Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2026 – 09:00 pm BST

PDB ID	:	6FXJ / pdb_00006fxj
Title	:	Structure of coproheme decarboxylase from Listeria monocytogenes in complex with iron coproporphyrin III
Authors	:	Hofbauer, S.; Pfanzagl, V.; Mlynek, G.
Deposited on	:	2018-03-09
Resolution	:	1.79 Å(reported)

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

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

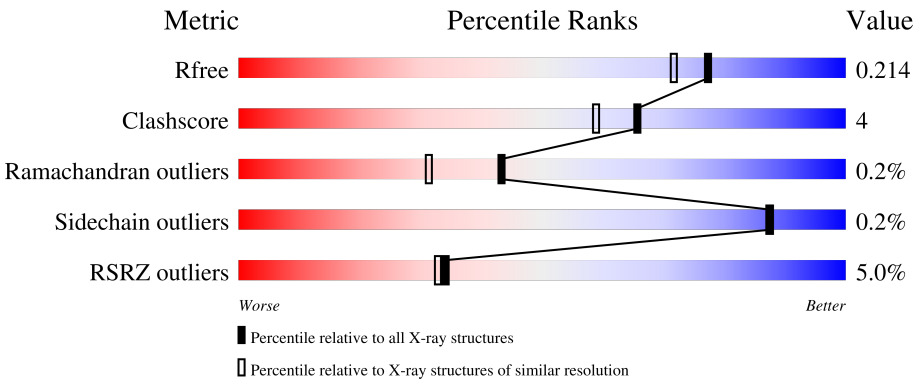
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	251	2%, 95%, 5%
1	B	251	7%, 90%, 5%, 6%
1	C	251	8%, 83%, 10%, •, 6%
1	D	251	2%, 92%, 7%
1	E	251	5%, 89%, 6%, 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21321 atoms, of which 9872 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.

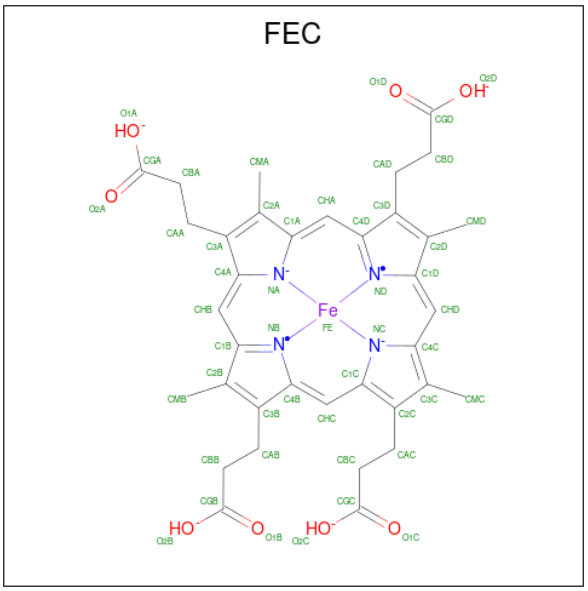
- Molecule 1 is a protein called Putative heme-dependent peroxidase lmo2113.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	251	4120	1336	2030	351	393	10	0	16	0
1	B	237	3912	1272	1934	328	370	8	23	11	0
1	C	237	3855	1254	1903	327	363	8	0	4	0
1	D	250	4030	1312	1984	342	383	9	0	4	0
1	E	238	3931	1280	1941	334	368	8	0	10	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

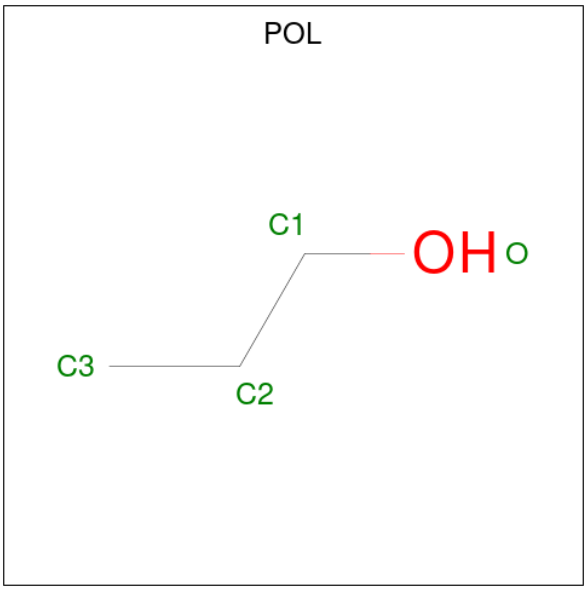
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	1	1	1	0	0

- Molecule 3 is 1,3,5,8-TETRAMETHYL-PORPHINE-2,4,6,7-TETRAPROPIONIC ACID FERROUS COMPLEX (CCD ID: FEC) (formula: $C_{36}H_{36}FeN_4O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			49	36	1	4	8		
3	B	1	Total	C	Fe	N	O	0	0
			49	36	1	4	8		
3	C	1	Total	C	Fe	N	O	0	0
			49	36	1	4	8		
3	D	1	Total	C	Fe	N	O	0	0
			49	36	1	4	8		
3	E	1	Total	C	Fe	N	O	0	0
			49	36	1	4	8		

- Molecule 4 is N-PROPANOL (CCD ID: POL) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	B	1	12	3	8	1	0	0
			Total	C	H	O		
4	B	1	12	3	8	1	0	0
			Total	C	H	O		
4	C	1	12	3	8	1	0	0
			Total	C	H	O		
4	C	1	12	3	8	1	0	0
			Total	C	H	O		
4	C	1	12	3	8	1	0	0
			Total	C	H	O		
4	D	1	12	3	8	1	0	0
			Total	C	H	O		
4	D	1	12	3	8	1	0	0
			Total	C	H	O		
4	D	1	12	3	8	1	0	0
			Total	C	H	O		
4	E	1	12	3	8	1	0	0
			Total	C	H	O		
4	E	1	12	3	8	1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	D	1	1	1	0	0

- Molecule 6 is water.

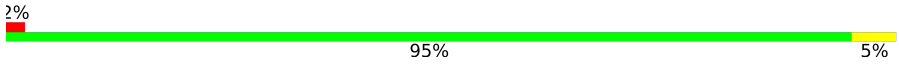
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	247	247	247	0	0
			Total	O		
6	B	186	186	186	0	0
			Total	O		
6	C	198	198	198	0	0
			Total	O		
6	D	273	273	273	0	0
			Total	O		
6	E	196	196	196	0	0

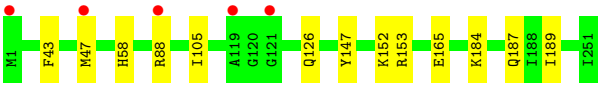
3 Residue-property plots (i)

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: Putative heme-dependent peroxidase lmo2113

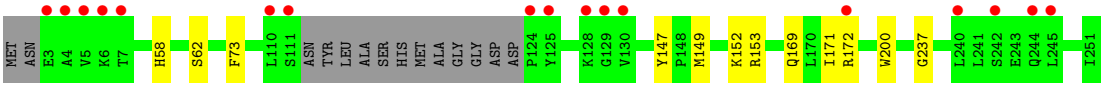
Chain A:





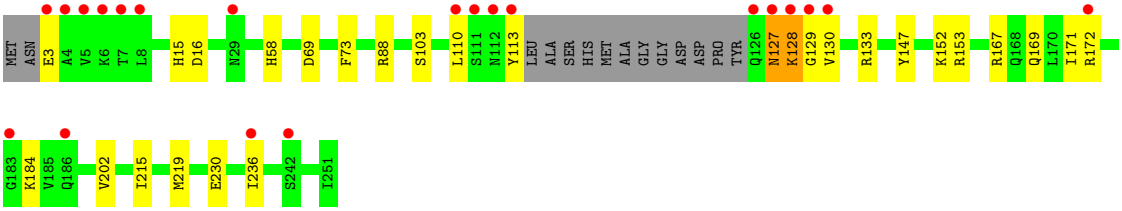
• Molecule 1: Putative heme-dependent peroxidase lmo2113

Chain B:



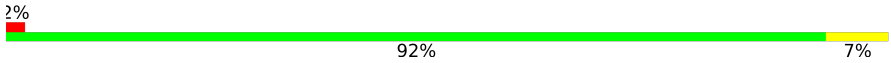
• Molecule 1: Putative heme-dependent peroxidase lmo2113

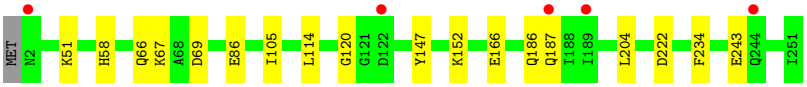
Chain C:



