



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:47 PM UTC

PDB ID : 2WDQ / pdb_00002wdq
Title : E. coli succinate:quinone oxidoreductase (SQR) with carboxin bound
Authors : Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on : 2009-03-25
Resolution : 2.40 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 ⓘ 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	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

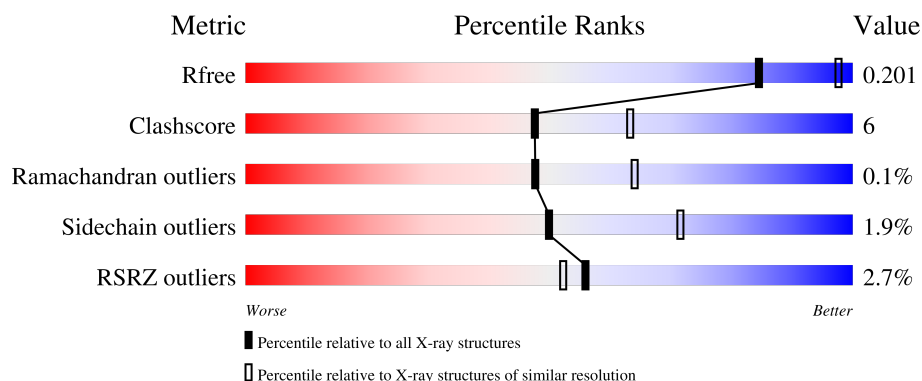
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	588	% 87% 12% .
1	E	588	% 90% 10%
1	I	588	88% 12%
2	B	238	% 92% 6% .
2	F	238	95% 5% .

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Mol	Chain	Length	Quality of chain
2	J	238	 90% 9%
3	C	129	 16% 84% 10% 6%
3	G	129	 9% 83% 11% 6%
3	K	129	 7% 84% 10% 6%
4	D	115	 6% 77% 12% 9%
4	H	115	 13% 79% 10% 9%
4	L	115	 5% 80% 10% 9%

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
6	TEO	E	1589	-	-	X	-
6	TEO	I	1589	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26034 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 SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4522	2812	821	861	28			
1	E	588	Total	C	N	O	S	0	0	0
			4522	2812	821	861	28			
1	I	588	Total	C	N	O	S	0	0	0
			4522	2812	821	861	28			

- Molecule 2 is a protein called SUCCINATE DEHYDROGENASE IRON-SULFUR SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1869	1172	329	348	20			
2	F	238	Total	C	N	O	S	0	0	0
			1869	1172	329	348	20			
2	J	238	Total	C	N	O	S	0	0	0
			1869	1172	329	348	20			

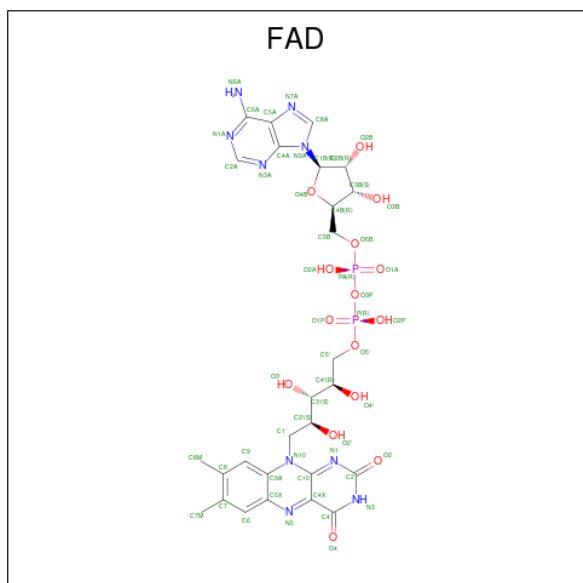
- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	121	Total	C	N	O	S	0	0	0
			933	619	151	158	5			
3	G	121	Total	C	N	O	S	0	0	0
			933	619	151	158	5			
3	K	121	Total	C	N	O	S	0	0	0
			933	619	151	158	5			

- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT.

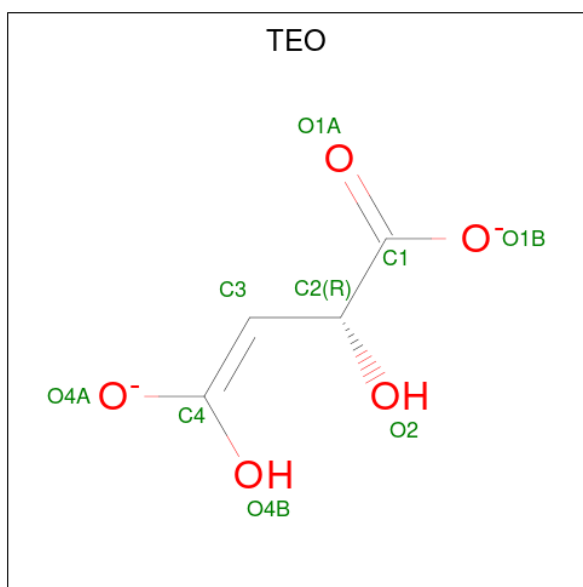
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total 836	C 577	N 123	O 133	S 3	0	0	0
4	H	105	Total 836	C 577	N 123	O 133	S 3	0	0	0
4	L	105	Total 836	C 577	N 123	O 133	S 3	0	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	I	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is MALATE LIKE INTERMEDIATE (CCD ID: TEO) (formula: $C_4H_4O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		
6	E	1	Total	C	O	0	0
			9	4	5		
6	I	1	Total	C	O	0	0
			9	4	5		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

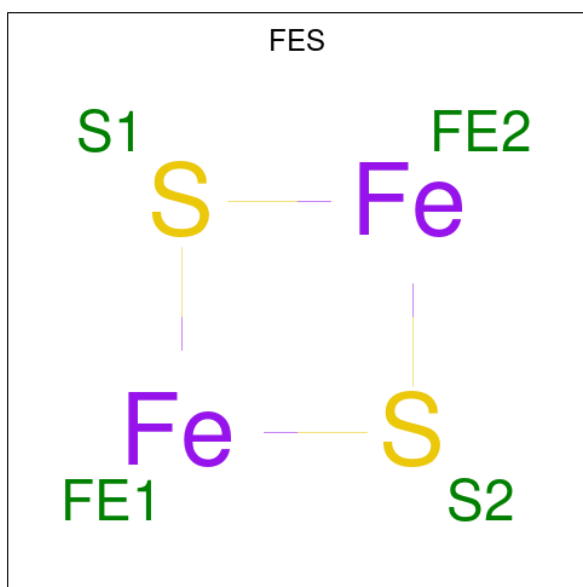
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		
7	E	1	Total	Na	0	0
			1	1		
7	I	1	Total	Na	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



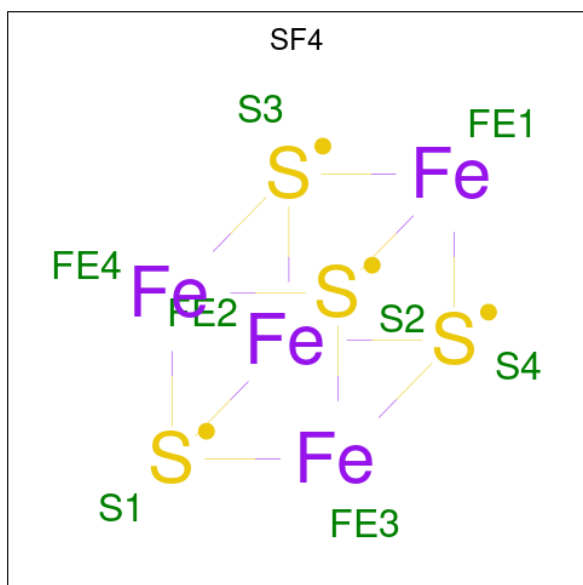
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			4	2	2		

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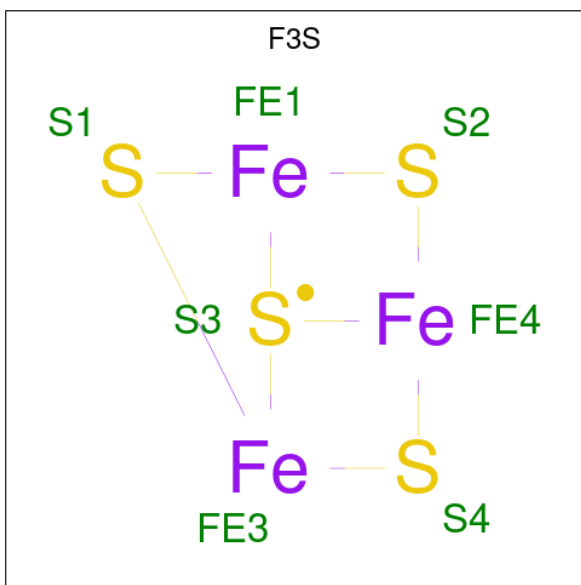
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	Fe	S	0	0
			4	2	2		
9	J	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



