wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 04:50 PM EDT

PDB ID	:	1NF6
Title	:	X-ray structure of the Desulfovibrio desulfuricans bacterioferritin: the diiron site in different catalytic states ("cycled" structure: reduced in solution and allowed to reoxidise before crystallisation)
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	:	2002-12-13
Resolution	:	2.35 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:

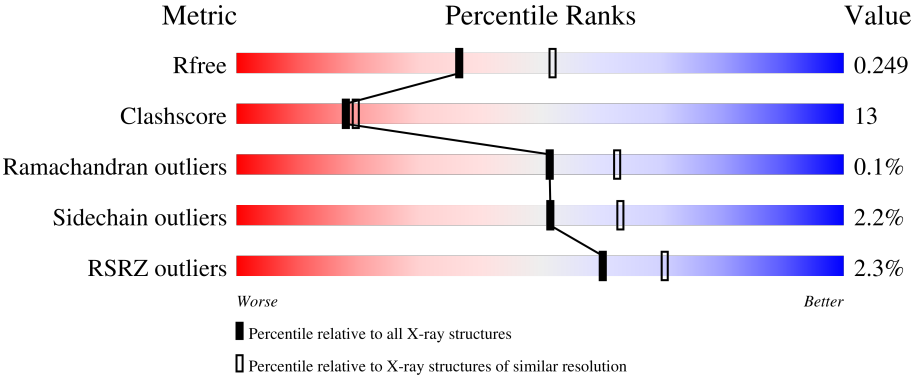
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	3% 74% 21% • 5%
1	B	179	3% 71% 23% • 5%
1	C	179	3% 72% 22% • 5%
1	D	179	4% 75% 18% • 5%
1	E	179	2% 66% 27% • 5%

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Mol	Chain	Length	Quality of chain
1	F	179	3% 70% 25%
1	G	179	2% 69% 25% 6%
1	H	179	2% 79% 16% 5%
1	I	179	% 75% 20% 5%
1	J	179	2% 71% 22% 5%
1	K	179	% 73% 21% 6%
1	L	179	% 77% 17% 5%
1	M	179	2% 75% 17% 6%
1	N	179	% 73% 20% 5%
1	O	179	2% 66% 28% 6%
1	P	179	2% 69% 26% 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	I	1804	-	-	X	-
3	SO4	J	2004	-	-	X	-
3	SO4	L	2204	-	-	X	-
3	SO4	N	1204	-	-	X	-
5	GOL	P	2615	-	X	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 23933 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.

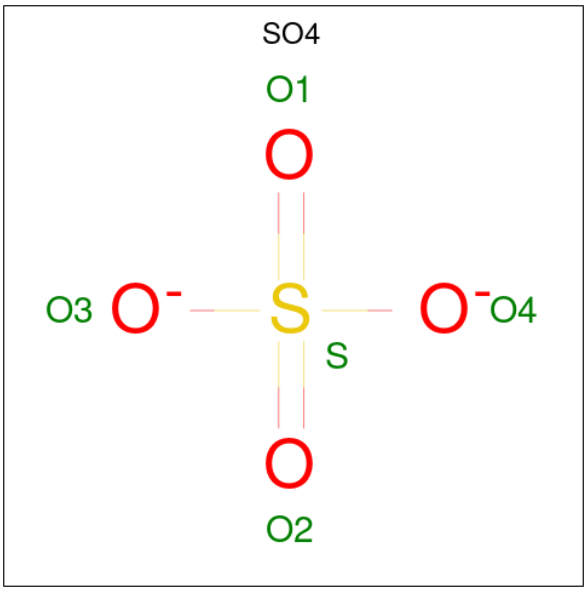
- Molecule 1 is a protein called bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	170	1324	824	228	266	6	0	0	0
1	B	170	1321	824	228	263	6	0	0	0
1	C	170	1324	824	228	266	6	0	0	0
1	D	170	1320	822	227	265	6	0	0	0
1	E	170	1315	820	225	264	6	0	0	0
1	F	171	1319	821	225	267	6	0	0	0
1	G	169	1324	825	226	267	6	0	1	0
1	H	170	1328	828	229	265	6	0	0	0
1	I	170	1318	820	224	268	6	0	0	0
1	J	170	1333	833	230	264	6	0	1	0
1	K	169	1321	823	226	266	6	0	0	0
1	L	170	1325	825	229	265	6	0	1	0
1	M	169	1316	820	226	264	6	0	0	0
1	N	170	1317	820	227	264	6	0	0	0
1	O	169	1313	817	224	266	6	0	0	0
1	P	170	1328	827	228	267	6	0	0	0

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

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

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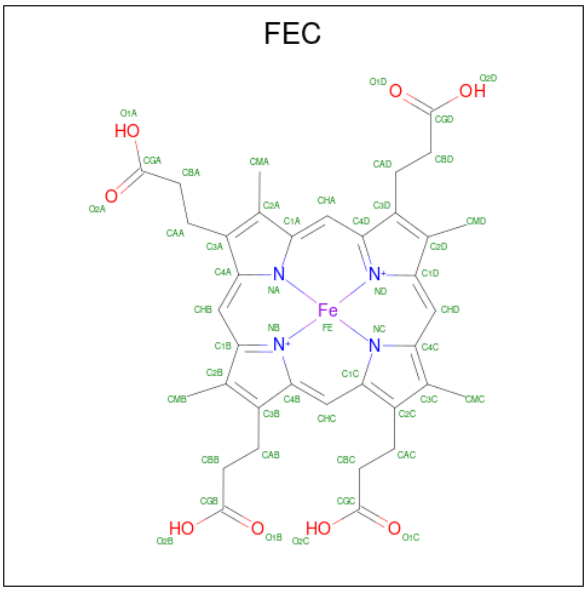
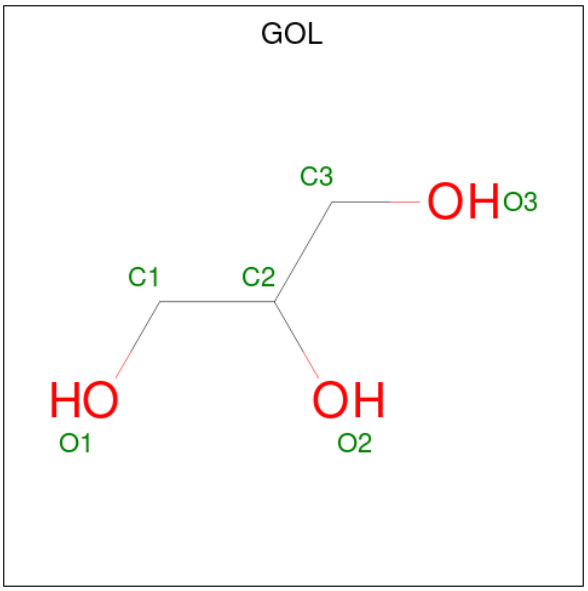
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	1	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0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

- Molecule 4 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		
4	A	1	98	72	2	8	16	0	1
			Total	C	Fe	N	O		
4	C	1	98	72	2	8	16	0	1
			Total	C	Fe	N	O		
4	F	1	98	72	2	8	16	0	1
			Total	C	Fe	N	O		
4	G	1	98	72	2	8	16	0	1
			Total	C	Fe	N	O		
4	I	1	98	72	2	8	16	0	1
			Total	C	Fe	N	O		
4	K	1	98	72	2	8	16	0	1
			Total	C	Fe	N	O		
4	N	1	98	72	2	8	16	0	1
			Total	C	Fe	N	O		
4	O	1	98	72	2	8	16	0	1

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	121	121	121	0	0
6	B	115	115	115	0	0
6	C	92	92	92	0	0
6	D	114	114	114	0	0
6	E	92	92	92	0	0
6	F	112	112	112	0	0
6	G	130	130	130	0	0
6	H	97	97	97	0	0
6	I	132	132	132	0	0
6	J	113	113	113	0	0
6	K	133	133	133	0	0

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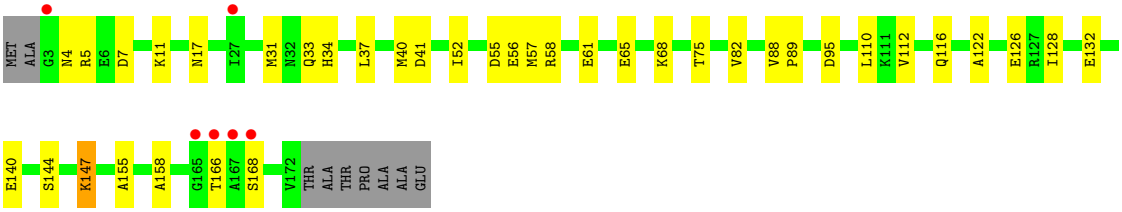
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	L	131	131	131	0	0
			Total	O		
6	M	128	128	128	0	0
			Total	O		
6	N	119	119	119	0	0
			Total	O		
6	O	77	77	77	0	0
			Total	O		
6	P	105	105	105	0	0

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.

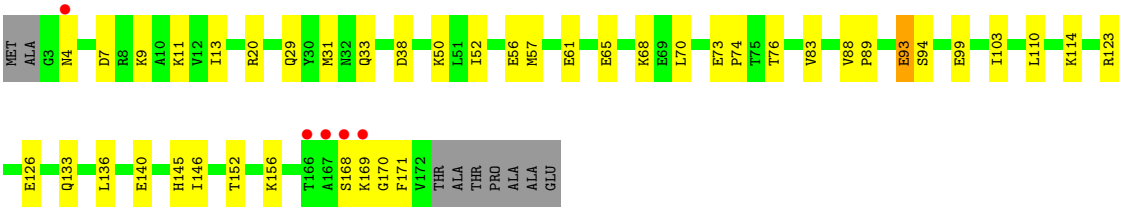
- Molecule 1: bacterioferritin

Chain A:



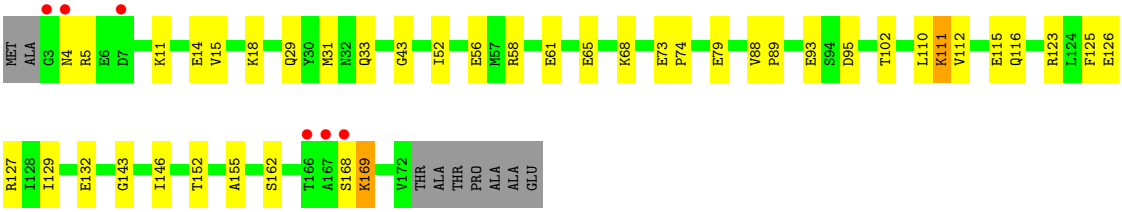
- Molecule 1: bacterioferritin

Chain B:



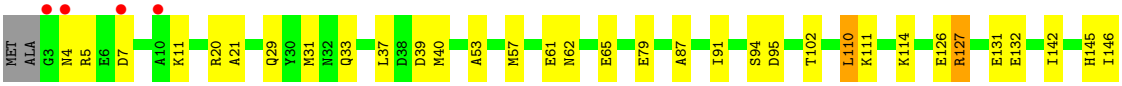
- Molecule 1: bacterioferritin

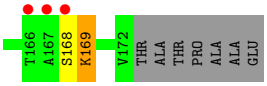
Chain C:



- Molecule 1: bacterioferritin

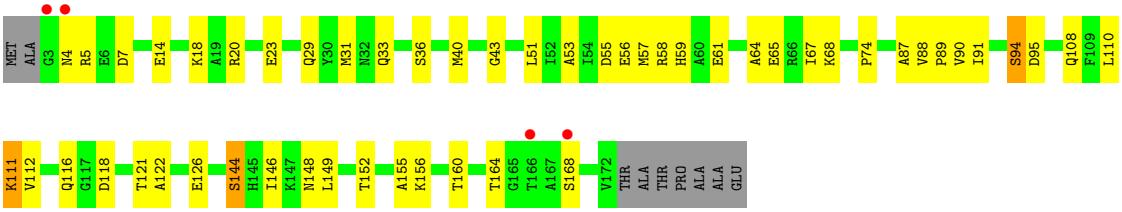
Chain D:





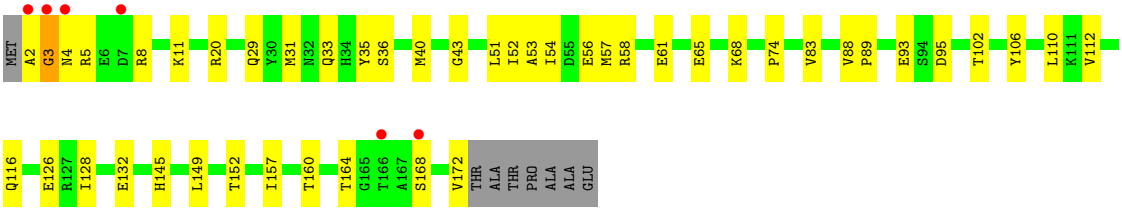
• Molecule 1: bacterioferritin

Chain E:



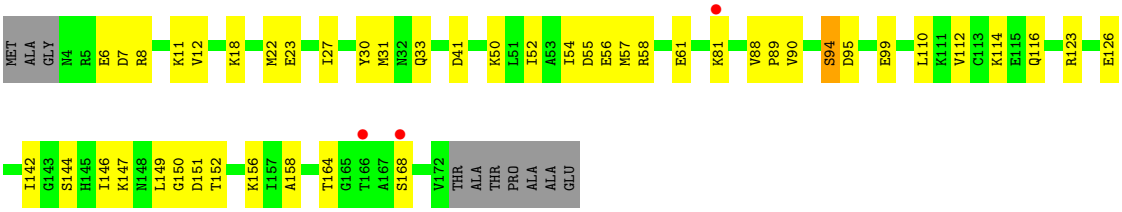
• Molecule 1: bacterioferritin

Chain F:



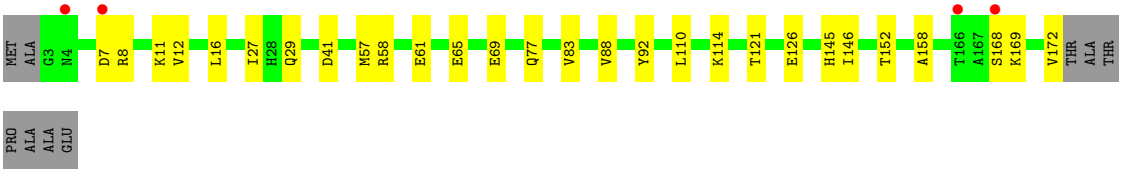
• Molecule 1: bacterioferritin

Chain G:



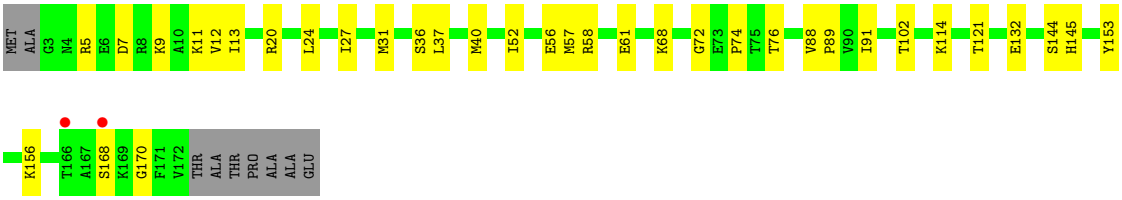
• Molecule 1: bacterioferritin

Chain H:



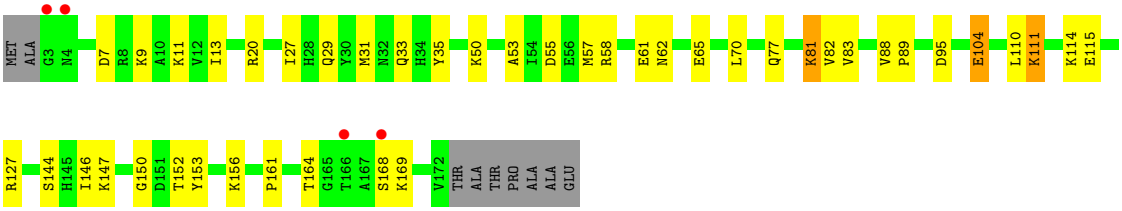
• Molecule 1: bacterioferritin

Chain I:



• Molecule 1: bacterioferritin

Chain J:

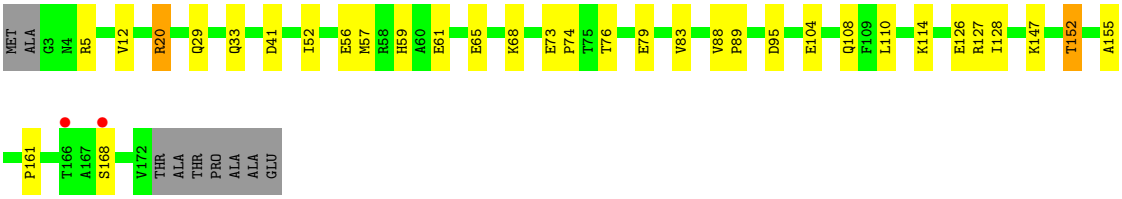


• Molecule 1: bacterioferritin

Chain K:

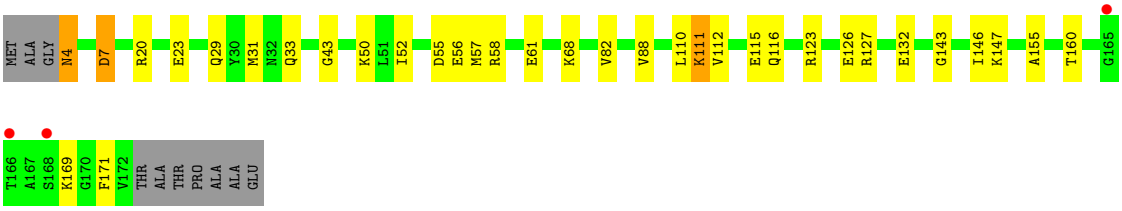
• Molecule 1: bacterioferritin

Chain L:



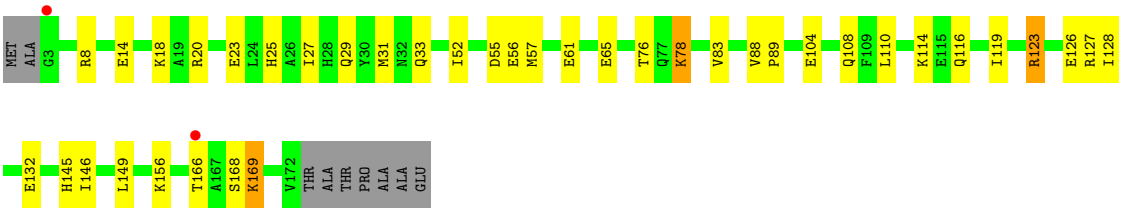
• Molecule 1: bacterioferritin

Chain M:



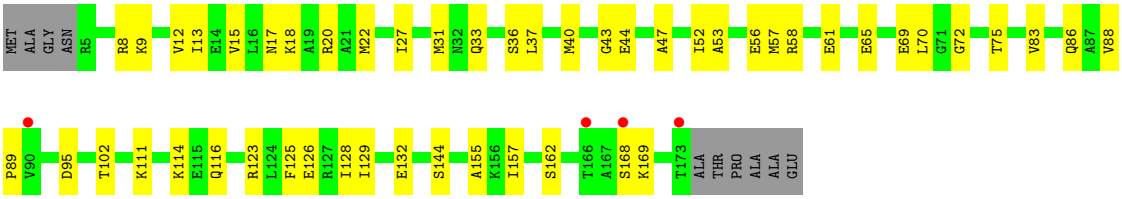
• Molecule 1: bacterioferritin

Chain N:



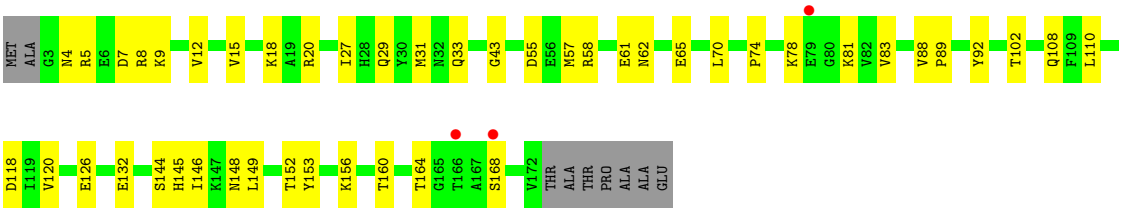
- Molecule 1: bacterioferritin

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	225.79Å 225.79Å 225.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 29.91 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-2.35) 96.1 (29.91-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 2.36Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.197 , 0.267 0.189 , 0.249	Depositor DCC
R_{free} test set	3041 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.048 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23933	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.83% 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, SO4, FE, GOL

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	0.27	0/1344	0.72	0/1813
1	B	0.27	0/1341	0.67	0/1808
1	C	0.27	0/1344	0.71	0/1813
1	D	0.27	0/1340	0.73	0/1808
1	E	0.27	0/1335	0.72	0/1802
1	F	0.27	0/1339	0.71	0/1809
1	G	0.28	0/1349	0.70	0/1818
1	H	0.27	0/1348	0.69	1/1816 (0.1%)
1	I	0.27	0/1338	0.72	0/1807
1	J	0.27	0/1357	0.71	0/1828
1	K	0.27	0/1341	0.70	0/1809
1	L	0.27	0/1350	0.72	0/1821
1	M	0.27	0/1336	0.66	0/1803
1	N	0.28	0/1337	0.72	0/1805
1	O	0.27	0/1333	0.70	0/1801
1	P	0.27	0/1348	0.74	1/1817 (0.1%)
All	All	0.27	0/21480	0.71	2/28978 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	92	TYR	CA-CB-CG	-5.36	103.22	113.40
1	P	92	TYR	CA-CB-CG	-5.04	103.82	113.40

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	1324	0	1277	39	0
1	B	1321	0	1280	40	0
1	C	1324	0	1277	41	0
1	D	1320	0	1271	35	0
1	E	1315	0	1264	43	0
1	F	1319	0	1260	39	0
1	G	1324	0	1280	40	0
1	H	1328	0	1293	26	0
1	I	1318	0	1259	37	0
1	J	1333	0	1304	47	0
1	K	1321	0	1274	33	0
1	L	1325	0	1279	38	0
1	M	1316	0	1268	28	0
1	N	1317	0	1264	44	0
1	O	1313	0	1252	38	1
1	P	1328	0	1286	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	1	0
3	D	5	0	0	1	0
3	E	10	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	10	0	0	0	0
3	G	10	0	0	1	0
3	H	10	0	0	1	0
3	I	15	0	0	4	0
3	J	10	0	0	0	6
3	K	20	0	0	1	0
3	L	10	0	0	3	8
3	M	15	0	0	1	0
3	N	15	0	0	2	0
3	O	5	0	0	0	0
3	P	5	0	0	1	0
4	A	98	0	64	17	0
4	C	98	0	64	17	0
4	F	98	0	64	18	0
4	G	98	0	64	15	0
4	I	98	0	64	23	0
4	K	98	0	64	17	0
4	N	98	0	64	21	0
4	O	98	0	64	19	0
5	P	6	0	4	4	0
6	A	121	0	0	6	0
6	B	115	0	0	3	0
6	C	92	0	0	2	0
6	D	114	0	0	8	0
6	E	92	0	0	1	0
6	F	112	0	0	7	0
6	G	130	0	0	2	0
6	H	97	0	0	5	0
6	I	132	0	0	4	0
6	J	113	0	0	9	0
6	K	133	0	0	6	0
6	L	131	0	0	8	0
6	M	128	0	0	3	0
6	N	119	0	0	2	0
6	O	77	0	0	0	0
6	P	105	0	0	7	0
All	All	23933	0	20904	578	15

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 13.

The worst 5 of 578 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:L:114:LYS:HD3	3:L:2204:SO4:O4	1.30	1.31
5:P:2615:GOL:C1	6:P:8947:HOH:O	1.82	1.25
1:L:114:LYS:CE	3:L:2204:SO4:O4	2.14	0.95
1:P:29:GLN:HE22	1:P:83:VAL:H	1.15	0.95
1:H:110:LEU:HD11	1:H:126:GLU:HG3	1.49	0.94

The worst 5 of 15 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:J:2004:SO4:O3	3:J:2004:SO4:O4[8_555]	0.24	1.96
3:J:2004:SO4:O1	3:J:2004:SO4:O3[8_555]	0.29	1.91
3:J:2004:SO4:O1	3:J:2004:SO4:O4[11_455]	0.30	1.90
3:L:2204:SO4:O2	3:L:2204:SO4:O4[6_555]	0.32	1.88
3:L:2204:SO4:O1	3:L:2204:SO4:O2[6_555]	0.45	1.75

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	168/179 (94%)	165 (98%)	3 (2%)	0	100	100
1	B	168/179 (94%)	163 (97%)	5 (3%)	0	100	100
1	C	168/179 (94%)	166 (99%)	2 (1%)	0	100	100
1	D	168/179 (94%)	163 (97%)	5 (3%)	0	100	100
1	E	168/179 (94%)	163 (97%)	5 (3%)	0	100	100
1	F	169/179 (94%)	166 (98%)	2 (1%)	1 (1%)	25	27
1	G	168/179 (94%)	161 (96%)	5 (3%)	2 (1%)	13	11
1	H	168/179 (94%)	162 (96%)	6 (4%)	0	100	100
1	I	168/179 (94%)	165 (98%)	3 (2%)	0	100	100
1	J	169/179 (94%)	166 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	167/179 (93%)	164 (98%)	3 (2%)	0	100	100
1	L	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
1	M	167/179 (93%)	165 (99%)	2 (1%)	0	100	100
1	N	168/179 (94%)	165 (98%)	3 (2%)	0	100	100
1	O	167/179 (93%)	165 (99%)	2 (1%)	0	100	100
1	P	168/179 (94%)	162 (96%)	6 (4%)	0	100	100
All	All	2688/2864 (94%)	2627 (98%)	58 (2%)	3 (0%)	51	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	3	GLY
1	G	151	ASP
1	G	150	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/145 (94%)	136 (99%)	1 (1%)	84	91
1	B	136/145 (94%)	133 (98%)	3 (2%)	52	63
1	C	137/145 (94%)	135 (98%)	2 (2%)	65	76
1	D	136/145 (94%)	131 (96%)	5 (4%)	34	42
1	E	135/145 (93%)	132 (98%)	3 (2%)	52	63
1	F	135/145 (93%)	134 (99%)	1 (1%)	84	91
1	G	138/145 (95%)	132 (96%)	6 (4%)	29	35
1	H	138/145 (95%)	136 (99%)	2 (1%)	67	78
1	I	136/145 (94%)	135 (99%)	1 (1%)	84	91
1	J	139/145 (96%)	134 (96%)	5 (4%)	35	43
1	K	137/145 (94%)	134 (98%)	3 (2%)	52	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	137/145 (94%)	134 (98%)	3 (2%)	52	63
1	M	136/145 (94%)	132 (97%)	4 (3%)	42	52
1	N	135/145 (93%)	132 (98%)	3 (2%)	52	63
1	O	135/145 (93%)	133 (98%)	2 (2%)	65	76
1	P	138/145 (95%)	134 (97%)	4 (3%)	42	52
All	All	2185/2320 (94%)	2137 (98%)	48 (2%)	52	63

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	152	THR
1	M	4	ASN
1	K	7	ASP
1	L	20	ARG
1	M	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	33	GLN
1	N	62	ASN
1	L	29	GLN
1	M	32	ASN
1	N	145	HIS

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 67 ligands modelled in this entry, 16 are monoatomic - leaving 51 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	N	1204	-	4,4,4	2.02	1 (25%)	6,6,6	0.89	0
3	SO4	O	2501	-	4,4,4	1.86	1 (25%)	6,6,6	0.94	0
3	SO4	M	2301	-	4,4,4	1.89	1 (25%)	6,6,6	0.93	0
4	FEC	A	1005[A]	1	40,56,56	1.20	3 (7%)	42,90,90	1.75	12 (28%)
3	SO4	A	1003	-	4,4,4	2.00	1 (25%)	6,6,6	0.84	0
3	SO4	K	2101	-	4,4,4	1.92	1 (25%)	6,6,6	0.94	0
4	FEC	G	1704[A]	1	40,56,56	1.21	2 (5%)	42,90,90	1.73	13 (30%)
3	SO4	M	2303	-	4,4,4	1.94	1 (25%)	6,6,6	0.81	0
3	SO4	J	2004	-	4,4,4	1.93	1 (25%)	6,6,6	0.92	0
3	SO4	A	1004	-	4,4,4	1.88	1 (25%)	6,6,6	0.92	0
3	SO4	L	2201	-	4,4,4	1.91	1 (25%)	6,6,6	0.92	0
4	FEC	O	2502[B]	1	40,56,56	1.20	3 (7%)	42,90,90	1.79	14 (33%)
3	SO4	L	2204	1	4,4,4	1.95	1 (25%)	6,6,6	0.87	0
3	SO4	B	1201	-	4,4,4	1.88	1 (25%)	6,6,6	0.92	0
4	FEC	F	1604[B]	1	40,56,56	1.22	4 (10%)	42,90,90	1.94	12 (28%)
3	SO4	N	2402	-	4,4,4	2.02	1 (25%)	6,6,6	0.89	0
3	SO4	J	2001	-	4,4,4	1.89	1 (25%)	6,6,6	0.84	0
3	SO4	F	1603	-	4,4,4	1.94	1 (25%)	6,6,6	0.86	0
3	SO4	E	1501	-	4,4,4	1.92	1 (25%)	6,6,6	0.96	0
4	FEC	O	2502[A]	1	40,56,56	1.21	4 (10%)	42,90,90	1.74	11 (26%)
4	FEC	I	1903[B]	1	40,56,56	1.23	4 (10%)	42,90,90	1.71	14 (33%)
3	SO4	G	1701	-	4,4,4	2.18	1 (25%)	6,6,6	0.78	0
4	FEC	N	2403[B]	1	40,56,56	1.24	3 (7%)	42,90,90	1.67	13 (30%)
4	FEC	K	2104[B]	1	40,56,56	1.22	3 (7%)	42,90,90	1.75	11 (26%)
4	FEC	C	1305[B]	1	40,56,56	1.23	4 (10%)	42,90,90	1.79	13 (30%)
4	FEC	F	1604[A]	1	40,56,56	1.22	4 (10%)	42,90,90	1.84	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	H	1802	-	4,4,4	1.94	1 (25%)	6,6,6	0.87	0
3	SO4	K	1604	-	4,4,4	1.94	1 (25%)	6,6,6	0.86	0
3	SO4	C	1304	-	4,4,4	1.99	1 (25%)	6,6,6	0.88	0
3	SO4	D	1401	-	4,4,4	1.99	1 (25%)	6,6,6	0.88	0
3	SO4	E	1404	-	4,4,4	1.93	1 (25%)	6,6,6	0.93	0
3	SO4	G	1703	-	4,4,4	2.02	1 (25%)	6,6,6	0.89	0
3	SO4	I	1901	-	4,4,4	1.93	1 (25%)	6,6,6	0.92	0
3	SO4	A	1001	-	4,4,4	1.80	1 (25%)	6,6,6	0.95	0
3	SO4	C	1302	-	4,4,4	1.91	1 (25%)	6,6,6	0.88	0
3	SO4	K	2103	-	4,4,4	1.91	1 (25%)	6,6,6	0.92	0
4	FEC	I	1903[A]	1	40,56,56	1.22	4 (10%)	42,90,90	1.74	11 (26%)
3	SO4	P	2601	-	4,4,4	1.90	1 (25%)	6,6,6	0.90	0
3	SO4	F	1601	-	4,4,4	2.02	1 (25%)	6,6,6	0.84	0
4	FEC	N	2403[A]	1	40,56,56	1.24	3 (7%)	42,90,90	1.73	14 (33%)
4	FEC	K	2104[A]	1	40,56,56	1.25	4 (10%)	42,90,90	1.79	10 (23%)
4	FEC	C	1305[A]	1	40,56,56	1.24	4 (10%)	42,90,90	1.75	11 (26%)
3	SO4	K	2102	-	4,4,4	1.94	1 (25%)	6,6,6	0.86	0
3	SO4	H	1801	-	4,4,4	1.83	1 (25%)	6,6,6	0.84	0
3	SO4	M	2302	-	4,4,4	2.00	1 (25%)	6,6,6	0.85	0
3	SO4	N	2401	-	4,4,4	1.94	1 (25%)	6,6,6	0.82	0
4	FEC	A	1005[B]	1	40,56,56	1.22	4 (10%)	42,90,90	1.81	13 (30%)
5	GOL	P	2615	-	5,5,5	4.54	5 (100%)	5,5,5	4.83	3 (60%)
4	FEC	G	1704[B]	1	40,56,56	1.26	4 (10%)	42,90,90	1.78	12 (28%)
3	SO4	I	1804	-	4,4,4	1.95	2 (50%)	6,6,6	0.80	0
3	SO4	I	1902	-	4,4,4	1.96	2 (50%)	6,6,6	0.80	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
4	FEC	N	2403[B]	1	-	6/20/120/120	-
4	FEC	C	1305[A]	1	-	7/20/120/120	-
4	FEC	K	2104[B]	1	-	9/20/120/120	-
4	FEC	C	1305[B]	1	-	9/20/120/120	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FEC	F	1604[A]	1	-	10/20/120/120	-
4	FEC	F	1604[B]	1	-	12/20/120/120	-
4	FEC	A	1005[A]	1	-	10/20/120/120	-
4	FEC	A	1005[B]	1	-	6/20/120/120	-
5	GOL	P	2615	-	-	2/4/4/4	-
4	FEC	G	1704[A]	1	-	5/20/120/120	-
4	FEC	O	2502[A]	1	-	10/20/120/120	-
4	FEC	G	1704[B]	1	-	14/20/120/120	-
4	FEC	O	2502[B]	1	-	12/20/120/120	-
4	FEC	I	1903[A]	1	-	8/20/120/120	-
4	FEC	I	1903[B]	1	-	9/20/120/120	-
4	FEC	N	2403[A]	1	-	7/20/120/120	-
4	FEC	K	2104[A]	1	-	10/20/120/120	-

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	2615	GOL	C3-C2	-7.27	1.21	1.51
5	P	2615	GOL	O1-C1	4.52	1.61	1.42
3	G	1701	SO4	O1-S	3.98	1.67	1.46
5	P	2615	GOL	O3-C3	3.65	1.57	1.42
3	G	1703	SO4	O1-S	3.65	1.65	1.46

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	2615	GOL	O3-C3-C2	8.20	149.53	110.20
4	F	1604[B]	FEC	CBC-CAC-C2C	7.13	124.63	112.60
4	F	1604[A]	FEC	CBC-CAC-C2C	6.77	124.01	112.60
5	P	2615	GOL	O2-C2-C3	6.33	137.00	109.12
4	K	2104[A]	FEC	CBC-CAC-C2C	5.67	122.17	112.60

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1005[A]	FEC	C3C-C2C-CAC-CBC
4	A	1005[A]	FEC	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
4	A	1005[B]	FEC	C3C-C2C-CAC-CBC
4	A	1005[B]	FEC	C1C-C2C-CAC-CBC
4	C	1305[B]	FEC	C3C-C2C-CAC-CBC

There are no ring outliers.

