Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2026 – 04:31 pm BST

PDB ID	:	7Q4F / pdb_00007q4f
Title	:	Structure of coproheme decarboxylase from Corynebacterium diptht heriae W183Y mutant in complex with coproheme
Authors	:	Michlits, H.; Valente, N.; Mlynek, G.; Hofbauer, S.
Deposited on	:	2021-10-30
Resolution	:	2.15 Å(reported)

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

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

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

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

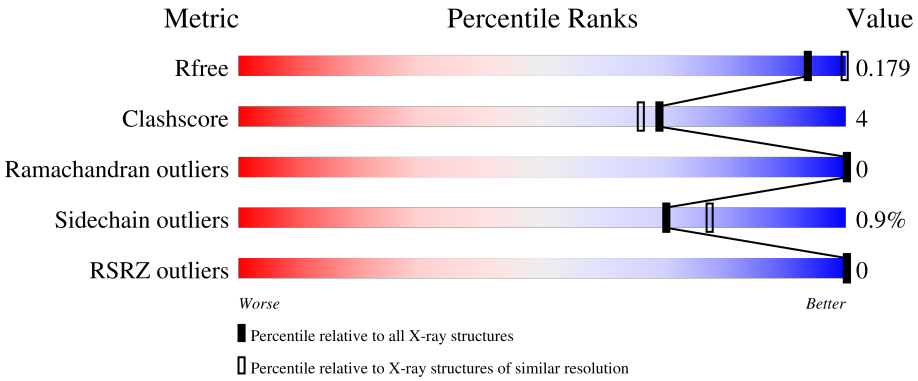
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	237	89% 8% .
1	B	237	87% 10% .
1	C	237	93% . .
1	D	237	87% 10% .
1	E	237	88% 9% .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19594 atoms, of which 9271 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 Coproheme decarboxylase from Corynebacterium diphtheriae W183Y mutant in complex with coproheme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	H	N	O	S	0	0	0
			3678	1198	1804	329	339	8			
1	B	230	Total	C	H	N	O	S	0	1	0
			3693	1203	1810	330	342	8			
1	C	230	Total	C	H	N	O	S	0	0	0
			3678	1198	1804	329	339	8			
1	D	230	Total	C	H	N	O	S	0	0	0
			3678	1198	1804	329	339	8			
1	E	230	Total	C	H	N	O	S	0	6	0
			3736	1213	1835	336	344	8			

There are 20 discrepancies between the modelled and reference sequences:

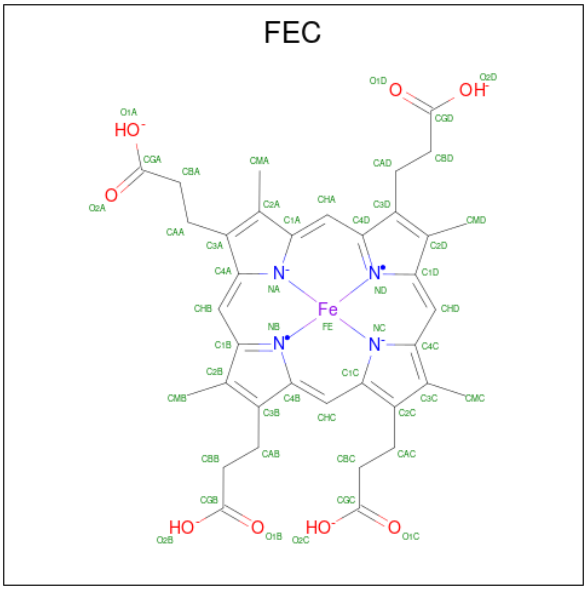
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A2T1BSE4
A	0	PRO	-	expression tag	UNP A0A2T1BSE4
A	183	TYR	TRP	engineered mutation	UNP A0A2T1BSE4
A	235	GLY	-	expression tag	UNP A0A2T1BSE4
B	-1	GLY	-	expression tag	UNP A0A2T1BSE4
B	0	PRO	-	expression tag	UNP A0A2T1BSE4
B	183	TYR	TRP	engineered mutation	UNP A0A2T1BSE4
B	235	GLY	-	expression tag	UNP A0A2T1BSE4
C	-1	GLY	-	expression tag	UNP A0A2T1BSE4
C	0	PRO	-	expression tag	UNP A0A2T1BSE4
C	183	TYR	TRP	engineered mutation	UNP A0A2T1BSE4
C	235	GLY	-	expression tag	UNP A0A2T1BSE4
D	-1	GLY	-	expression tag	UNP A0A2T1BSE4
D	0	PRO	-	expression tag	UNP A0A2T1BSE4
D	183	TYR	TRP	engineered mutation	UNP A0A2T1BSE4
D	235	GLY	-	expression tag	UNP A0A2T1BSE4
E	-1	GLY	-	expression tag	UNP A0A2T1BSE4
E	0	PRO	-	expression tag	UNP A0A2T1BSE4

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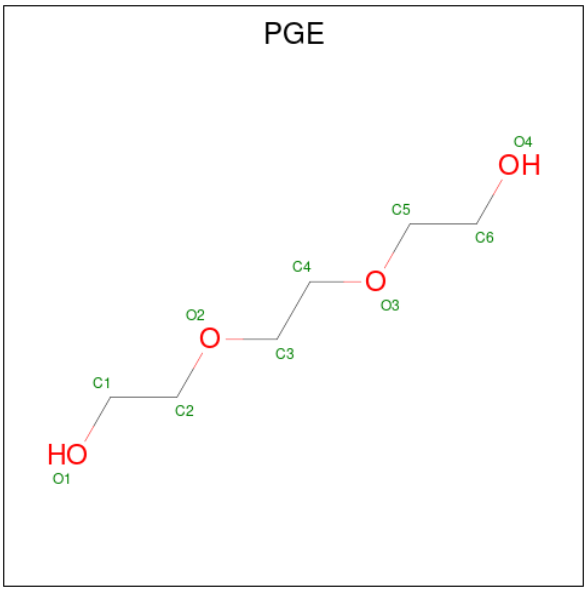
Chain	Residue	Modelled	Actual	Comment	Reference
E	183	TYR	TRP	engineered mutation	UNP A0A2T1BSE4
E	235	GLY	-	expression tag	UNP A0A2T1BSE4

- Molecule 2 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).



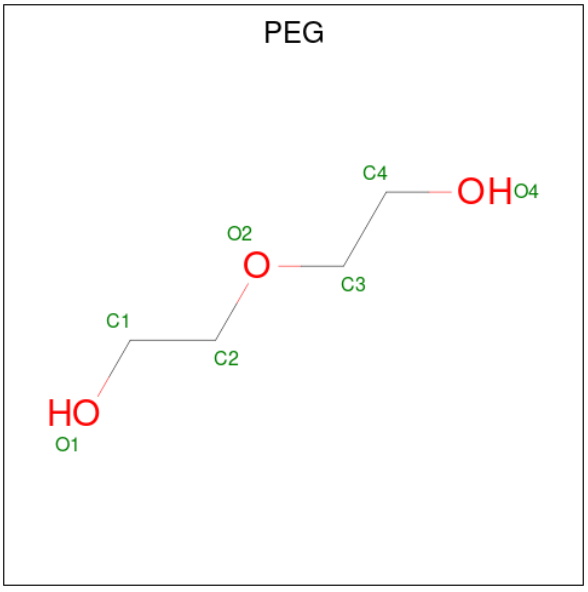
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			85	36	1	36	4	8		
2	B	1	Total	C	Fe	H	N	O	0	0
			85	36	1	36	4	8		
2	C	1	Total	C	Fe	H	N	O	0	0
			85	36	1	36	4	8		
2	D	1	Total	C	Fe	H	N	O	0	0
			85	36	1	36	4	8		
2	E	1	Total	C	Fe	H	N	O	0	0
			85	36	1	36	4	8		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	E	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	146	Total O 146 146	0	0
5	B	134	Total O 134 134	0	0
5	C	134	Total O 134 134	0	0
5	D	107	Total O 107 107	0	0
5	E	127	Total O 127 127	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: Coproheme decarboxylase from Corynebacterium diphtheriae W183Y mutant in complex with coproheme

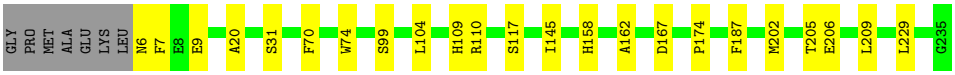
Chain A:



• Molecule 1: Coproheme decarboxylase from Corynebacterium diphtheriae W183Y mutant in complex with coproheme

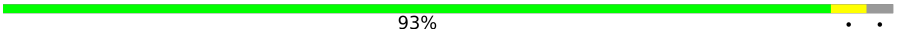
Chain B:

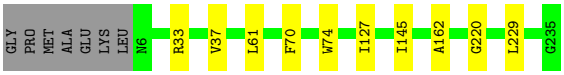




• Molecule 1: Coproheme decarboxylase from Corynebacterium diphtheriae W183Y mutant in complex with coproheme

Chain C:





• Molecule 1: Coproheme decarboxylase from Corynebacterium diphtheriae W183Y mutant in complex with coproheme

Chain D:

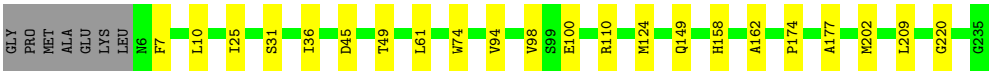




• Molecule 1: Coproheme decarboxylase from Corynebacterium diphtheriae W183Y mutant in complex with coproheme

Chain E:




GLY
PRO
MET
ALA
GLU
LYS
LEU
N6
F7
L10
I25
S31
I36
D45
T49
L61
W74
V94
V98
S99
E100
R110
M124
Q149
H158
A162
P174
A177
M202
L209
G220
G235

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 1 2	Depositor
Cell constants a, b, c, α, β, γ	141.81Å 141.81Å 124.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.51 – 2.15 43.51 – 2.15	Depositor EDS
% Data completeness (in resolution range)	91.1 (43.51-2.15) 91.1 (43.51-2.15)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.88 (at 2.00Å)	Xtriage
Refinement program	PDB-REDO, PHENIX dev_4380	Depositor
R, R_{free}	0.140 , 0.182 0.144 , 0.179	Depositor DCC
R_{free} test set	1999 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.285 for -h,-k,l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	19594	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, FEC, PEG

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	0.14	0/1924	0.29	0/2604
1	B	0.15	0/1933	0.29	0/2616
1	C	0.13	0/1924	0.27	0/2604
1	D	0.13	0/1924	0.28	0/2604
1	E	0.13	0/1979	0.28	0/2677
All	All	0.14	0/9684	0.28	0/13105

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1874	1804	1804	13	0
1	B	1883	1810	1809	17	0
1	C	1874	1804	1804	9	0
1	D	1874	1804	1804	17	0
1	E	1901	1835	1801	15	0
2	A	49	36	32	2	0
2	B	49	36	32	3	0
2	C	49	36	32	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	49	36	32	2	0
2	E	49	36	32	2	0
3	A	10	14	14	0	0
4	B	7	10	10	0	0
4	E	7	10	10	0	0
5	A	146	0	0	2	0
5	B	134	0	0	3	0
5	C	134	0	0	0	0
5	D	107	0	0	0	0
5	E	127	0	0	1	1
All	All	10323	9271	9216	67	1

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 (67) 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:145:ILE:HD11	1:B:209:LEU:HD21	1.62	0.80
1:D:162:ALA:HB1	2:D:401:FEC:HMC1	1.66	0.77
1:B:162:ALA:CB	2:B:401:FEC:HMC1	2.18	0.74
1:E:162:ALA:HB1	2:E:401:FEC:HMC2	1.71	0.72
1:D:224:SER:OG	1:D:228:GLU:OE1	2.11	0.67
1:B:162:ALA:HB1	2:B:401:FEC:HMC1	1.78	0.66
1:A:162:ALA:CB	2:A:401:FEC:HMC1	2.28	0.63
1:D:67:GLU:HA	1:D:67:GLU:OE1	1.96	0.63
1:D:162:ALA:HB3	2:D:401:FEC:HAC1	1.81	0.62
1:E:7:PHE:CE1	1:E:124:MET:HE1	2.36	0.61
1:A:162:ALA:HB1	2:A:401:FEC:HMC1	1.83	0.61
1:D:158:HIS:O	1:D:202:MET:HE1	2.02	0.59
1:A:232:VAL:O	5:A:501:HOH:O	2.17	0.58
1:E:149[B]:GLN:NE2	5:E:503:HOH:O	2.38	0.57
1:E:162:ALA:CB	2:E:401:FEC:HMC2	2.34	0.56
1:B:70:PHE:HB3	1:B:229:LEU:HD11	1.86	0.56
1:B:6:ASN:N	5:B:508:HOH:O	2.39	0.55
1:E:25:ILE:HD11	1:E:100:GLU:HG3	1.89	0.55
1:B:158:HIS:O	1:B:202:MET:HE1	2.06	0.55
1:B:99:SER:OG	5:B:501:HOH:O	2.18	0.55
1:E:10:LEU:HD13	1:E:124:MET:HE3	1.89	0.54
1:C:162:ALA:CB	2:C:401:FEC:HMC2	2.38	0.54
1:A:29:LEU:HD23	1:A:33:ARG:CZ	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:NH1	1:A:230:VAL:O	2.43	0.52
1:D:35:GLU:OE1	1:D:35:GLU:N	2.42	0.51
1:E:158:HIS:O	1:E:202:MET:HE1	2.11	0.50
1:E:25:ILE:HD12	1:E:98:VAL:O	2.11	0.50
1:C:162:ALA:HB1	2:C:401:FEC:HMC2	1.94	0.50
1:D:163:ARG:HH11	1:D:163:ARG:HG3	1.77	0.49
1:A:70:PHE:HB3	1:A:229:LEU:HD11	1.96	0.48
1:C:61:LEU:HD23	1:C:220:GLY:HA3	1.96	0.47
1:D:127:ILE:H	1:D:127:ILE:HD12	1.79	0.47
1:D:67:GLU:OE1	1:D:67:GLU:CA	2.61	0.47
1:C:162:ALA:HB3	2:C:401:FEC:HAC1	1.96	0.47
1:E:25:ILE:HD12	1:E:98:VAL:C	2.40	0.46
1:D:199:MET:HG3	1:E:177:ALA:HB2	1.96	0.46
1:B:7:PHE:CE2	1:B:117:SER:HA	2.51	0.45
1:A:209:LEU:HD21	1:C:145:ILE:HD11	2.00	0.44
1:E:45:ASP:O	1:E:49:THR:HG23	2.18	0.43
1:A:145:ILE:HG21	1:B:205:THR:O	2.18	0.43
1:D:109:HIS:HA	1:D:173:VAL:HG13	2.00	0.43
1:A:69:ASP:OD1	5:A:502:HOH:O	2.21	0.43
1:B:110:ARG:HB2	1:B:174:PRO:HG2	2.01	0.43
1:B:20:ALA:HA	1:B:104:LEU:HD23	2.01	0.42
1:D:61:LEU:HD11	1:D:71:MET:HB2	2.01	0.42
1:D:70:PHE:HB3	1:D:229:LEU:HD11	2.02	0.42
1:D:61:LEU:HD23	1:D:220:GLY:HA3	2.01	0.42
1:E:110:ARG:HB2	1:E:174:PRO:HG2	2.02	0.42
1:B:109:HIS:O	5:B:502:HOH:O	2.21	0.42
1:C:70:PHE:HB2	1:C:229:LEU:HD21	2.00	0.42
1:C:33:ARG:O	1:C:37:VAL:HG23	2.20	0.42
1:D:147:ASP:HB3	1:D:150:LYS:HG3	2.02	0.42
1:A:19:PHE:CE1	1:A:134:VAL:HG21	2.55	0.42
1:C:70:PHE:CB	1:C:229:LEU:HD21	2.49	0.42
1:B:206:GLU:O	1:B:206:GLU:HG3	2.19	0.41
1:A:158:HIS:O	1:A:202:MET:HE1	2.21	0.41
1:E:36:ILE:CG1	1:E:94:VAL:HG11	2.51	0.41
1:E:61:LEU:HD23	1:E:220:GLY:HA3	2.02	0.41
2:C:401:FEC:HBB1	2:C:401:FEC:HHC	2.03	0.41
1:B:187:PHE:CZ	2:B:401:FEC:C2D	3.03	0.41
1:D:140:SER:HA	1:D:212:ARG:HG3	2.03	0.41
1:B:167:ASP:OD1	1:B:167:ASP:N	2.50	0.40
1:C:127:ILE:H	1:C:127:ILE:HD12	1.86	0.40
1:A:126:GLU:OE1	1:A:169:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ASN:O	1:B:9:GLU:HB3	2.21	0.40
1:B:145:ILE:HD11	1:E:209:LEU:HD21	2.03	0.40
1:D:167:ASP:OD1	1:D:167:ASP:N	2.46	0.40

All (1) 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)
5:E:591:HOH:O	5:E:591:HOH:O[4_555]	2.06	0.14

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	228/237 (96%)	221 (97%)	7 (3%)	0	100	100
1	B	229/237 (97%)	220 (96%)	9 (4%)	0	100	100
1	C	228/237 (96%)	223 (98%)	5 (2%)	0	100	100
1	D	228/237 (96%)	224 (98%)	4 (2%)	0	100	100
1	E	234/237 (99%)	229 (98%)	5 (2%)	0	100	100
All	All	1147/1185 (97%)	1117 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/196 (97%)	189 (99%)	2 (1%)	68	75
1	B	192/196 (98%)	190 (99%)	2 (1%)	68	75
1	C	191/196 (97%)	190 (100%)	1 (0%)	81	87
1	D	191/196 (97%)	189 (99%)	2 (1%)	68	75
1	E	197/196 (100%)	195 (99%)	2 (1%)	68	75
All	All	962/980 (98%)	953 (99%)	9 (1%)	70	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	TRP
1	A	188	GLU
1	B	31	SER
1	B	74	TRP
1	C	74	TRP
1	D	31	SER
1	D	74	TRP
1	E	31	SER
1	E	74	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	B	149	GLN
1	C	41	GLN
1	D	39	GLN
1	D	160	GLN
1	D	231	ASN
1	E	39	GLN
1	E	41	GLN

