wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 09:18 PM EDT

PDB ID	:	3BCC
Title	:	STIGMATELLIN AND ANTIMYCIN BOUND CYTOCHROME BC1 COMPLEX FROM CHICKEN
Authors	:	Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.; Crofts, A.R.; Berry, E.A.; Kim, S.-H.
Deposited on	:	1998-03-23
Resolution	:	3.70 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:

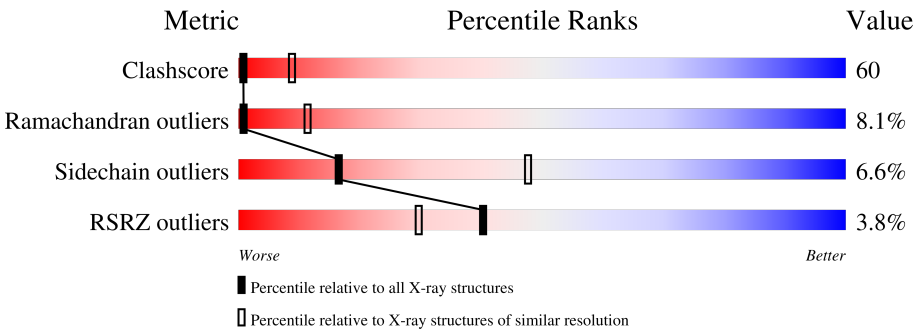
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.70 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))
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	446	3%; 29%, 61%, 8% ••
2	B	422	7%; 30%, 56%, 10% • •
3	C	380	%; 21%, 66%, 12% •
4	D	241	%; 29%, 63%, 8%
5	E	196	13%; 31%, 59%, 9% •
6	F	109	38%, 45%, 8% • 8%

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Mol	Chain	Length	Quality of chain
7	G	81	35% 52% 7%
8	H	78	% 42% 40% 15%
9	I	33	61% 39%
10	J	62	2% 44% 42% 8% 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
14	FES	E	197	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 15645 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 UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3423	2147	601	657	18	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	TYR	THR	conflict	UNP P31800
A	23	VAL	LEU	conflict	UNP P31800
A	59	LEU	VAL	conflict	UNP P31800
A	72	GLN	GLY	conflict	UNP P31800
A	91	SER	THR	conflict	UNP P31800
A	106	VAL	LEU	conflict	UNP P31800
A	135	VAL	LEU	conflict	UNP P31800
A	136	ARG	GLN	conflict	UNP P31800
A	147	GLU	ASP	conflict	UNP P31800
A	162	GLY	PRO	conflict	UNP P31800
A	174	ILE	VAL	conflict	UNP P31800
A	188	THR	ARG	conflict	UNP P31800
A	191	THR	LYS	conflict	UNP P31800
A	203	VAL	LEU	conflict	UNP P31800
A	206	GLN	ARG	conflict	UNP P31800
A	210	GLU	ASP	conflict	UNP P31800
A	217	GLY	SER	conflict	UNP P31800
A	219	VAL	LEU	conflict	UNP P31800
A	220	PRO	SER	conflict	UNP P31800
A	221	PHE	GLY	conflict	UNP P31800
A	225	ASP	GLU	conflict	UNP P31800
A	233	LYS	PRO	conflict	UNP P31800
A	242	ARG	CYS	conflict	UNP P31800
A	267	LEU	ASN	conflict	UNP P31800
A	282	ARG	CYS	conflict	UNP P31800
A	288	LEU	ALA	conflict	UNP P31800
A	290	SER	LEU	conflict	UNP P31800

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Chain	Residue	Modelled	Actual	Comment	Reference
A	299	VAL	ALA	conflict	UNP P31800
A	311	SER	ASN	conflict	UNP P31800
A	315	SER	ALA	conflict	UNP P31800
A	316	GLU	ASP	conflict	UNP P31800
A	320	PHE	LEU	conflict	UNP P31800
A	322	PHE	ALA	conflict	UNP P31800
A	323	TYR	HIS	conflict	UNP P31800
A	328	ARG	HIS	conflict	UNP P31800
A	349	ILE	ALA	conflict	UNP P31800
A	350	SER	THR	conflict	UNP P31800
A	360	PHE	LEU	conflict	UNP P31800
A	382	GLU	SER	conflict	UNP P31800
A	393	GLU	ALA	conflict	UNP P31800
A	397	GLU	SER	conflict	UNP P31800
A	399	LEU	ILE	conflict	UNP P31800
A	406	MET	VAL	conflict	UNP P31800
A	415	ILE	PHE	conflict	UNP P31800
A	425	PRO	PHE	conflict	UNP P31800

- Molecule 2 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	406	2994	1878	518	591	7	0	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ILE	PHE	conflict	UNP P23004
B	28	LYS	ARG	conflict	UNP P23004
B	42	SER	ALA	conflict	UNP P23004
B	44	GLY	ALA	conflict	UNP P23004
B	46	THR	ARG	conflict	UNP P23004
B	49	VAL	LEU	conflict	UNP P23004
B	61	SER	ASN	conflict	UNP P23004
B	99	GLU	THR	conflict	UNP P23004
B	117	GLU	ASP	conflict	UNP P23004
B	134	PRO	ARG	conflict	UNP P23004
B	139	ASP	ALA	conflict	UNP P23004
B	145	LYS	ARG	conflict	UNP P23004
B	152	PHE	LEU	conflict	UNP P23004
B	157	THR	ALA	conflict	UNP P23004

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Chain	Residue	Modelled	Actual	Comment	Reference
B	174	ASP	ASN	conflict	UNP P23004
B	188	SER	PRO	conflict	UNP P23004
B	194	PHE	TYR	conflict	UNP P23004
B	207	VAL	ILE	conflict	UNP P23004
B	218	ASN	GLN	conflict	UNP P23004
B	223	LEU	PHE	conflict	UNP P23004
B	240	ARG	HIS	conflict	UNP P23004
B	257	ILE	LEU	conflict	UNP P23004
B	266	GLY	SER	conflict	UNP P23004
B	282	ASN	GLY	conflict	UNP P23004
B	304	LEU	SER	conflict	UNP P23004
B	332	TYR	SER	conflict	UNP P23004
B	335	GLN	ASP	conflict	UNP P23004
B	352	VAL	LEU	conflict	UNP P23004
B	355	GLU	PRO	conflict	UNP P23004
B	356	ASN	ASP	conflict	UNP P23004
B	367	LYS	GLY	conflict	UNP P23004
B	380	GLU	ASP	conflict	UNP P23004
B	393	ASN	THR	conflict	UNP P23004
B	412	LYS	ASN	conflict	UNP P23004
B	420	ARG	GLY	conflict	UNP P23004
B	421	GLN	ARG	conflict	UNP P23004
B	436	VAL	ILE	conflict	UNP P23004

- Molecule 3 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	379	3002	2013	473	504	12	0	0	0

- Molecule 4 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1899	1214	326	345	14	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	17	PRO	LEU	conflict	UNP P00125
D	143	VAL	LEU	conflict	UNP P00125
D	167	ASP	GLU	conflict	UNP P00125

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Chain	Residue	Modelled	Actual	Comment	Reference
D	216	VAL	LEU	conflict	UNP P00125
D	221	TYR	ALA	conflict	UNP P00125

- Molecule 5 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1512	953	266	285	8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	ASN	ASP	conflict	UNP P13272
E	17	PRO	GLU	conflict	UNP P13272
E	18	ASP	VAL	conflict	UNP P13272
E	19	ASP	LEU	conflict	UNP P13272
E	20	TYR	ASP	conflict	UNP P13272
E	26	ARG	LYS	conflict	UNP P13272
E	29	ASP	SER	conflict	UNP P13272
E	30	PRO	GLU	conflict	UNP P13272
E	31	SER	ALA	conflict	UNP P13272
E	42	VAL	THR	conflict	UNP P13272
E	45	LEU	VAL	conflict	UNP P13272
E	56	THR	SER	conflict	UNP P13272