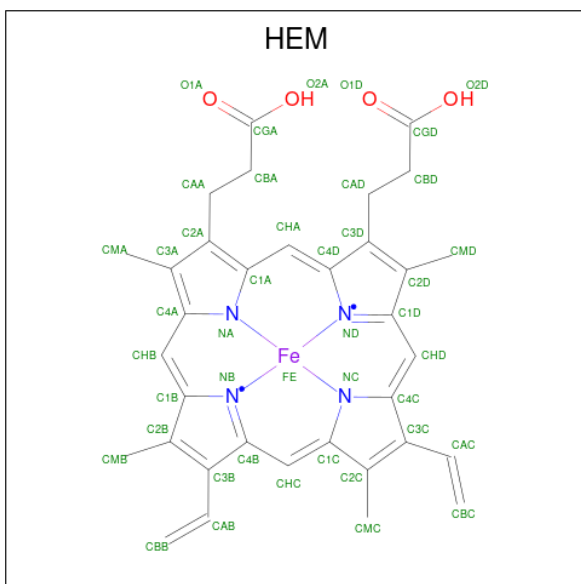
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			8	4	4		
10	F	1	Total	Fe	S	0	0
			8	4	4		
10	J	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 11 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



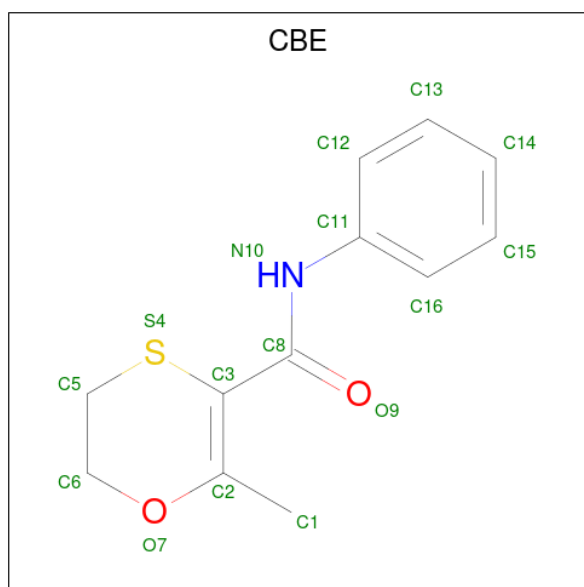
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			7	3	4		
11	F	1	Total	Fe	S	0	0
			7	3	4		
11	J	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
12	G	1	Total	C	Fe	N	O	
			43	34	1	4	4	
12	K	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 13 is 2-METHYL-N-PHENYL-5,6-DIHYDRO-1,4-OXATHIINE-3-CARBOXAMIDE (CCD ID: CBE) (formula: $C_{12}H_{13}NO_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	S	
			16	12	1	2	1	
13	G	1	Total	C	N	O	S	
			16	12	1	2	1	
13	K	1	Total	C	N	O	S	
			16	12	1	2	1	

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	258	Total	O		
			258	258	0	0
14	B	128	Total	O		
			128	128	0	0
14	C	22	Total	O		
			22	22	0	0

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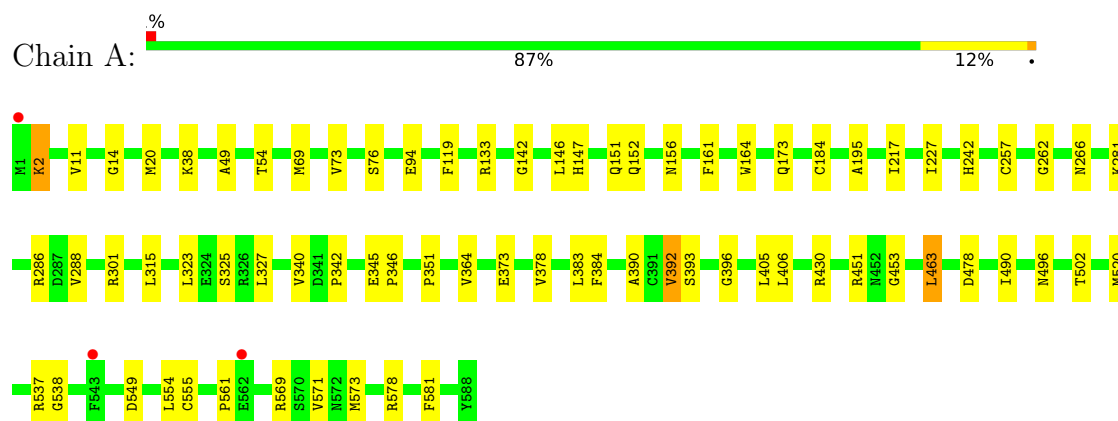
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	D	10	Total 10	O 10	0	0
14	E	234	Total 234	O 234	0	0
14	F	116	Total 116	O 116	0	0
14	G	17	Total 17	O 17	0	0
14	H	4	Total 4	O 4	0	0
14	I	197	Total 197	O 197	0	0
14	J	107	Total 107	O 107	0	0
14	K	17	Total 17	O 17	0	0
14	L	6	Total 6	O 6	0	0

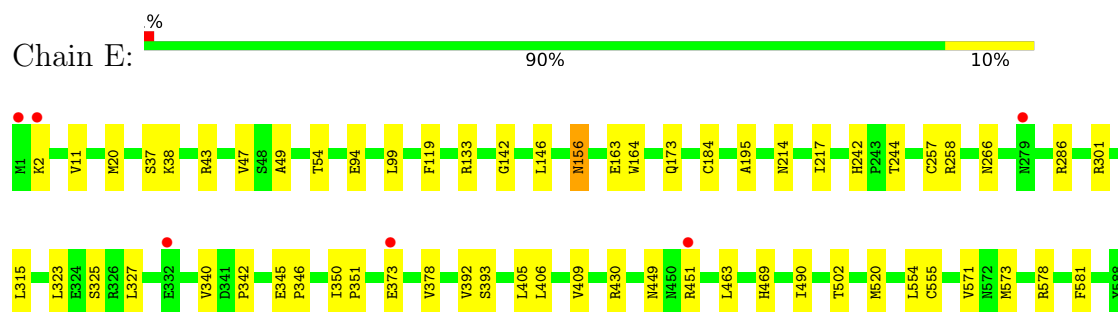
3 Residue-property plots [i](#)

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.

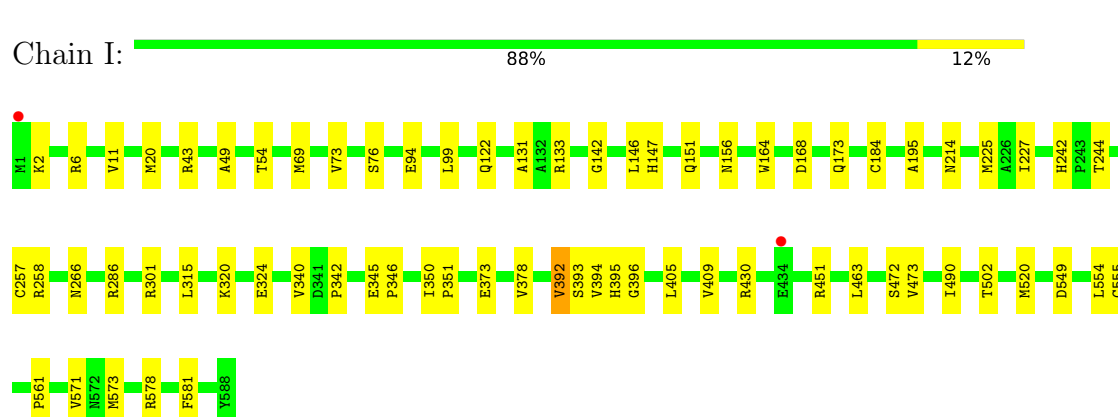
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT



