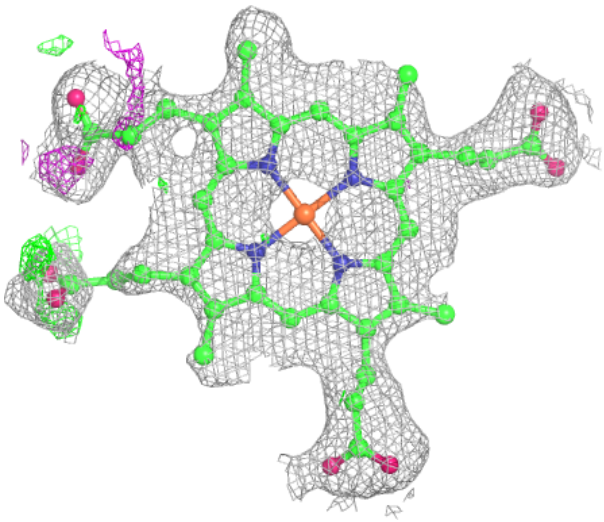


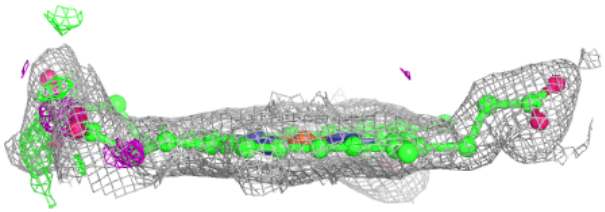


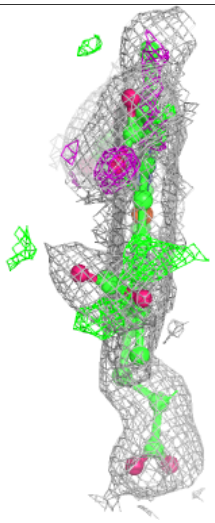
Electron density around FEC G 1608 (A): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around FEC G 1608 (B):

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

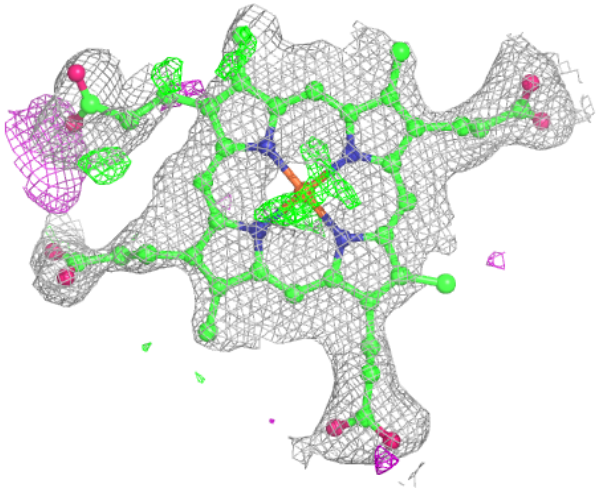


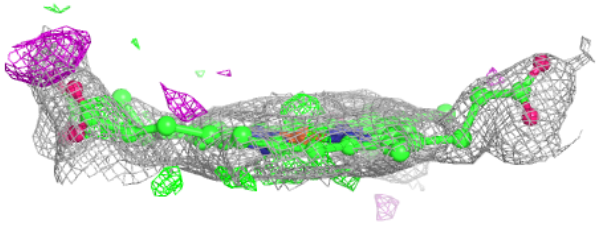


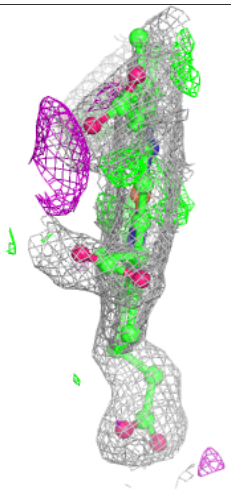


Electron density around FEC P 2507 (A):