- Molecule 6 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	100	875	557	153	162	3	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	29	TYR	LEU	conflict	UNP P00129
F	38	TYR	HIS	conflict	UNP P00129
F	59	MET	VAL	conflict	UNP P00129
F	69	ASN	SER	conflict	UNP P00129
F	87	VAL	LYS	conflict	UNP P00129
F	88	PRO	SER	conflict	UNP P00129
F	108	ASP	ALA	conflict	UNP P00129

- Molecule 7 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	78	626	411	114	100	1	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	13	LEU	VAL	conflict	UNP P13271
G	25	PRO	ALA	conflict	UNP P13271
G	34	VAL	ILE	conflict	UNP P13271
G	38	TRP	LEU	conflict	UNP P13271
G	41	LEU	THR	conflict	UNP P13271
G	53	LEU	VAL	conflict	UNP P13271
G	58	LEU	VAL	conflict	UNP P13271
G	78	VAL	GLU	conflict	UNP P13271

- Molecule 8 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	66	490	301	88	96	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	59	PHE	LEU	conflict	UNP P00126

- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	33	159	92	33	34	0	0	0

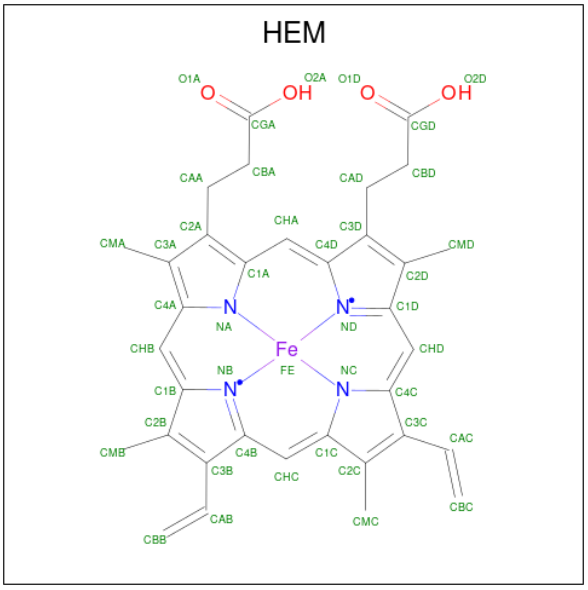
- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	59	459	299	78	82	0	0	0

There is a discrepancy between the modelled and reference sequences:

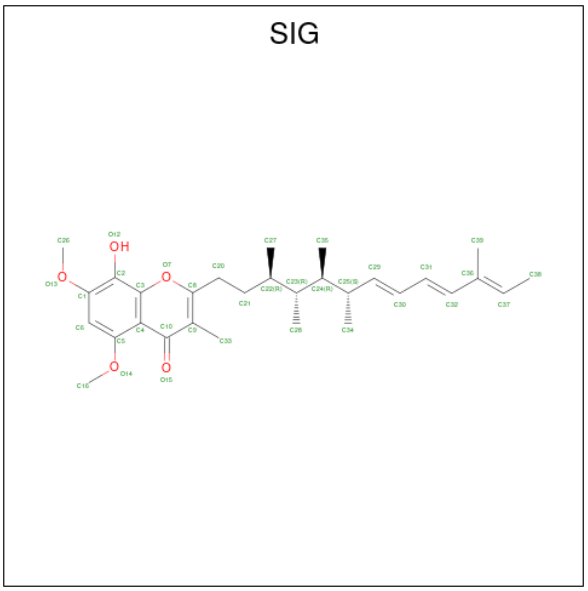
Chain	Residue	Modelled	Actual	Comment	Reference
J	30	LEU	PHE	conflict	UNP P00130

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



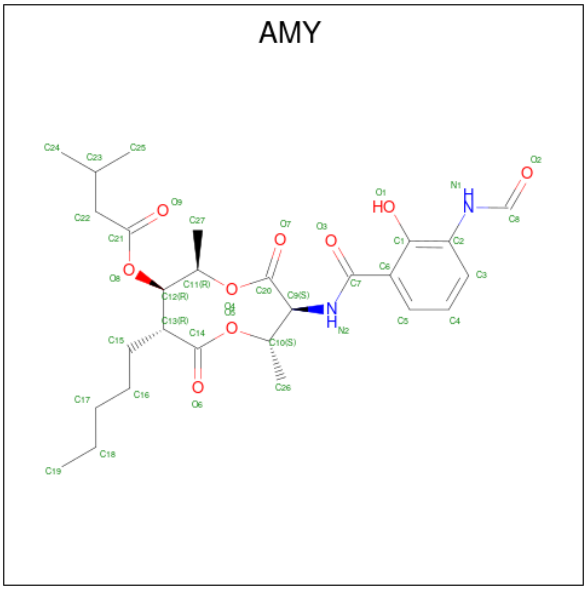
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
11	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
11	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
11	D	1	43	34	1	4	4	0	0

- Molecule 12 is STIGMATELLIN (three-letter code: SIG) (formula: $C_{30}H_{42}O_5$).



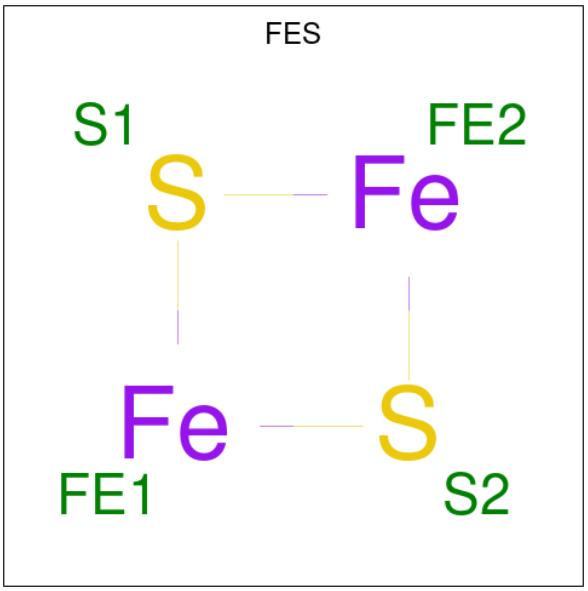
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	C	1	35	30	5	0	0

- Molecule 13 is ANTIMYCIN (three-letter code: AMY) (formula: $C_{27}H_{38}N_2O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	C	1	38	27	2	9	0	0

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



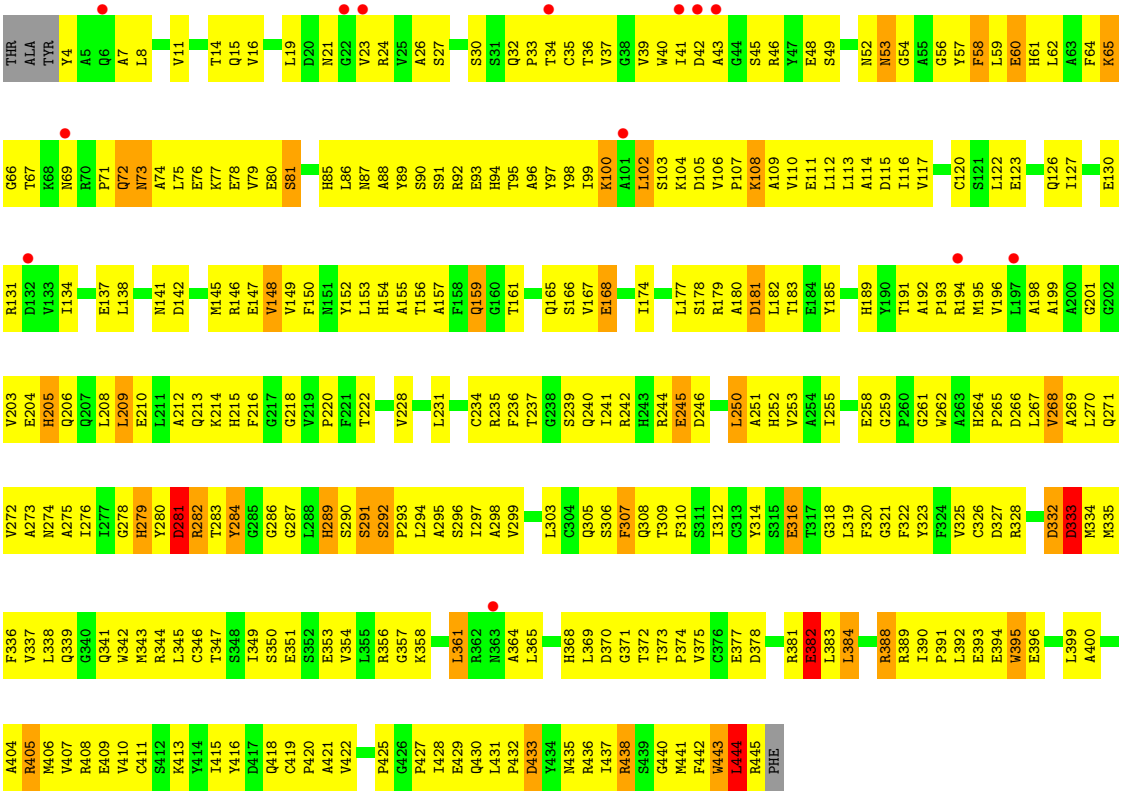
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
14	E	1	4	2	2	0	0

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.