• Molecule 1: Putative heme-dependent peroxidase lmo2113

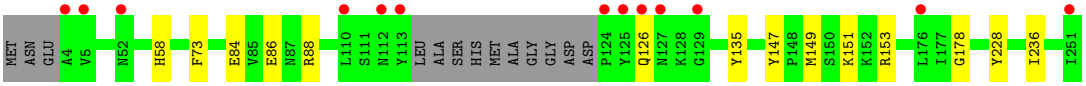
Chain D:





• Molecule 1: Putative heme-dependent peroxidase lmo2113

Chain E:


MET
ASN
GLU
A4
V5
N52
H58
F73
E84
V85
E86
N87
R88
L110
S111
N112
Y113
LEU
ALA
SER
HIS
MET
ALA
GLY
GLY
ASP
ASP
P124
Y125
Q126
N127
K128
G129
Y135
Y147
P148
M149
S150
K151
K152
R153
L176
I177
G178
Y228
I236
I251

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.87Å 129.11Å 77.92Å 90.00° 105.96° 90.00°	Depositor
Resolution (Å)	48.89 – 1.79 48.89 – 1.79	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.89-1.79) 83.7 (48.89-1.79)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 1.79Å)	Xtriage
Refinement program	PHENIX dev_2719, PHENIX dev_2719	Depositor
R, R_{free}	0.186 , 0.214 0.188 , 0.214	Depositor DCC
R_{free} test set	2005 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.970	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21321	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: POL, FEC, CL, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.21	0/2188	0.39	0/2954
1	B	0.20	0/2068	0.39	0/2787
1	C	0.21	0/2014	0.36	0/2717
1	D	0.21	0/2108	0.40	0/2846
1	E	0.20	0/2091	0.37	0/2818
All	All	0.21	0/10469	0.38	0/14122

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2090	2030	1967	14	0
1	B	1978	1934	1883	9	0
1	C	1952	1903	1891	24	0
1	D	2046	1984	1967	17	0
1	E	1990	1941	1883	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	1	0	0	0	0
3	A	49	0	32	3	0
3	B	49	0	32	4	0
3	C	49	0	32	9	0
3	D	49	0	31	5	0
3	E	49	0	32	5	0
4	B	8	16	16	0	0
4	C	12	24	24	0	0
4	D	12	24	24	0	0
4	E	8	16	16	1	0
5	D	1	0	0	0	0
6	A	247	0	0	4	0
6	B	186	0	0	1	0
6	C	198	0	0	5	0
6	D	273	0	0	10	0
6	E	196	0	0	8	0
All	All	11449	9872	9830	78	0

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

All (78) 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:A:147:TYR:OH	3:A:302:FEC:HAD1	1.69	0.92
1:D:147:TYR:OH	3:D:302:FEC:HAD1	1.69	0.91
1:D:120:GLY:O	6:D:401:HOH:O	1.90	0.88
1:D:186:GLN:OE1	6:D:402:HOH:O	1.92	0.87
1:A:165:GLU:OE2	6:A:401:HOH:O	1.97	0.83
1:A:187[A]:GLN:OE1	6:A:402:HOH:O	1.98	0.81
1:A:126:GLN:NE2	6:A:403:HOH:O	2.13	0.80
1:E:86:GLU:OE2	6:E:401:HOH:O	1.99	0.79
1:B:147:TYR:OH	3:B:302:FEC:HAD1	1.81	0.79
3:C:302:FEC:O2D	3:C:302:FEC:HMD3	1.82	0.79
1:E:147:TYR:OH	3:E:302:FEC:HAD1	1.83	0.78
1:C:219:MET:SD	3:C:302:FEC:HBA2	2.24	0.78
1:C:127:ASN:O	1:C:130:VAL:N	2.18	0.76
1:C:184:LYS:NZ	6:C:403:HOH:O	2.17	0.76
1:D:51:LYS:NZ	6:D:403:HOH:O	1.93	0.73
1:B:149:MET:SD	3:B:302:FEC:HBD1	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASP:OD1	6:C:401:HOH:O	2.08	0.72
1:E:84:GLU:OE1	6:E:404:HOH:O	2.08	0.70
1:D:243:GLU:O	6:D:404:HOH:O	2.08	0.70
1:C:128:LYS:NZ	6:C:404:HOH:O	2.26	0.69
1:C:169:GLN:OE1	1:C:172[A]:ARG:NH1	2.25	0.68
1:E:149:MET:SD	3:E:302:FEC:HBD1	2.33	0.67
4:E:303:POL:O	6:E:403:HOH:O	2.08	0.66
1:D:166:GLU:OE1	6:D:405:HOH:O	2.14	0.66
1:C:3:GLU:OE2	6:C:402:HOH:O	2.14	0.65
1:E:88[B]:ARG:NH2	6:E:409:HOH:O	2.30	0.64
1:E:135:TYR:OH	6:E:405:HOH:O	2.16	0.63
1:C:88:ARG:HD3	6:C:545:HOH:O	2.00	0.61
1:A:184:LYS:NZ	6:A:404:HOH:O	2.14	0.59
1:D:67:LYS:NZ	1:D:234:PHE:O	2.37	0.58
1:D:86:GLU:OE2	6:D:406:HOH:O	2.18	0.57
1:C:147:TYR:OH	3:C:302:FEC:O1A	2.22	0.56
1:E:126:GLN:NE2	6:E:402:HOH:O	2.01	0.56
1:A:47:MET:HE2	1:A:58:HIS:CG	2.42	0.55
1:A:43:PHE:CE1	1:A:47:MET:SD	3.00	0.54
1:C:215:ILE:HD11	3:C:302:FEC:HMB3	1.90	0.54
1:B:152:LYS:NZ	1:E:153:ARG:O	2.41	0.53
1:D:147:TYR:CZ	3:D:302:FEC:HAD1	2.45	0.52
1:B:169:GLN:OE1	1:B:172:ARG:NH1	2.44	0.51
1:E:178:GLY:CA	3:E:302:FEC:HMC2	2.43	0.48
1:A:152:LYS:NZ	1:B:153:ARG:O	2.46	0.48
1:C:202:VAL:HG21	3:C:302:FEC:HMA3	1.96	0.48
1:A:105:ILE:HG21	1:C:236:ILE:HD11	1.96	0.48
1:A:153:ARG:O	1:C:152:LYS:NZ	2.46	0.48
3:E:302:FEC:HHB	6:E:406:HOH:O	2.14	0.48
3:C:302:FEC:HBB1	3:C:302:FEC:HHC	1.96	0.47
1:A:187[B]:GLN:OE1	1:A:189[B]:ILE:HD11	2.14	0.47
1:C:153:ARG:O	1:D:152:LYS:NZ	2.47	0.47
3:D:302:FEC:HMB3	6:D:420:HOH:O	2.15	0.47
1:C:113:TYR:CG	1:C:171:ILE:HD13	2.50	0.47
1:B:200:TRP:CZ2	3:B:302:FEC:HBA1	2.50	0.46
1:A:147:TYR:HH	3:A:302:FEC:HAD1	1.78	0.46
3:C:302:FEC:O1A	3:C:302:FEC:CMA	2.63	0.46
1:C:219:MET:SD	3:C:302:FEC:O2A	2.74	0.46
1:D:222:ASP:OD1	6:D:407:HOH:O	2.21	0.46
1:C:202:VAL:HG11	3:C:302:FEC:HAA1	1.98	0.45
1:E:58:HIS:HA	1:E:73:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:CD2	1:A:88:ARG:NH1	2.85	0.44
1:D:204:LEU:HD11	3:D:302:FEC:HMD1	1.99	0.44
1:D:105:ILE:HG21	1:E:236:ILE:HD11	2.00	0.44
1:A:147:TYR:CZ	3:A:302:FEC:HAD1	2.50	0.44
1:B:58:HIS:HA	1:B:73:PHE:O	2.18	0.43
1:D:187[A]:GLN:N	1:D:187[A]:GLN:OE1	2.52	0.43
1:C:113:TYR:CD2	1:C:171:ILE:HD13	2.54	0.43
1:D:69:ASP:OD1	6:D:408:HOH:O	2.21	0.43
1:B:171:ILE:HD13	6:B:432:HOH:O	2.19	0.43
1:C:167:ARG:O	1:C:171:ILE:HD12	2.19	0.42
1:C:110:LEU:HD11	1:C:133:ARG:HB3	2.02	0.42
1:C:58:HIS:HA	1:C:73:PHE:O	2.19	0.42
1:B:62[A]:SER:O	1:B:237:GLY:CA	2.68	0.41
1:C:127:ASN:O	1:C:129:GLY:N	2.53	0.41
1:D:58:HIS:HB2	6:D:458:HOH:O	2.21	0.41
3:D:302:FEC:HHA	3:D:302:FEC:HAD2	1.92	0.40
1:E:151[A]:LYS:HA	1:E:228:TYR:O	2.21	0.40
1:C:15:HIS:O	1:C:103:SER:HA	2.20	0.40
3:E:302:FEC:HAA1	6:E:406:HOH:O	2.21	0.40
3:B:302:FEC:CBD	3:B:302:FEC:HHA	2.50	0.40
1:C:16:ASP:OD1	1:D:66:GLN:NE2	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	262/251 (104%)	259 (99%)	3 (1%)	0	100 100
1	B	243/251 (97%)	240 (99%)	3 (1%)	0	100 100
1	C	237/251 (94%)	232 (98%)	3 (1%)	2 (1%)	16 6
1	D	252/251 (100%)	248 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	244/251 (97%)	241 (99%)	3 (1%)	0	100	100
All	All	1238/1255 (99%)	1220 (98%)	16 (1%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	LYS
1	C	127	ASN