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

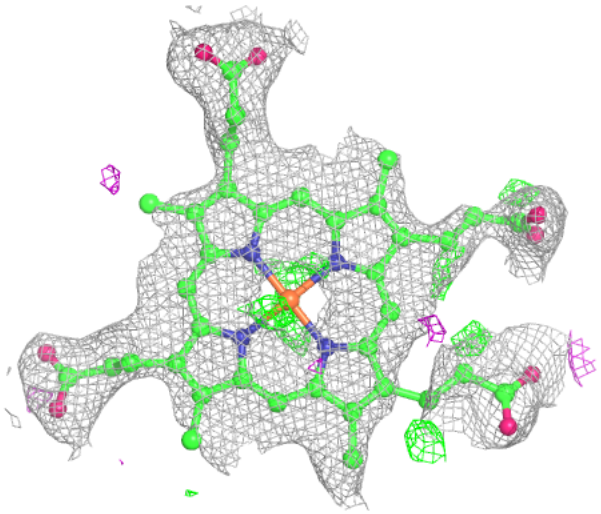


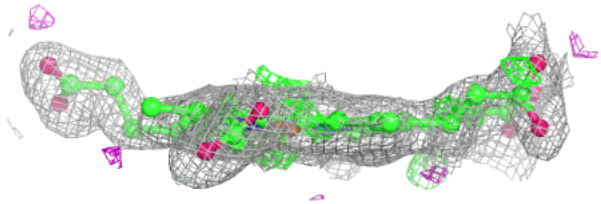


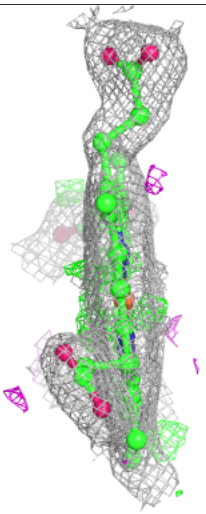


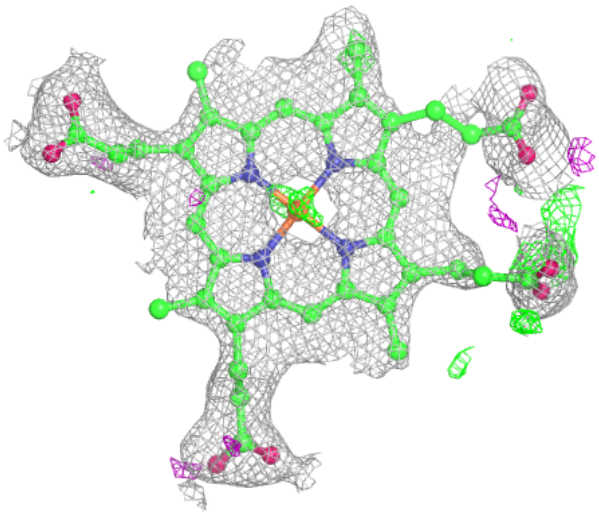
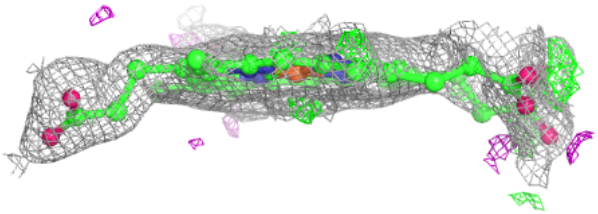
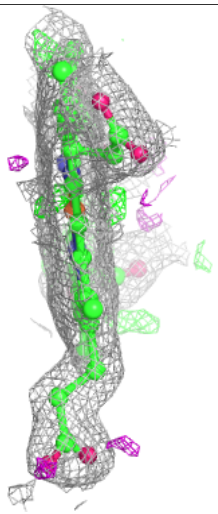
Electron density around FEC P 2507 (B):