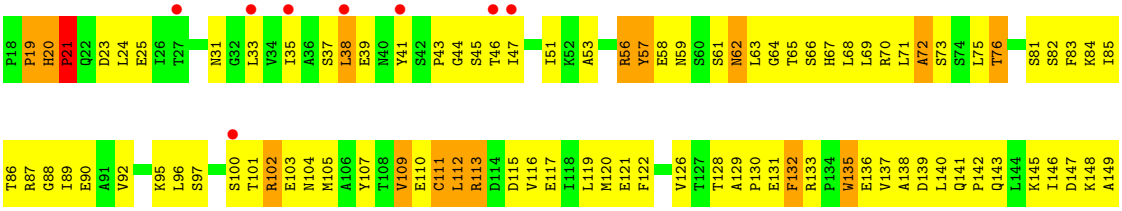
• Molecule 1: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

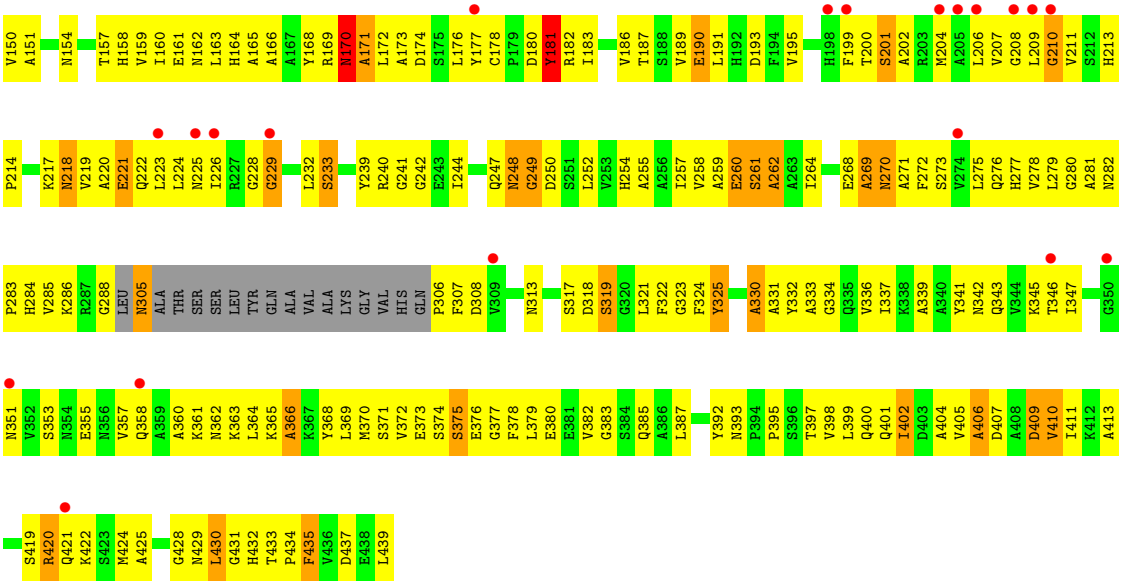
Chain A:



• Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

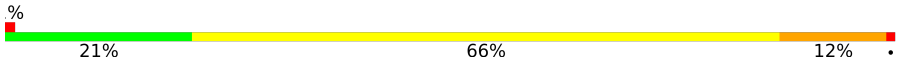
Chain B:

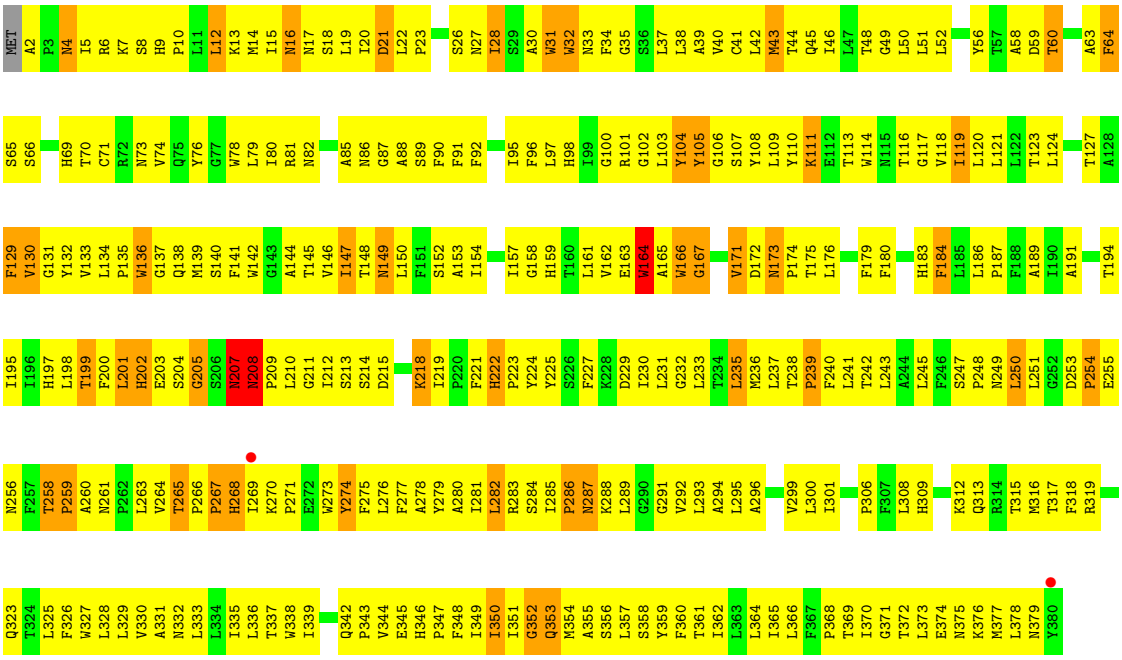




- Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

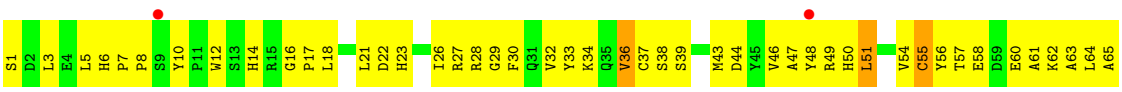
Chain C:

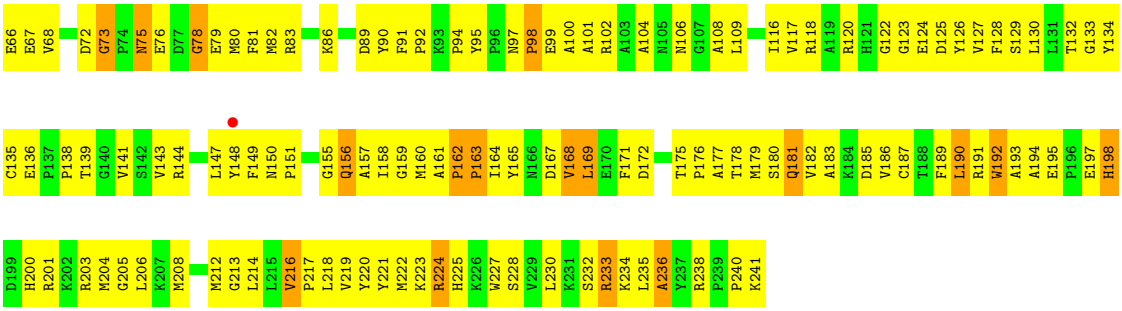




- Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

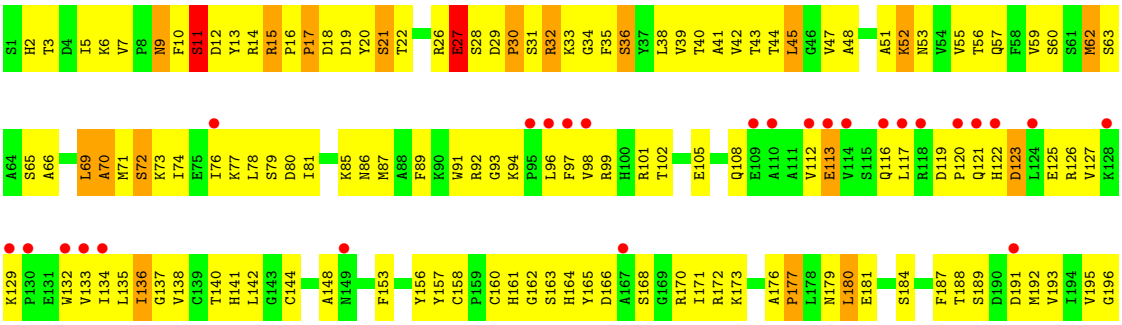
Chain D:





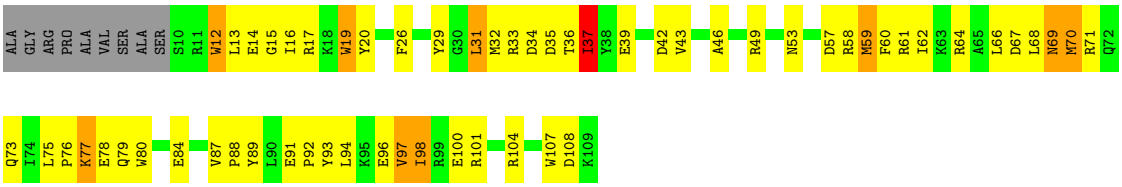
- Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain E:



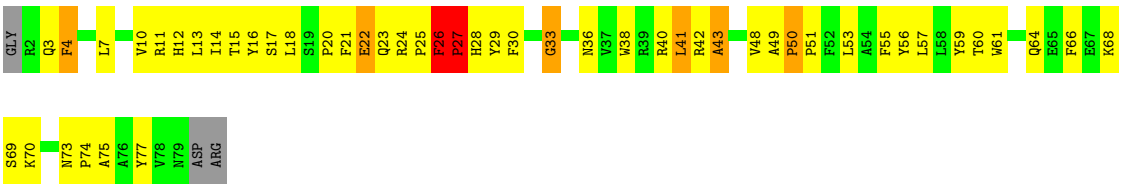
- Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain F:



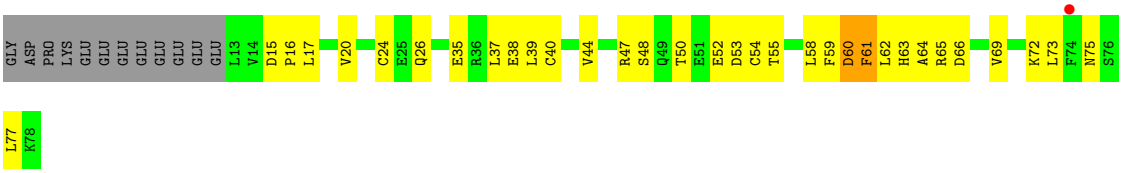
- Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain G:



- Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain H:



• Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain I:

• Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.18Å 179.73Å 238.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.70 86.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.8 (12.00-3.70) 77.4 (86.13-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	0.71 (at 3.19Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.289 , 0.321 0.288 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	82.7	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	15645	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: SIG, AMY, HEM, FES

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	0.50	0/3495	0.77	1/4742 (0.0%)
2	B	0.49	0/3046	0.73	0/4132
3	C	0.60	0/3104	0.86	1/4252 (0.0%)
4	D	0.54	0/1960	0.80	2/2665 (0.1%)
5	E	0.58	1/1548 (0.1%)	0.77	1/2095 (0.0%)
6	F	0.52	0/896	0.74	0/1206
7	G	0.57	0/648	1.16	3/882 (0.3%)
8	H	0.43	0/495	0.67	0/669
10	J	0.58	0/470	0.79	1/635 (0.2%)
All	All	0.54	1/15662 (0.0%)	0.80	9/21278 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6	LYS	CD-CE	6.62	1.67	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	26	PHE	C-N-CD	-20.16	76.25	120.60
7	G	26	PHE	C-N-CA	12.85	175.99	122.00
7	G	27	PRO	CA-N-CD	-7.88	100.47	111.50
1	A	287	GLY	N-CA-C	-6.79	96.12	113.10
4	D	76	GLU	N-CA-C	-6.20	94.27	111.00

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	3423	0	3286	448	0
2	B	2994	0	2906	327	0
3	C	3002	0	3036	487	0
4	D	1899	0	1822	254	1
5	E	1512	0	1483	185	0
6	F	875	0	839	88	1
7	G	626	0	591	67	0
8	H	490	0	445	45	0
9	I	159	0	43	21	0
10	J	459	0	424	55	0
11	C	86	0	60	23	0
11	D	43	0	30	6	0
12	C	35	0	42	13	0
13	C	38	0	36	15	0
14	E	4	0	0	2	0
All	All	15645	0	15043	1851	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 60.

The worst 5 of 1851 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:SER:HB3	11:C:382:HEM:HBD1	1.22	1.17
3:C:316:MET:SD	3:C:319:ARG:HG3	1.90	1.11
1:A:36:THR:HG22	1:A:100:LYS:HB3	1.31	1.11
3:C:146:VAL:HG23	3:C:147:ILE:H	1.15	1.08
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.14	1.07

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)
4:D:165:TYR:OH	6:F:14:GLU:OE2[3_555]	2.18	0.02

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	440/446 (99%)	310 (70%)	103 (23%)	27 (6%)	1	18
2	B	404/422 (96%)	281 (70%)	83 (20%)	40 (10%)	0	8
3	C	377/380 (99%)	235 (62%)	106 (28%)	36 (10%)	0	8
4	D	239/241 (99%)	175 (73%)	47 (20%)	17 (7%)	1	15
5	E	194/196 (99%)	141 (73%)	39 (20%)	14 (7%)	1	14
6	F	98/109 (90%)	74 (76%)	17 (17%)	7 (7%)	1	15
7	G	76/81 (94%)	52 (68%)	17 (22%)	7 (9%)	1	9
8	H	64/78 (82%)	42 (66%)	19 (30%)	3 (5%)	2	23
10	J	57/62 (92%)	37 (65%)	13 (23%)	7 (12%)	0	4
All	All	1949/2015 (97%)	1347 (69%)	444 (23%)	158 (8%)	1	11

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	282	ARG
1	A	284	TYR
1	A	289	HIS
2	B	19	PRO

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	359/376 (96%)	336 (94%)	23 (6%)	17	48
2	B	307/336 (91%)	286 (93%)	21 (7%)	16	47
3	C	326/329 (99%)	304 (93%)	22 (7%)	16	47
4	D	201/207 (97%)	192 (96%)	9 (4%)	27	57
5	E	165/169 (98%)	151 (92%)	14 (8%)	10	40
6	F	90/98 (92%)	82 (91%)	8 (9%)	9	37
7	G	60/72 (83%)	53 (88%)	7 (12%)	5	26
8	H	51/74 (69%)	51 (100%)	0	100	100
10	J	41/52 (79%)	39 (95%)	2 (5%)	25	56
All	All	1600/1713 (93%)	1494 (93%)	106 (7%)	16	48