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	229/216 (106%)	229 (100%)	0	100	100
1	B	217/216 (100%)	217 (100%)	0	100	100
1	C	210/216 (97%)	209 (100%)	1 (0%)	81	80
1	D	218/216 (101%)	217 (100%)	1 (0%)	81	80
1	E	217/216 (100%)	217 (100%)	0	100	100
All	All	1091/1080 (101%)	1089 (100%)	2 (0%)	87	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	230	GLU
1	D	114	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	168	GLN
1	E	83	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
4	POL	E	304	-	3,3,3	0.40	0	2,2,2	0.39	0
4	POL	C	304	-	3,3,3	0.42	0	2,2,2	0.32	0
4	POL	D	303	-	3,3,3	0.42	0	2,2,2	0.30	0
4	POL	D	304	-	3,3,3	0.42	0	2,2,2	0.36	0
4	POL	D	305	-	3,3,3	0.41	0	2,2,2	0.34	0
4	POL	C	305	-	3,3,3	0.42	0	2,2,2	0.33	0
3	FEC	D	302	1	56,56,56	1.46	8 (14%)	76,90,90	1.39	11 (14%)
4	POL	B	304	-	3,3,3	0.43	0	2,2,2	0.31	0
3	FEC	A	302	1	56,56,56	1.46	6 (10%)	76,90,90	1.39	13 (17%)
4	POL	B	303	-	3,3,3	0.42	0	2,2,2	0.30	0
4	POL	C	303	-	3,3,3	0.41	0	2,2,2	0.31	0
3	FEC	B	302	-	56,56,56	1.46	7 (12%)	76,90,90	1.46	11 (14%)
4	POL	E	303	-	3,3,3	0.41	0	2,2,2	0.31	0
3	FEC	E	302	1	56,56,56	1.46	6 (10%)	76,90,90	1.38	10 (13%)
3	FEC	C	302	-	56,56,56	1.50	8 (14%)	76,90,90	1.53	16 (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	POL	E	304	-	-	0/1/1/1	-
4	POL	C	304	-	-	0/1/1/1	-
4	POL	D	303	-	-	0/1/1/1	-
4	POL	D	304	-	-	1/1/1/1	-
4	POL	D	305	-	-	0/1/1/1	-
4	POL	C	305	-	-	0/1/1/1	-
3	FEC	D	302	1	-	6/20/100/100	-
4	POL	B	304	-	-	1/1/1/1	-
3	FEC	A	302	1	-	9/20/100/100	-
4	POL	B	303	-	-	1/1/1/1	-
4	POL	C	303	-	-	0/1/1/1	-
3	FEC	B	302	-	-	11/20/100/100	-
4	POL	E	303	-	-	1/1/1/1	-
3	FEC	E	302	1	-	8/20/100/100	-
3	FEC	C	302	-	-	8/20/100/100	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	FEC	C3B-C2B	6.40	1.50	1.36
3	B	302	FEC	C3B-C2B	6.32	1.50	1.36
3	E	302	FEC	C3B-C2B	6.26	1.50	1.36
3	A	302	FEC	C3B-C2B	6.14	1.49	1.36
3	D	302	FEC	C3B-C2B	6.02	1.49	1.36
3	C	302	FEC	FE-NB	3.84	2.06	1.94
3	E	302	FEC	FE-NB	3.64	2.06	1.94
3	A	302	FEC	FE-NB	3.54	2.05	1.94
3	B	302	FEC	FE-NB	3.44	2.05	1.94
3	D	302	FEC	FE-NB	3.35	2.05	1.94
3	D	302	FEC	CMA-C2A	2.76	1.56	1.50
3	A	302	FEC	CMA-C2A	2.66	1.56	1.50
3	E	302	FEC	CMA-C2A	2.48	1.56	1.50
3	C	302	FEC	CMD-C2D	2.44	1.56	1.50
3	B	302	FEC	CMA-C2A	2.42	1.55	1.50
3	B	302	FEC	CMD-C2D	2.41	1.55	1.50
3	A	302	FEC	CMD-C2D	2.38	1.55	1.50
3	E	302	FEC	CMC-C3C	2.33	1.55	1.50
3	C	302	FEC	CMA-C2A	2.33	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	FEC	CMC-C3C	2.32	1.55	1.50
3	E	302	FEC	CMD-C2D	2.32	1.55	1.50
3	B	302	FEC	CMC-C3C	2.32	1.55	1.50
3	D	302	FEC	CMD-C2D	2.31	1.55	1.50
3	D	302	FEC	CMC-C3C	2.29	1.55	1.50
3	C	302	FEC	CMC-C3C	2.28	1.55	1.50
3	D	302	FEC	CAD-C3D	2.23	1.57	1.51
3	D	302	FEC	C2C-C3C	-2.21	1.32	1.38
3	E	302	FEC	CAD-C3D	2.15	1.56	1.51
3	A	302	FEC	FE-NA	2.13	2.02	1.95
3	C	302	FEC	CAD-C3D	2.12	1.56	1.51
3	B	302	FEC	CAD-C3D	2.11	1.56	1.51
3	C	302	FEC	C2C-C3C	-2.09	1.33	1.38
3	D	302	FEC	FE-NA	2.02	2.02	1.95
3	C	302	FEC	CAC-C2C	2.02	1.56	1.51
3	B	302	FEC	CAC-C2C	2.02	1.56	1.51