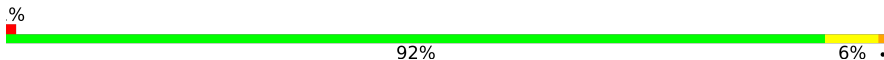
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT



• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT



- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain B: 



- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain F: 



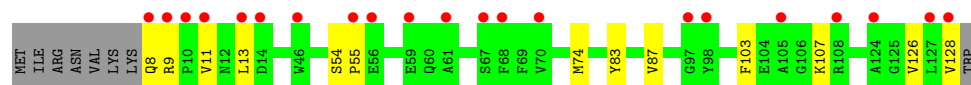
- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain J: 



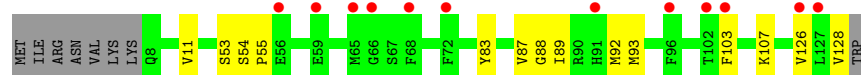
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain C: 



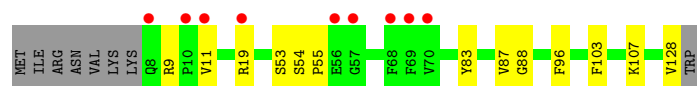
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain G: 



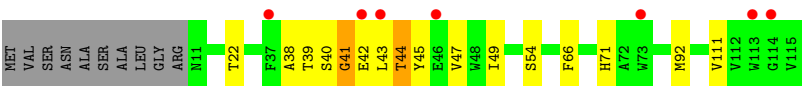
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain K: 

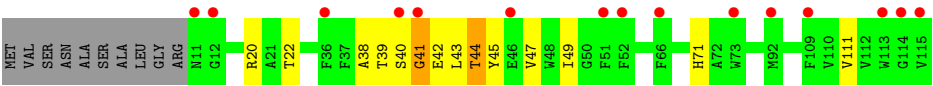
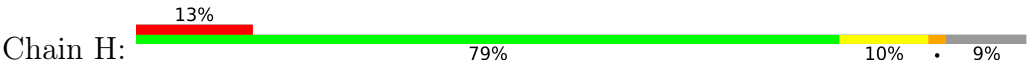


- Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

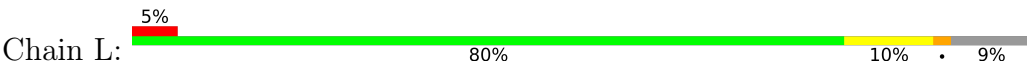
Chain D: 



● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT



● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.40Å 178.46Å 200.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	133.63 – 2.40 133.43 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (133.63-2.40) 99.5 (133.43-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.171 , 0.200 0.172 , 0.201	Depositor DCC
R_{free} test set	8380 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26034	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: FAD, HEM, SO4, SF4, FES, CBE, TEO, NA, F3S

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	0.89	3/4611 (0.1%)	0.94	2/6237 (0.0%)
1	E	0.84	2/4611 (0.0%)	0.92	1/6237 (0.0%)
1	I	0.77	0/4611	0.88	2/6237 (0.0%)
2	B	0.86	1/1908 (0.1%)	0.93	1/2578 (0.0%)
2	F	0.82	0/1908	0.91	0/2578
2	J	0.82	0/1908	0.90	1/2578 (0.0%)
3	C	0.68	0/953	0.78	0/1293
3	G	0.67	0/953	0.79	0/1293
3	K	0.66	0/953	0.81	1/1293 (0.1%)
4	D	0.72	0/859	0.80	0/1175
4	H	0.65	0/859	0.80	1/1175 (0.1%)
4	L	0.66	0/859	0.77	0/1175
All	All	0.80	6/24993 (0.0%)	0.89	9/33849 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	449	ASN	CG-ND2	-6.60	1.19	1.33
1	E	156	ASN	CG-ND2	-6.07	1.20	1.33
1	A	152	GLN	CD-NE2	-5.76	1.21	1.33
1	A	288	VAL	CA-CB	5.39	1.60	1.54
1	A	390	ALA	CA-CB	-5.32	1.45	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	9	ARG	N-CA-C	6.71	118.35	109.83
2	B	213	VAL	CB-CA-C	-6.43	103.46	112.14
1	I	244	THR	N-CA-C	5.71	116.59	108.54
1	E	244	THR	N-CA-C	5.64	117.27	109.54
1	I	392	VAL	N-CA-C	5.57	116.35	110.72

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	4522	0	4426	49	0
1	E	4522	0	4426	44	0
1	I	4522	0	4426	50	0
2	B	1869	0	1850	13	0
2	F	1869	0	1850	9	0
2	J	1869	0	1850	18	0
3	C	933	0	979	16	0
3	G	933	0	979	14	0
3	K	933	0	979	11	0
4	D	836	0	875	13	0
4	H	836	0	875	13	0
4	L	836	0	875	11	0
5	A	53	0	29	6	0
5	E	53	0	30	7	0
5	I	53	0	29	7	0
6	A	9	0	3	3	0
6	E	9	0	3	4	0
6	I	9	0	3	4	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
8	A	5	0	0	0	0
8	E	5	0	0	0	0
8	I	5	0	0	0	0
9	B	4	0	0	0	0
9	F	4	0	0	0	0
9	J	4	0	0	0	0
10	B	8	0	0	0	0
10	F	8	0	0	0	0
10	J	8	0	0	1	0
11	B	7	0	0	0	0
11	F	7	0	0	0	0
11	J	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	43	0	30	6	0
12	G	43	0	30	5	0
12	K	43	0	30	6	0
13	C	16	0	13	2	0
13	G	16	0	13	1	0
13	K	16	0	13	2	0
14	A	258	0	0	5	0
14	B	128	0	0	1	0
14	C	22	0	0	1	0
14	D	10	0	0	1	0
14	E	234	0	0	3	0
14	F	116	0	0	0	0
14	G	17	0	0	0	0
14	H	4	0	0	0	0
14	I	197	0	0	3	0
14	J	107	0	0	1	0
14	K	17	0	0	1	0
14	L	6	0	0	0	0
All	All	26034	0	24616	278	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 6.

The worst 5 of 278 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:502:THR:HG22	14:A:2215:HOH:O	1.41	1.17
1:I:490:ILE:HG22	1:I:520:MET:HE1	1.34	1.10
12:C:1129:HEM:HHD	12:C:1129:HEM:HBC2	1.35	1.09
1:E:490:ILE:HG22	1:E:520:MET:HE1	1.38	0.99
1:I:490:ILE:CG2	1:I:520:MET:HE1	1.99	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	586/588 (100%)	571 (97%)	15 (3%)	0	100	100
1	E	586/588 (100%)	571 (97%)	15 (3%)	0	100	100
1	I	586/588 (100%)	572 (98%)	14 (2%)	0	100	100
2	B	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
2	F	236/238 (99%)	227 (96%)	9 (4%)	0	100	100
2	J	236/238 (99%)	229 (97%)	7 (3%)	0	100	100
3	C	119/129 (92%)	116 (98%)	3 (2%)	0	100	100
3	G	119/129 (92%)	115 (97%)	4 (3%)	0	100	100
3	K	119/129 (92%)	115 (97%)	4 (3%)	0	100	100
4	D	103/115 (90%)	96 (93%)	6 (6%)	1 (1%)	12	20
4	H	103/115 (90%)	96 (93%)	6 (6%)	1 (1%)	12	20
4	L	103/115 (90%)	97 (94%)	5 (5%)	1 (1%)	12	20
All	All	3132/3210 (98%)	3033 (97%)	96 (3%)	3 (0%)	48	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	41	GLY
4	L	41	GLY
4	D	41	GLY

5.3.2 Protein sidechains ⓘ

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	473/473 (100%)	465 (98%)	8 (2%)	53	74
1	E	473/473 (100%)	466 (98%)	7 (2%)	57	77
1	I	473/473 (100%)	469 (99%)	4 (1%)	73	86
2	B	208/208 (100%)	203 (98%)	5 (2%)	43	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	208/208 (100%)	202 (97%)	6 (3%)	37	60
2	J	208/208 (100%)	201 (97%)	7 (3%)	32	54
3	C	101/109 (93%)	100 (99%)	1 (1%)	68	84
3	G	101/109 (93%)	100 (99%)	1 (1%)	68	84
3	K	101/109 (93%)	100 (99%)	1 (1%)	68	84
4	D	88/96 (92%)	84 (96%)	4 (4%)	24	42
4	H	88/96 (92%)	86 (98%)	2 (2%)	44	66
4	L	88/96 (92%)	85 (97%)	3 (3%)	32	54
All	All	2610/2658 (98%)	2561 (98%)	49 (2%)	50	71