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	208	ASN
4	D	169	LEU
7	G	22	GLU
3	C	254	PRO
3	C	350	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	16	ASN
3	C	261	ASN
7	G	64	GLN
3	C	17	ASN
3	C	86	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
11	HEM	C	382	3	41,50,50	1.94	9 (21%)	45,82,82	2.55	17 (37%)
11	HEM	C	381	3	41,50,50	1.83	11 (26%)	45,82,82	3.09	22 (48%)
14	FES	E	197	5	0,4,4	-	-	-		
11	HEM	D	242	4	41,50,50	1.91	8 (19%)	45,82,82	2.65	17 (37%)
13	AMY	C	384	-	39,39,39	3.94	17 (43%)	35,53,53	4.14	12 (34%)
12	SIG	C	383	-	32,36,36	1.58	6 (18%)	40,50,50	2.31	10 (25%)

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
11	HEM	C	382	3	-	6/12/54/54	-
11	HEM	C	381	3	-	6/12/54/54	-
14	FES	E	197	5	-	-	0/1/1/1
11	HEM	D	242	4	-	8/12/54/54	-
13	AMY	C	384	-	-	15/37/52/52	0/1/2/2
12	SIG	C	383	-	-	16/29/30/30	0/2/2/2

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	384	AMY	O6-C14	12.13	1.51	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	384	AMY	O7-C20	10.35	1.47	1.21
13	C	384	AMY	O5-C14	8.62	1.54	1.34
13	C	384	AMY	C27-C11	-7.71	1.33	1.51
11	D	242	HEM	C3C-C2C	-6.43	1.31	1.40

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	384	AMY	O5-C14-O6	-13.11	107.56	124.08
13	C	384	AMY	O4-C20-O7	-12.87	107.87	124.08
11	D	242	HEM	CBA-CAA-C2A	10.21	130.05	112.62
11	C	381	HEM	C1B-NB-C4B	-8.91	95.87	105.07
12	C	383	SIG	C20-C8-C9	8.49	132.42	120.39

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	381	HEM	C2B-C3B-CAB-CBB
11	C	381	HEM	C4B-C3B-CAB-CBB
11	C	382	HEM	C1A-C2A-CAA-CBA
11	C	382	HEM	C2B-C3B-CAB-CBB
11	C	382	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

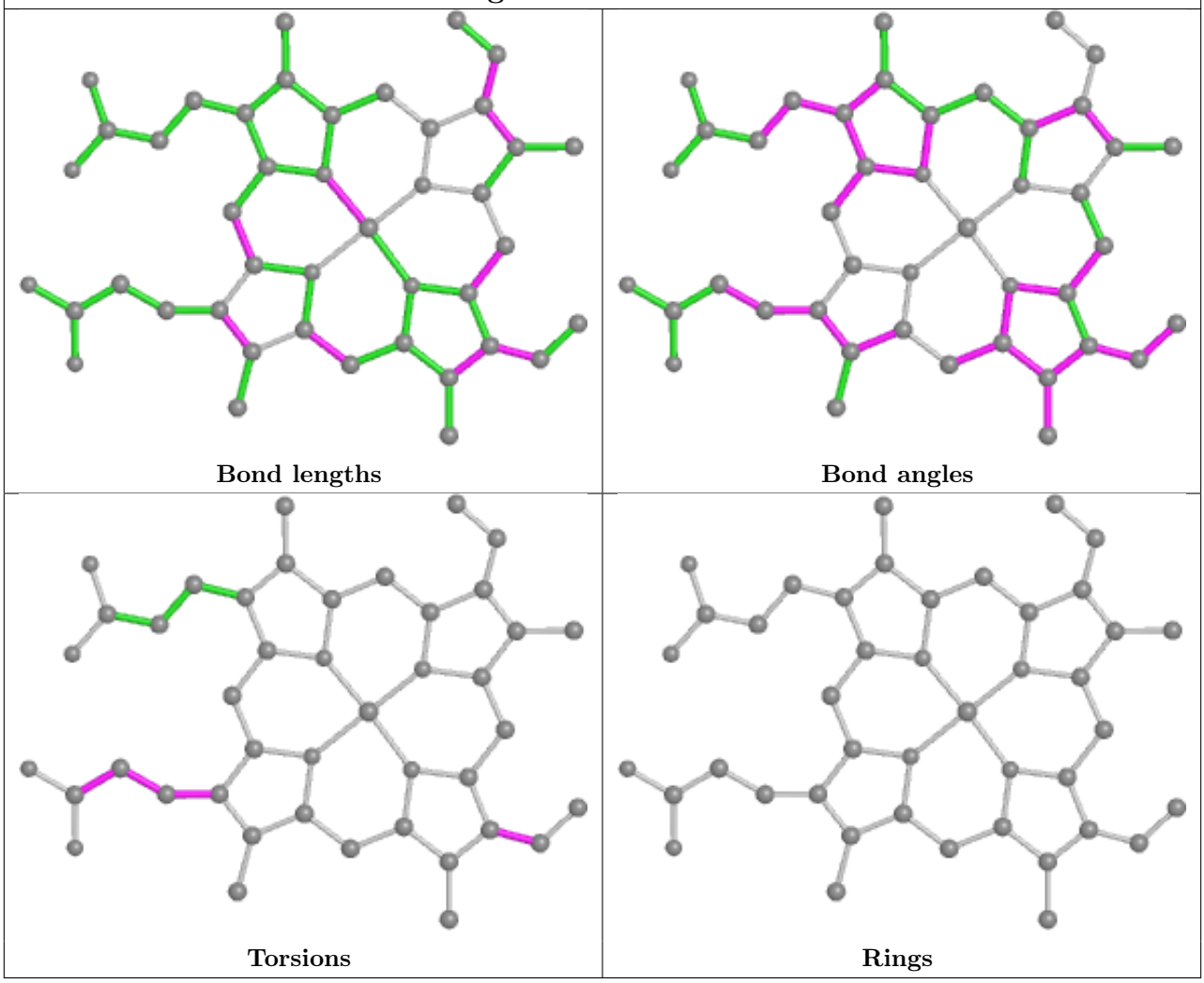
6 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	382	HEM	11	0
11	C	381	HEM	12	0
14	E	197	FES	2	0
11	D	242	HEM	6	0
13	C	384	AMY	15	0
12	C	383	SIG	13	0

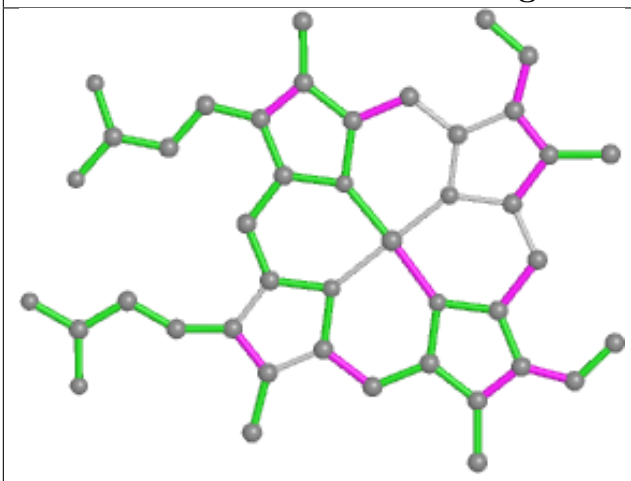
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