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



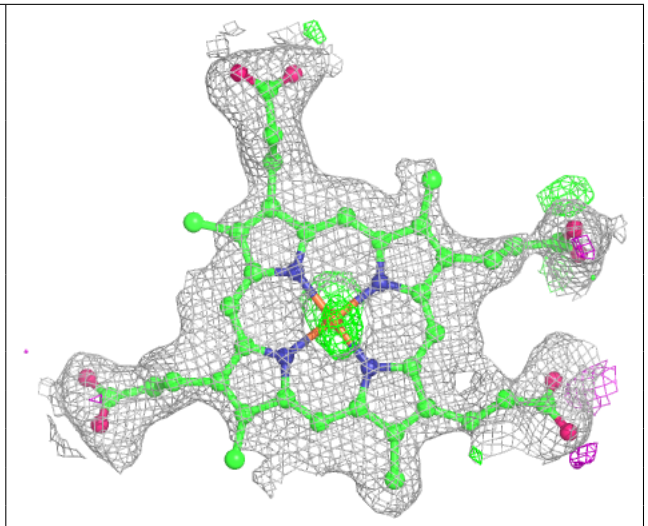


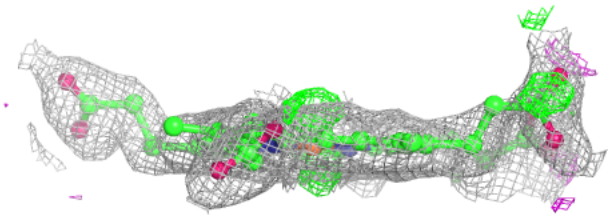


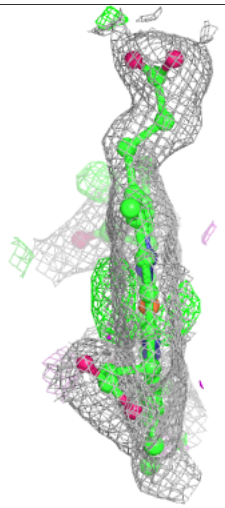
Electron density around FEC B 1107 (A): 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around FEC L 2108 (B):

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

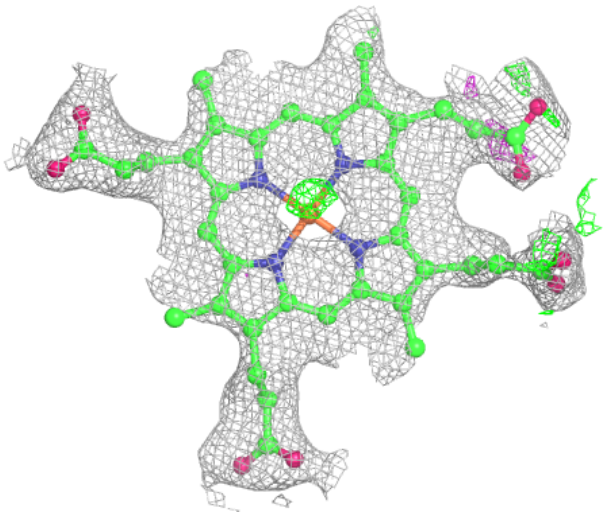


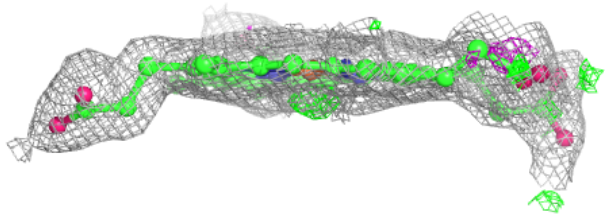


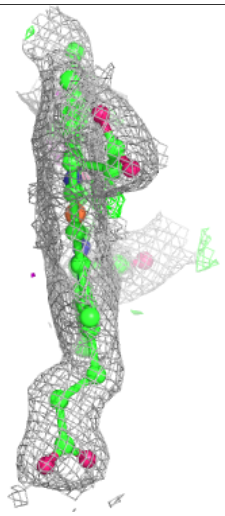


Electron density around FEC M 2207 (A):