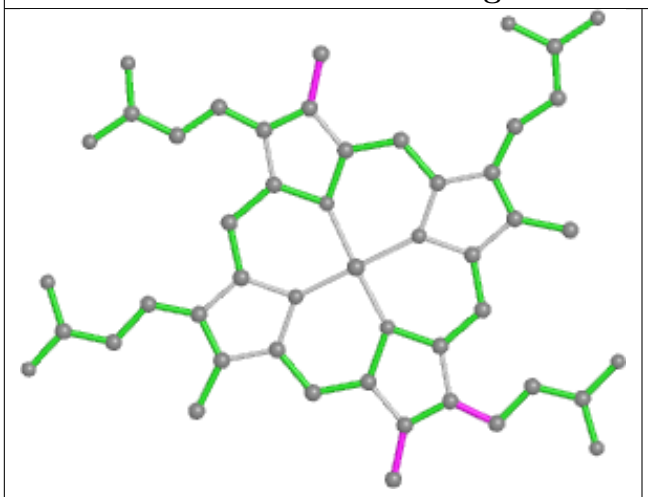
29 monomers are involved in 182 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1204	SO4	2	0
4	A	1005[A]	FEC	9	0
4	G	1704[A]	FEC	8	0
3	J	2004	SO4	0	6
4	O	2502[B]	FEC	12	0
3	L	2204	SO4	3	8
4	F	1604[B]	FEC	10	0
4	O	2502[A]	FEC	7	0
4	I	1903[B]	FEC	11	0
3	G	1701	SO4	1	0
4	N	2403[B]	FEC	12	0
4	K	2104[B]	FEC	7	0
4	C	1305[B]	FEC	9	0
4	F	1604[A]	FEC	8	0
3	H	1802	SO4	1	0
3	K	1604	SO4	1	0
3	D	1401	SO4	1	0
3	E	1404	SO4	0	1
3	C	1302	SO4	1	0
4	I	1903[A]	FEC	12	0
3	P	2601	SO4	1	0
4	N	2403[A]	FEC	9	0
4	K	2104[A]	FEC	10	0
4	C	1305[A]	FEC	8	0
3	M	2302	SO4	1	0
4	A	1005[B]	FEC	8	0
5	P	2615	GOL	4	0
4	G	1704[B]	FEC	7	0
3	I	1804	SO4	4	0

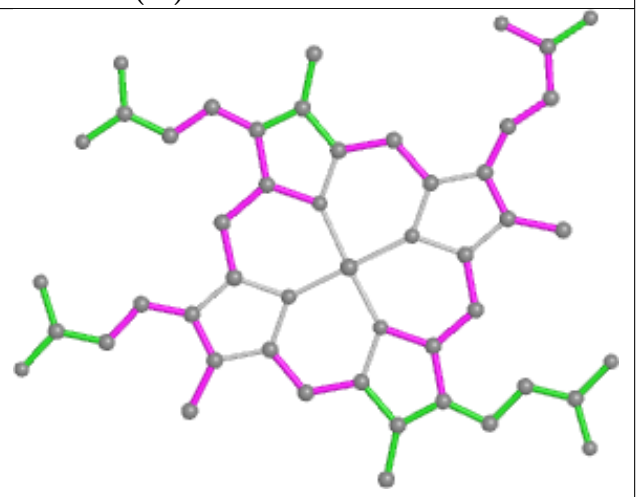
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

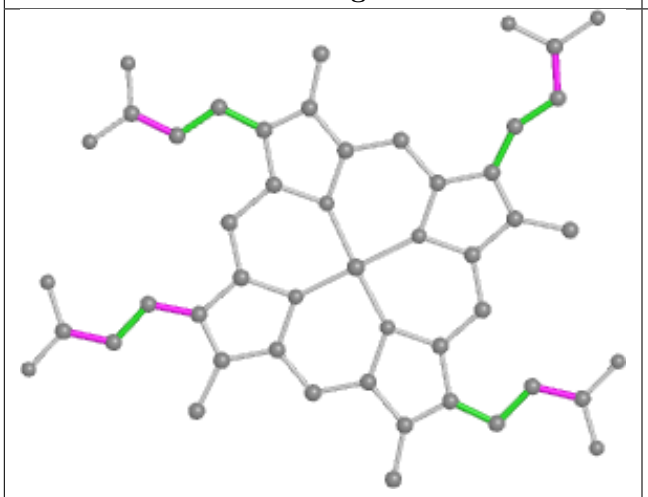
Ligand FEC A 1005 (A)



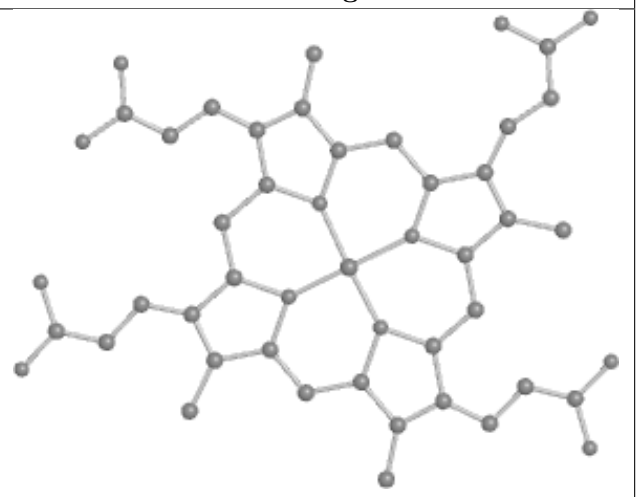
Bond lengths



Bond angles

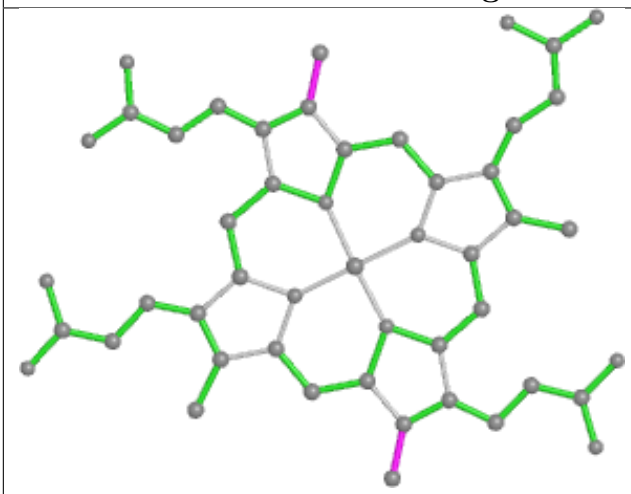


Torsions



Rings

Ligand FEC G 1704 (A)



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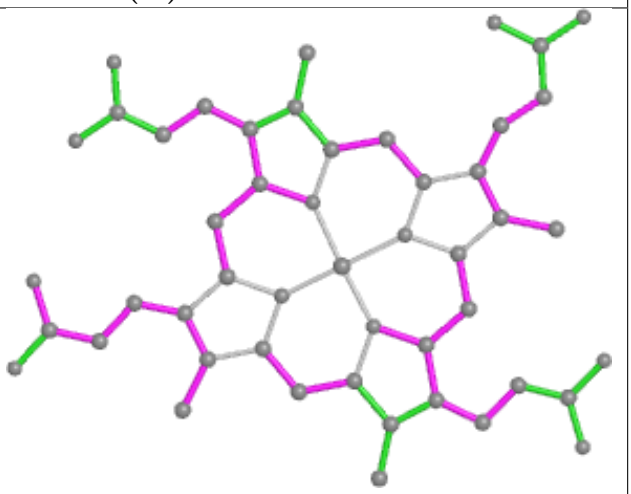

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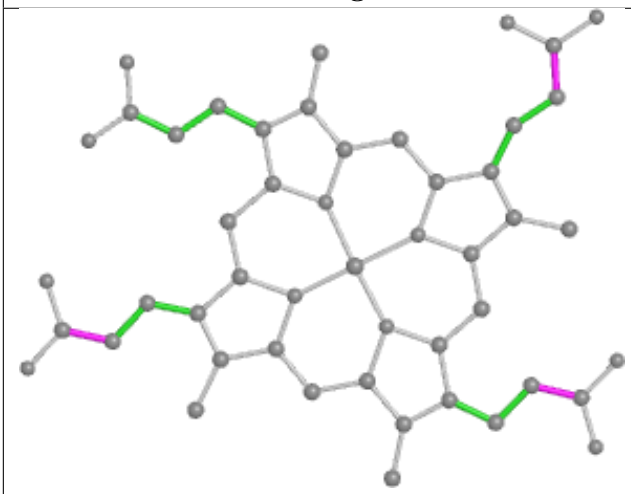
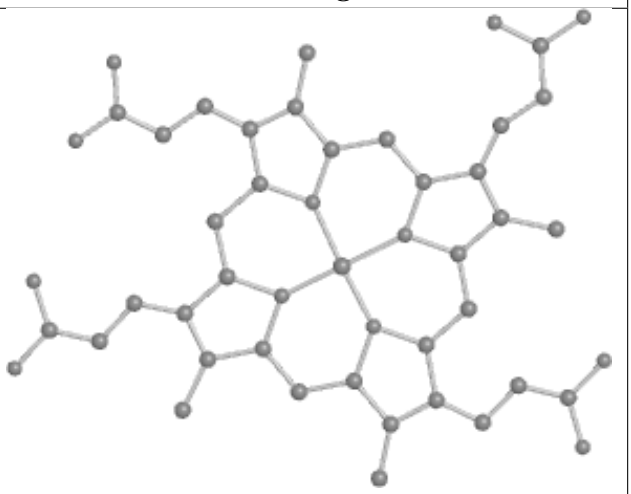
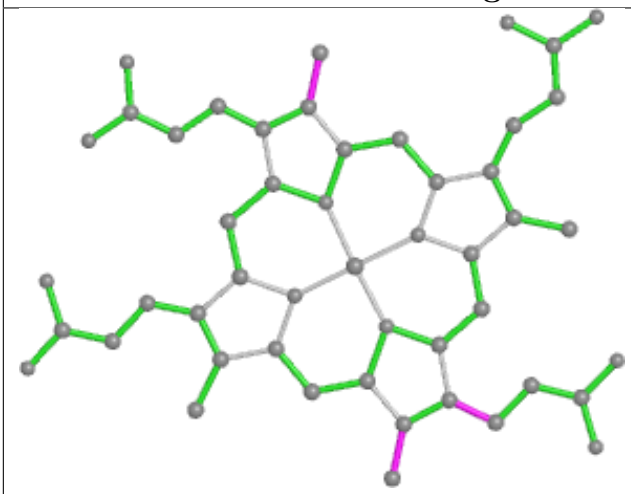


Torsions



Rings

Ligand FEC O 2502 (B)



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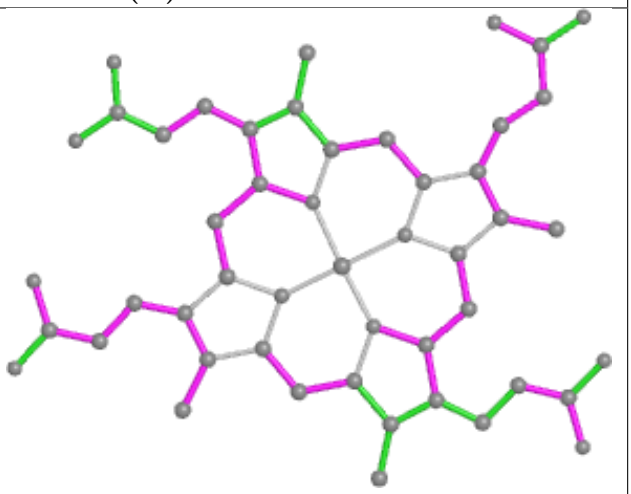
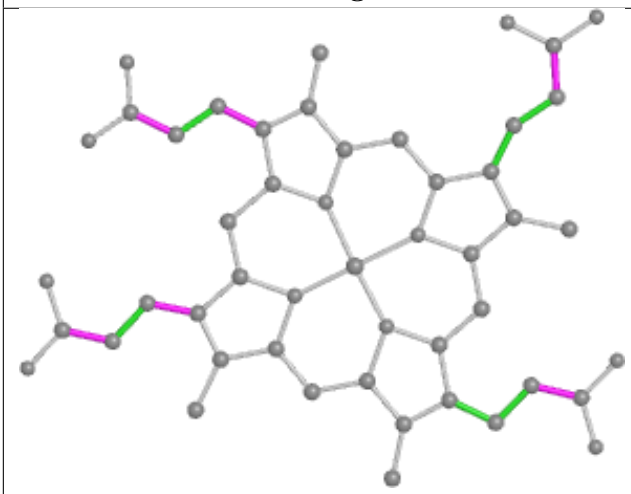


Bond angles



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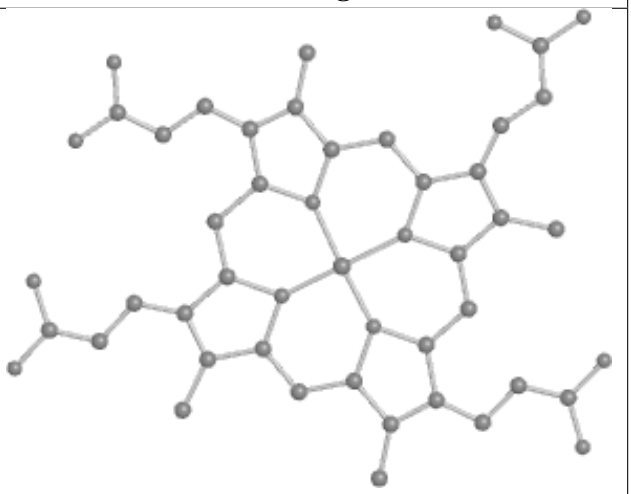
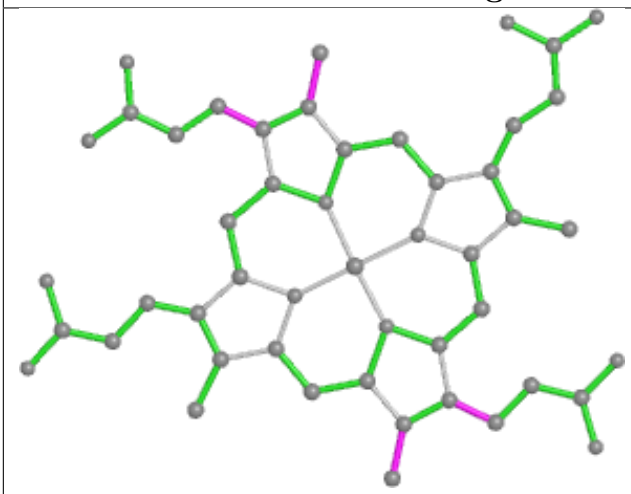


Rings

Ligand FEC F 1604 (B)



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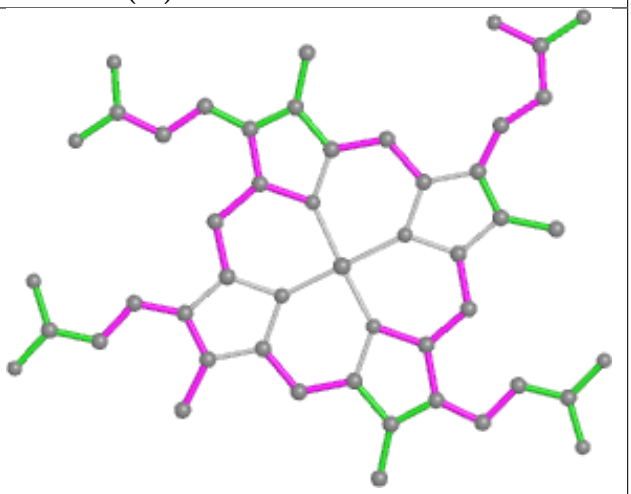
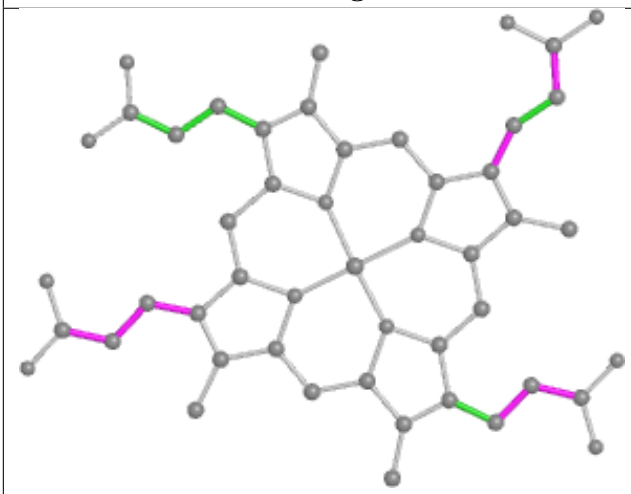
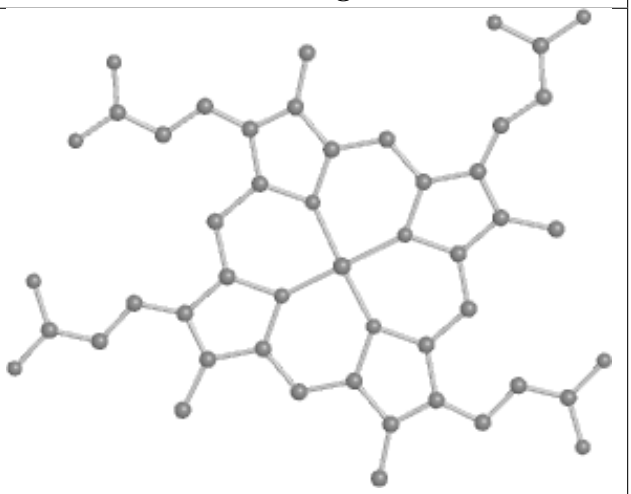