5.3.3 RNA

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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FEC	E	401	1	56,56,56	0.92	4 (7%)	76,90,90	1.43	14 (18%)
4	PEG	B	402	-	6,6,6	0.10	0	5,5,5	0.11	0
2	FEC	D	401	1	56,56,56	0.90	4 (7%)	76,90,90	1.42	15 (19%)
2	FEC	C	401	1	56,56,56	0.90	4 (7%)	76,90,90	1.41	13 (17%)
4	PEG	E	402	-	6,6,6	0.12	0	5,5,5	0.10	0
2	FEC	B	401	1	56,56,56	0.93	5 (8%)	76,90,90	1.47	13 (17%)
3	PGE	A	402	-	9,9,9	0.30	0	8,8,8	0.35	0
2	FEC	A	401	1	56,56,56	0.92	4 (7%)	76,90,90	1.42	14 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FEC	E	401	1	-	9/20/100/100	-
4	PEG	B	402	-	-	1/4/4/4	-
2	FEC	D	401	1	-	10/20/100/100	-
2	FEC	C	401	1	-	12/20/100/100	-
4	PEG	E	402	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FEC	B	401	1	-	8/20/100/100	-
3	PGE	A	402	-	-	3/7/7/7	-
2	FEC	A	401	1	-	9/20/100/100	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	FEC	CMB-C2B	2.47	1.56	1.50
2	A	401	FEC	CMA-C2A	2.46	1.56	1.50
2	C	401	FEC	CMA-C2A	2.45	1.56	1.50
2	C	401	FEC	CMB-C2B	2.43	1.55	1.50
2	A	401	FEC	CMD-C2D	2.43	1.55	1.50
2	B	401	FEC	CMA-C2A	2.42	1.55	1.50
2	D	401	FEC	CMA-C2A	2.41	1.55	1.50
2	D	401	FEC	CMB-C2B	2.41	1.55	1.50
2	B	401	FEC	CMB-C2B	2.41	1.55	1.50
2	D	401	FEC	CMD-C2D	2.39	1.55	1.50
2	C	401	FEC	CMD-C2D	2.39	1.55	1.50
2	E	401	FEC	CMA-C2A	2.37	1.55	1.50
2	A	401	FEC	CMB-C2B	2.35	1.55	1.50
2	E	401	FEC	CMD-C2D	2.34	1.55	1.50
2	B	401	FEC	CMD-C2D	2.26	1.55	1.50
2	B	401	FEC	CMC-C3C	2.21	1.55	1.50
2	C	401	FEC	CMC-C3C	2.20	1.55	1.50
2	A	401	FEC	CMC-C3C	2.13	1.55	1.50
2	D	401	FEC	CMC-C3C	2.09	1.55	1.50
2	E	401	FEC	CMC-C3C	2.09	1.55	1.50
2	B	401	FEC	C4B-C3B	-2.07	1.41	1.45

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	FEC	CHA-C4D-ND	4.71	129.53	124.42
2	C	401	FEC	CHA-C4D-ND	4.33	129.12	124.42
2	B	401	FEC	CHB-C4A-NA	4.30	129.09	124.44
2	A	401	FEC	C1D-ND-C4D	3.88	109.08	105.07
2	E	401	FEC	C1D-ND-C4D	3.86	109.06	105.07
2	A	401	FEC	CHA-C4D-ND	3.80	128.55	124.42
2	D	401	FEC	CHA-C4D-ND	3.79	128.54	124.42
2	E	401	FEC	CHA-C4D-ND	3.79	128.54	124.42
2	C	401	FEC	CHB-C4A-NA	3.73	128.47	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	FEC	C1D-ND-C4D	3.63	108.82	105.07
2	D	401	FEC	C4A-NA-C1A	3.59	108.87	105.35
2	E	401	FEC	C4A-NA-C1A	3.56	108.83	105.35
2	A	401	FEC	C4A-NA-C1A	3.53	108.80	105.35
2	B	401	FEC	CHC-C4B-NB	3.50	128.69	124.37
2	B	401	FEC	C1D-ND-C4D	3.44	108.63	105.07
2	D	401	FEC	CHB-C4A-NA	3.19	127.89	124.44
2	C	401	FEC	C4A-NA-C1A	3.18	108.47	105.35
2	B	401	FEC	C4A-NA-C1A	3.18	108.46	105.35
2	E	401	FEC	CHB-C4A-NA	3.15	127.85	124.44
2	C	401	FEC	CHC-C4B-NB	3.15	128.26	124.37
2	C	401	FEC	C1D-ND-C4D	3.14	108.32	105.07
2	E	401	FEC	C4B-NB-C1B	3.00	108.17	105.07
2	A	401	FEC	CHB-C4A-NA	2.92	127.59	124.44
2	A	401	FEC	CHB-C1B-C2B	2.84	129.42	124.98
2	E	401	FEC	CHB-C1B-C2B	2.80	129.35	124.98
2	D	401	FEC	CHB-C1B-C2B	2.78	129.32	124.98
2	A	401	FEC	C4B-NB-C1B	2.73	107.89	105.07
2	A	401	FEC	CHC-C4B-NB	2.68	127.68	124.37
2	C	401	FEC	C4B-NB-C1B	2.68	107.84	105.07
2	B	401	FEC	CHB-C1B-C2B	2.66	129.13	124.98
2	D	401	FEC	CHC-C4B-NB	2.64	127.63	124.37
2	C	401	FEC	CHB-C1B-C2B	2.59	129.03	124.98
2	D	401	FEC	C4B-NB-C1B	2.59	107.75	105.07
2	E	401	FEC	CHC-C4B-NB	2.58	127.55	124.37
2	E	401	FEC	C3A-C4A-NA	-2.54	107.86	110.32
2	D	401	FEC	C3A-C4A-NA	-2.53	107.86	110.32
2	A	401	FEC	C1C-CHC-C4B	-2.53	120.34	126.34
2	B	401	FEC	C1C-CHC-C4B	-2.52	120.36	126.34
2	A	401	FEC	C3A-C4A-NA	-2.51	107.88	110.32
2	D	401	FEC	C1C-CHC-C4B	-2.51	120.38	126.34
2	E	401	FEC	C1C-CHC-C4B	-2.51	120.39	126.34
2	C	401	FEC	C1C-CHC-C4B	-2.48	120.45	126.34
2	A	401	FEC	C4C-CHD-C1D	-2.35	120.78	126.34
2	D	401	FEC	C4C-CHD-C1D	-2.34	120.79	126.34
2	E	401	FEC	C1A-CHA-C4D	-2.34	121.01	126.06
2	E	401	FEC	C4C-CHD-C1D	-2.33	120.80	126.34
2	D	401	FEC	C1A-CHA-C4D	-2.33	121.03	126.06
2	A	401	FEC	C1A-CHA-C4D	-2.32	121.06	126.06
2	B	401	FEC	C1A-CHA-C4D	-2.30	121.09	126.06
2	C	401	FEC	C4C-CHD-C1D	-2.30	120.89	126.34
2	A	401	FEC	C1C-NC-C4C	2.30	107.60	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	FEC	C1C-NC-C4C	2.30	107.60	105.35
2	C	401	FEC	C3A-C4A-NA	-2.29	108.09	110.32
2	D	401	FEC	C4A-CHB-C1B	-2.29	121.11	126.06
2	C	401	FEC	C1A-CHA-C4D	-2.28	121.14	126.06
2	A	401	FEC	C4A-CHB-C1B	-2.27	121.17	126.06
2	B	401	FEC	C4A-CHB-C1B	-2.25	121.20	126.06
2	E	401	FEC	C4A-CHB-C1B	-2.25	121.21	126.06
2	B	401	FEC	C4C-CHD-C1D	-2.22	121.06	126.34
2	C	401	FEC	C4A-CHB-C1B	-2.22	121.27	126.06
2	B	401	FEC	C4B-NB-C1B	2.19	107.33	105.07
2	A	401	FEC	C2D-C1D-ND	-2.18	107.25	109.84
2	B	401	FEC	CHD-C4C-NC	2.17	127.84	123.85
2	E	401	FEC	C2D-C1D-ND	-2.15	107.29	109.84
2	B	401	FEC	C3A-C4A-NA	-2.15	108.23	110.32
2	D	401	FEC	C2D-C1D-ND	-2.11	107.33	109.84
2	E	401	FEC	C3D-C4D-ND	-2.09	108.33	110.36
2	D	401	FEC	C3D-C4D-ND	-2.08	108.34	110.36
2	C	401	FEC	CHD-C4C-NC	2.06	127.63	123.85