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

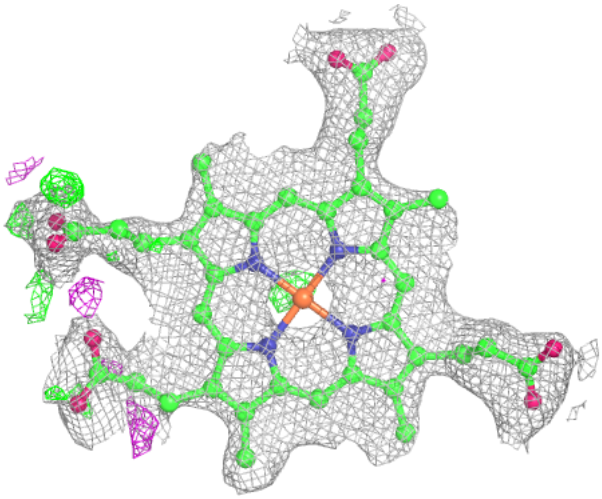


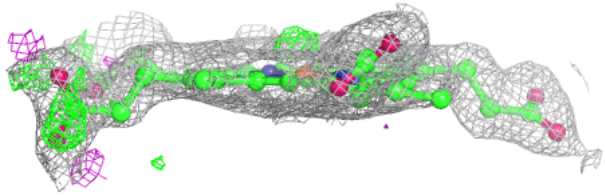


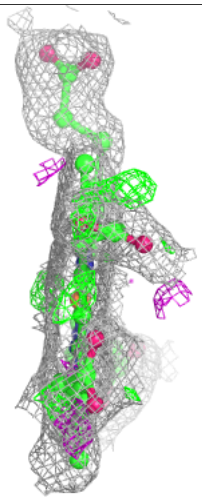


Electron density around FEC M 2207 (B):

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

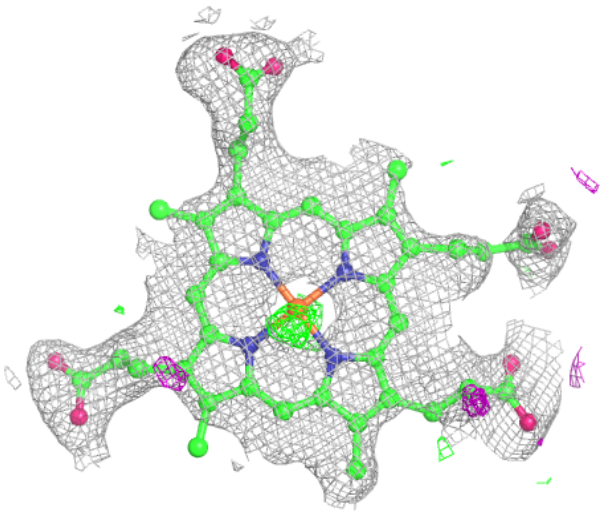


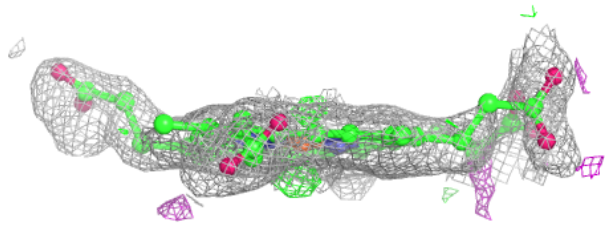


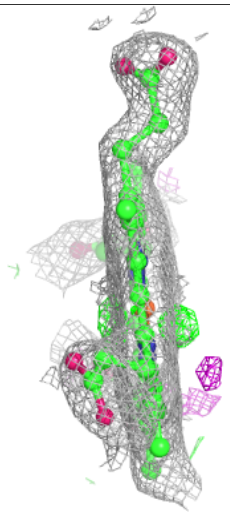


Electron density around FEC I 1807 (A):