Bond angles

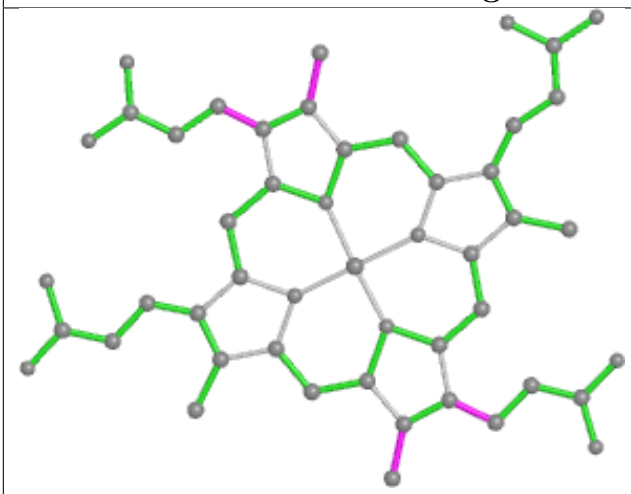


Torsions



Rings

Ligand FEC O 2502 (A)



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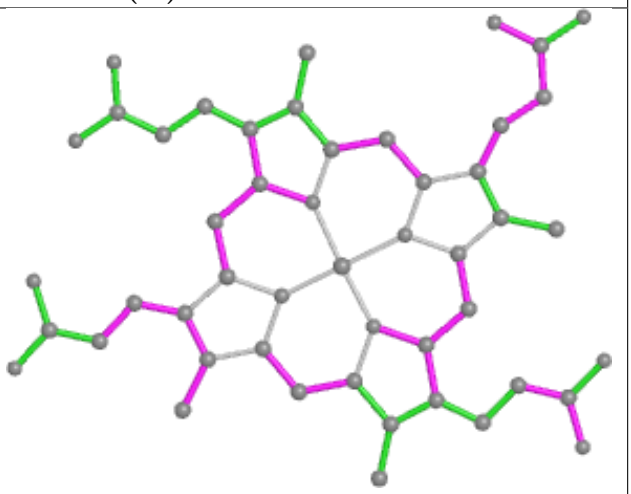
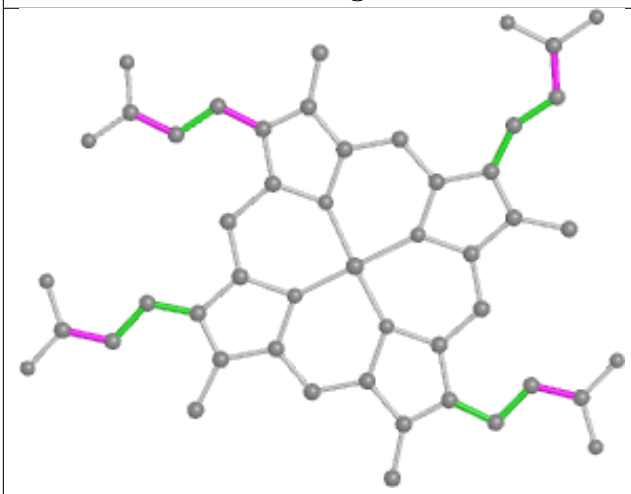
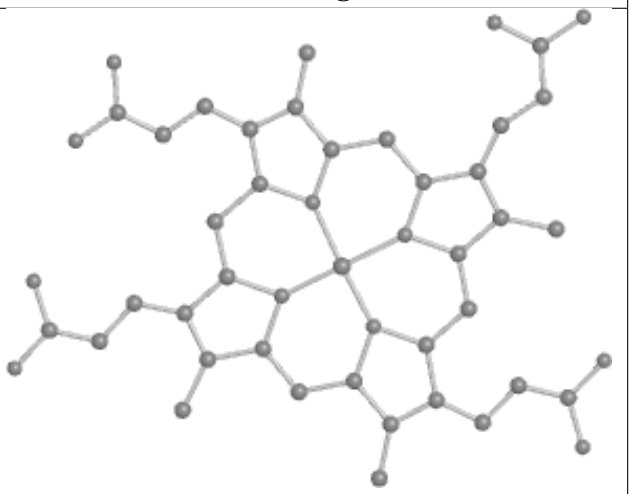


Bond angles

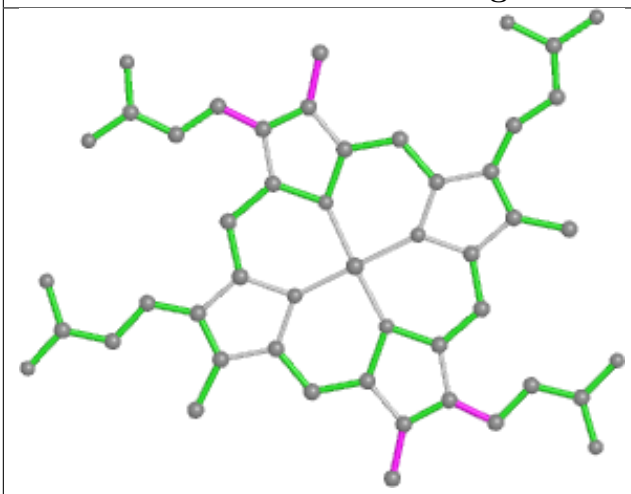


Torsions



Rings

Ligand FEC I 1903 (B)



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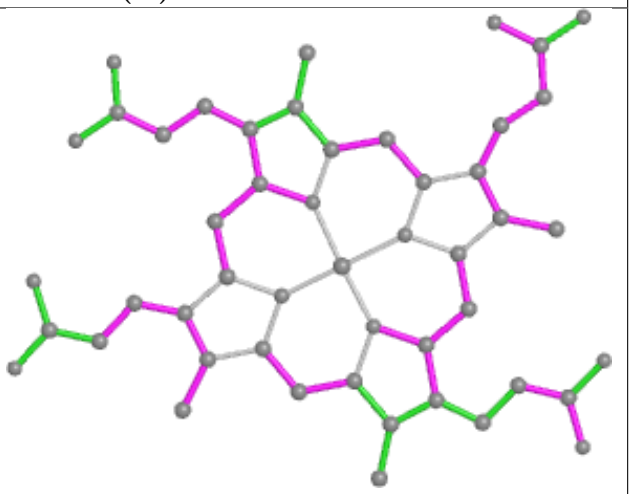
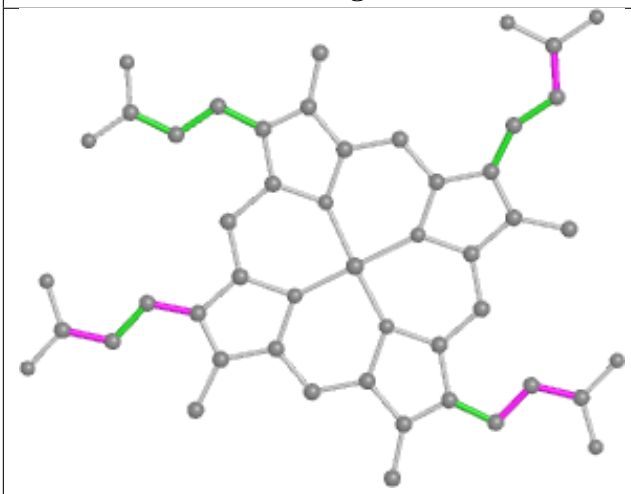


Bond angles



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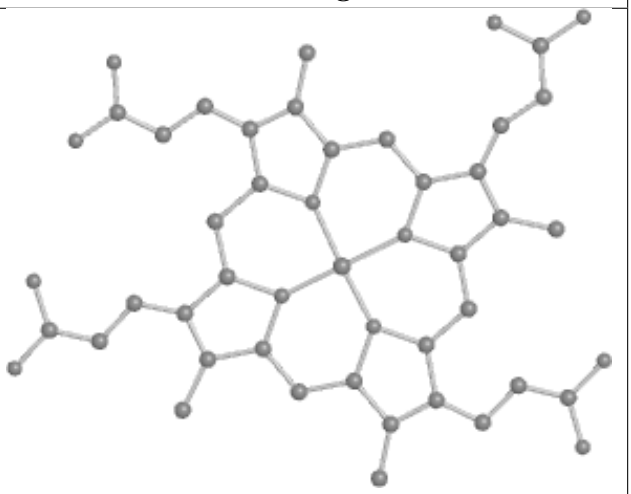
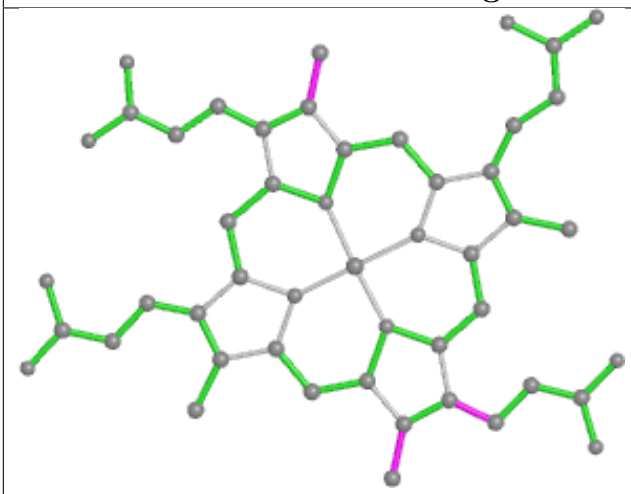


Rings

Ligand FEC N 2403 (B)



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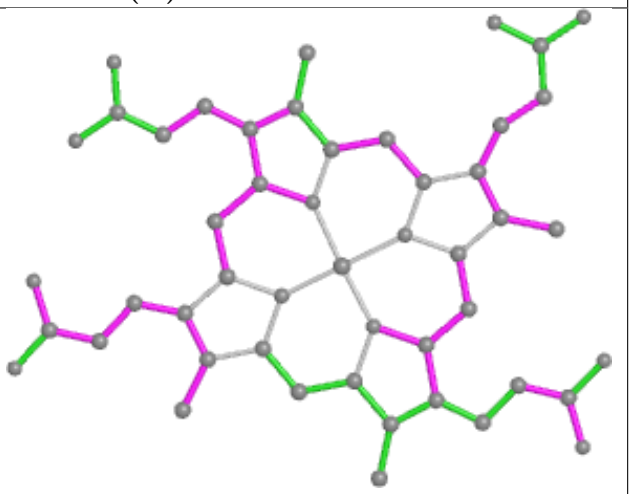

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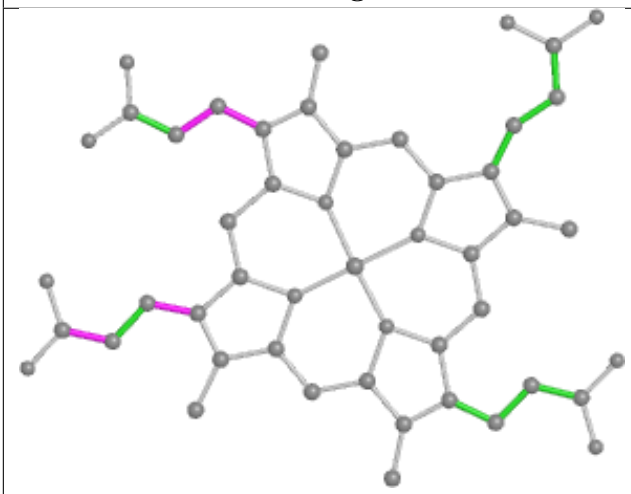
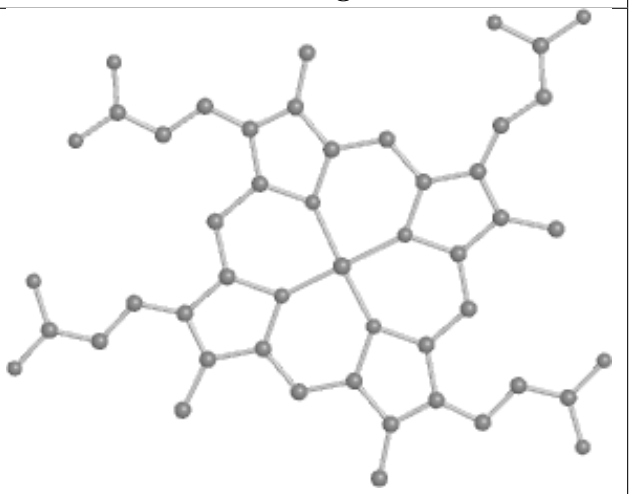
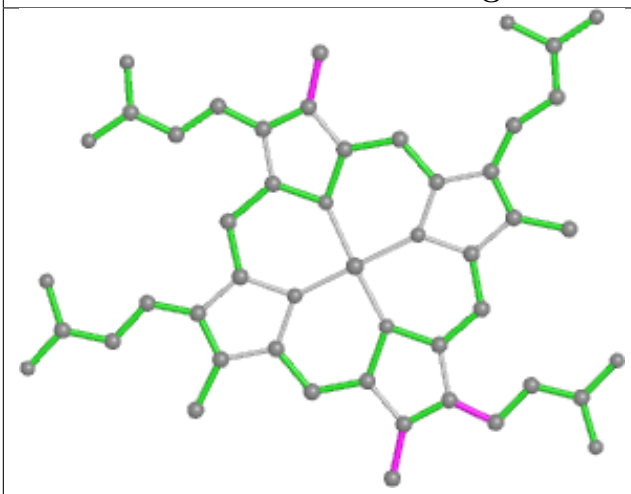


Torsions



Rings

Ligand FEC K 2104 (B)



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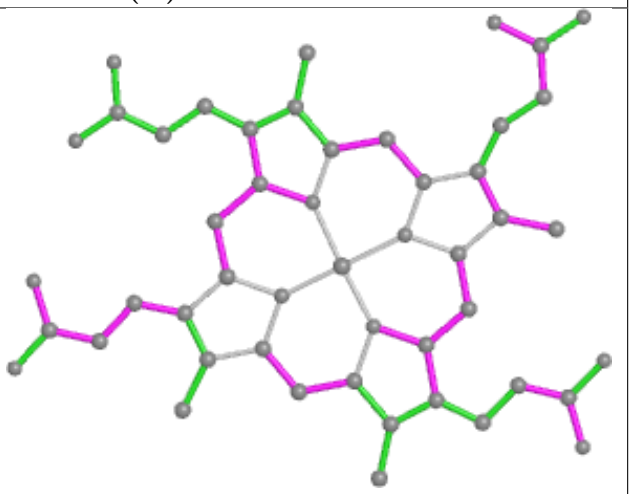

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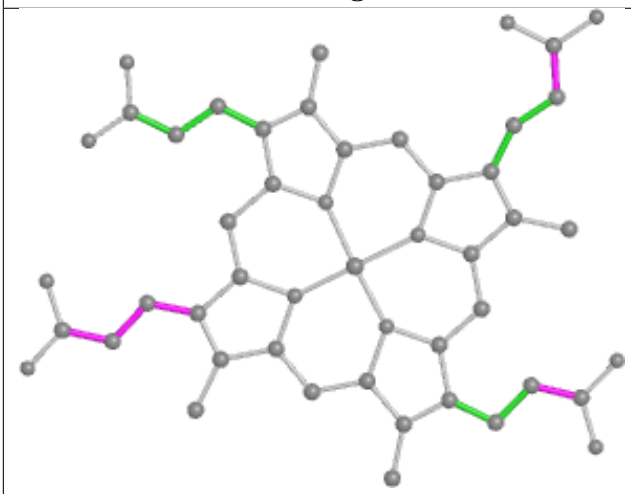

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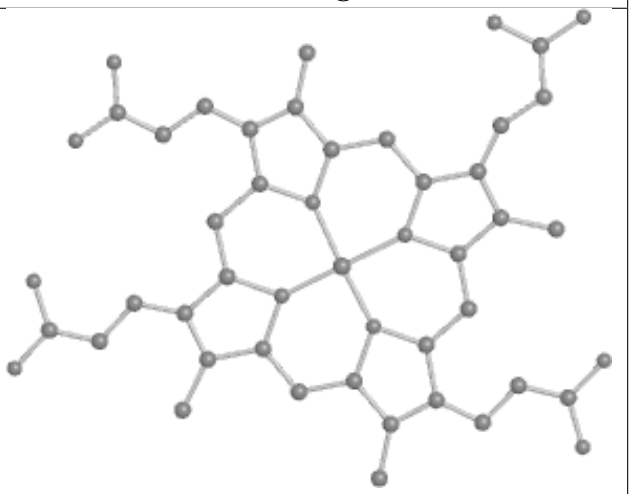
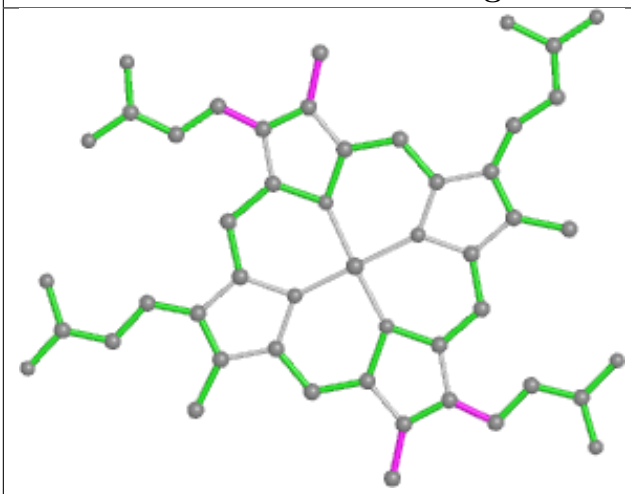