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PGE	O1-C1-C2-O2
4	E	402	PEG	O1-C1-C2-O2
2	B	401	FEC	C3A-CAA-CBA-CGA
2	C	401	FEC	C3A-CAA-CBA-CGA
2	D	401	FEC	C3A-CAA-CBA-CGA
2	E	401	FEC	C2C-CAC-CBC-CGC
4	B	402	PEG	O1-C1-C2-O2
4	E	402	PEG	O2-C3-C4-O4
2	A	401	FEC	C3A-CAA-CBA-CGA
2	B	401	FEC	C4D-C3D-CAD-CBD
2	E	401	FEC	C3A-CAA-CBA-CGA
2	C	401	FEC	C4B-C3B-CAB-CBB
2	C	401	FEC	C4D-C3D-CAD-CBD
2	B	401	FEC	C2D-C3D-CAD-CBD
3	A	402	PGE	C4-C3-O2-C2
2	C	401	FEC	C2D-C3D-CAD-CBD
4	E	402	PEG	C1-C2-O2-C3
2	D	401	FEC	C3B-CAB-CBB-CGB
2	C	401	FEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	C	401	FEC	C3B-CAB-CBB-CGB
2	E	401	FEC	CAC-CBC-CGC-O2C
2	A	401	FEC	CAD-CBD-CGD-O1D
2	D	401	FEC	CAC-CBC-CGC-O1C
2	A	401	FEC	CAC-CBC-CGC-O2C
2	E	401	FEC	CAA-CBA-CGA-O2A
2	E	401	FEC	CAC-CBC-CGC-O1C
2	E	401	FEC	CAD-CBD-CGD-O1D
2	E	401	FEC	CAB-CBB-CGB-O1B
2	A	401	FEC	CAC-CBC-CGC-O1C
2	A	401	FEC	CAA-CBA-CGA-O2A
2	B	401	FEC	CAB-CBB-CGB-O1B
2	C	401	FEC	CAB-CBB-CGB-O2B
2	D	401	FEC	CAD-CBD-CGD-O1D
2	A	401	FEC	CAD-CBD-CGD-O2D
2	A	401	FEC	CAB-CBB-CGB-O2B
2	D	401	FEC	CAA-CBA-CGA-O2A
2	D	401	FEC	CAA-CBA-CGA-O1A
2	E	401	FEC	CAD-CBD-CGD-O2D
2	C	401	FEC	CAA-CBA-CGA-O1A
2	C	401	FEC	CAD-CBD-CGD-O2D
3	A	402	PGE	O3-C5-C6-O4
2	B	401	FEC	CAB-CBB-CGB-O2B
2	E	401	FEC	CAB-CBB-CGB-O2B
2	D	401	FEC	C4B-C3B-CAB-CBB
2	D	401	FEC	CAD-CBD-CGD-O2D
2	C	401	FEC	CAB-CBB-CGB-O1B
2	A	401	FEC	CAB-CBB-CGB-O1B
2	D	401	FEC	CAC-CBC-CGC-O2C
2	C	401	FEC	CAD-CBD-CGD-O1D
2	B	401	FEC	CAD-CBD-CGD-O1D
2	B	401	FEC	CAA-CBA-CGA-O1A
2	C	401	FEC	CAC-CBC-CGC-O2C
2	A	401	FEC	CAA-CBA-CGA-O1A
2	B	401	FEC	CAD-CBD-CGD-O2D
2	D	401	FEC	CAB-CBB-CGB-O1B

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	FEC	2	0

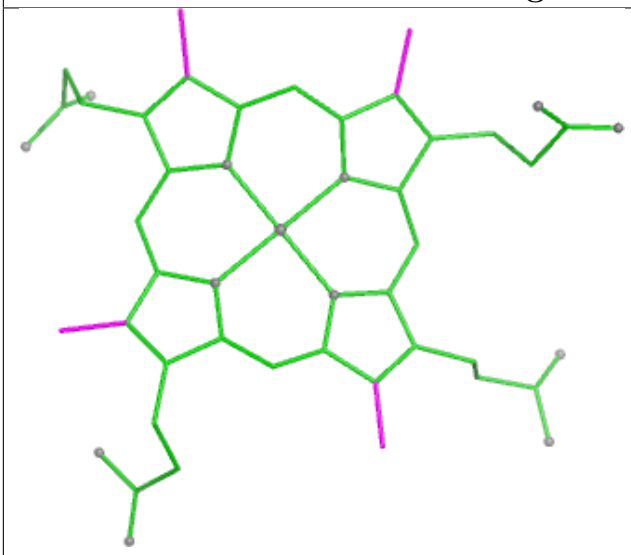
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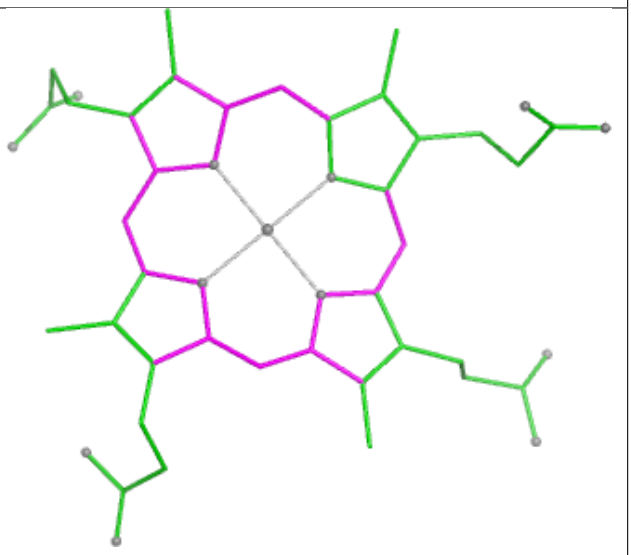
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	FEC	2	0
2	C	401	FEC	4	0
2	B	401	FEC	3	0
2	A	401	FEC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