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	FEC	CBD-CAD-C3D	4.43	124.93	112.63
3	B	302	FEC	C4B-NB-C1B	4.04	109.25	105.07
3	B	302	FEC	CAD-C3D-C4D	-3.78	118.06	124.66
3	B	302	FEC	CAD-C3D-C2D	3.76	134.88	127.88
3	C	302	FEC	CBA-CAA-C3A	3.72	122.95	112.63
3	E	302	FEC	C4B-NB-C1B	3.71	108.90	105.07
3	A	302	FEC	C4B-NB-C1B	3.65	108.85	105.07
3	B	302	FEC	CBD-CAD-C3D	3.62	122.68	112.63
3	D	302	FEC	CBD-CAD-C3D	3.61	122.65	112.63
3	E	302	FEC	CAD-C3D-C2D	3.40	134.22	127.88
3	E	302	FEC	CBD-CAD-C3D	3.40	122.07	112.63
3	E	302	FEC	O1A-CGA-O2A	3.36	131.68	123.30
3	A	302	FEC	O1A-CGA-O2A	3.31	131.55	123.30
3	E	302	FEC	CAD-C3D-C4D	-3.25	118.98	124.66
3	B	302	FEC	O1A-CGA-O2A	3.23	131.35	123.30
3	A	302	FEC	CBD-CAD-C3D	3.21	121.56	112.63
3	C	302	FEC	C4B-NB-C1B	3.20	108.38	105.07
3	D	302	FEC	C4B-NB-C1B	3.17	108.35	105.07
3	C	302	FEC	CMD-C2D-C1D	-3.09	120.33	125.04
3	D	302	FEC	CAD-C3D-C2D	3.05	133.55	127.88
3	D	302	FEC	CAD-C3D-C4D	-3.03	119.36	124.66
3	E	302	FEC	O2A-CGA-CBA	-2.99	113.49	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	FEC	O2A-CGA-CBA	-2.93	113.68	123.08
3	D	302	FEC	O1A-CGA-O2A	2.90	130.52	123.30
3	A	302	FEC	C1B-C2B-C3B	-2.84	103.97	106.96
3	E	302	FEC	O1D-CGD-CBD	-2.80	114.09	123.08
3	C	302	FEC	O1D-CGD-CBD	-2.76	114.20	123.08
3	B	302	FEC	O1D-CGD-CBD	-2.74	114.28	123.08
3	A	302	FEC	O2D-CGD-O1D	2.68	129.99	123.30
3	C	302	FEC	O2D-CGD-O1D	2.68	129.99	123.30
3	D	302	FEC	C1B-C2B-C3B	-2.60	104.22	106.96
3	B	302	FEC	O2D-CGD-O1D	2.59	129.74	123.30
3	D	302	FEC	O2D-CGD-O1D	2.58	129.73	123.30
3	B	302	FEC	CBA-CAA-C3A	2.58	119.80	112.63
3	C	302	FEC	CHA-C1A-NA	2.54	127.19	124.44
3	B	302	FEC	O2A-CGA-CBA	-2.54	114.91	123.08
3	C	302	FEC	C1B-C2B-C3B	-2.54	104.28	106.96
3	B	302	FEC	C1B-C2B-C3B	-2.53	104.29	106.96
3	C	302	FEC	O2C-CGC-CBC	2.49	122.04	114.03
3	A	302	FEC	CBB-CAB-C3B	-2.49	105.70	112.63
3	D	302	FEC	O1D-CGD-CBD	-2.49	115.09	123.08
3	D	302	FEC	O2A-CGA-CBA	-2.46	115.18	123.08
3	E	302	FEC	C1B-C2B-C3B	-2.44	104.39	106.96
3	E	302	FEC	O2D-CGD-O1D	2.44	129.38	123.30
3	B	302	FEC	O2C-CGC-CBC	2.43	121.84	114.03
3	C	302	FEC	CBB-CAB-C3B	-2.43	105.89	112.63
3	A	302	FEC	CAD-C3D-C4D	-2.41	120.44	124.66
3	A	302	FEC	CAD-C3D-C2D	2.39	132.32	127.88
3	A	302	FEC	CAA-C3A-C4A	-2.35	120.46	124.89
3	C	302	FEC	O1A-CGA-O2A	2.33	129.10	123.30
3	D	302	FEC	O2C-CGC-CBC	2.30	121.42	114.03
3	C	302	FEC	CAC-C2C-C1C	2.21	129.24	124.89
3	C	302	FEC	CMD-C2D-C3D	2.20	132.09	126.12
3	A	302	FEC	O2C-CGC-CBC	2.19	121.06	114.03
3	C	302	FEC	O2A-CGA-CBA	-2.19	116.05	123.08
3	C	302	FEC	C4A-NA-C1A	2.17	107.47	105.35
3	A	302	FEC	C4A-NA-C1A	2.17	107.47	105.35
3	E	302	FEC	O2C-CGC-CBC	2.13	120.89	114.03
3	A	302	FEC	O1D-CGD-CBD	-2.10	116.33	123.08
3	D	302	FEC	CAA-C3A-C4A	-2.09	120.95	124.89
3	C	302	FEC	CHC-C4B-NB	2.04	126.89	124.37

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	FEC	C2C-CAC-CBC-CGC
3	B	302	FEC	C2A-C3A-CAA-CBA
3	B	302	FEC	C4A-C3A-CAA-CBA
3	A	302	FEC	C1C-C2C-CAC-CBC
3	C	302	FEC	C2C-CAC-CBC-CGC
3	C	302	FEC	C2D-C3D-CAD-CBD
3	C	302	FEC	C4D-C3D-CAD-CBD
3	A	302	FEC	C2C-CAC-CBC-CGC
3	B	302	FEC	C3D-CAD-CBD-CGD
3	C	302	FEC	C3A-CAA-CBA-CGA
3	D	302	FEC	C2C-CAC-CBC-CGC
3	E	302	FEC	C3D-CAD-CBD-CGD
3	B	302	FEC	C3A-CAA-CBA-CGA
3	B	302	FEC	C4D-C3D-CAD-CBD
3	A	302	FEC	C3C-C2C-CAC-CBC
4	E	303	POL	O-C1-C2-C3
3	A	302	FEC	CAC-CBC-CGC-O1C
3	C	302	FEC	CAC-CBC-CGC-O2C
3	D	302	FEC	CAC-CBC-CGC-O1C
3	A	302	FEC	CAA-CBA-CGA-O1A
3	A	302	FEC	CAA-CBA-CGA-O2A
3	C	302	FEC	CAC-CBC-CGC-O1C
3	D	302	FEC	CAC-CBC-CGC-O2C
3	E	302	FEC	CAC-CBC-CGC-O2C
3	A	302	FEC	CAC-CBC-CGC-O2C
3	C	302	FEC	CAA-CBA-CGA-O2A
3	B	302	FEC	CAB-CBB-CGB-O1B
4	B	303	POL	O-C1-C2-C3
4	B	304	POL	O-C1-C2-C3
4	D	304	POL	O-C1-C2-C3
3	E	302	FEC	CAC-CBC-CGC-O1C
3	B	302	FEC	CAB-CBB-CGB-O2B
3	C	302	FEC	CAA-CBA-CGA-O1A
3	E	302	FEC	CAB-CBB-CGB-O2B
3	A	302	FEC	CAD-CBD-CGD-O2D
3	E	302	FEC	CAB-CBB-CGB-O1B
3	E	302	FEC	CAA-CBA-CGA-O1A
3	E	302	FEC	CAA-CBA-CGA-O2A
3	B	302	FEC	C2D-C3D-CAD-CBD
3	A	302	FEC	CAD-CBD-CGD-O1D
3	B	302	FEC	CAC-CBC-CGC-O1C
3	B	302	FEC	CAC-CBC-CGC-O2C
3	D	302	FEC	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
3	E	302	FEC	C4D-C3D-CAD-CBD
3	D	302	FEC	CAA-CBA-CGA-O1A
3	D	302	FEC	CAA-CBA-CGA-O2A

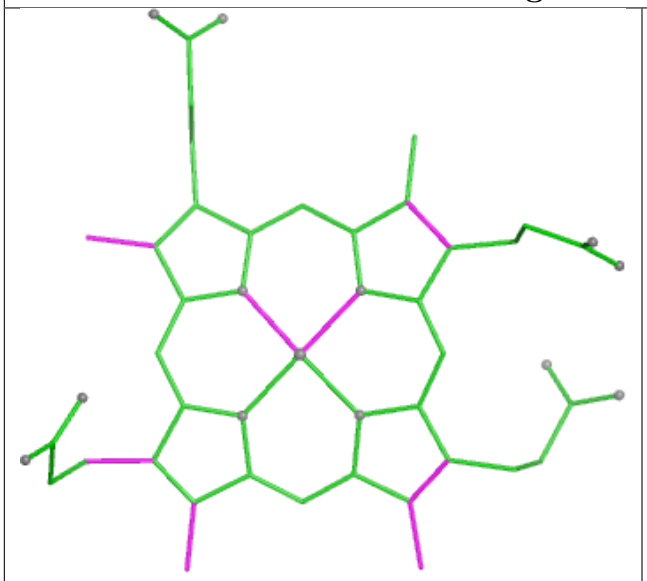
There are no ring outliers.

6 monomers are involved in 27 short contacts:

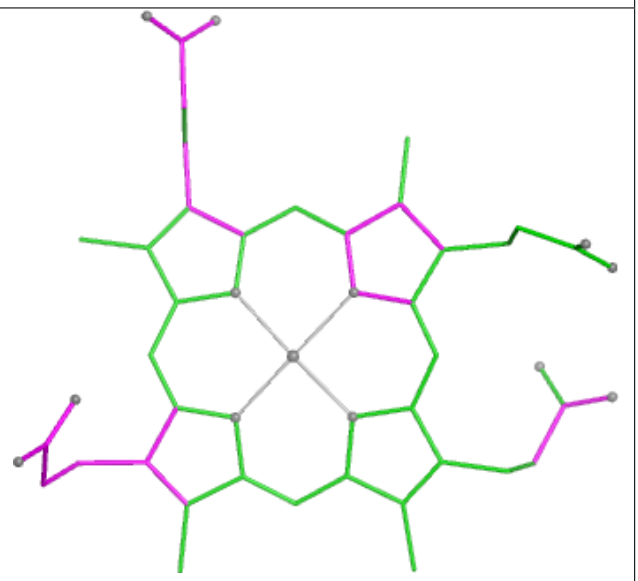
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	FEC	5	0
3	A	302	FEC	3	0
3	B	302	FEC	4	0
4	E	303	POL	1	0
3	E	302	FEC	5	0
3	C	302	FEC	9	0

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.