Rings

Ligand FEC C 1305 (B)



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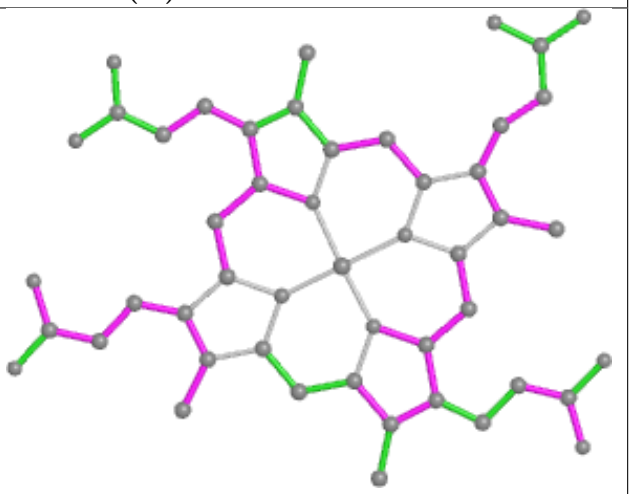
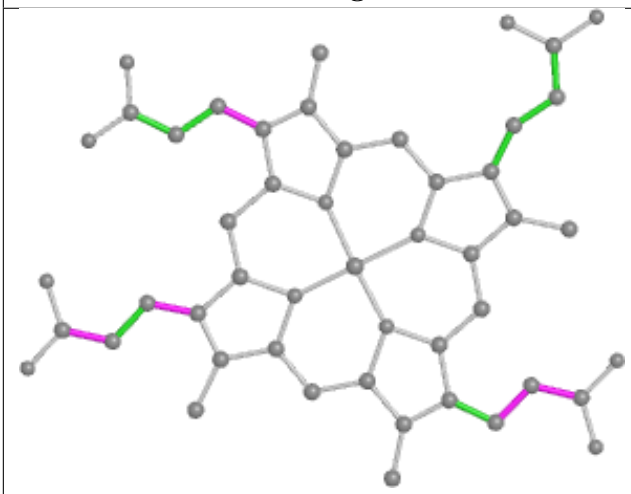
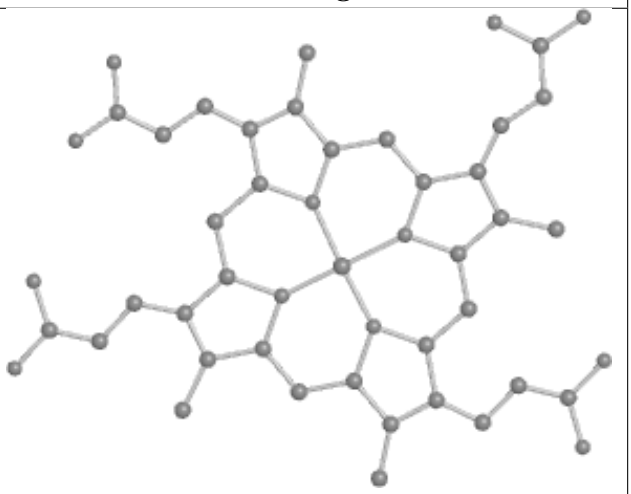


Bond angles

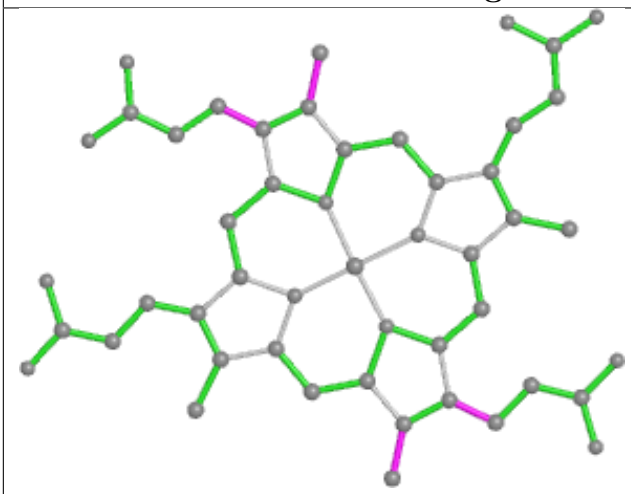


Torsions



Rings

Ligand FEC F 1604 (A)



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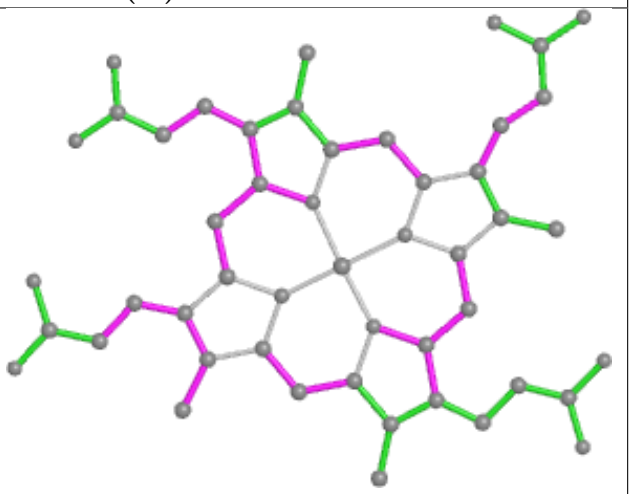
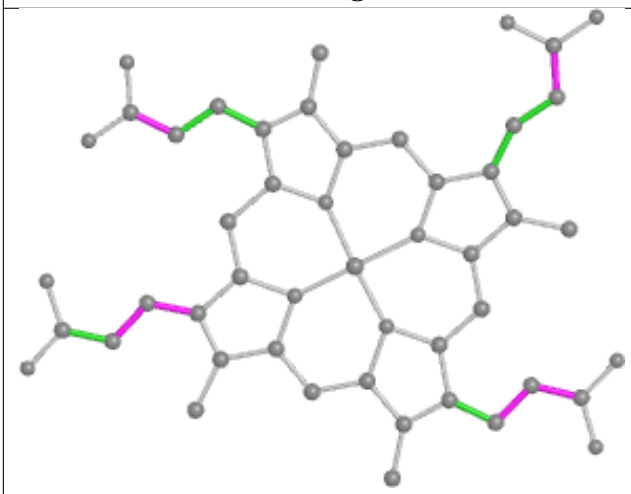


Bond angles



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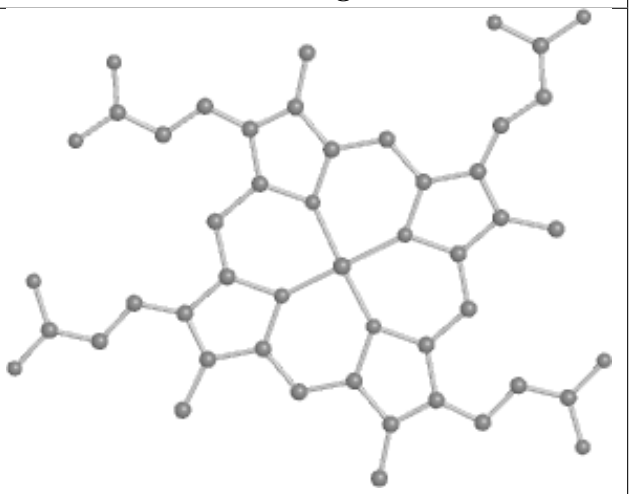
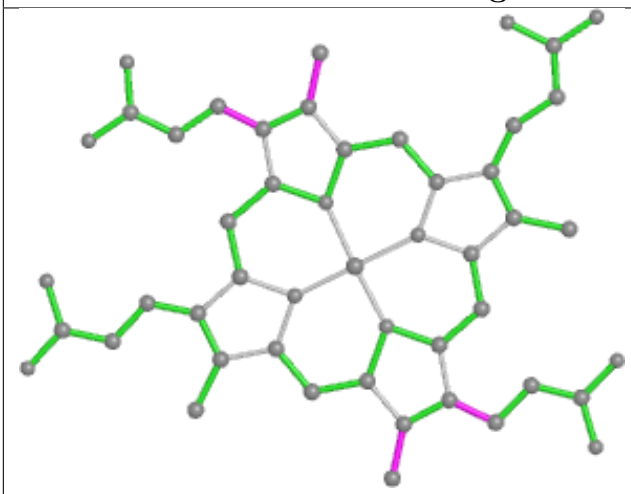


Rings

Ligand FEC I 1903 (A)



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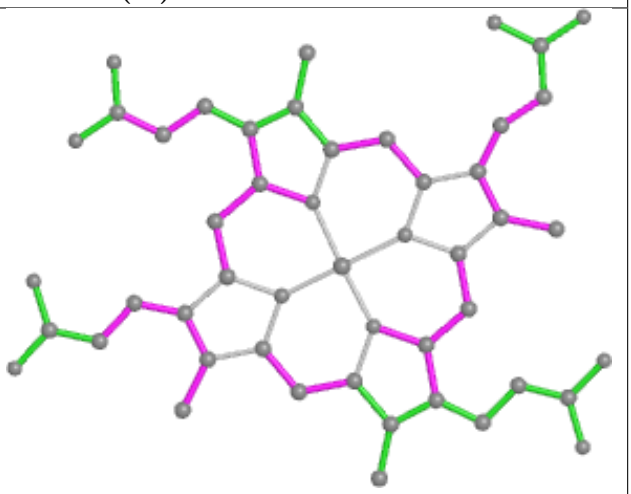
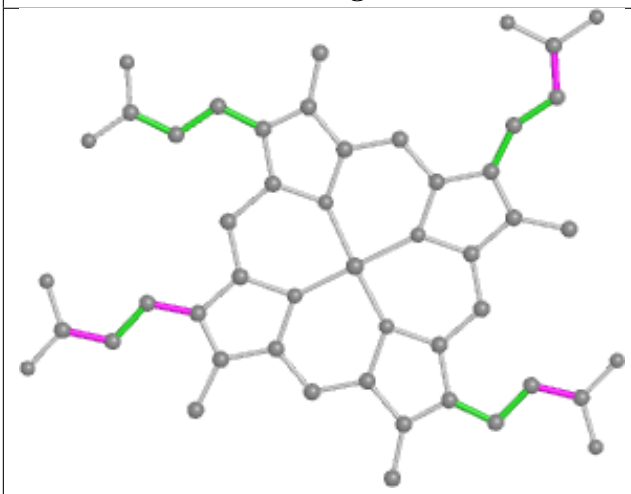
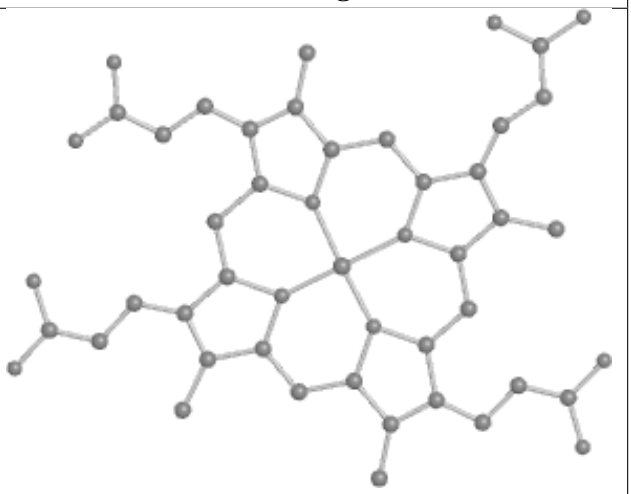


Bond angles

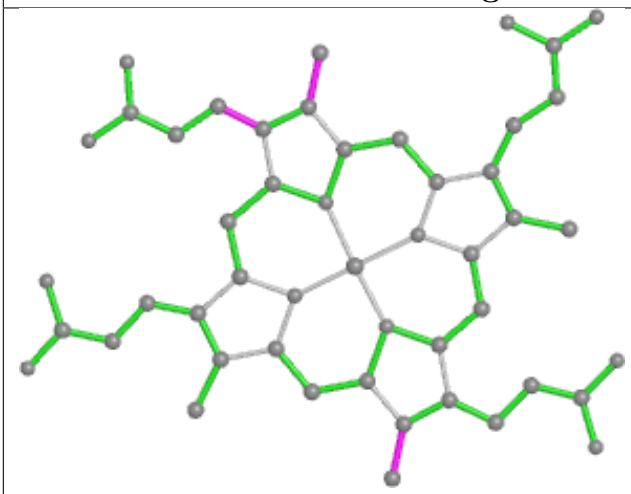


Torsions

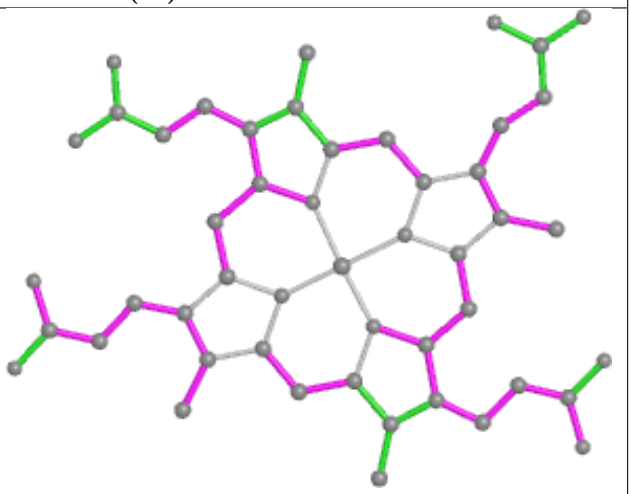


Rings

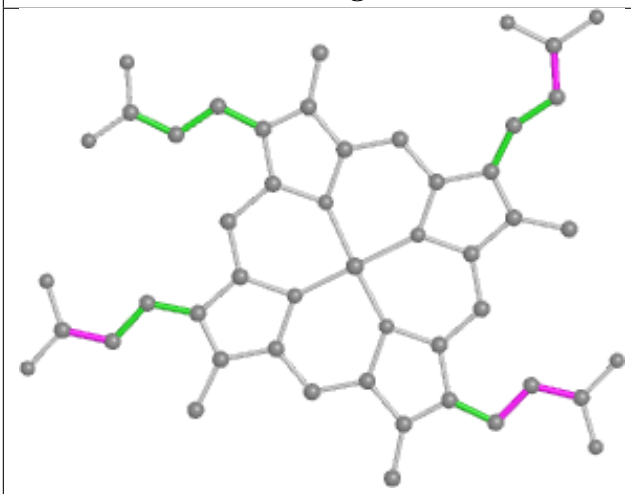
Ligand FEC N 2403 (A)