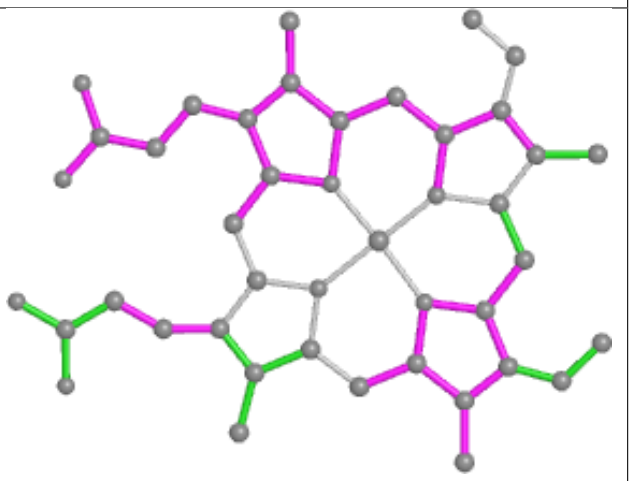
Ligand HEM C 382



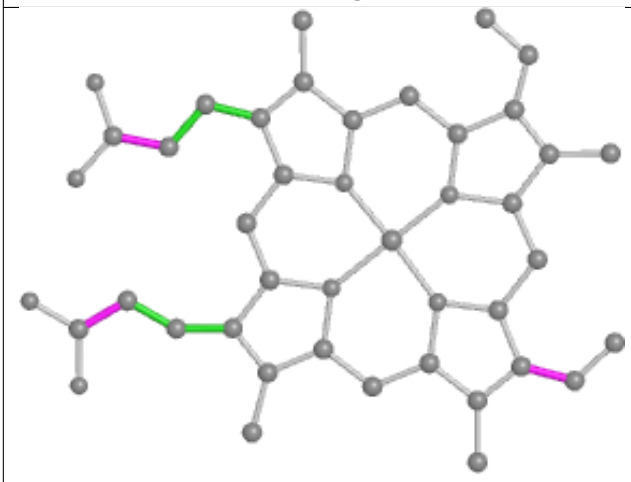
Ligand HEM C 381



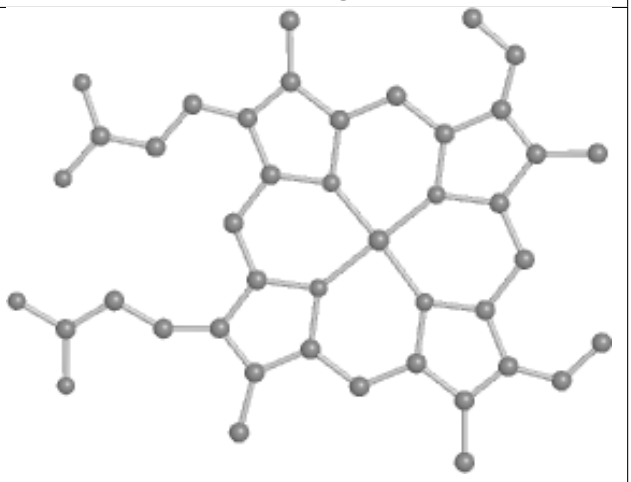
Bond lengths



Bond angles

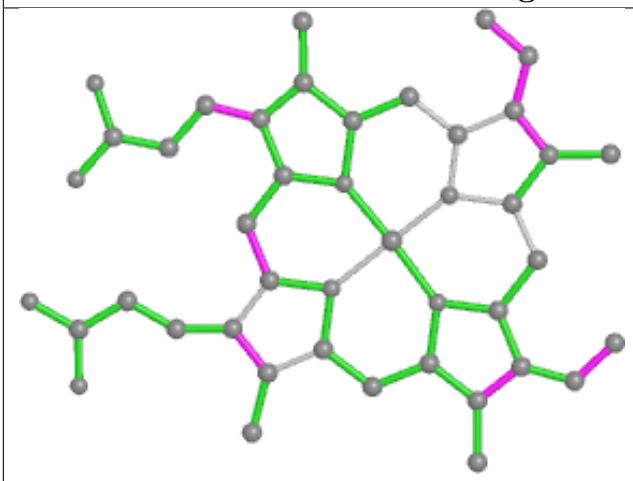


Torsions

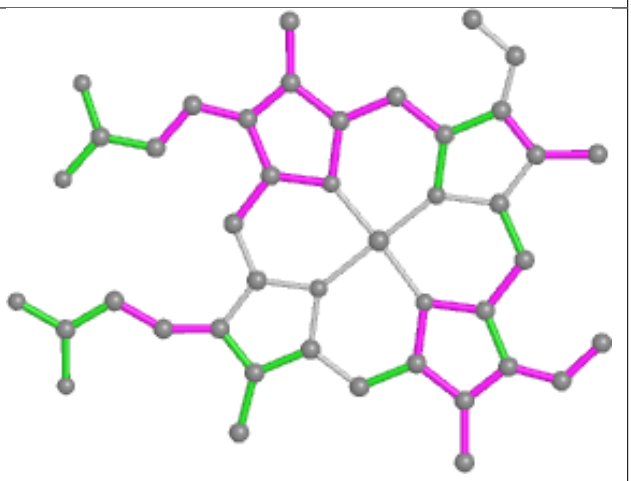


Rings

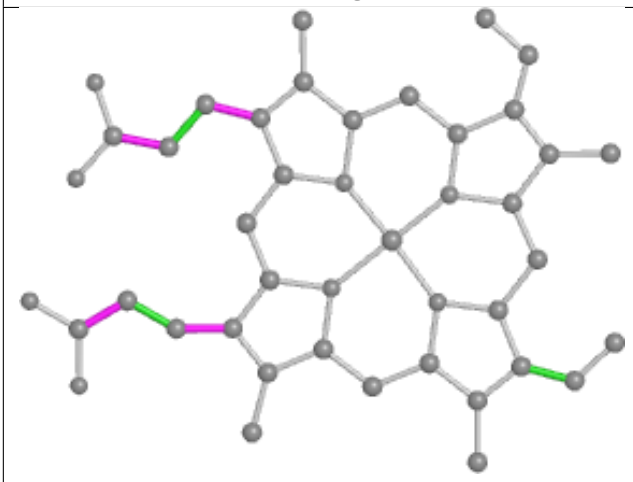
Ligand HEM D 242



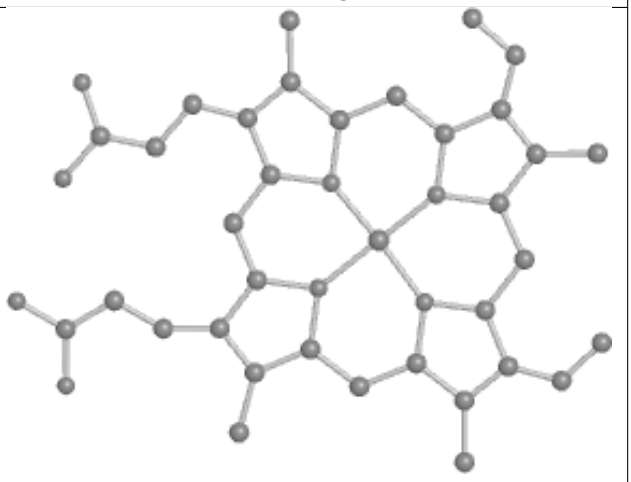
Bond lengths



Bond angles

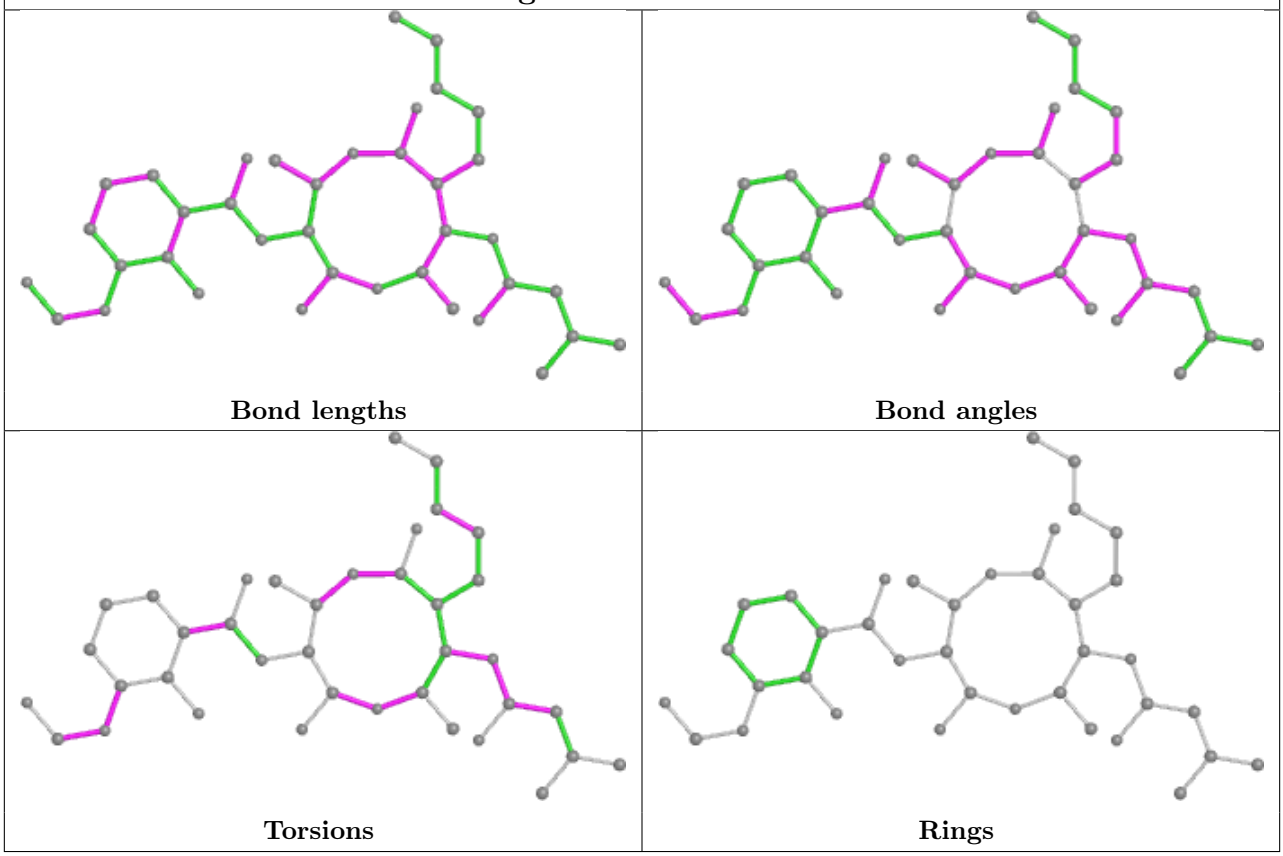


Torsions

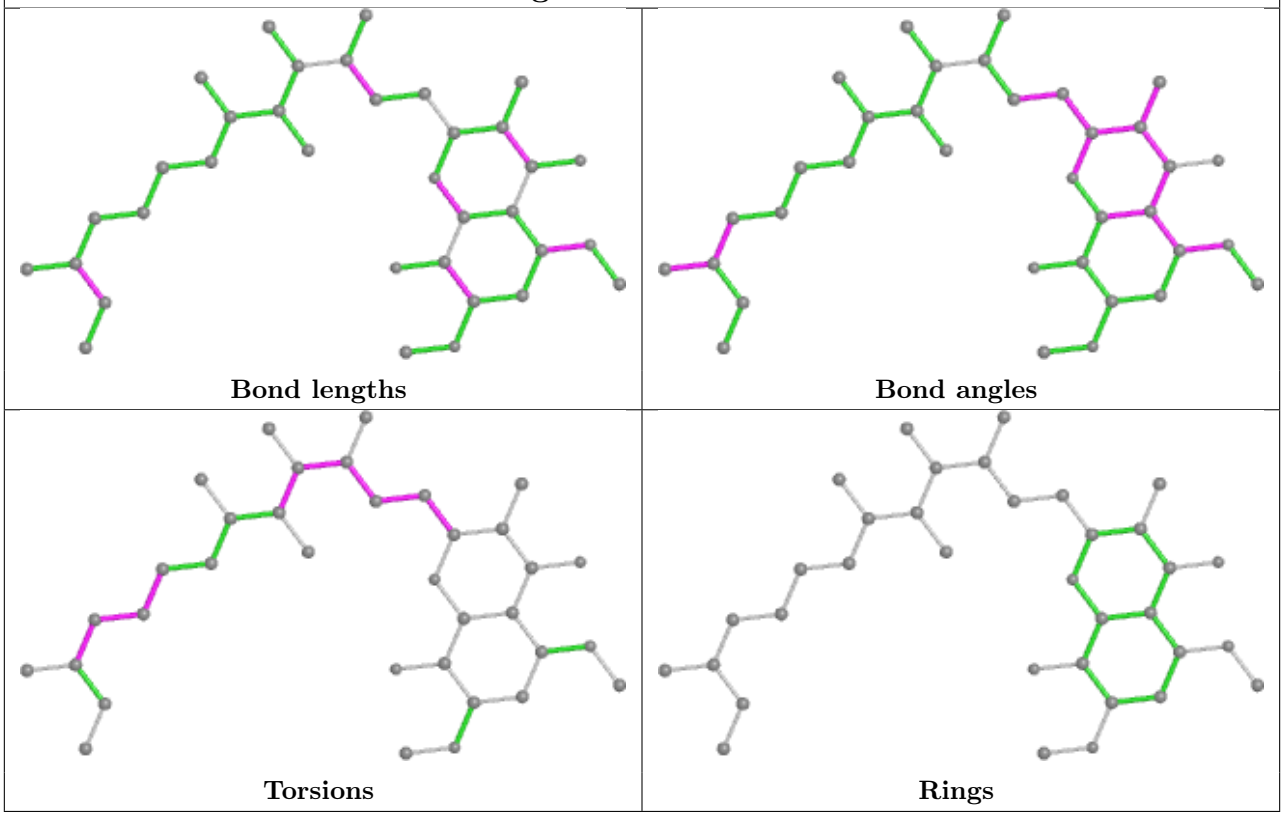


Rings

Ligand AMY C 384



Ligand SIG C 383



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	210:UNK	C	309:UNK	N	33.28
1	I	121:UNK	C	202:UNK	N	28.55

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	442/446 (99%)	0.13	13 (2%) 51 39	36, 84, 100, 100	0
2	B	406/422 (96%)	0.39	28 (6%) 16 11	58, 95, 100, 100	0
3	C	379/380 (99%)	-0.16	2 (0%) 91 85	13, 43, 72, 92	0
4	D	241/241 (100%)	-0.05	3 (1%) 79 69	27, 65, 95, 100	0