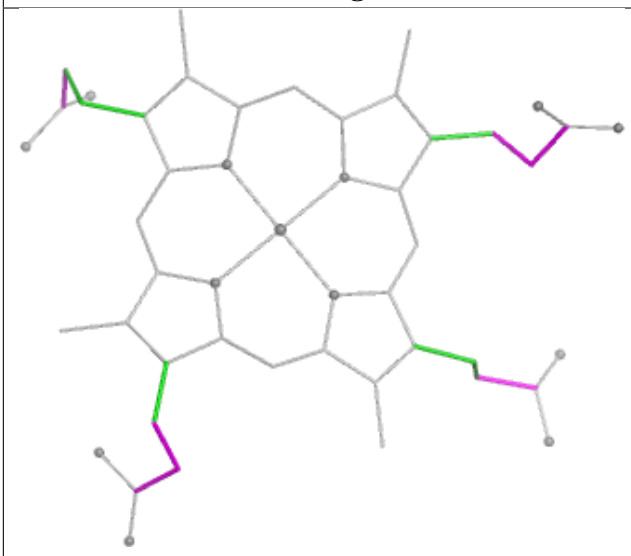
Ligand FEC E 401



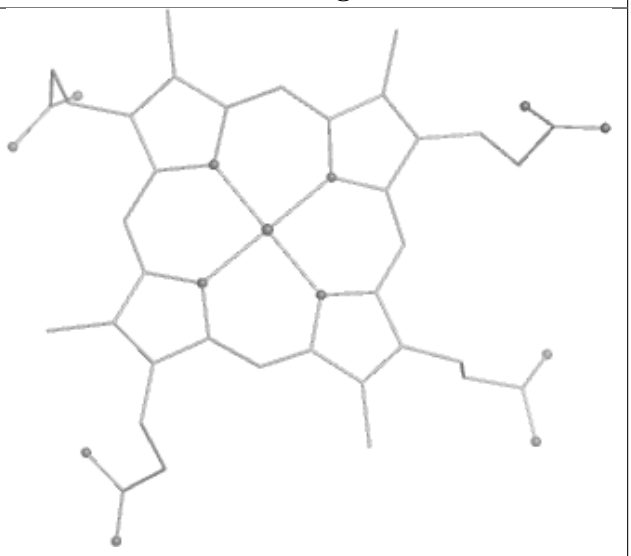
Bond lengths



Bond angles

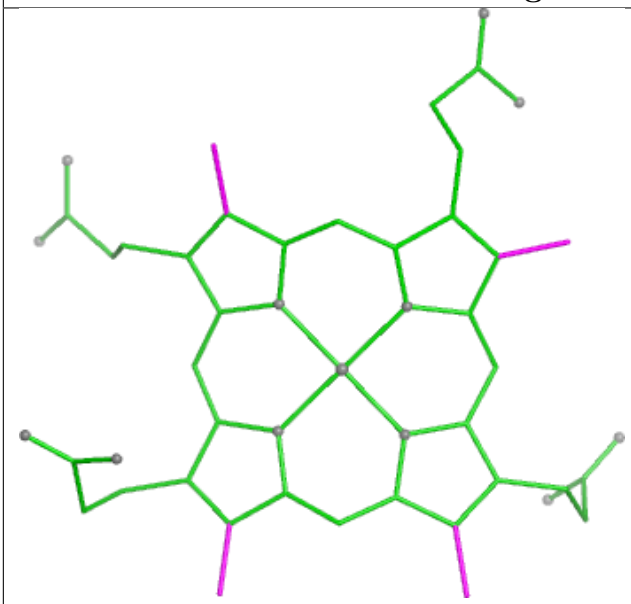


Torsions

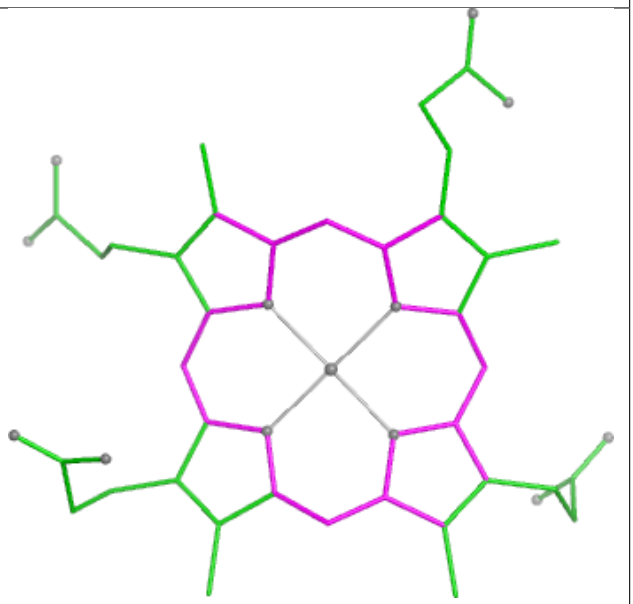


Rings

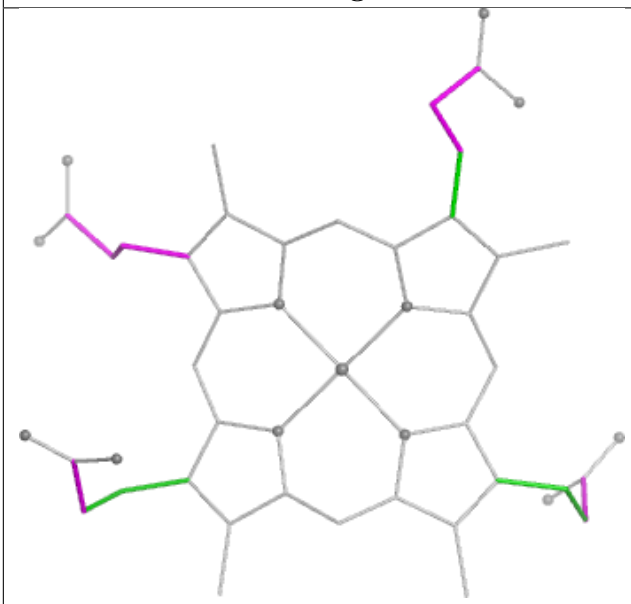
Ligand FEC D 401



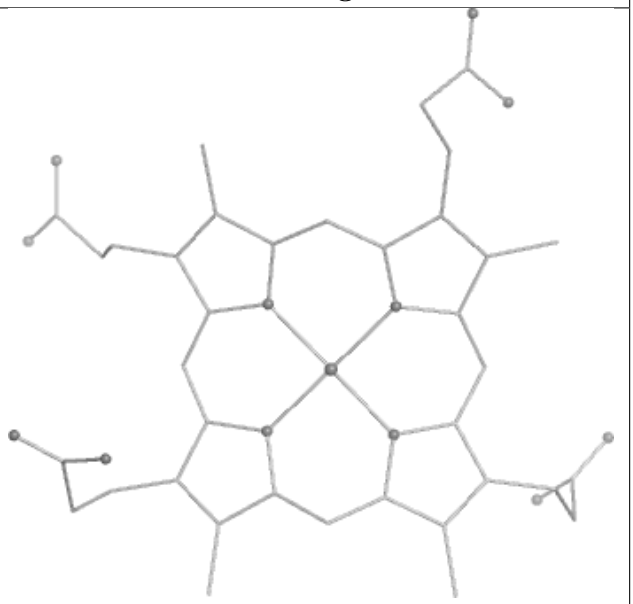
Bond lengths



Bond angles

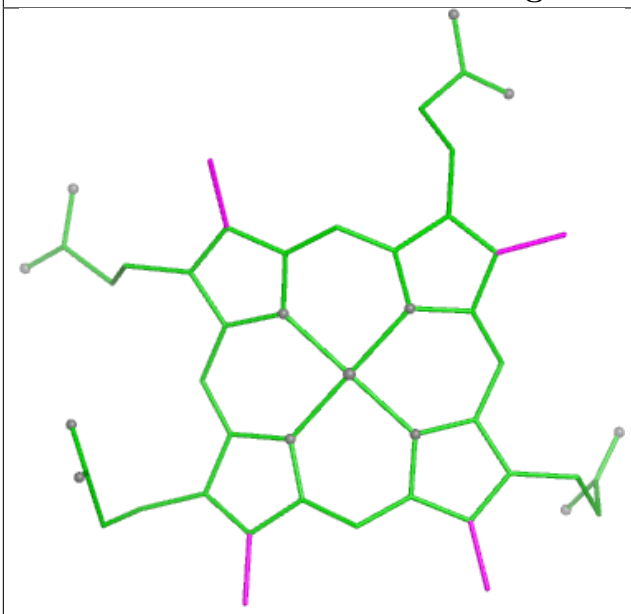


Torsions

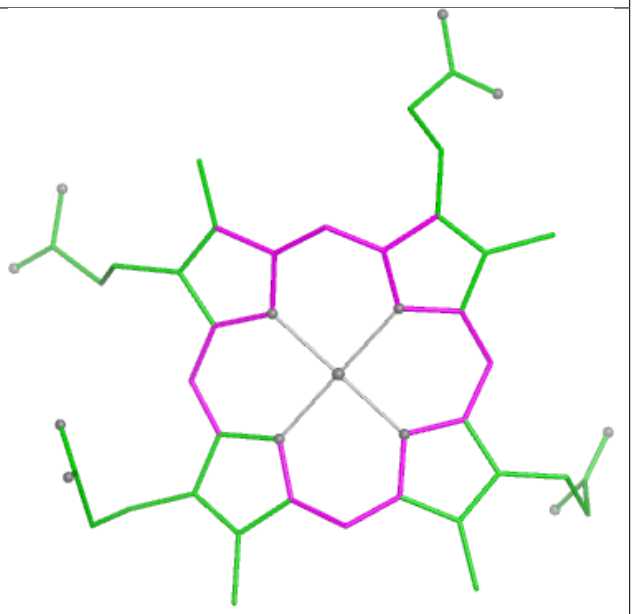


Rings

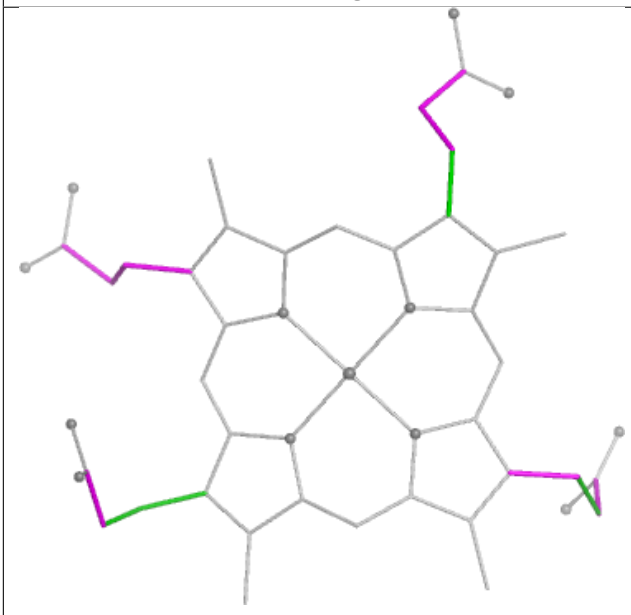
Ligand FEC C 401



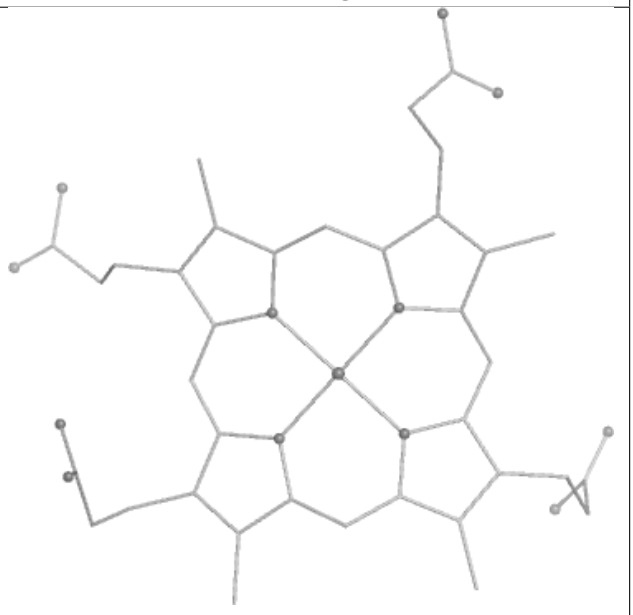
Bond lengths



Bond angles

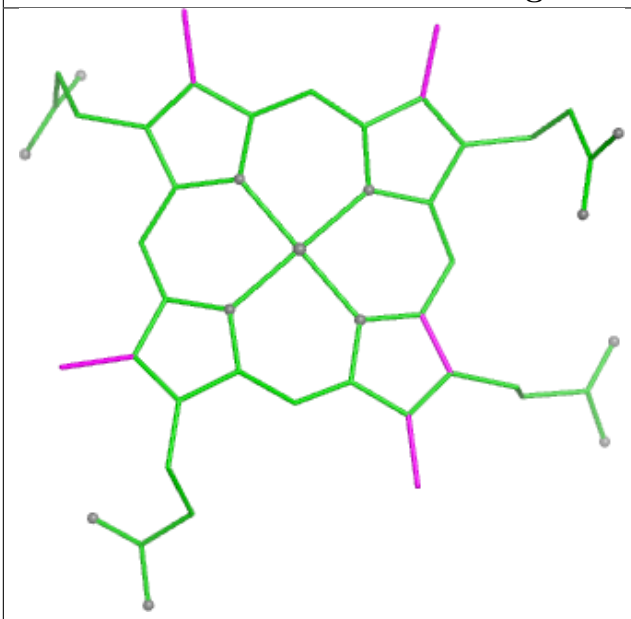


Torsions

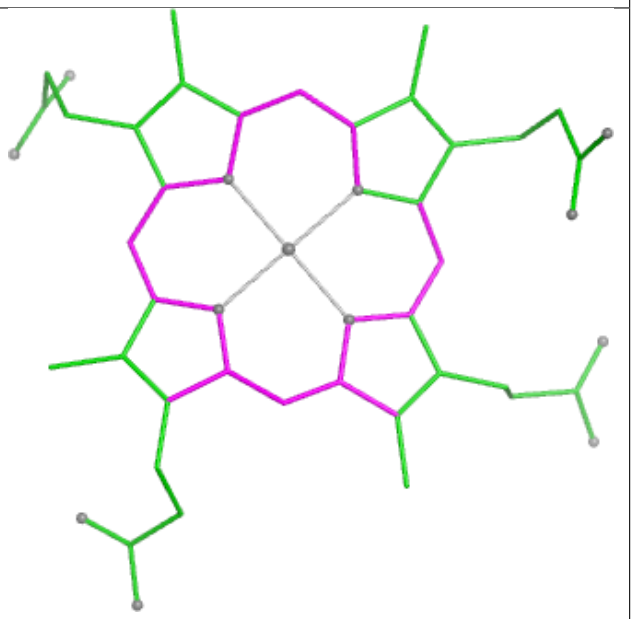


Rings

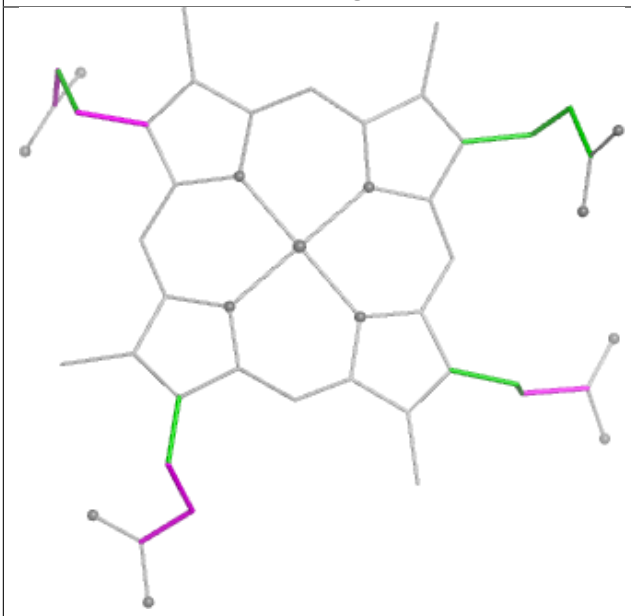