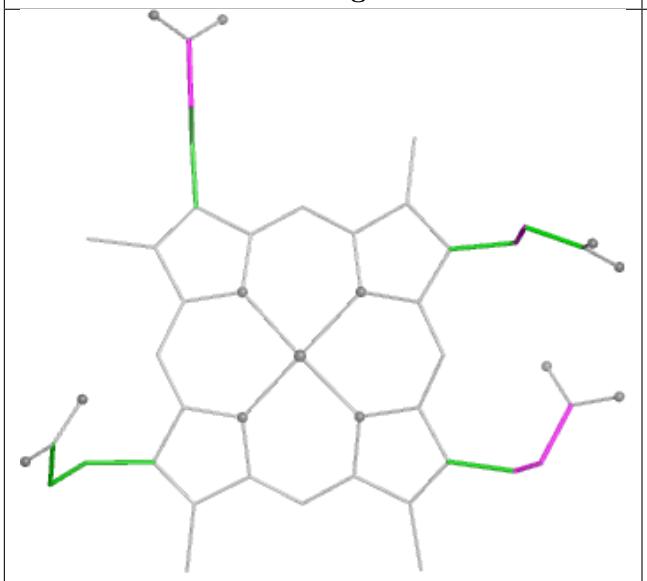
Ligand FEC D 302



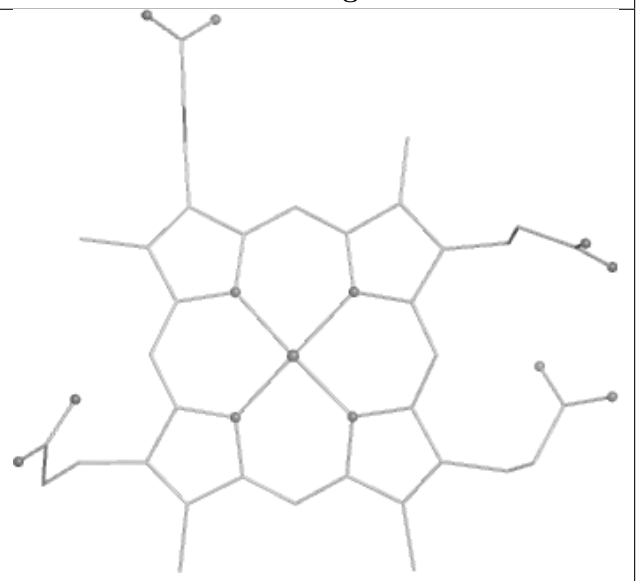
Bond lengths



Bond angles

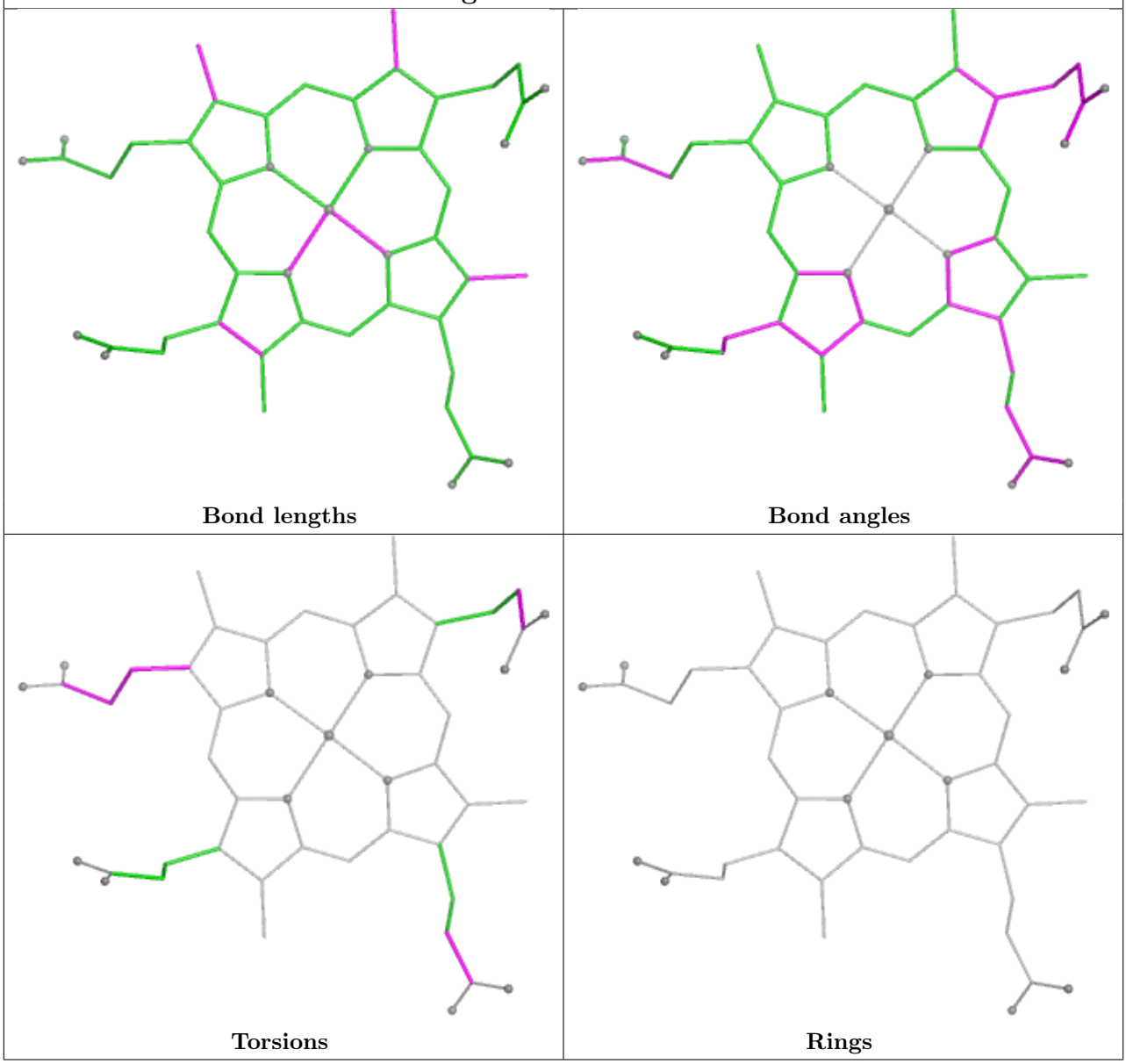


Torsions

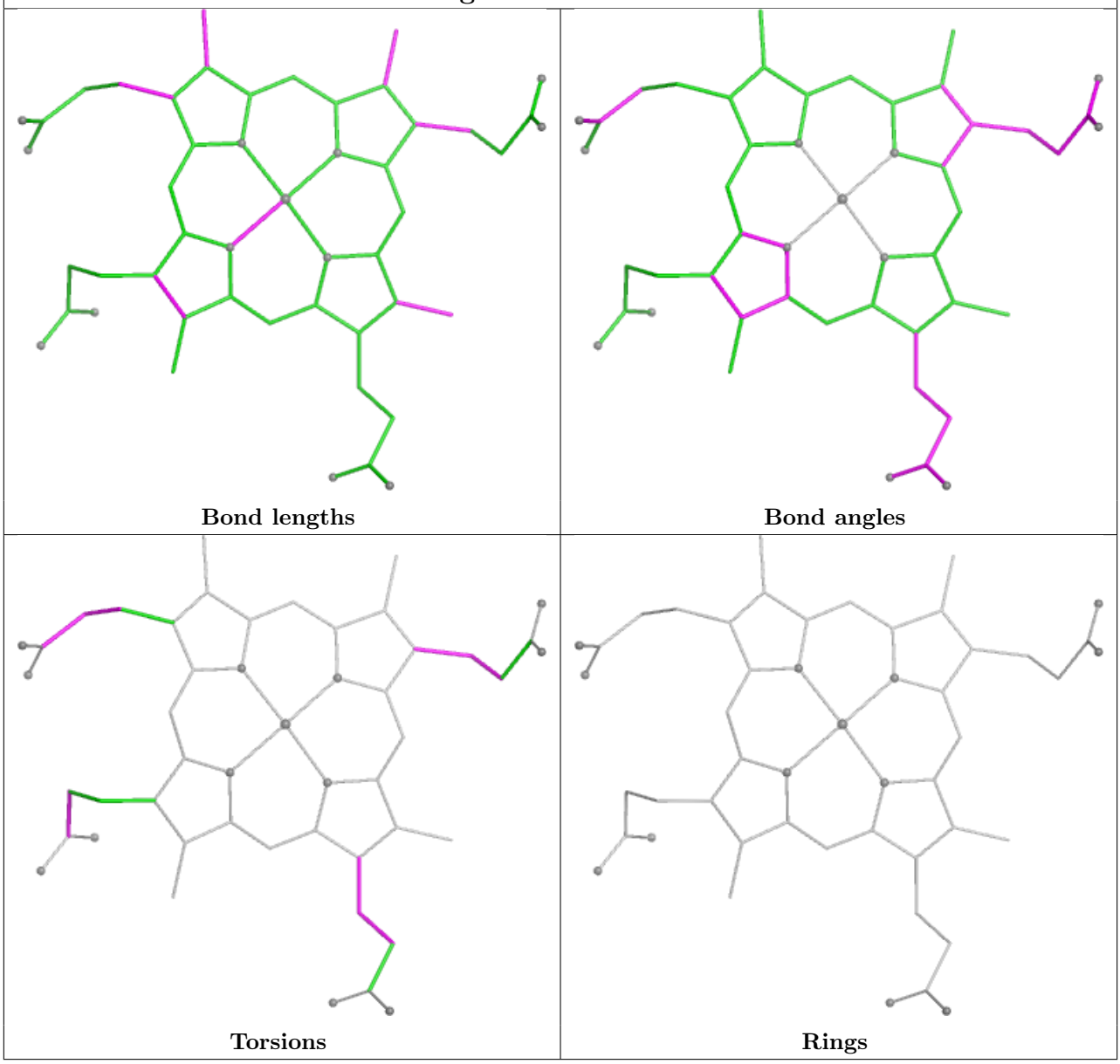


Rings

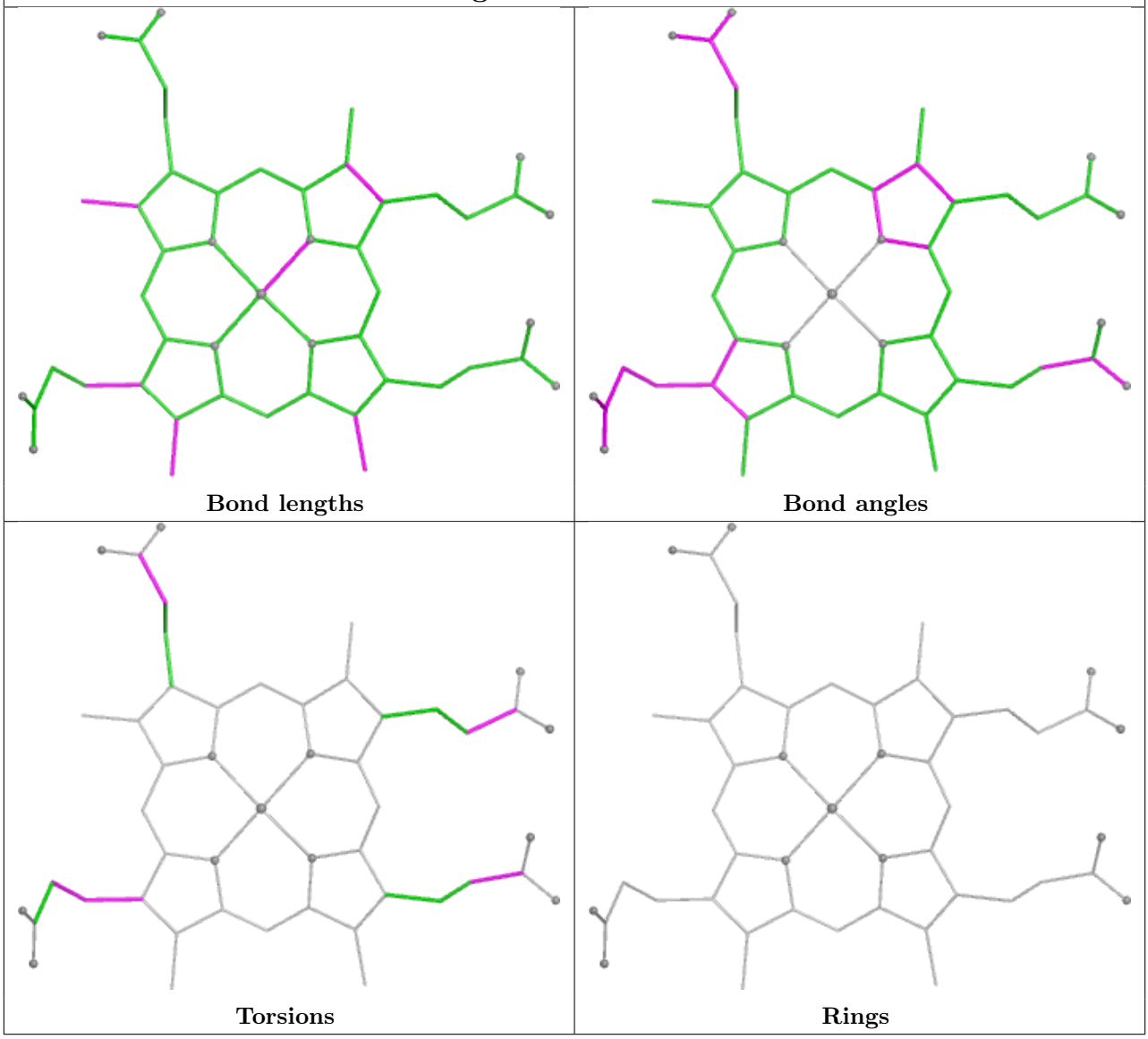
Ligand FEC A 302



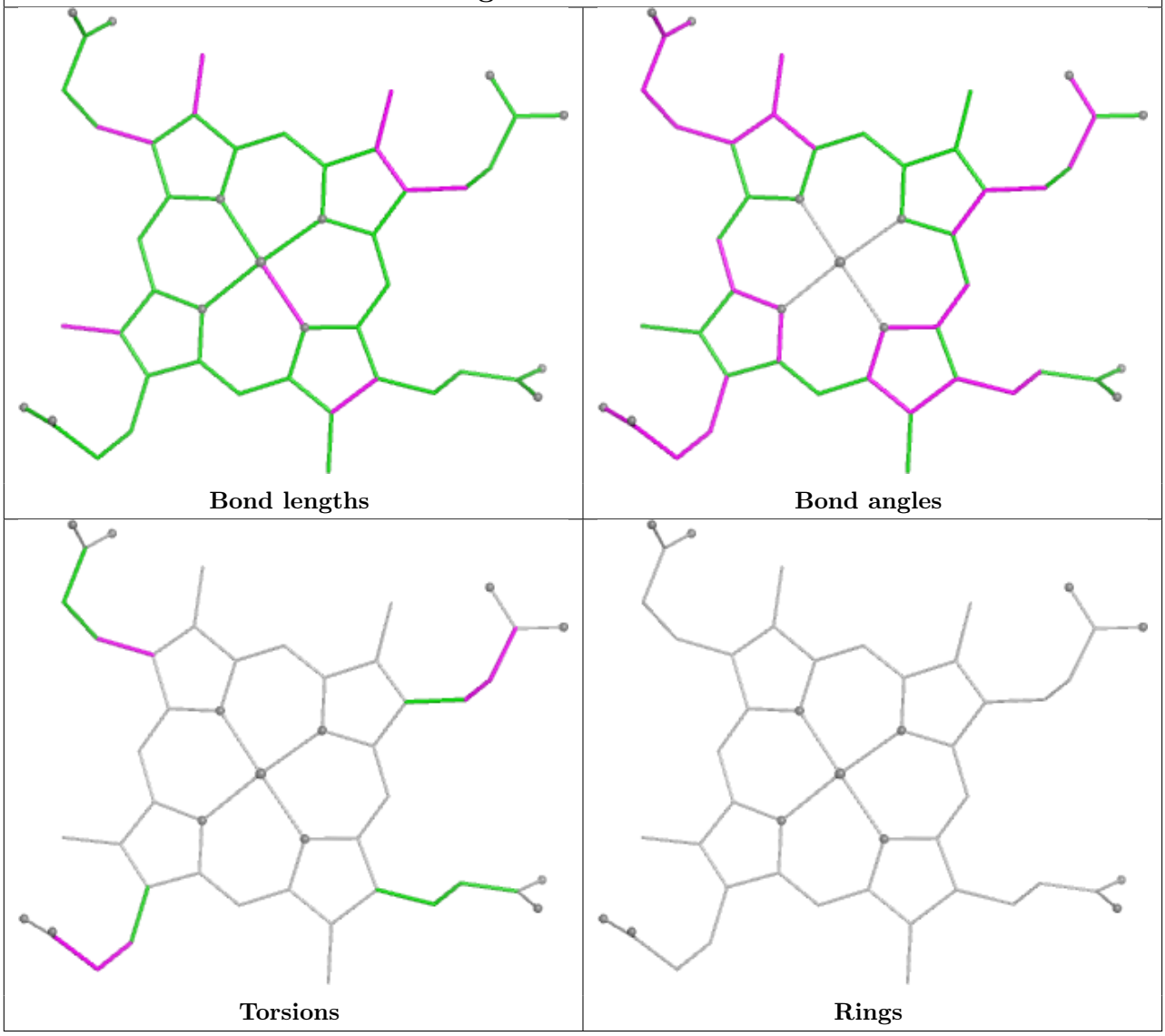
Ligand FEC B 302



Ligand FEC E 302



Ligand FEC C 302



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	251/251 (100%)	0.10	5 (1%)	65	65	12, 30, 55, 101	7 (2%)
1	B	237/251 (94%)	0.28	17 (7%)	21	20	13, 30, 67, 108	7 (2%)
1	C	237/251 (94%)	0.40	21 (8%)	15	13	20, 31, 72, 125	2 (0%)
1	D	250/251 (99%)	0.00	5 (2%)	65	65	18, 28, 53, 74	2 (0%)
1	E	238/251 (94%)	0.28	13 (5%)	30	29	12, 30, 71, 115	5 (2%)
All	All	1213/1255 (96%)	0.21	61 (5%)	34	33	12, 30, 63, 125	23 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	VAL	6.7
1	B	5	VAL	5.9
1	B	111[A]	SER	5.8
1	B	4	ALA	5.2
1	E	113	TYR	5.1
1	C	110	LEU	5.0
1	C	4	ALA	4.9
1	C	113	TYR	4.7
1	B	124	PRO	4.3
1	C	130	VAL	4.2
1	E	4	ALA	4.1
1	C	129	GLY	4.1
1	C	3	GLU	4.0