5	E	196/196 (100%)	0.53	26 (13%) 3 3	32, 95, 100, 100	0
6	F	100/109 (91%)	-0.20	0 100 100	39, 64, 93, 99	0
7	G	78/81 (96%)	-0.22	0 100 100	35, 74, 97, 99	0
8	H	66/78 (84%)	-0.18	1 (1%) 73 63	63, 91, 98, 100	0
9	I	0/33	-	-	-	-
10	J	59/62 (95%)	-0.13	1 (1%) 70 59	56, 71, 95, 100	0
All	All	1967/2048 (96%)	0.09	74 (3%) 40 30	13, 78, 100, 100	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	117	LEU	5.1
1	A	42	ASP	4.7
2	B	351	ASN	4.3
1	A	194	ARG	4.3
5	E	97	PHE	4.3

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)

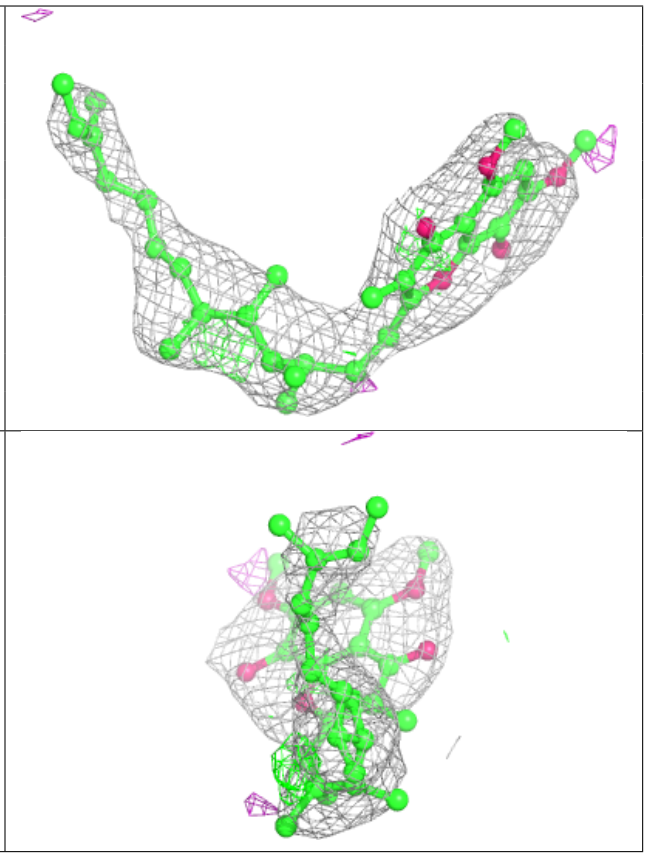
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	SIG	C	383	35/35	0.91	0.45	17,37,61,71	0
13	AMY	C	384	38/38	0.93	0.32	15,37,60,64	0
11	HEM	C	381	43/43	0.97	0.30	22,34,42,44	0
11	HEM	C	382	43/43	0.98	0.29	22,34,43,47	0
11	HEM	D	242	43/43	0.98	0.25	34,40,53,61	0
14	FES	E	197	4/4	0.98	0.20	71,84,87,88	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.