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	180	ARG
1	I	94	GLU
2	F	192	SER
4	H	43	LEU
1	I	378	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	109	GLN
3	K	30	HIS
2	F	237	ASN
2	J	135	GLN
2	F	235	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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$
6	TEO	E	1589	-	5,8,8	1.15	0	4,10,10	2.43	3 (75%)
8	SO4	I	1591	-	4,4,4	0.22	0	6,6,6	0.39	0
8	SO4	E	1591	-	4,4,4	0.34	0	6,6,6	0.30	0
13	CBE	G	1130	-	16,17,17	1.18	1 (6%)	17,22,22	1.97	3 (17%)
10	SF4	F	303	2	0,12,12	-	-	-		
9	FES	B	302	2	0,4,4	-	-	-		
10	SF4	B	303	2	0,12,12	-	-	-		
5	FAD	I	601	1	58,58,58	1.19	6 (10%)	85,89,89	1.75	21 (24%)
11	F3S	J	304	2	0,9,9	-	-	-		
12	HEM	C	1129	4,3	50,50,50	1.71	10 (20%)	67,82,82	1.38	10 (14%)
8	SO4	A	1591	-	4,4,4	0.33	0	6,6,6	0.16	0
6	TEO	I	1589	-	5,8,8	1.05	0	4,10,10	1.48	1 (25%)
12	HEM	K	1129	4,3	50,50,50	1.75	11 (22%)	67,82,82	1.45	10 (14%)
10	SF4	J	303	2	0,12,12	-	-	-		
11	F3S	B	304	2	0,9,9	-	-	-		
11	F3S	F	304	2	0,9,9	-	-	-		
5	FAD	A	601	1	58,58,58	1.13	5 (8%)	85,89,89	1.81	23 (27%)
9	FES	J	302	2	0,4,4	-	-	-		
12	HEM	G	1129	4,3	50,50,50	1.68	9 (18%)	67,82,82	1.46	11 (16%)
13	CBE	C	1130	-	16,17,17	1.12	1 (6%)	17,22,22	1.82	2 (11%)
5	FAD	E	601	1	58,58,58	1.05	3 (5%)	85,89,89	1.87	23 (27%)
9	FES	F	302	2	0,4,4	-	-	-		
13	CBE	K	1130	-	16,17,17	1.21	2 (12%)	17,22,22	1.57	2 (11%)
6	TEO	A	1589	-	5,8,8	1.38	0	4,10,10	2.18	1 (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
6	TEO	E	1589	-	-	4/6/8/8	-
13	CBE	G	1130	-	-	1/6/19/19	0/2/2/2
10	SF4	F	303	2	-	-	0/6/5/5
9	FES	B	302	2	-	-	0/1/1/1
10	SF4	B	303	2	-	-	0/6/5/5
5	FAD	I	601	1	-	3/34/50/50	0/6/6/6
11	F3S	J	304	2	-	-	0/3/3/3
12	HEM	C	1129	4,3	-	3/14/54/54	-
6	TEO	I	1589	-	-	1/6/8/8	-
12	HEM	K	1129	4,3	-	6/14/54/54	-
10	SF4	J	303	2	-	-	0/6/5/5
11	F3S	B	304	2	-	-	0/3/3/3
11	F3S	F	304	2	-	-	0/3/3/3
5	FAD	A	601	1	-	5/34/50/50	0/6/6/6
9	FES	J	302	2	-	-	0/1/1/1
12	HEM	G	1129	4,3	-	4/14/54/54	-
13	CBE	C	1130	-	-	1/6/19/19	0/2/2/2
5	FAD	E	601	1	-	5/34/50/50	0/6/6/6
9	FES	F	302	2	-	-	0/1/1/1
13	CBE	K	1130	-	-	2/6/19/19	0/2/2/2
6	TEO	A	1589	-	-	3/6/8/8	-

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1129	HEM	C3D-C2D	7.48	1.52	1.36
12	K	1129	HEM	C3D-C2D	6.98	1.51	1.36
12	G	1129	HEM	C3D-C2D	6.86	1.51	1.36
12	K	1129	HEM	FE-NB	4.83	2.09	1.94
12	G	1129	HEM	FE-NB	4.30	2.08	1.94

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	1130	CBE	O7-C2-C1	6.42	116.88	109.30
5	A	601	FAD	N3A-C2A-N1A	-6.33	119.00	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	601	FAD	N3A-C2A-N1A	-6.20	119.19	128.58
13	C	1130	CBE	O7-C2-C1	5.71	116.05	109.30
12	K	1129	HEM	C4D-ND-C1D	4.90	111.02	105.21

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	N10-C1'-C2'-C3'
5	E	601	FAD	PA-O3P-P-O5'
5	I	601	FAD	PA-O3P-P-O5'
6	A	1589	TEO	O2-C2-C3-C4

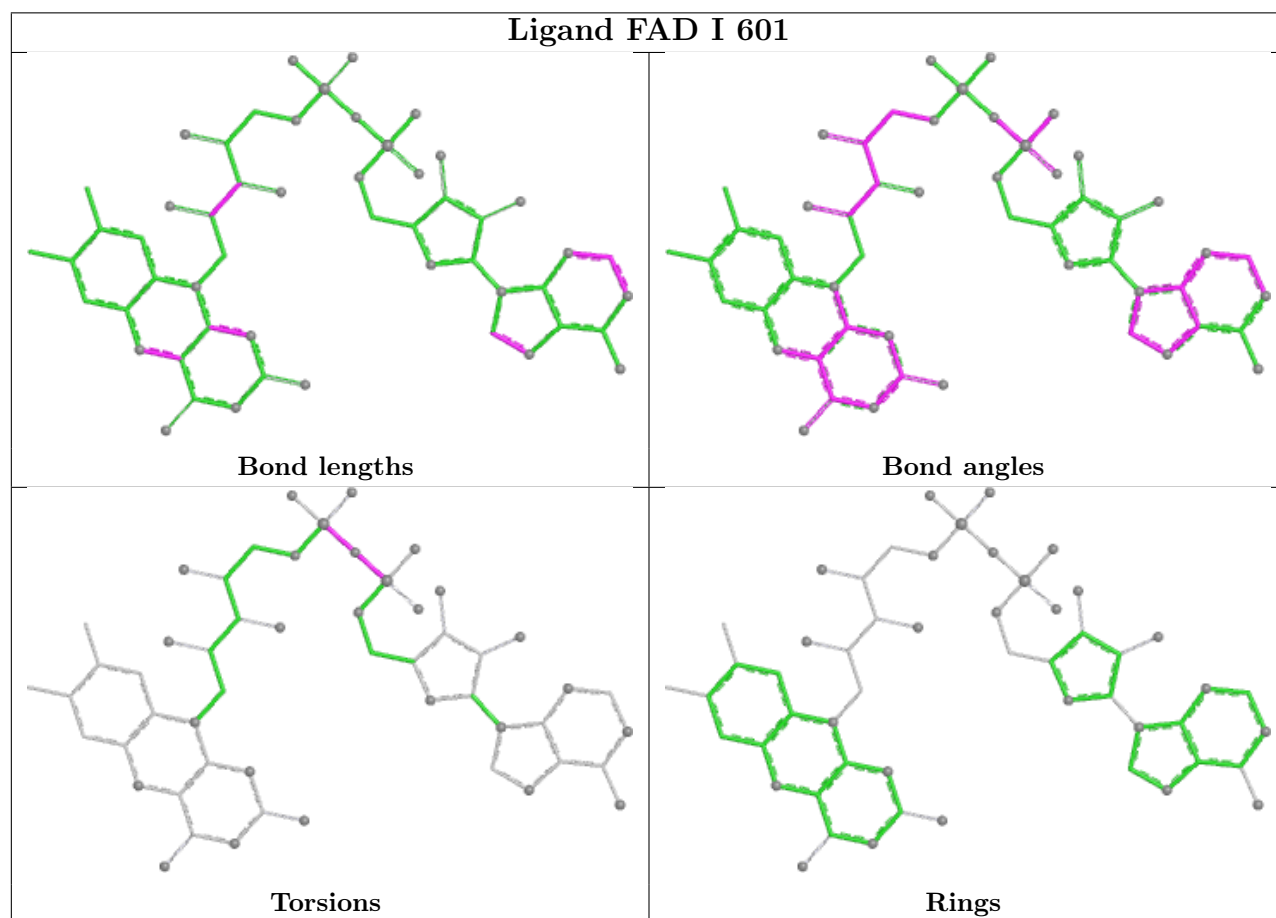
There are no ring outliers.