1	E	125	TYR	3.8
1	A	47	MET	3.7
1	E	124	PRO	3.6
1	C	7	THR	3.6
1	C	6	LYS	3.4
1	B	110	LEU	3.3
1	B	125	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	126	GLN	3.2
1	C	128	LYS	3.2
1	A	1	MET	3.1
1	B	7	THR	3.1
1	D	187[A]	GLN	3.0
1	E	5	VAL	3.0
1	C	112[A]	ASN	3.0
1	B	3	GLU	2.9
1	D	2	ASN	2.8
1	A	88	ARG	2.7
1	C	127	ASN	2.7
1	C	8	LEU	2.6
1	B	129	GLY	2.6
1	D	189	ILE	2.6
1	B	245	LEU	2.5
1	C	29	ASN	2.5
1	E	127	ASN	2.5
1	E	251	ILE	2.5
1	D	244	GLN	2.5
1	D	122	ASP	2.5
1	E	52	ASN	2.4
1	A	119	ALA	2.4
1	B	240[A]	LEU	2.4
1	C	186	GLN	2.3
1	E	112	ASN	2.3
1	B	130	VAL	2.3
1	E	176	LEU	2.3
1	B	6	LYS	2.2
1	E	129	GLY	2.2
1	C	111[A]	SER	2.2
1	C	242	SER	2.2
1	B	242[A]	SER	2.2
1	C	183	GLY	2.1
1	B	244	GLN	2.1
1	C	172[A]	ARG	2.1
1	C	236	ILE	2.1
1	A	121	GLY	2.1
1	B	128	LYS	2.1
1	B	172	ARG	2.1
1	E	110	LEU	2.1
1	E	126	GLN	2.0

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 oligosaccharides in this entry.

6.4 Ligands (i)

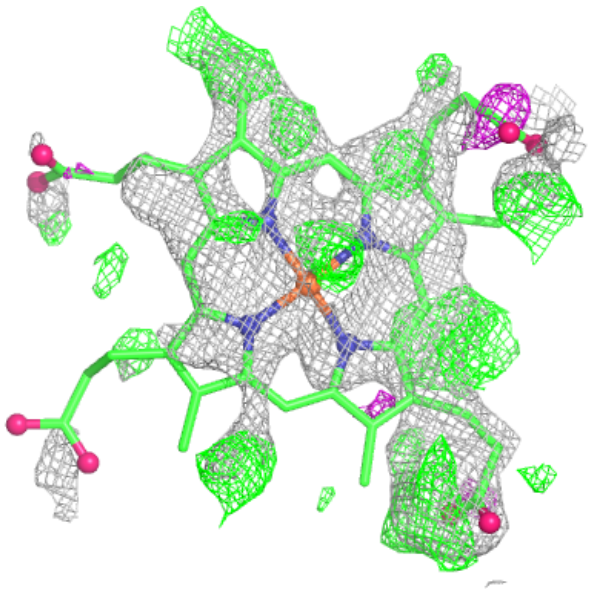
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

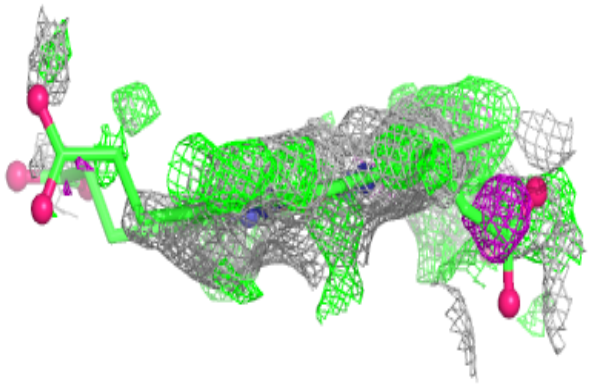