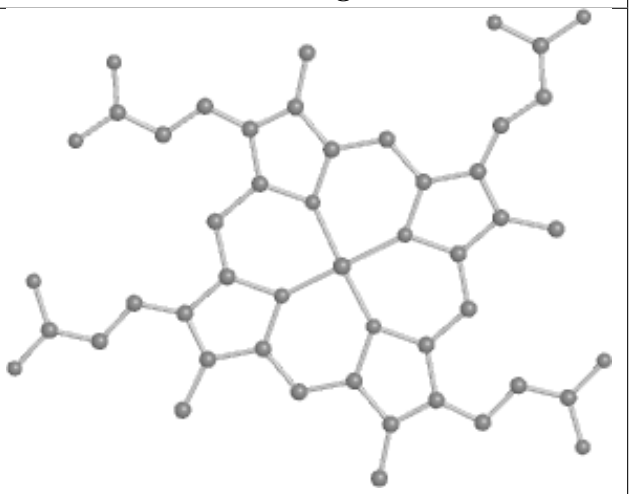
Bond lengths



Bond angles

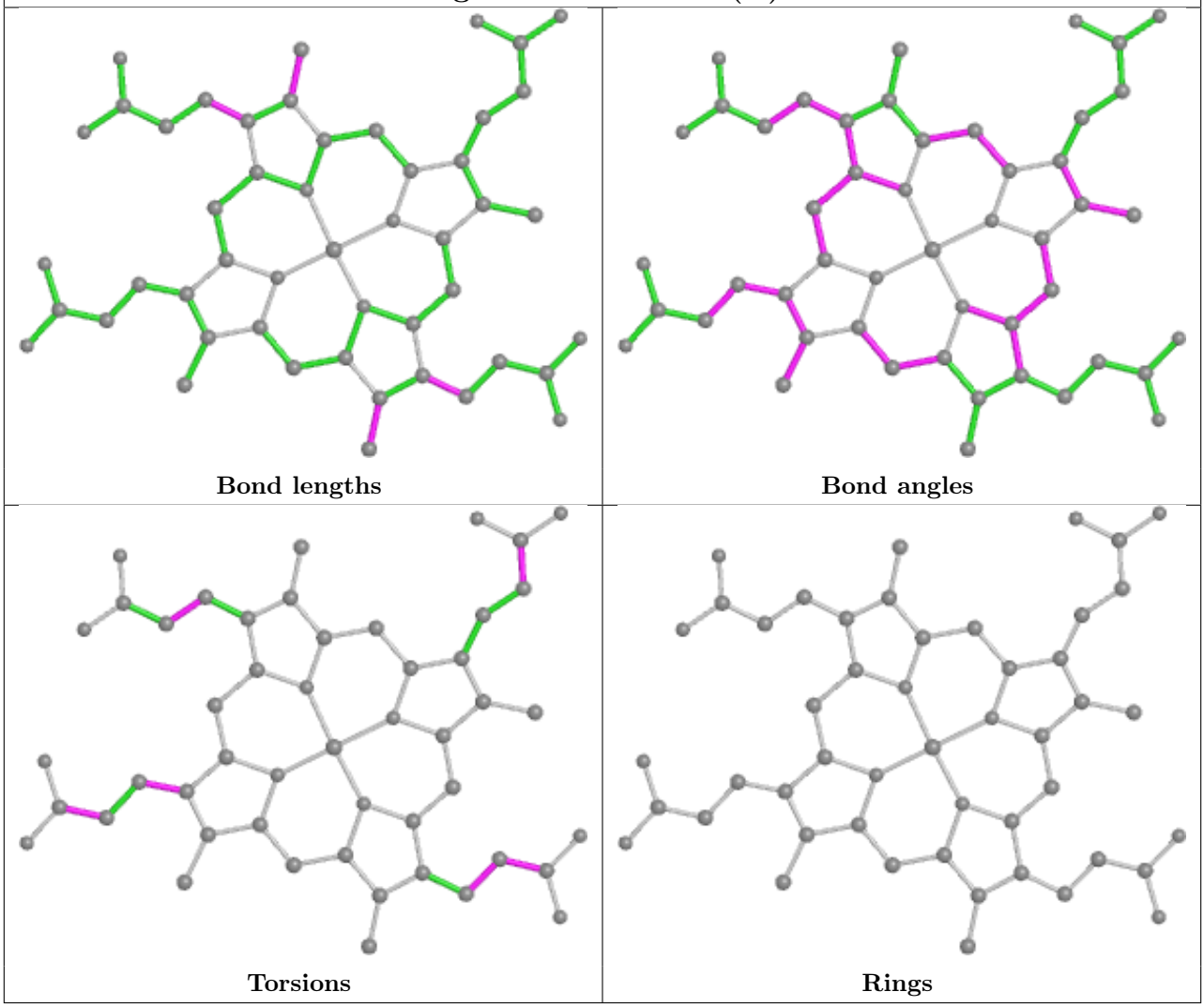


Torsions

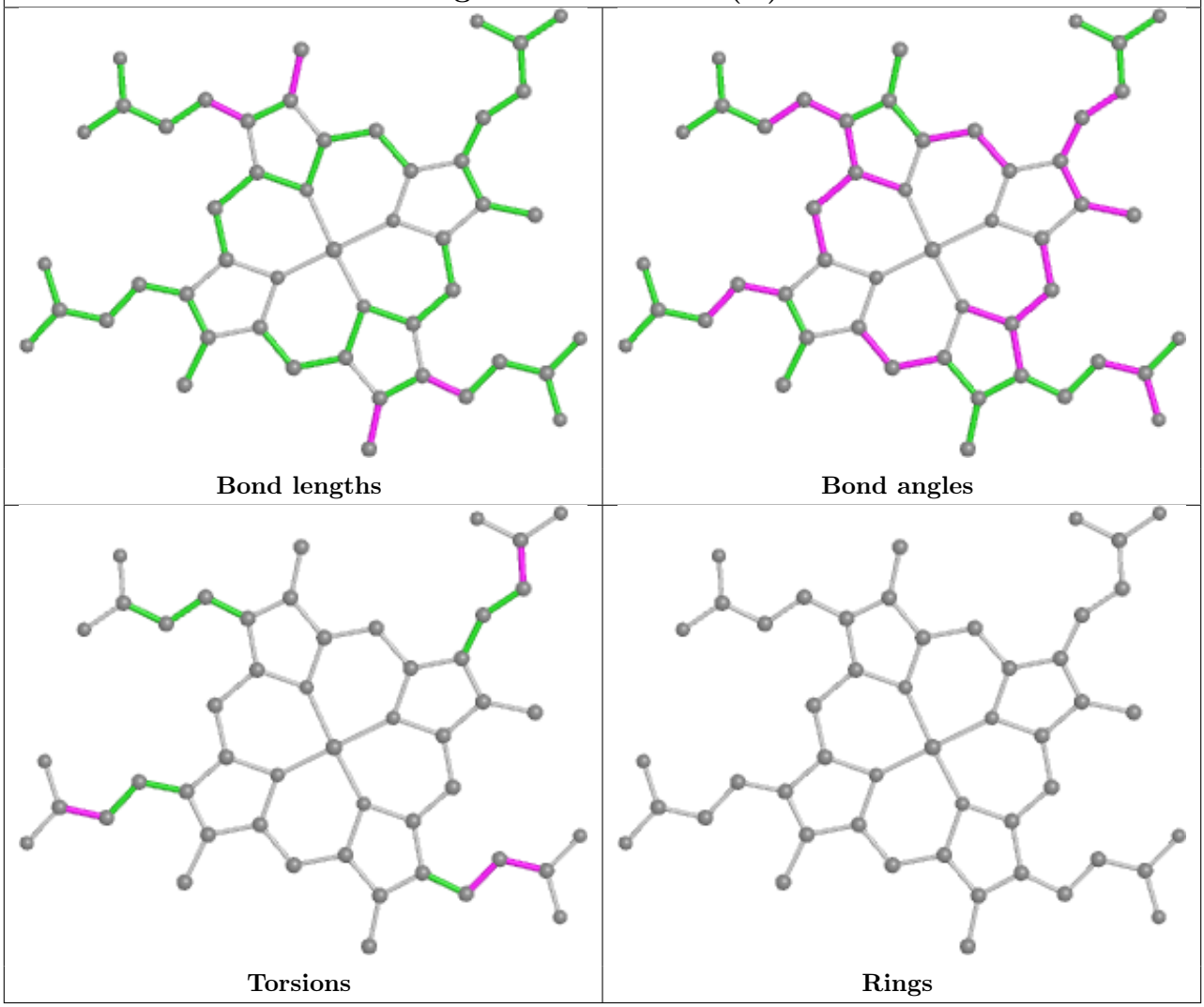


Rings

Ligand FEC K 2104 (A)



Ligand FEC C 1305 (A)



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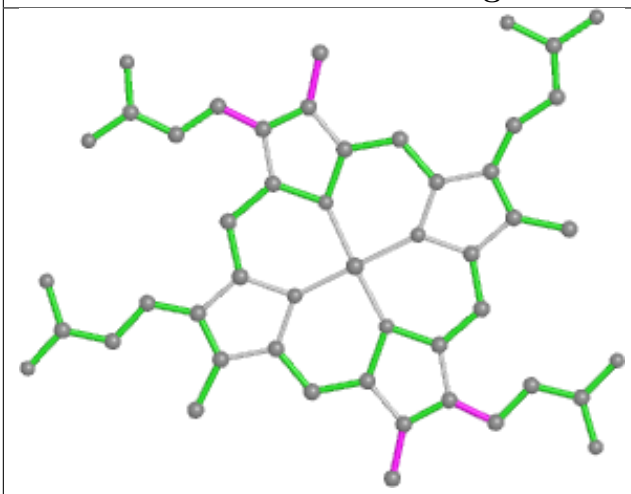
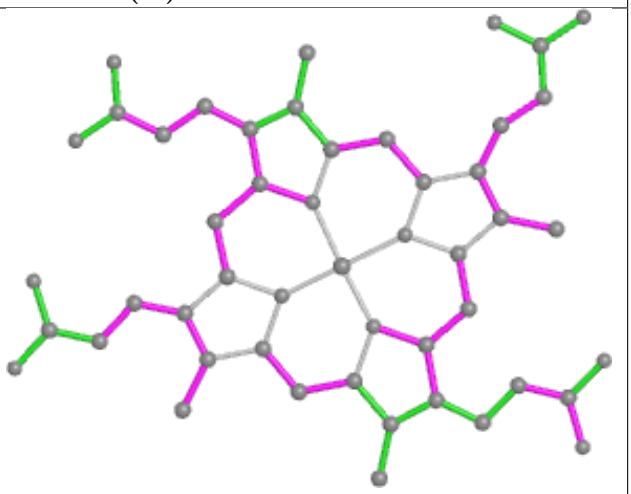
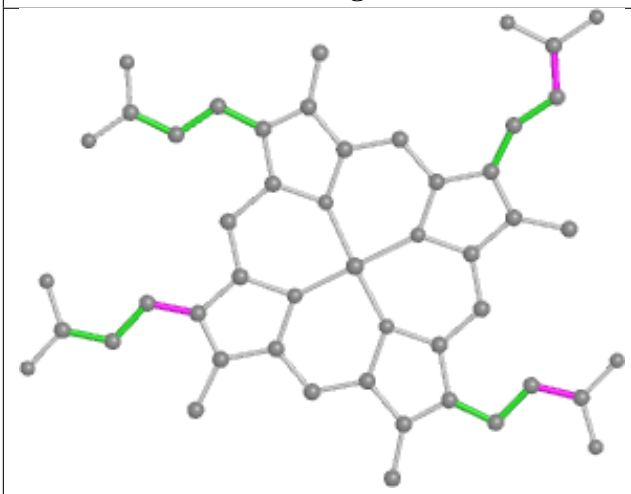


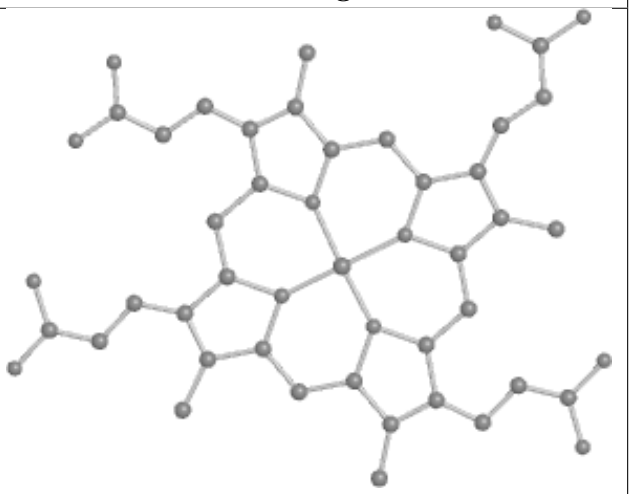
Bond lengths



Bond angles

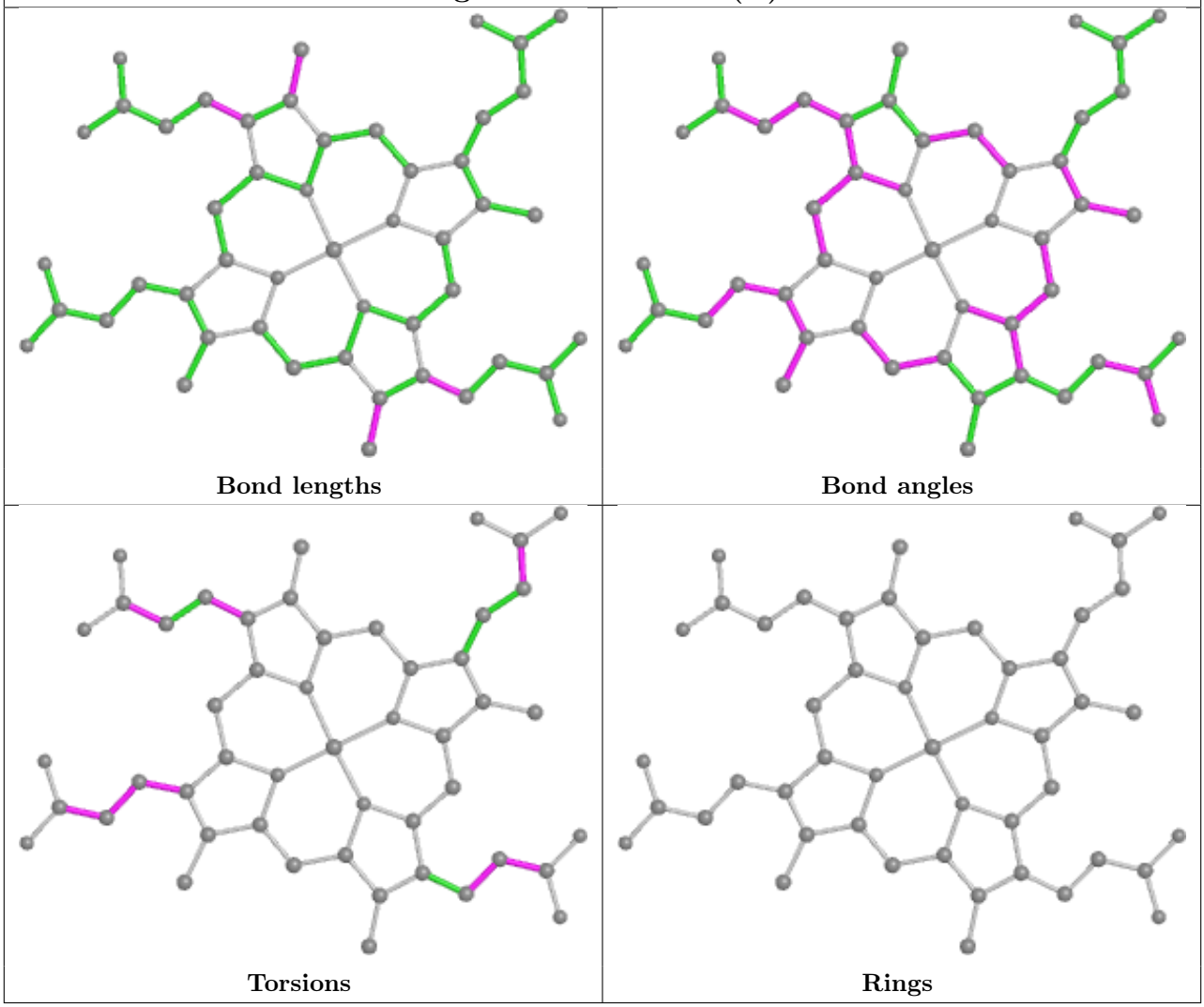


Torsions



Rings

Ligand FEC G 1704 (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	170/179 (94%)	-0.21	6 (3%)	44	56	17, 26, 40, 66	0
1	B	170/179 (94%)	-0.37	5 (2%)	51	62	17, 25, 40, 55	0
1	C	170/179 (94%)	-0.24	6 (3%)	44	56	17, 26, 41, 85	0
1	D	170/179 (94%)	-0.16	7 (4%)	37	49	17, 26, 40, 55	0
1	E	170/179 (94%)	-0.24	4 (2%)	59	68	17, 26, 40, 57	0
1	F	171/179 (95%)	-0.30	6 (3%)	44	56	17, 26, 43, 76	0
1	G	169/179 (94%)	-0.31	3 (1%)	68	77	17, 25, 40, 55	0
1	H	170/179 (94%)	-0.32	4 (2%)	59	68	17, 26, 41, 55	0
1	I	170/179 (94%)	-0.30	2 (1%)	79	86	17, 25, 40, 55	0
1	J	170/179 (94%)	-0.29	4 (2%)	59	68	17, 26, 41, 55	0
1	K	169/179 (94%)	-0.30	2 (1%)	79	86	16, 26, 41, 55	0
1	L	170/179 (94%)	-0.20	2 (1%)	79	86	17, 26, 39, 55	0
1	M	169/179 (94%)	-0.30	3 (1%)	68	77	17, 25, 40, 55	0
1	N	170/179 (94%)	-0.35	2 (1%)	79	86	17, 25, 38, 55	0
1	O	169/179 (94%)	-0.20	4 (2%)	59	68	17, 25, 41, 74	0
1	P	170/179 (94%)	-0.33	3 (1%)	68	77	17, 26, 41, 55	0
All	All	2717/2864 (94%)	-0.28	63 (2%)	60	70	16, 26, 41, 85	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	THR	5.7
1	A	166	THR	5.4
1	N	166	THR	5.1
1	E	166	THR	4.7
1	O	173	THR	4.6

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	G	1701	5/5	0.78	0.31	74,74,74,75	0
3	SO4	K	2103	5/5	0.79	0.23	69,69,69,71	0
3	SO4	C	1304	5/5	0.82	0.33	58,59,60,60	5
3	SO4	H	1802	5/5	0.83	0.36	72,72,73,73	0
3	SO4	M	2303	5/5	0.83	0.40	62,63,63,63	0
3	SO4	M	2302	5/5	0.84	0.46	73,73,73,74	0
3	SO4	I	1804	5/5	0.84	0.30	36,37,38,38	0
3	SO4	O	2501	5/5	0.85	0.21	70,70,71,71	0
3	SO4	N	1204	5/5	0.86	0.19	73,73,74,75	0
3	SO4	G	1703	5/5	0.86	0.25	73,73,74,75	0
3	SO4	K	2102	5/5	0.87	0.18	78,78,78,79	0
3	SO4	F	1601	5/5	0.87	0.24	66,66,67,67	0
3	SO4	D	1401	5/5	0.89	0.17	58,59,60,60	0
3	SO4	F	1603	5/5	0.89	0.29	78,78,78,79	0
3	SO4	E	1404	5/5	0.89	0.22	65,65,67,67	0
5	GOL	P	2615	6/6	0.89	0.21	27,31,47,67	0
3	SO4	K	1604	5/5	0.90	0.15	78,78,78,79	0
3	SO4	N	2401	5/5	0.90	0.17	62,63,63,63	0
3	SO4	H	1801	5/5	0.91	0.21	54,54,55,56	0
3	SO4	I	1901	5/5	0.91	0.18	61,61,62,63	0
3	SO4	N	2402	5/5	0.91	0.32	73,73,74,75	0
3	SO4	J	2001	5/5	0.91	0.18	66,67,67,69	0
3	SO4	P	2601	5/5	0.91	0.19	62,62,63,63	0
3	SO4	E	1501	5/5	0.91	0.22	67,68,68,68	0
3	SO4	L	2201	5/5	0.92	0.17	64,64,65,65	0
3	SO4	K	2101	5/5	0.93	0.17	51,53,53,54	0
3	SO4	B	1201	5/5	0.93	0.14	66,66,67,67	0