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

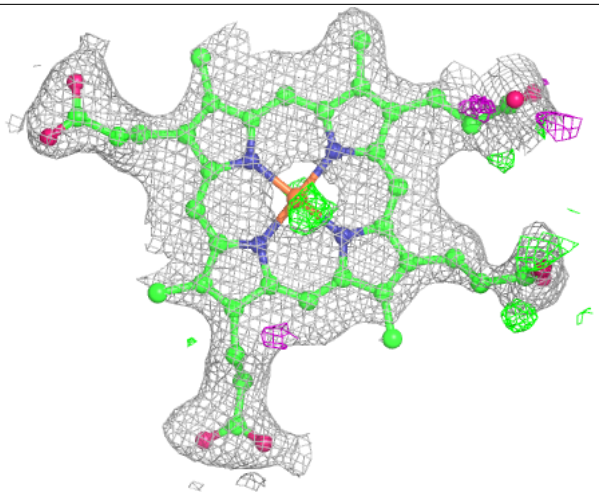


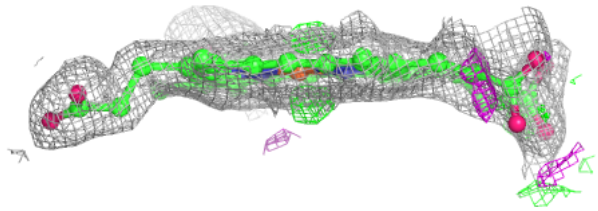


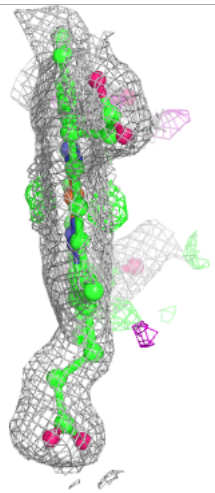


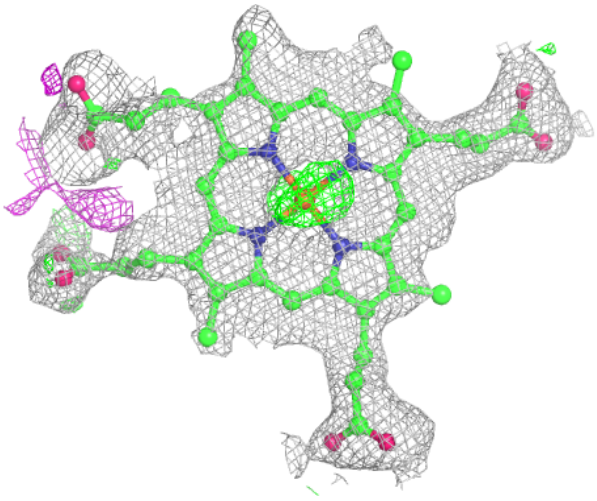
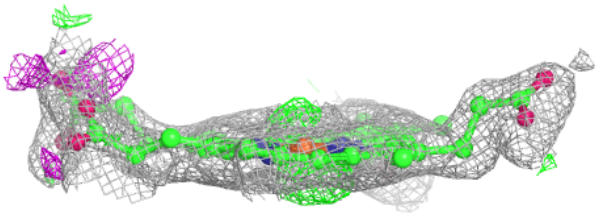
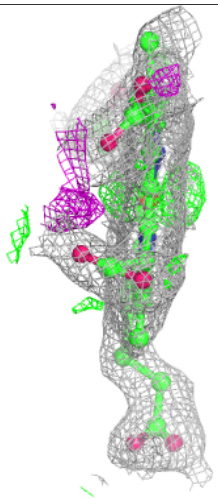
Electron density around FEC I 1807 (B):

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







Electron density around FEC L 2108 (A): 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.