Ligand FEC B 401



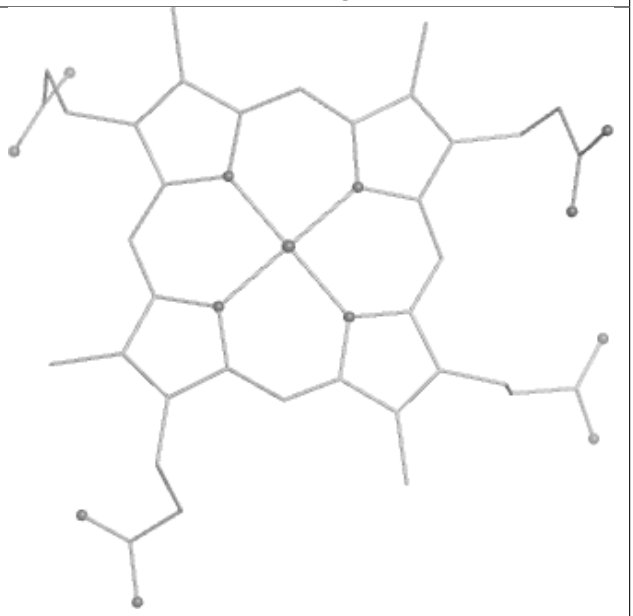
Bond lengths



Bond angles

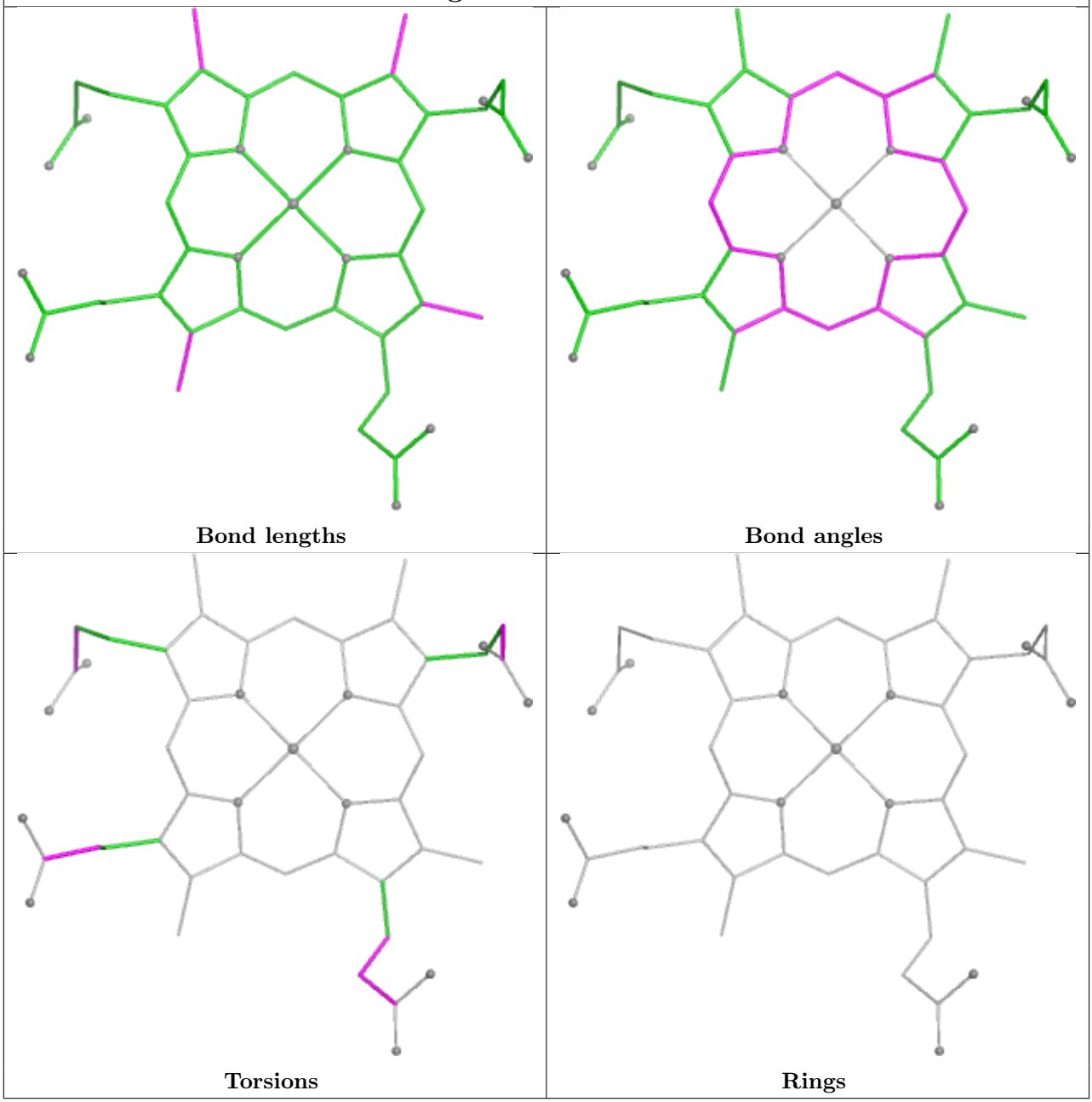


Torsions



Rings

Ligand FEC A 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	230/237 (97%)	-1.49	0	100	100	26, 42, 66, 75	0
1	B	230/237 (97%)	-1.50	0	100	100	22, 40, 69, 92	1 (0%)
1	C	230/237 (97%)	-1.45	0	100	100	29, 46, 65, 88	0
1	D	230/237 (97%)	-1.40	0	100	100	34, 54, 75, 95	0
1	E	230/237 (97%)	-1.40	0	100	100	20, 49, 76, 97	3 (1%)
All	All	1150/1185 (97%)	-1.45	0	100	100	20, 46, 73, 97	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGE	A	402	10/10	0.97	0.07	33,44,58,60	0
4	PEG	E	402	7/7	0.97	0.06	51,62,70,70	0
4	PEG	B	402	7/7	0.98	0.05	36,54,71,71	0