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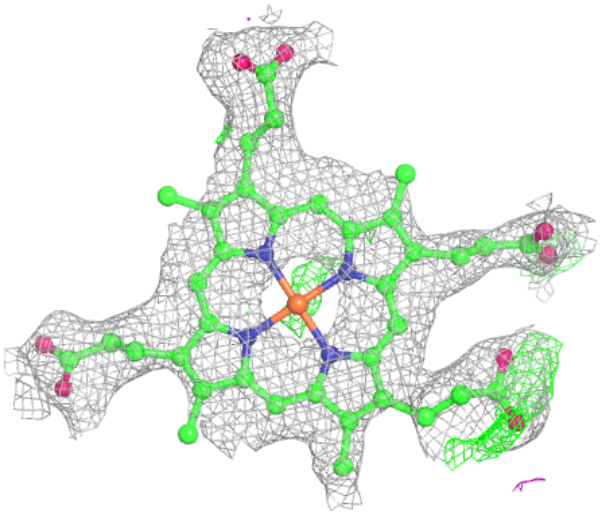
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	1302	5/5	0.93	0.35	73,73,73,75	0
3	SO4	A	1003	5/5	0.94	0.17	73,73,73,74	0
3	SO4	M	2301	5/5	0.94	0.15	51,51,52,53	0
4	FEC	F	1604[B]	49/49	0.95	0.19	17,19,26,27	49
4	FEC	F	1604[A]	49/49	0.95	0.19	16,19,26,27	49
4	FEC	C	1305[A]	49/49	0.96	0.18	16,19,26,27	49
4	FEC	C	1305[B]	49/49	0.96	0.18	13,20,25,31	49
3	SO4	L	2204	5/5	0.96	0.37	78,78,78,79	1
3	SO4	A	1001	5/5	0.96	0.15	53,54,54,55	0
4	FEC	G	1704[A]	49/49	0.96	0.21	16,19,26,27	49
4	FEC	G	1704[B]	49/49	0.96	0.21	10,19,26,27	49
4	FEC	K	2104[A]	49/49	0.96	0.20	16,19,25,27	49
4	FEC	K	2104[B]	49/49	0.96	0.20	10,19,26,27	49
4	FEC	N	2403[A]	49/49	0.96	0.20	16,19,26,27	49
4	FEC	N	2403[B]	49/49	0.96	0.20	11,19,24,29	49
3	SO4	I	1902	5/5	0.96	0.13	36,37,38,38	0
3	SO4	A	1004	5/5	0.97	0.12	66,66,67,67	5
4	FEC	A	1005[A]	49/49	0.97	0.20	16,19,26,27	49
4	FEC	I	1903[A]	49/49	0.97	0.18	16,19,26,28	49
4	FEC	I	1903[B]	49/49	0.97	0.18	16,19,26,29	49
4	FEC	A	1005[B]	49/49	0.97	0.20	14,19,25,27	49
3	SO4	J	2004	5/5	0.97	0.28	61,61,62,63	2
2	FE	N	200	1/1	0.97	0.06	28,28,28,28	0
2	FE	D	200	1/1	0.97	0.05	33,33,33,33	0
4	FEC	O	2502[A]	49/49	0.97	0.18	16,19,26,28	49
4	FEC	O	2502[B]	49/49	0.97	0.18	15,19,25,32	49
2	FE	F	200	1/1	0.97	0.03	31,31,31,31	0
2	FE	O	200	1/1	0.98	0.04	32,32,32,32	0
2	FE	M	200	1/1	0.99	0.06	27,27,27,27	0
2	FE	C	200	1/1	0.99	0.04	32,32,32,32	0
2	FE	A	200	1/1	0.99	0.03	30,30,30,30	0
2	FE	P	200	1/1	0.99	0.04	31,31,31,31	0
2	FE	E	200	1/1	0.99	0.02	31,31,31,31	0
2	FE	B	200	1/1	0.99	0.04	28,28,28,28	0
2	FE	G	200	1/1	0.99	0.03	29,29,29,29	0
2	FE	H	200	1/1	0.99	0.05	28,28,28,28	0
2	FE	J	200	1/1	0.99	0.04	30,30,30,30	0
2	FE	K	200	1/1	0.99	0.05	29,29,29,29	0
2	FE	L	200	1/1	0.99	0.06	29,29,29,29	0
2	FE	I	200	1/1	1.00	0.06	28,28,28,28	0

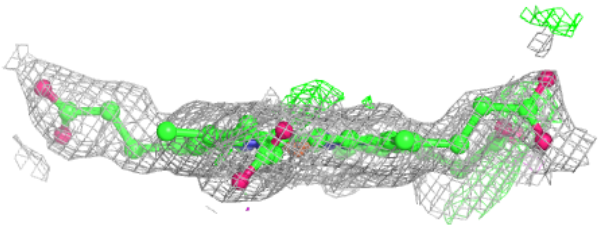
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

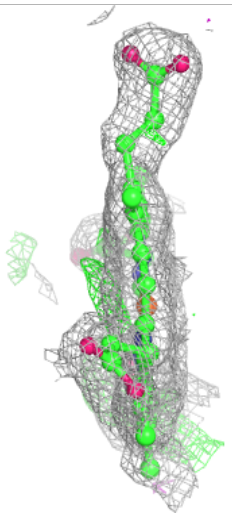
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FEC F 1604 (B):

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

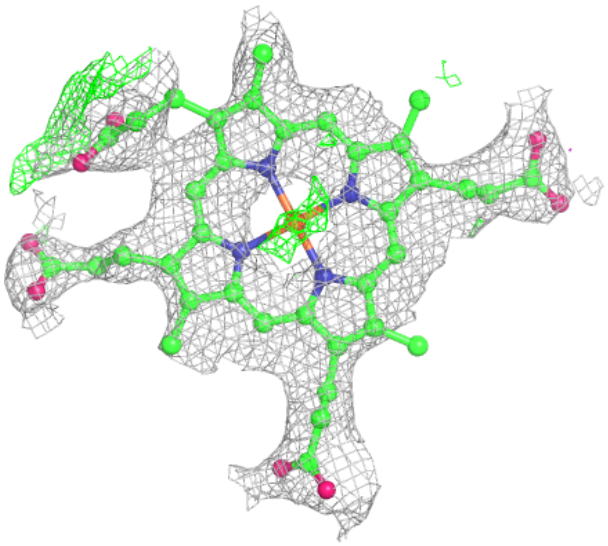


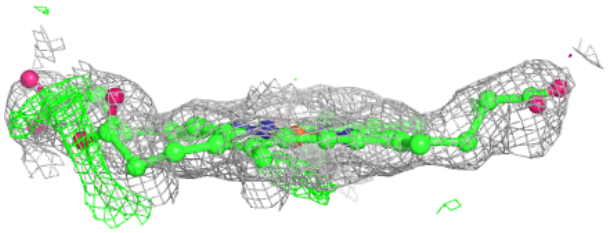


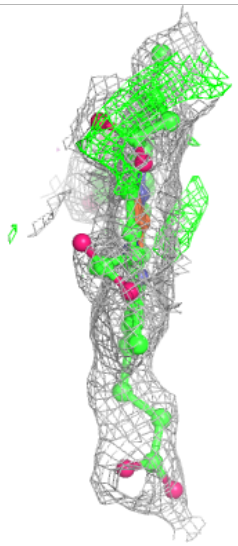


Electron density around FEC F 1604 (A):

$2mF_o$-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 C 1305 (A):

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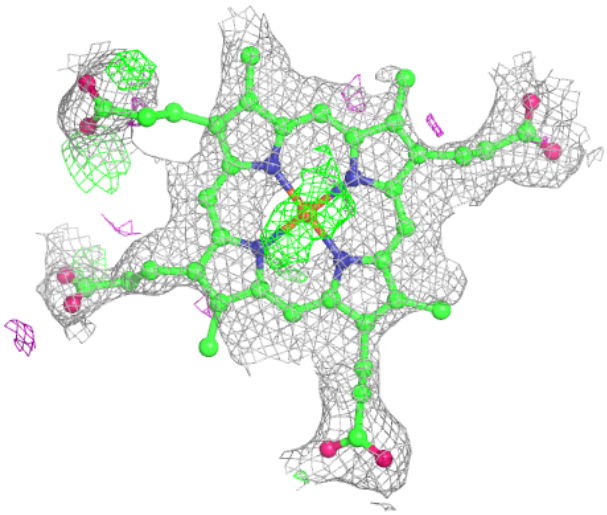
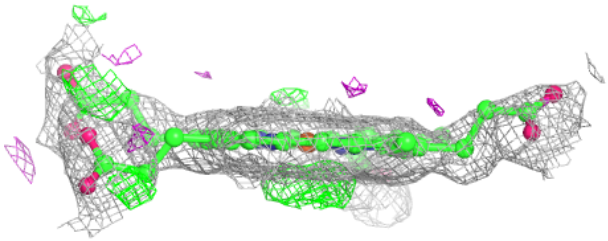
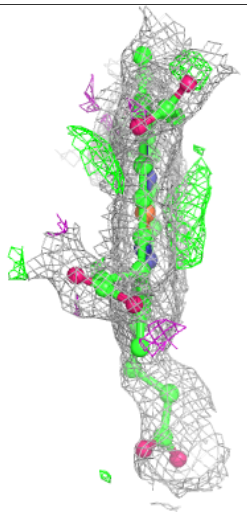
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around FEC C 1305 (B):

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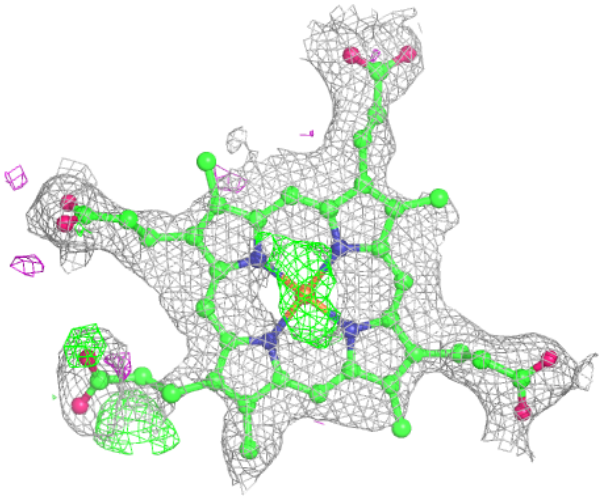
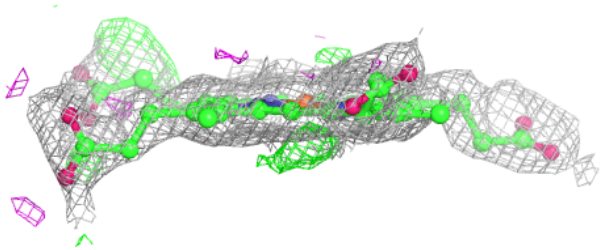
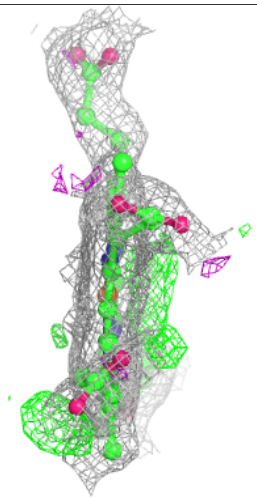
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around FEC G 1704 (A):

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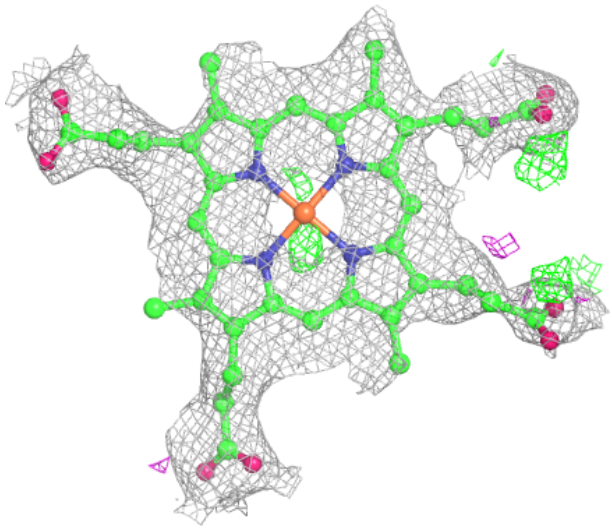
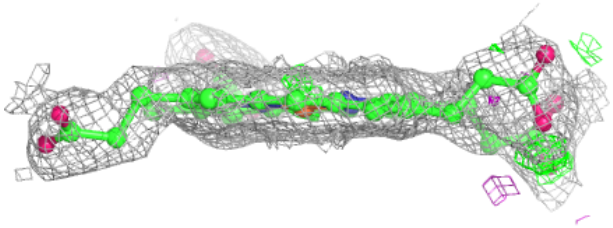
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around FEC G 1704 (B):

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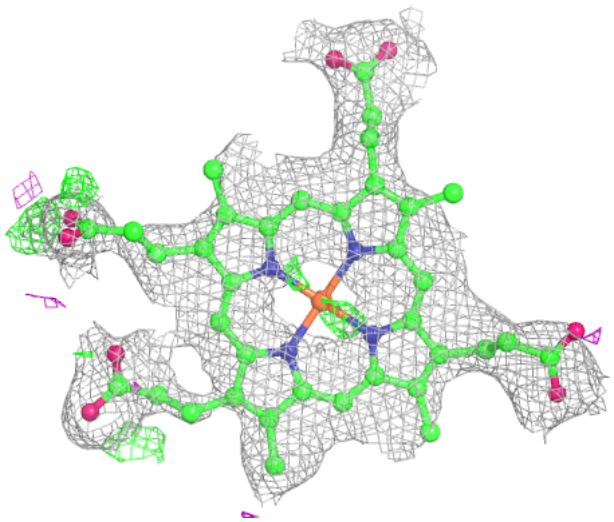
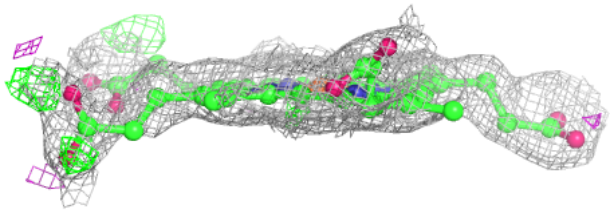
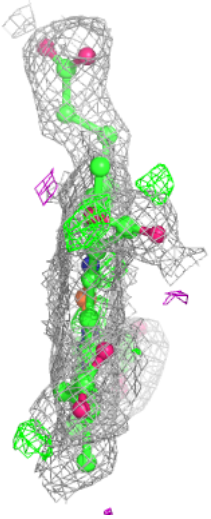
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around FEC K 2104 (A):

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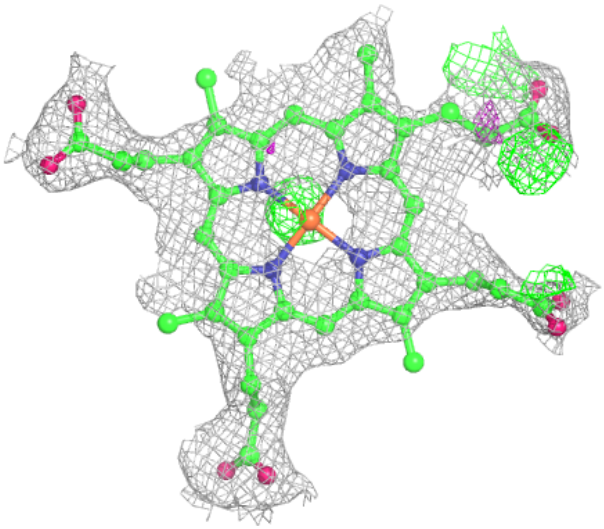
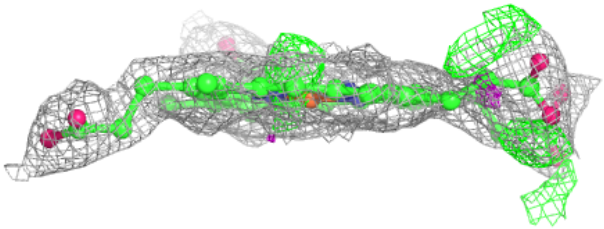
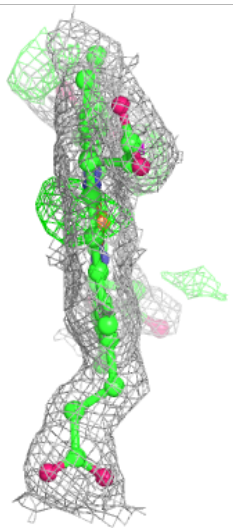
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