13 monomers are involved in 50 short contacts:

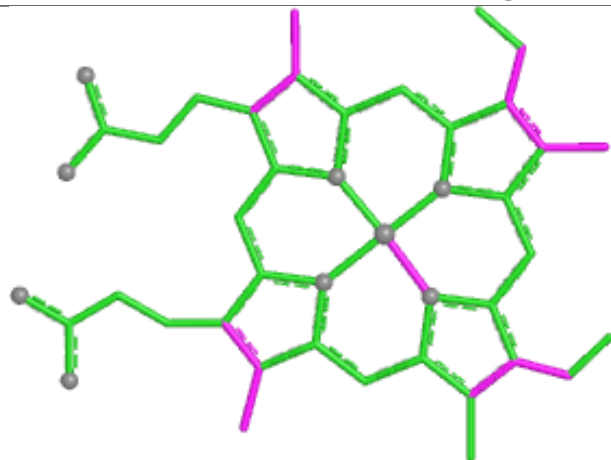
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1589	TEO	4	0
13	G	1130	CBE	1	0
5	I	601	FAD	7	0
12	C	1129	HEM	6	0
6	I	1589	TEO	4	0
12	K	1129	HEM	6	0
10	J	303	SF4	1	0
5	A	601	FAD	6	0
12	G	1129	HEM	5	0
13	C	1130	CBE	2	0
5	E	601	FAD	7	0
13	K	1130	CBE	2	0
6	A	1589	TEO	3	0

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 than 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.

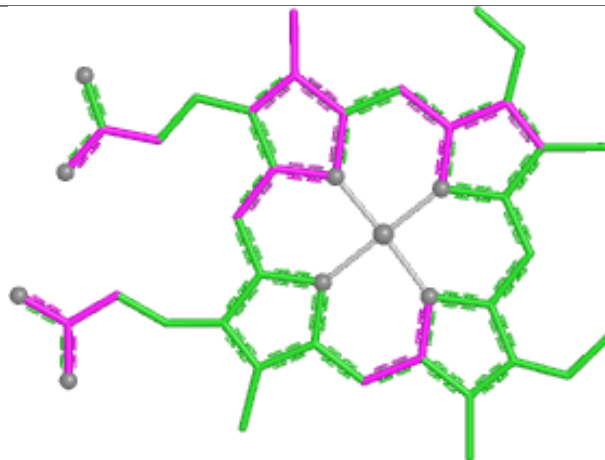
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



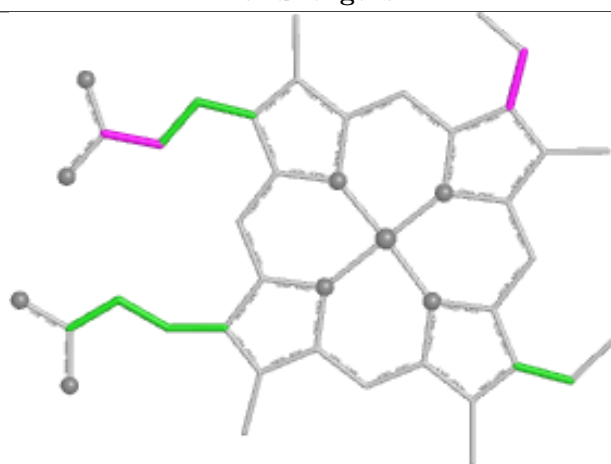
Ligand HEM C 1129



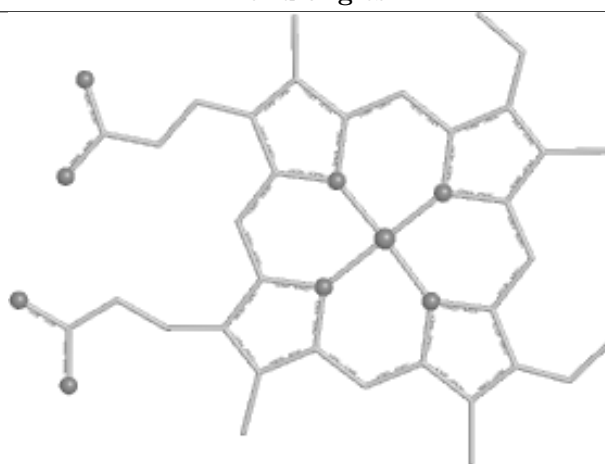
Bond lengths



Bond angles

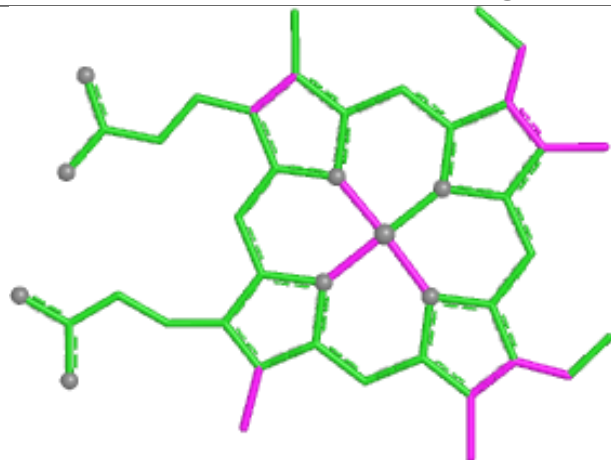


Torsions

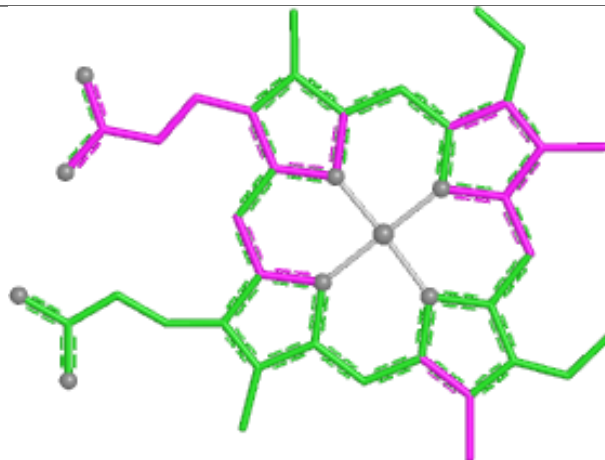


Rings

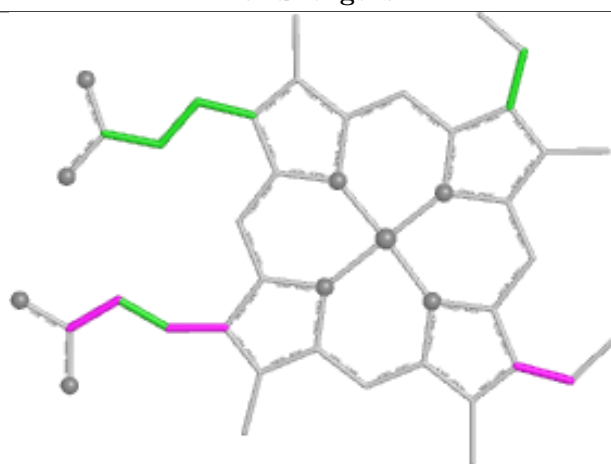
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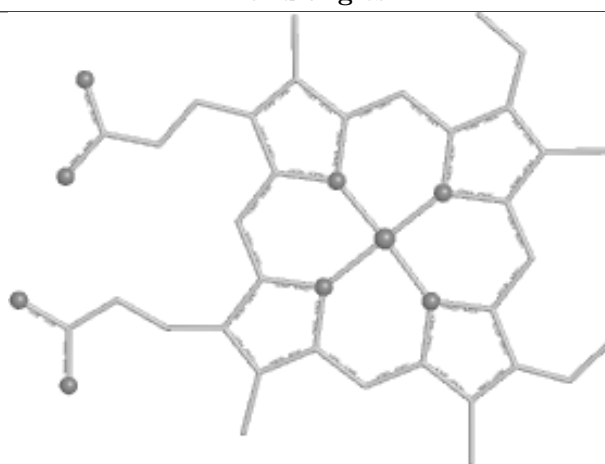
Bond lengths