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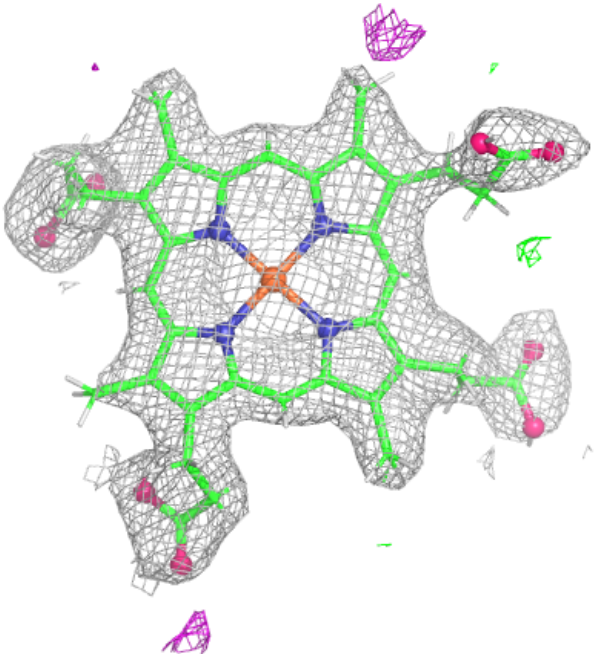
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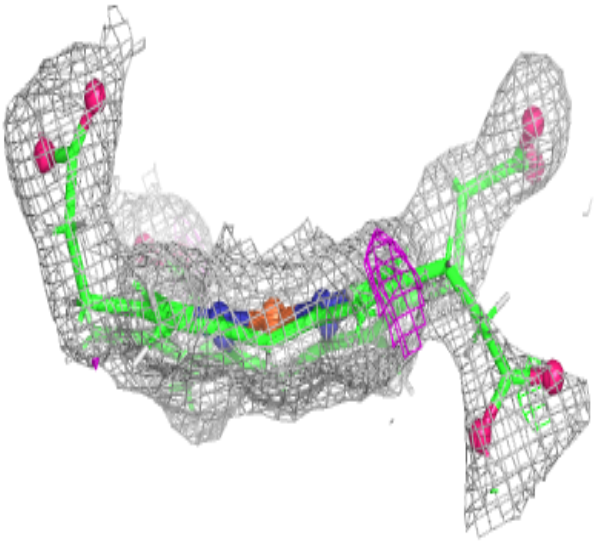
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FEC	E	401	49/49	0.99	0.04	36,47,66,72	0
2	FEC	D	401	49/49	0.99	0.04	40,56,77,88	0
2	FEC	C	401	49/49	1.00	0.03	37,49,68,81	0
2	FEC	A	401	49/49	1.00	0.03	32,43,55,66	0
2	FEC	B	401	49/49	1.00	0.03	34,44,64,71	0

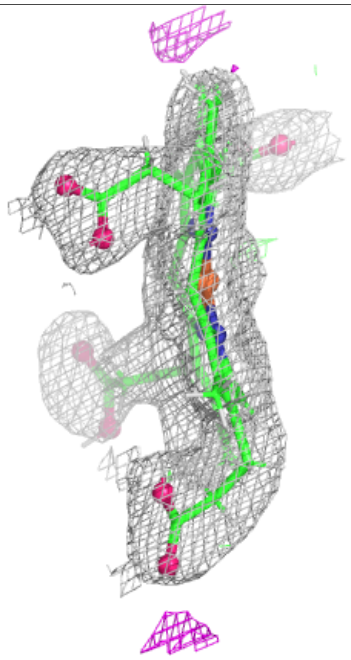
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FEC E 401:

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

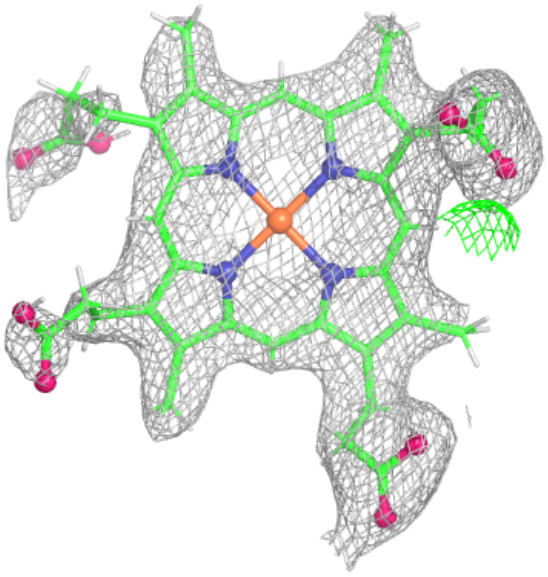


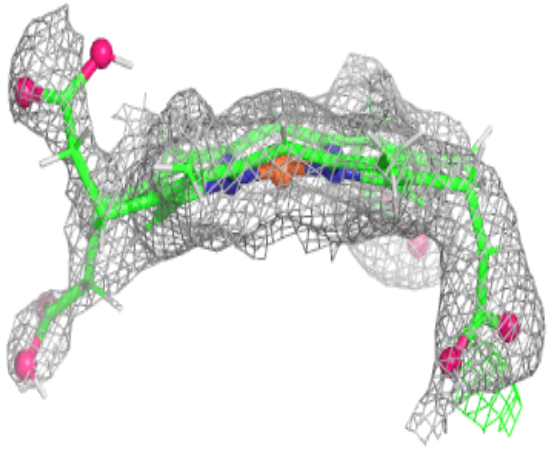


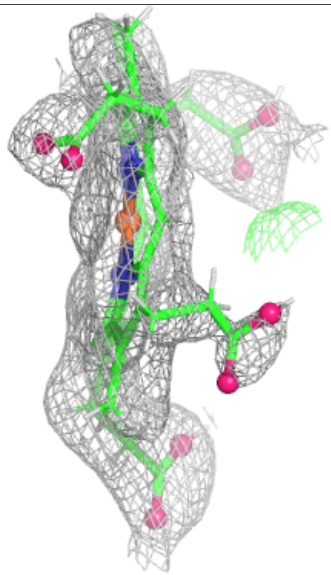


Electron density around FEC D 401:

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

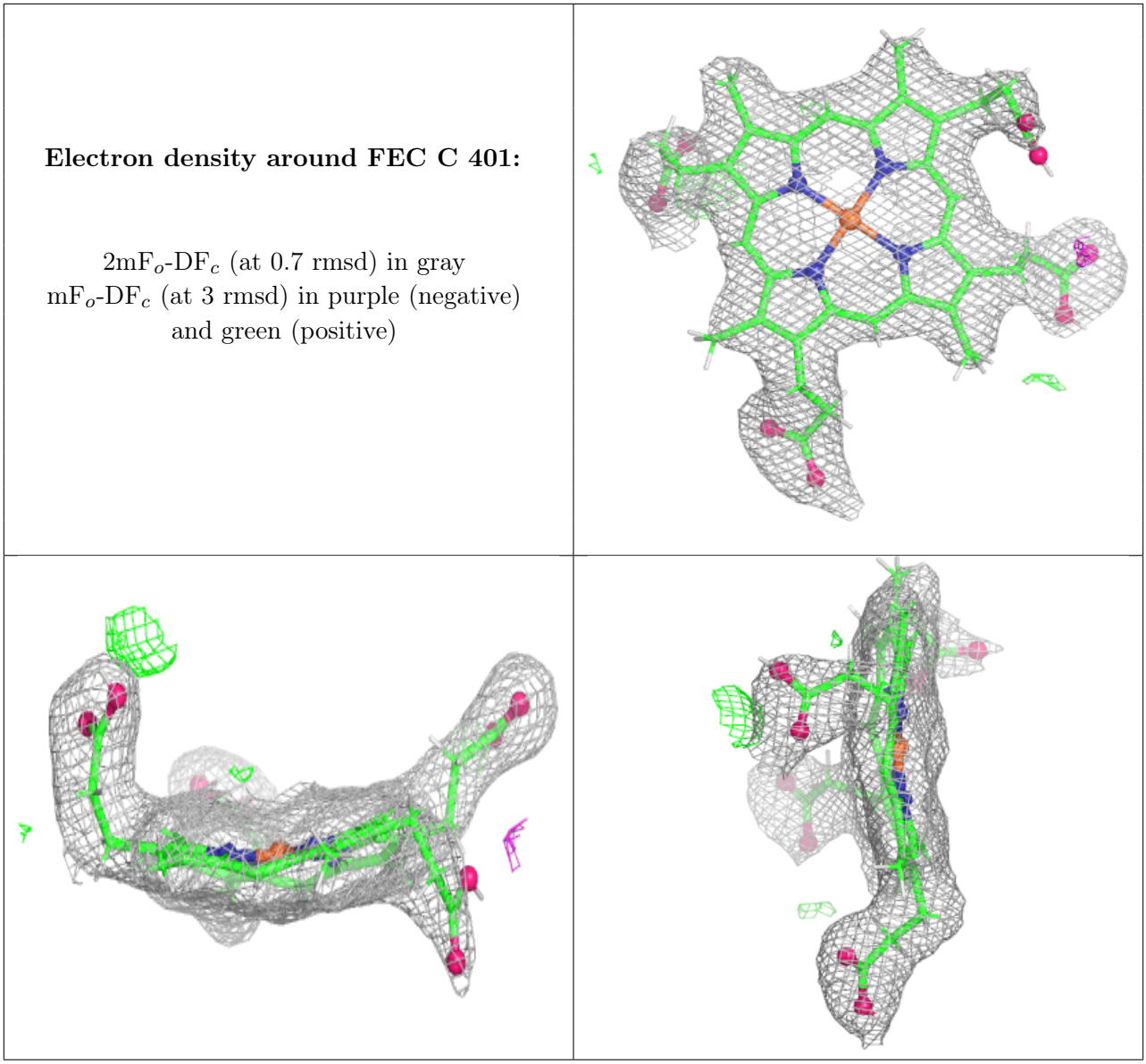






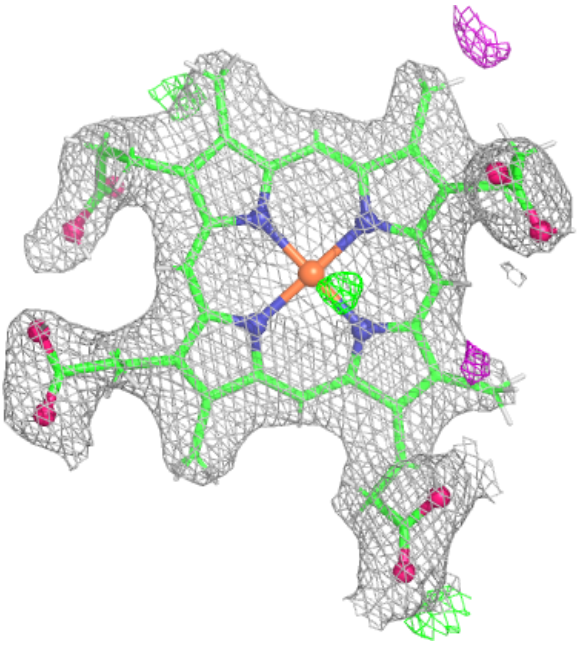
Electron density around FEC C 401:

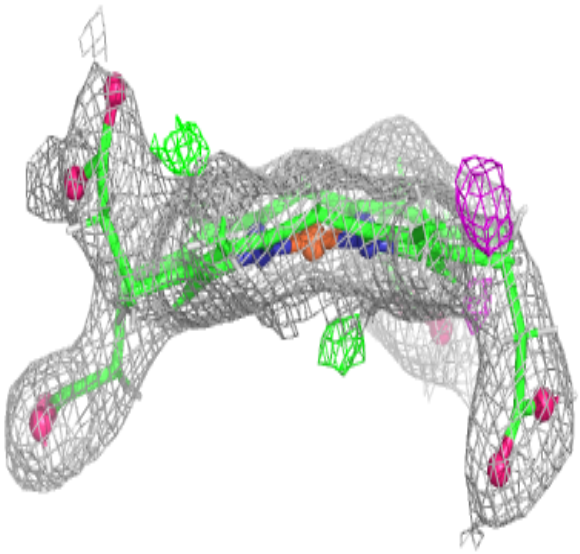
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

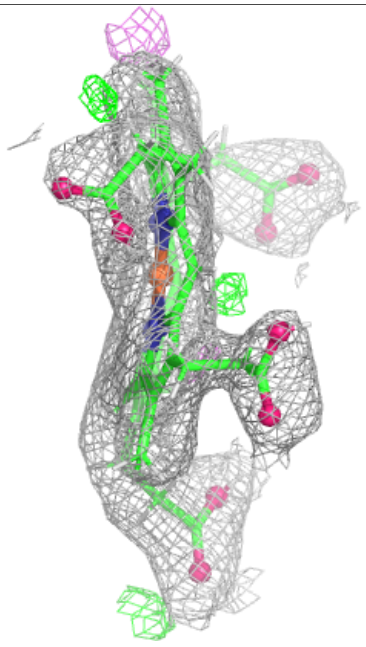


Electron density around FEC A 401:

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

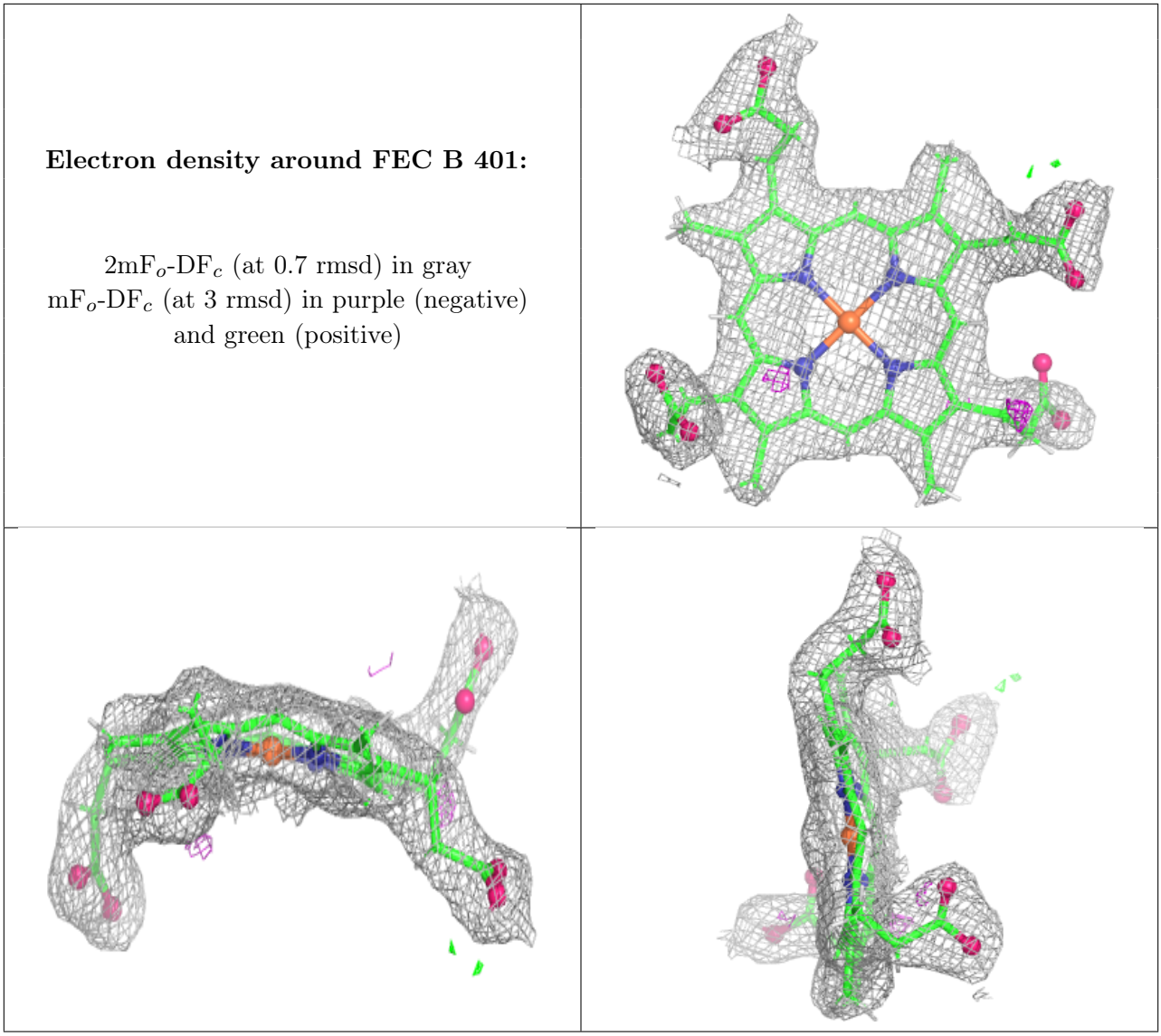






Electron density around FEC B 401:

$2mF_o$-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

There are no such residues in this entry.