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FEC	C	302	49/49	0.74	0.33	63,72,82,84	49
4	POL	C	305	4/4	0.75	0.16	57,68,70,70	0
4	POL	D	303	4/4	0.77	0.17	61,74,76,76	0
4	POL	B	304	4/4	0.78	0.22	56,68,70,70	0
4	POL	C	304	4/4	0.79	0.22	61,75,76,76	0
4	POL	D	304	4/4	0.80	0.17	51,62,63,63	0
4	POL	D	305	4/4	0.84	0.23	57,70,72,72	0
3	FEC	B	302	49/49	0.85	0.21	44,57,75,84	0
3	FEC	A	302	49/49	0.85	0.17	29,39,63,84	0
2	NA	D	306	1/1	0.86	0.24	56,56,56,56	0
4	POL	B	303	4/4	0.86	0.16	50,63,64,64	0
4	POL	E	304	4/4	0.86	0.14	51,62,62,63	0
4	POL	C	303	4/4	0.87	0.14	48,59,60,60	0
3	FEC	E	302	49/49	0.88	0.18	34,48,73,78	0
4	POL	E	303	4/4	0.89	0.13	42,53,54,54	0
5	CL	D	307	1/1	0.89	0.14	58,58,58,58	0
2	NA	C	306	1/1	0.93	0.07	36,36,36,36	0
3	FEC	D	302	49/49	0.94	0.14	28,33,51,66	0
2	NA	E	301	1/1	0.96	0.04	20,20,20,20	0
2	NA	C	301	1/1	0.97	0.05	22,22,22,22	0
2	NA	B	301	1/1	0.97	0.04	26,26,26,26	0
2	NA	A	301	1/1	0.98	0.04	24,24,24,24	0
2	NA	D	301	1/1	0.98	0.04	21,21,21,21	0

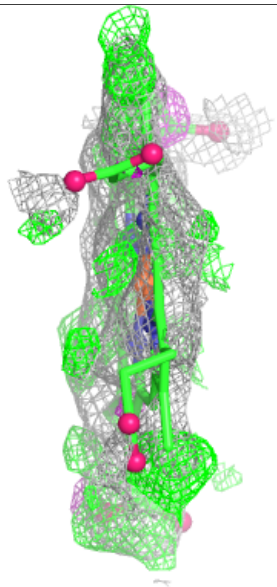
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FEC C 302:

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

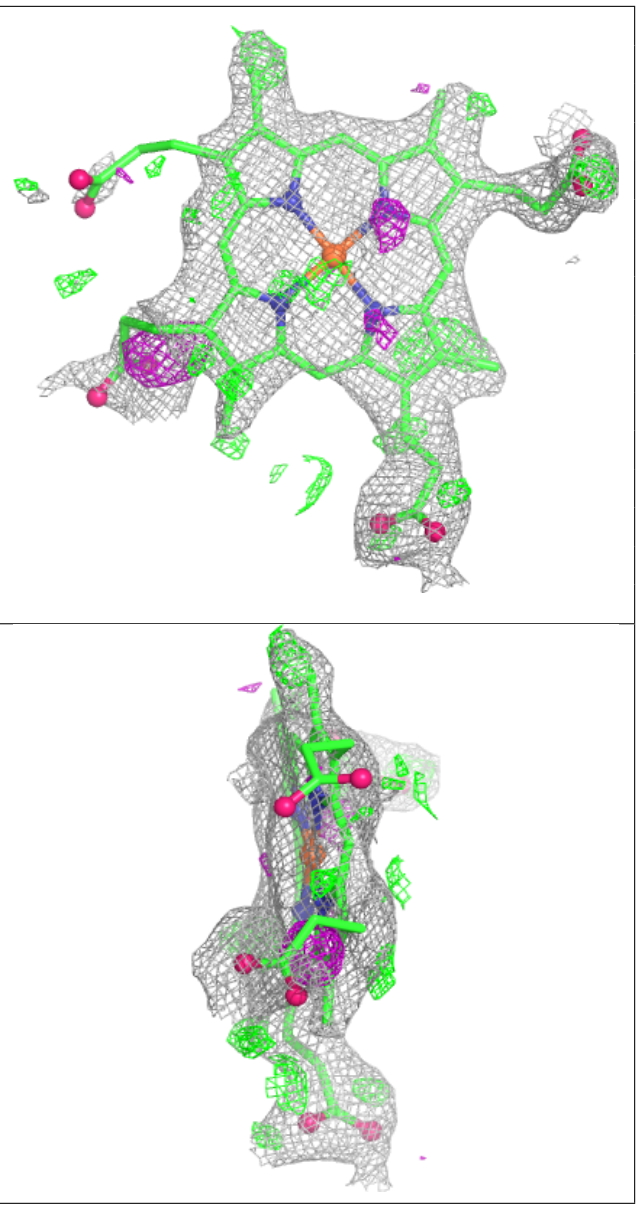






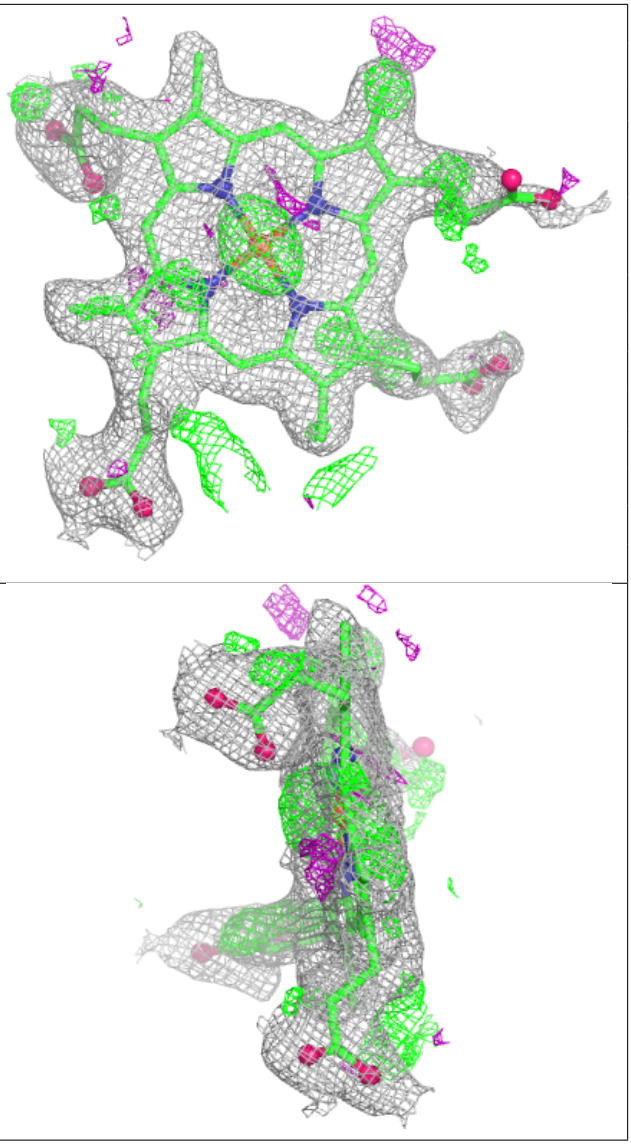
Electron density around FEC B 302:

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



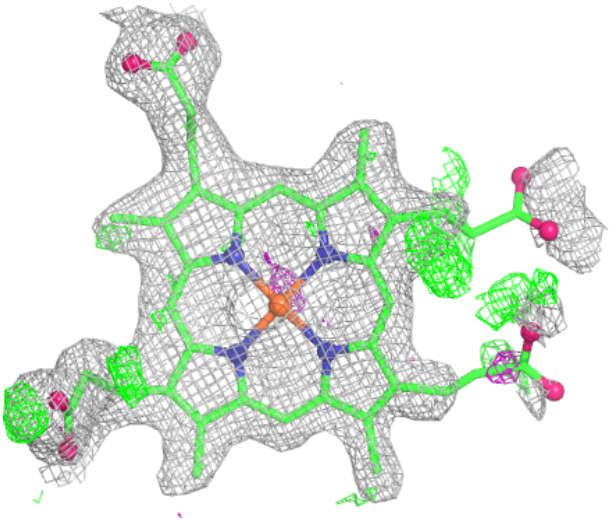
Electron density around FEC A 302:

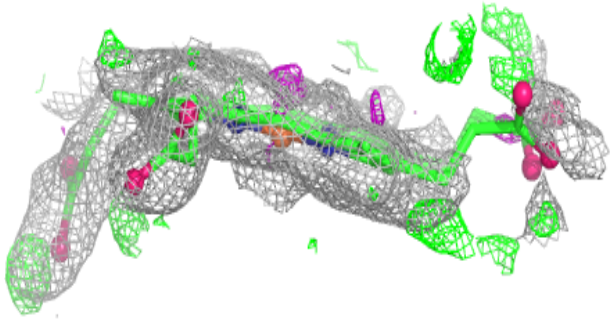
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

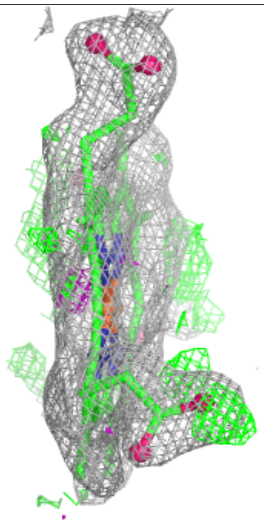


Electron density around FEC E 302:

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

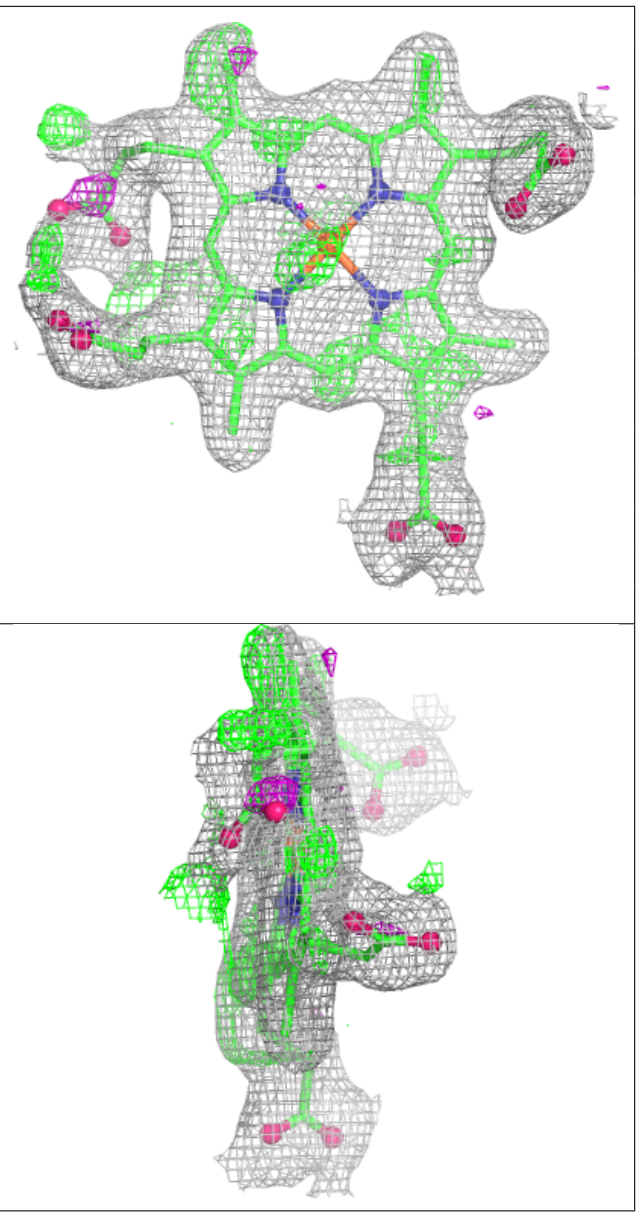






Electron density around FEC D 302:

$2mF_o$-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.