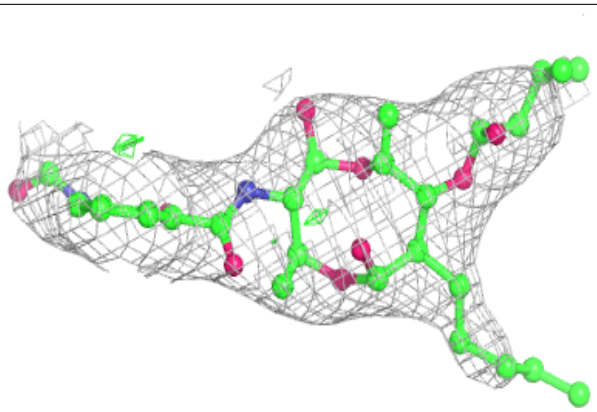
Electron density around SIG C 383:

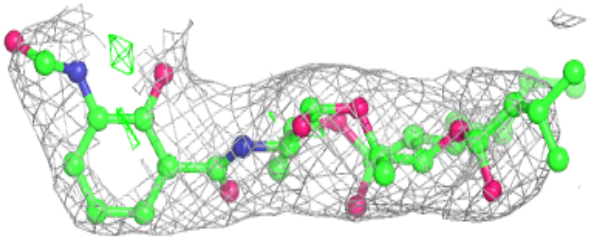
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

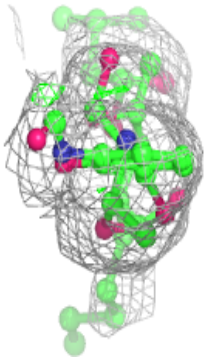


Electron density around AMY C 384:

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

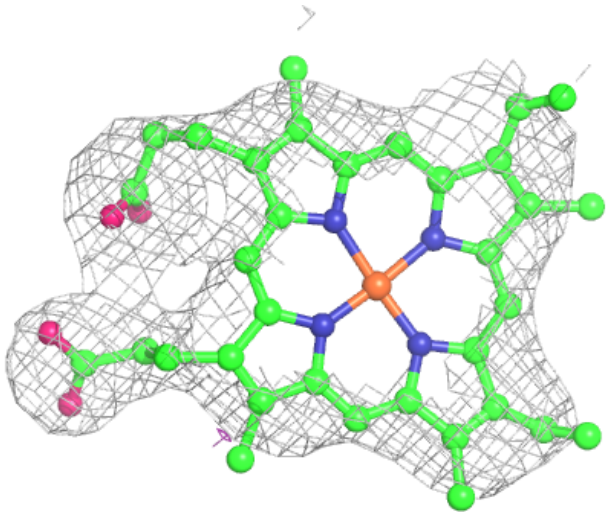


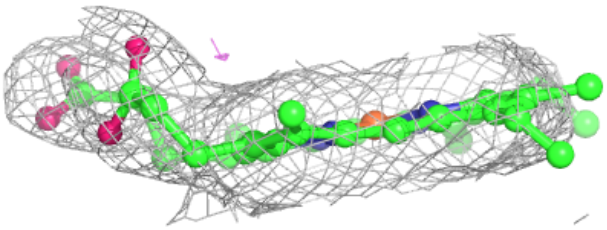


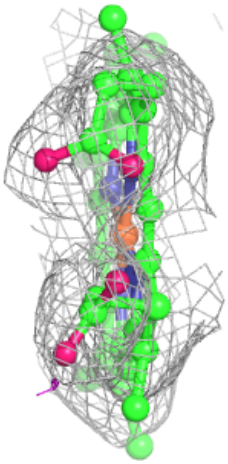


Electron density around HEM C 381:

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

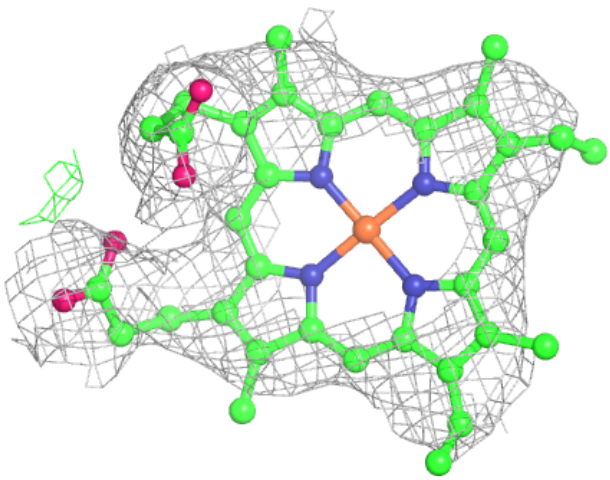


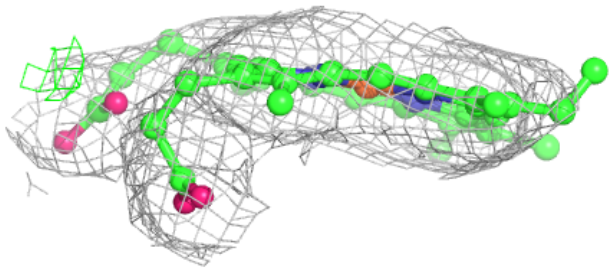


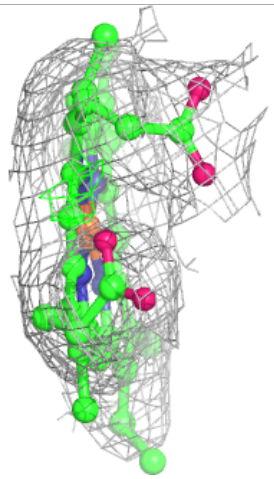


Electron density around HEM C 382:

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

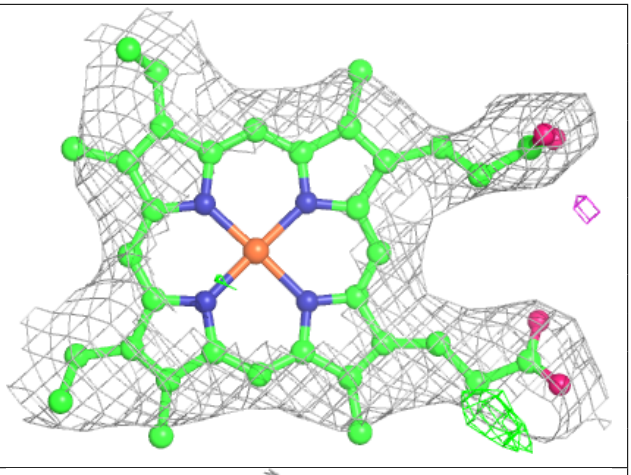


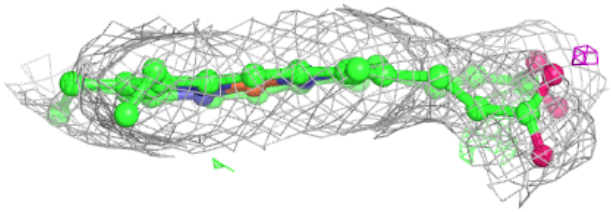


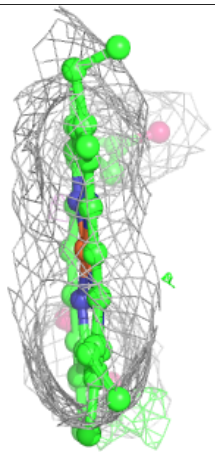


Electron density around HEM D 242:

$2mF_o$-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.