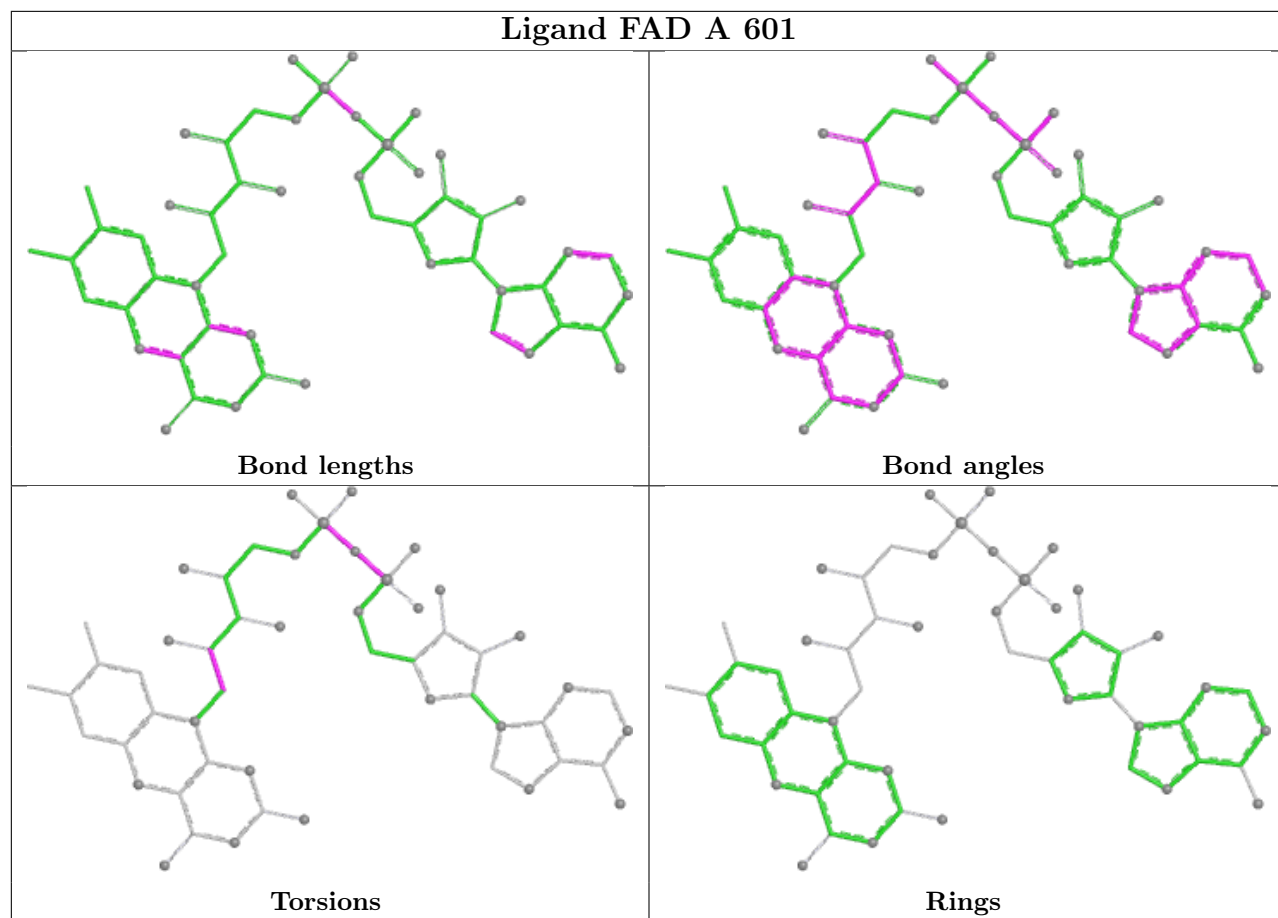
Bond angles



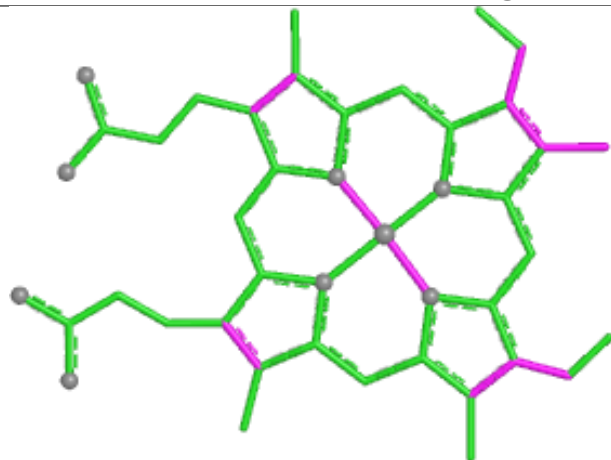
Torsions



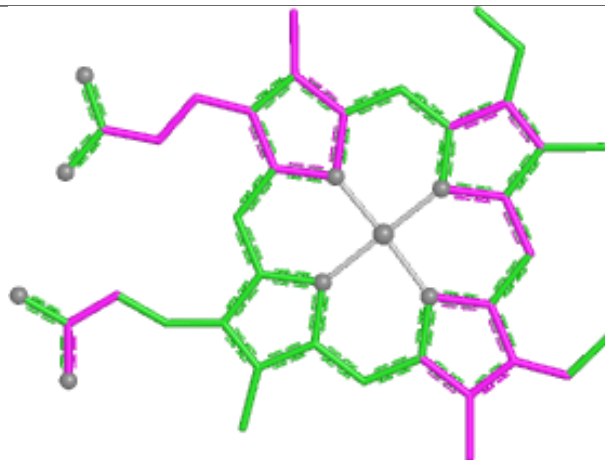
Rings



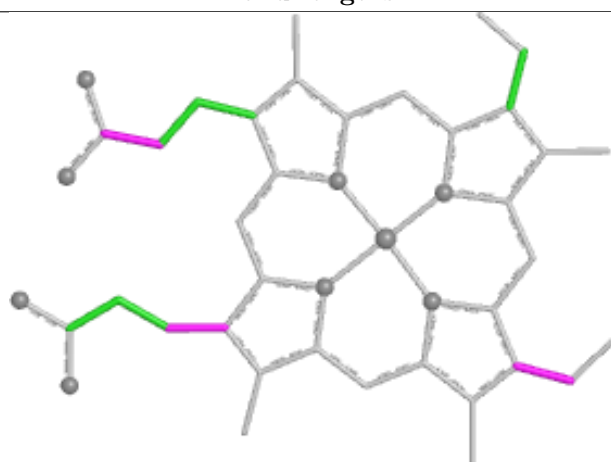
Ligand HEM G 1129



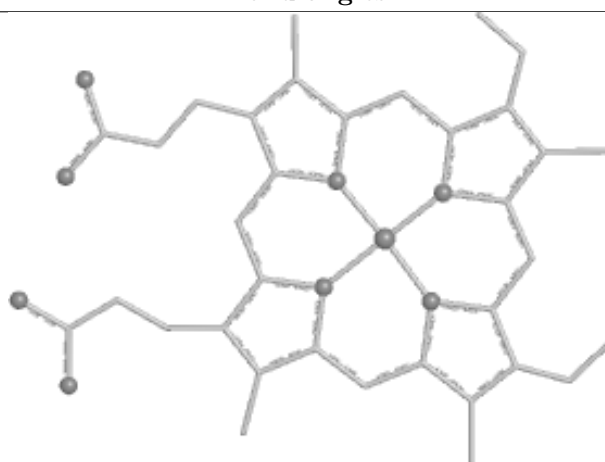
Bond lengths



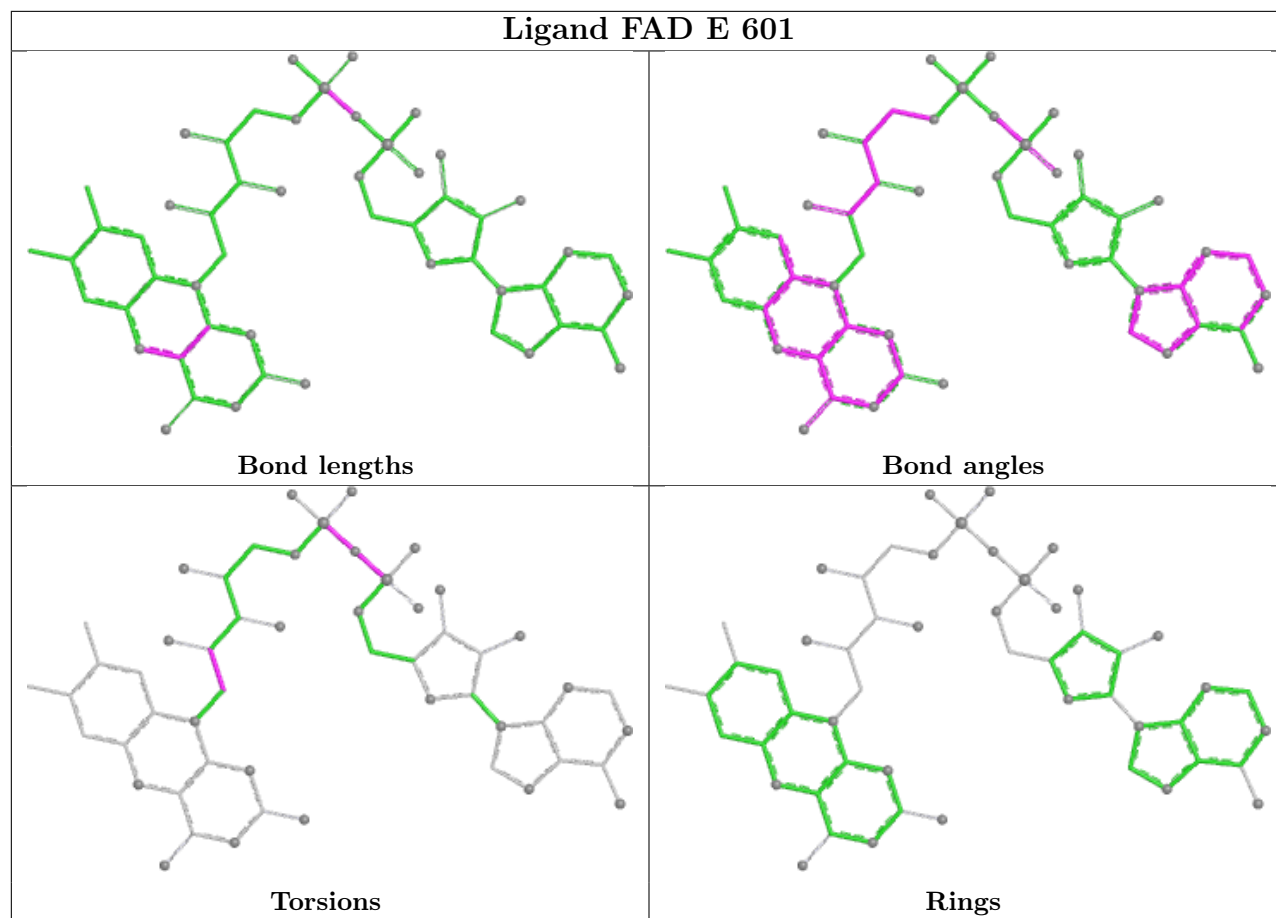
Bond angles



Torsions



Rings



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	588/588 (100%)	-0.17	3 (0%) 87 85	33, 39, 52, 72	0
1	E	588/588 (100%)	-0.04	6 (1%) 79 76	33, 39, 52, 72	0
1	I	588/588 (100%)	0.17	2 (0%) 90 88	33, 39, 52, 72	0
2	B	238/238 (100%)	-0.11	3 (1%) 75 71	28, 35, 49, 69	0
2	F	238/238 (100%)	-0.13	1 (0%) 88 86	28, 34, 49, 69	0
2	J	238/238 (100%)	-0.15	0 100 100	28, 35, 49, 69	0
3	C	121/129 (93%)	1.28	21 (17%) 4 3	45, 54, 67, 73	0
3	G	121/129 (93%)	0.95	12 (9%) 13 9	45, 54, 67, 73	0
3	K	121/129 (93%)	1.08	9 (7%) 20 17	45, 54, 67, 73	0
4	D	105/115 (91%)	0.64	7 (6%) 24 20	44, 49, 69, 72	0
4	H	105/115 (91%)	1.12	15 (14%) 6 5	44, 50, 69, 72	0
4	L	105/115 (91%)	0.72	6 (5%) 29 25	44, 49, 69, 72	0
All	All	3156/3210 (98%)	0.17	85 (2%) 56 52	28, 40, 61, 73	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	113	TRP	4.6
3	K	56	GLU	4.4
4	H	115	VAL	4.1
3	K	68	PHE	3.9
3	C	10	PRO	3.8

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