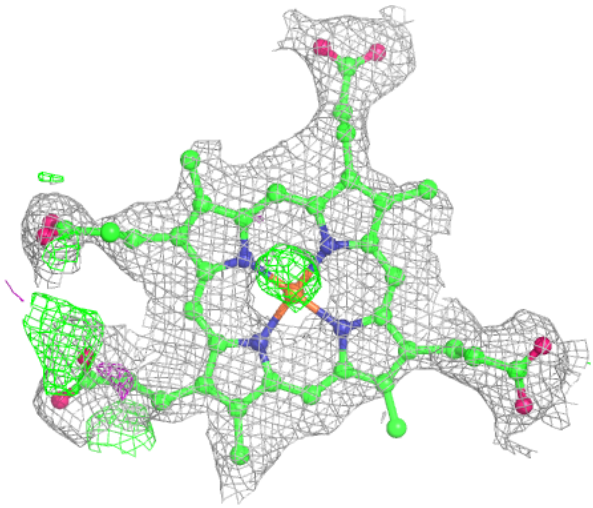


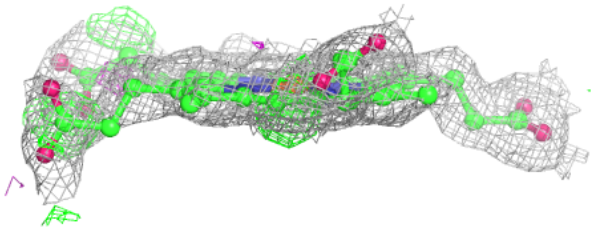


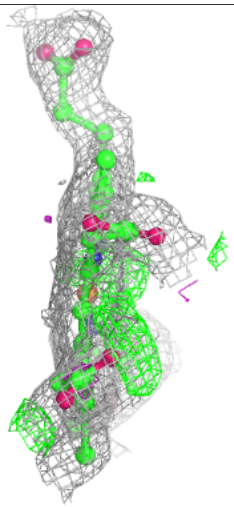


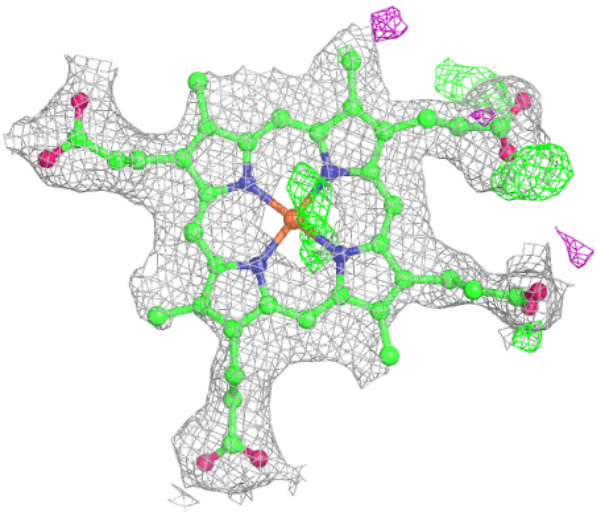
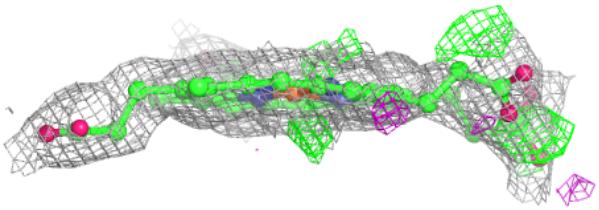
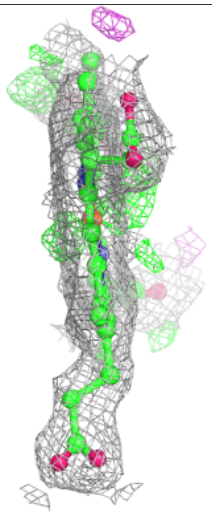
Electron density around FEC K 2104 (B):

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



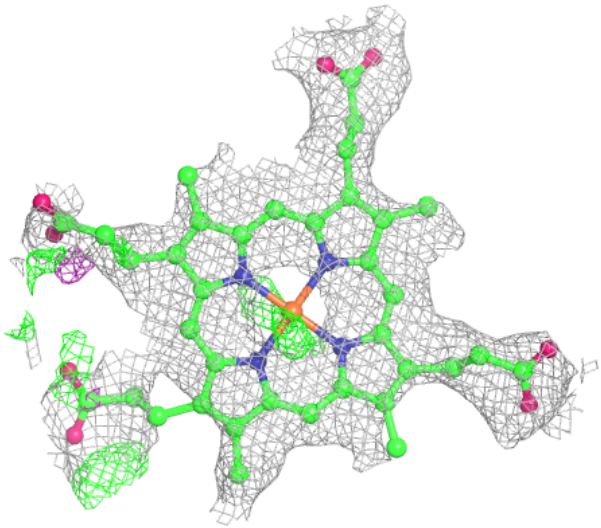


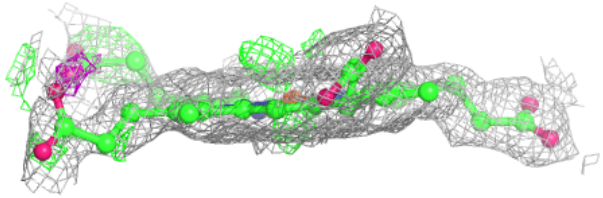


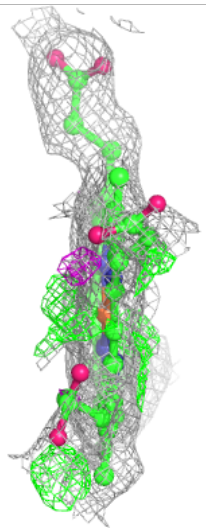
Electron density around FEC N 2403 (A): 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around FEC N 2403 (B):

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

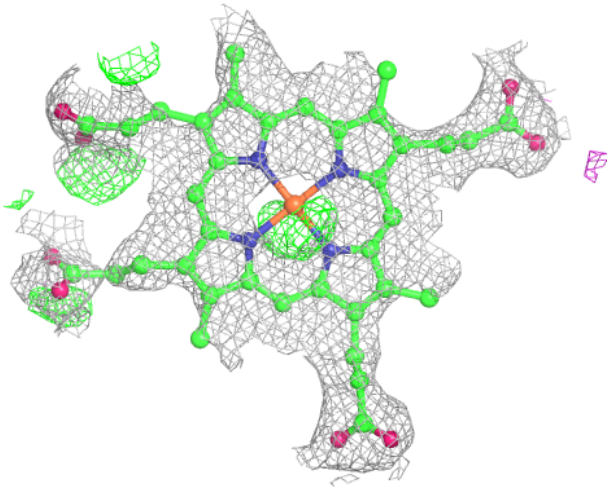


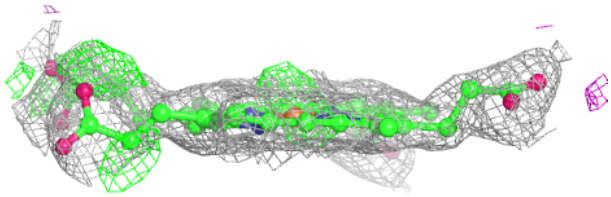


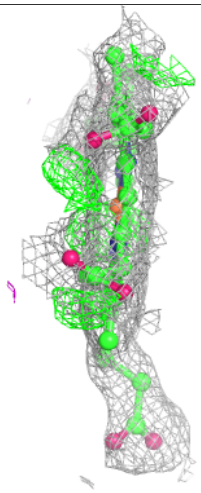


Electron density around FEC A 1005 (A):

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

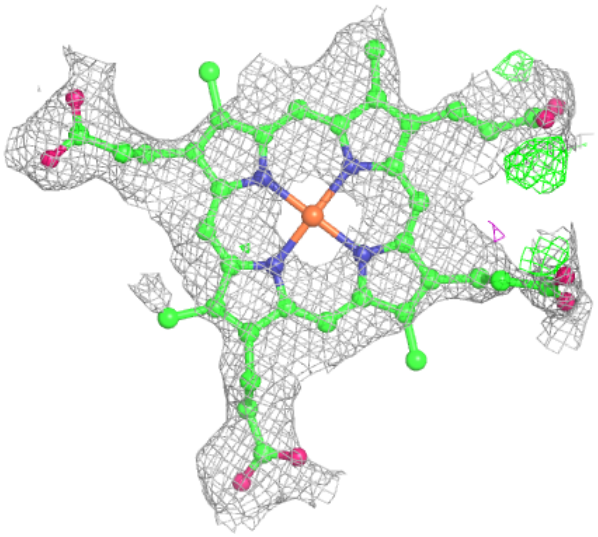


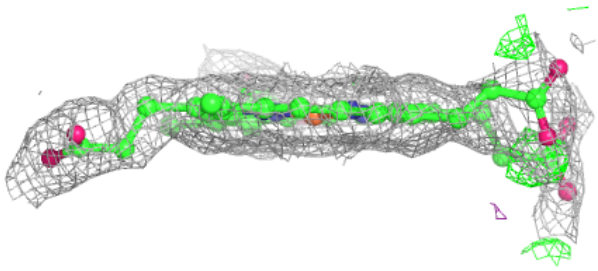


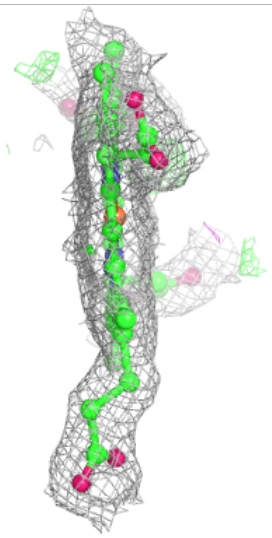


Electron density around FEC I 1903 (A):

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

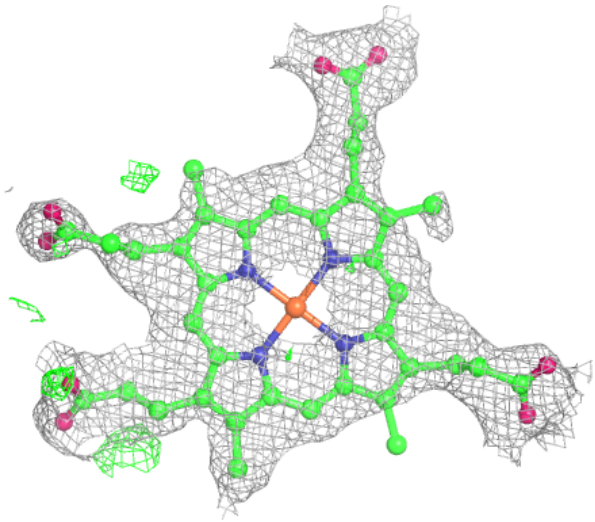


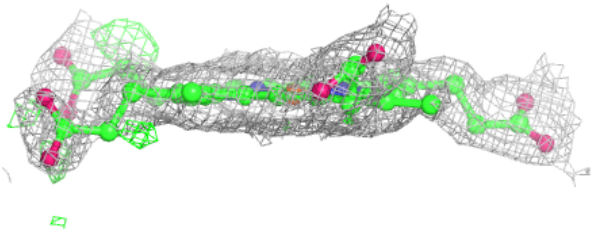


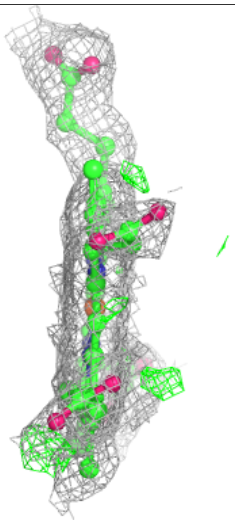


Electron density around FEC I 1903 (B):

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

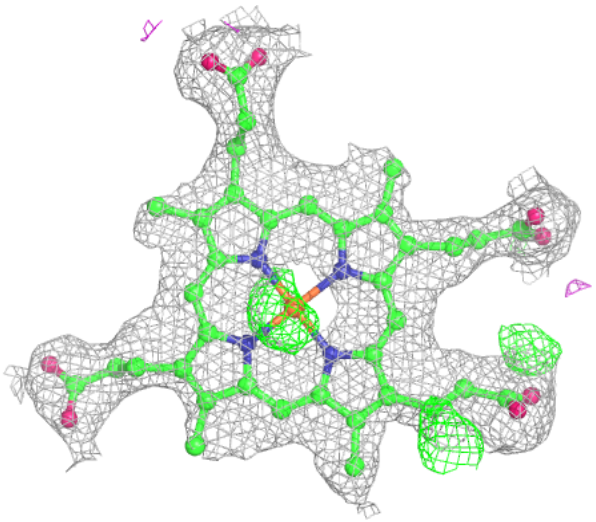


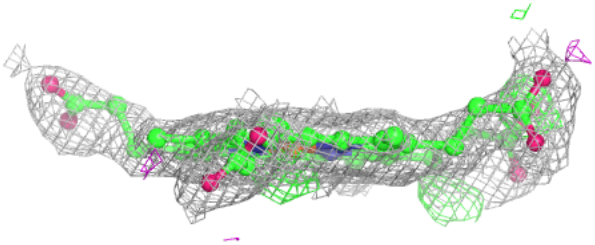




Electron density around FEC A 1005 (B):

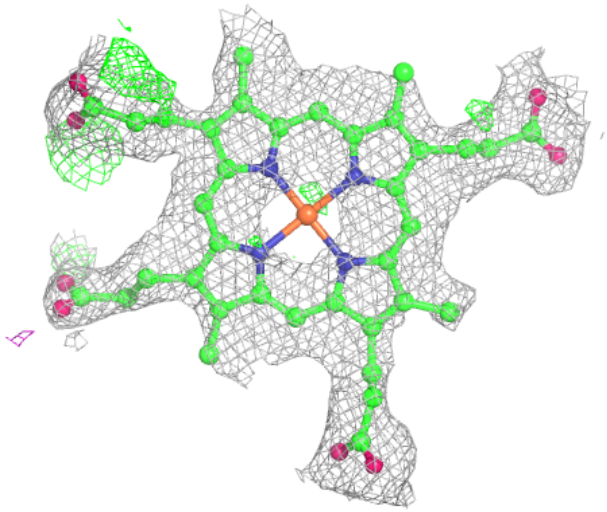
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

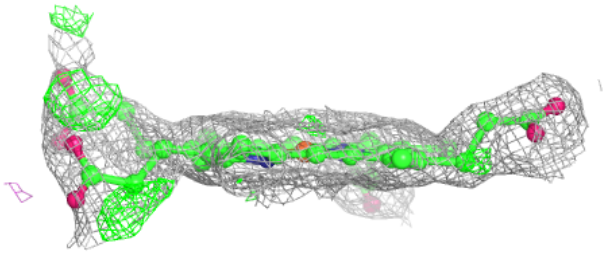


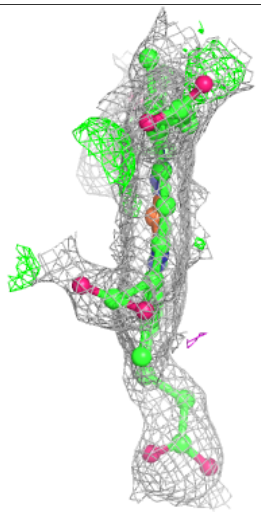


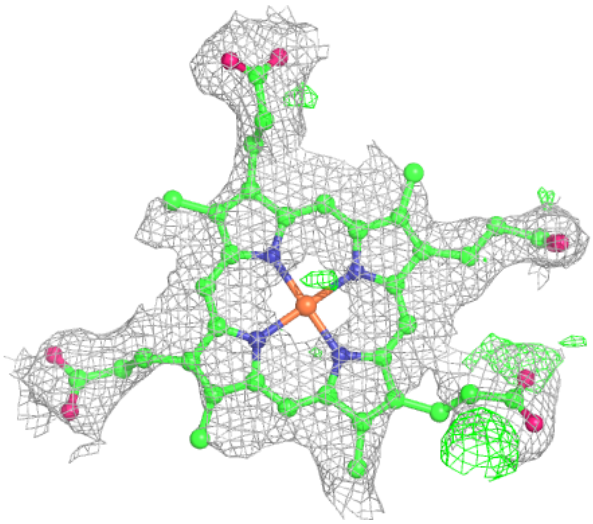
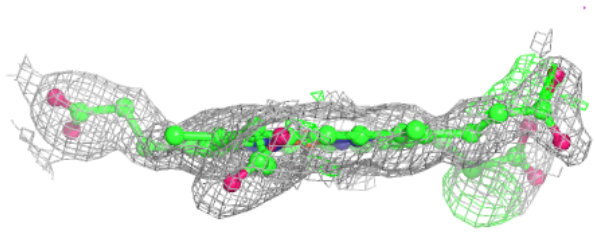
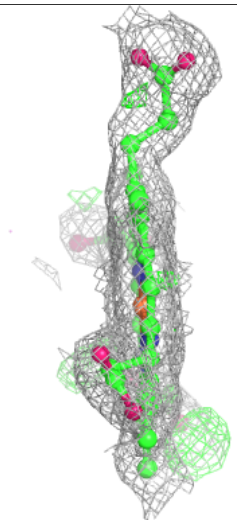
Electron density around FEC O 2502 (A):

$2mF_o$-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 O 2502 (B): $2mF_o$-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.