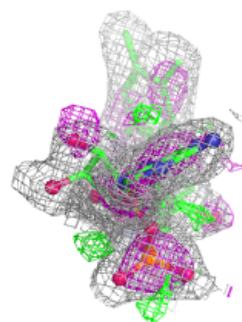
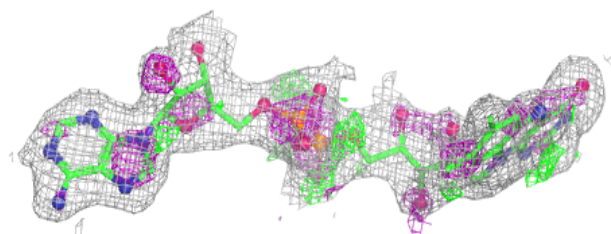
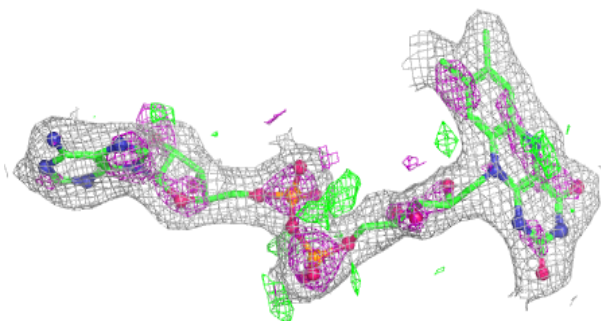
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	TEO	I	1589	9/9	0.91	0.17	45,46,49,51	0
6	TEO	A	1589	9/9	0.94	0.14	36,40,42,46	0
13	CBE	K	1130	16/16	0.94	0.12	39,44,47,47	0
8	SO4	A	1591	5/5	0.95	0.14	70,70,71,71	0
8	SO4	E	1591	5/5	0.95	0.17	66,66,68,69	0
13	CBE	G	1130	16/16	0.95	0.09	34,38,41,41	0
6	TEO	E	1589	9/9	0.95	0.13	32,35,37,40	0
5	FAD	A	601	53/53	0.96	0.09	21,29,34,37	0
5	FAD	E	601	53/53	0.96	0.09	25,30,38,40	0
8	SO4	I	1591	5/5	0.96	0.16	58,59,60,62	0
12	HEM	C	1129	43/43	0.96	0.10	36,40,53,57	0
12	HEM	K	1129	43/43	0.96	0.10	42,46,57,63	0
13	CBE	C	1130	16/16	0.96	0.08	37,39,42,43	0
5	FAD	I	601	53/53	0.96	0.10	29,33,41,43	0
7	NA	I	1590	1/1	0.96	0.10	29,29,29,29	0
10	SF4	F	303	8/8	0.97	0.06	30,31,32,33	0
12	HEM	G	1129	43/43	0.97	0.09	36,41,52,57	0
11	F3S	B	304	7/7	0.98	0.10	31,32,34,37	0
11	F3S	F	304	7/7	0.98	0.09	32,34,35,36	0
11	F3S	J	304	7/7	0.98	0.10	32,35,37,38	0
7	NA	E	1590	1/1	0.98	0.11	24,24,24,24	0
9	FES	F	302	4/4	0.98	0.10	28,28,29,31	0
9	FES	J	302	4/4	0.98	0.10	30,32,32,33	0
10	SF4	B	303	8/8	0.98	0.09	28,29,33,33	0
7	NA	A	1590	1/1	0.98	0.10	22,22,22,22	0
10	SF4	J	303	8/8	0.98	0.07	30,32,34,36	0
9	FES	B	302	4/4	0.99	0.10	29,29,31,31	0

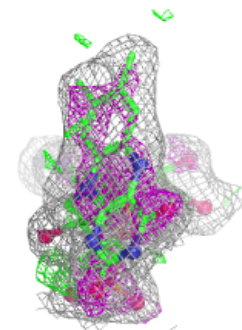
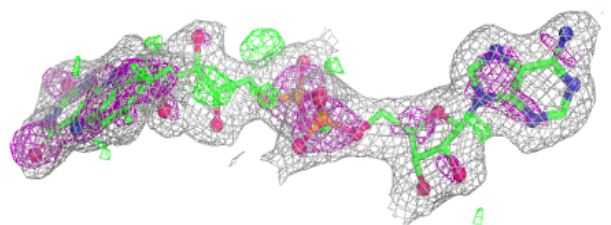
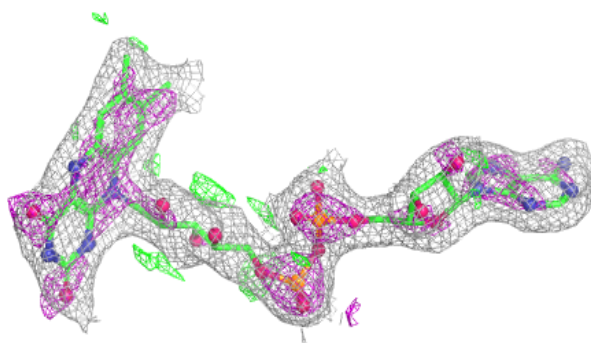
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 601:

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

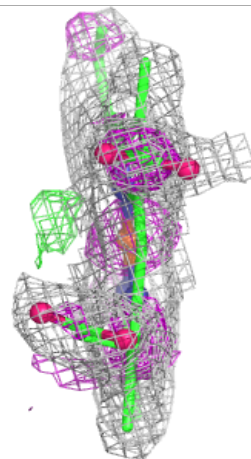
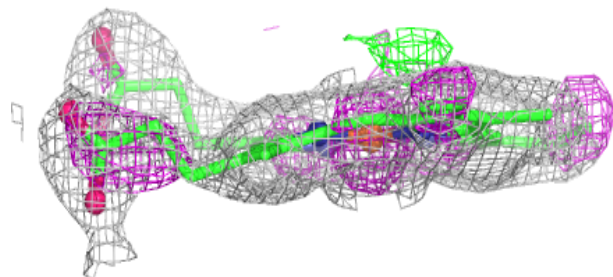
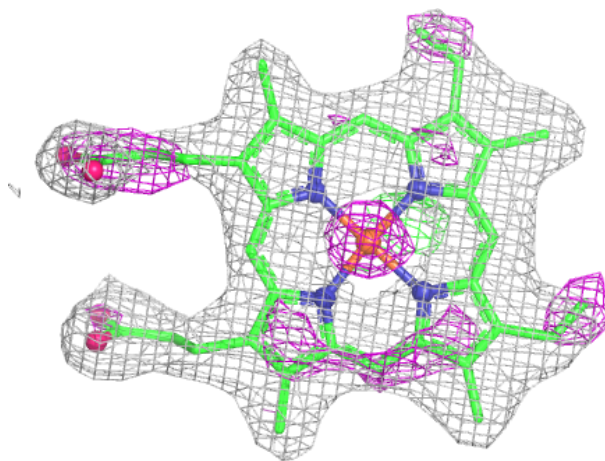
**Electron density around FAD E 601:**

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



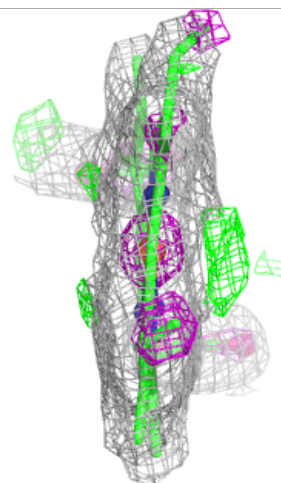
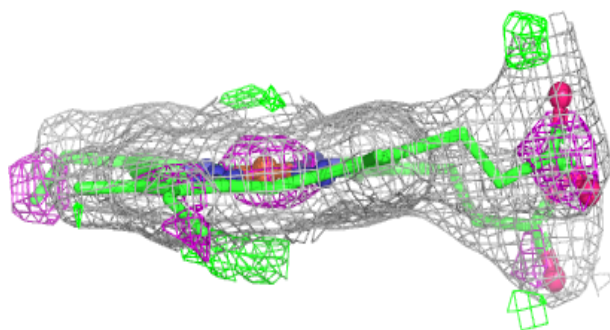
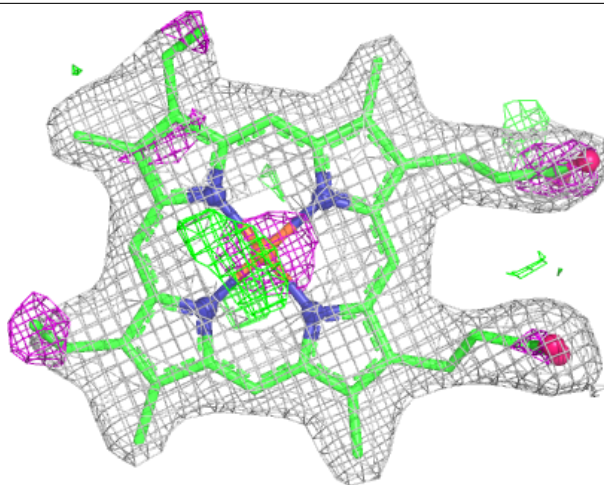
Electron density around HEM C 1129:

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



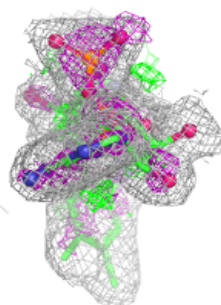
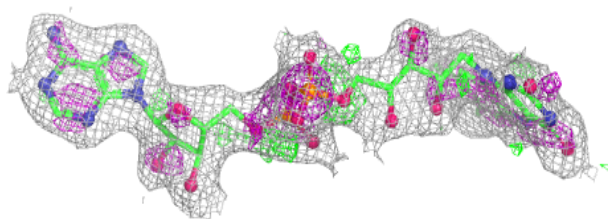
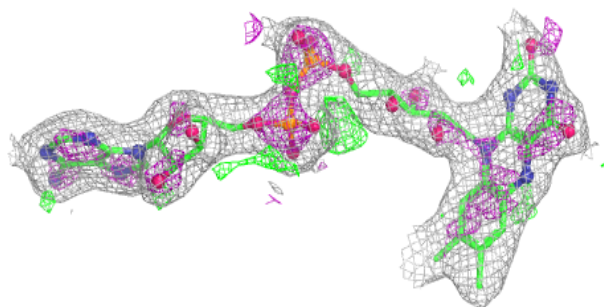
Electron density around HEM K 1129:

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

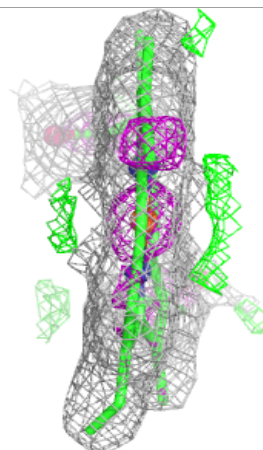
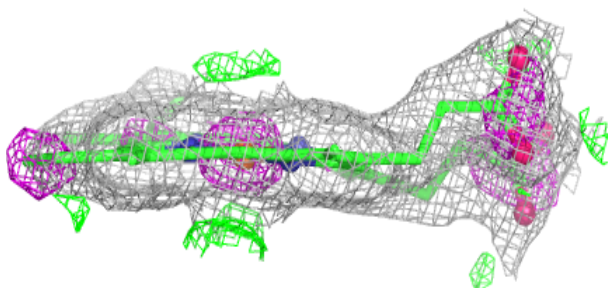
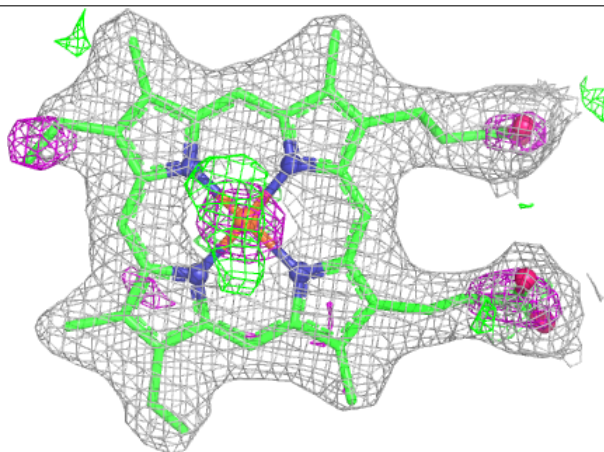


Electron density around FAD I 601:

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

**Electron density around HEM G 1129:**

$2mF_o-DF_c$ (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.