Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 03:53 pm GMT

PDB ID	:	2WDQ
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

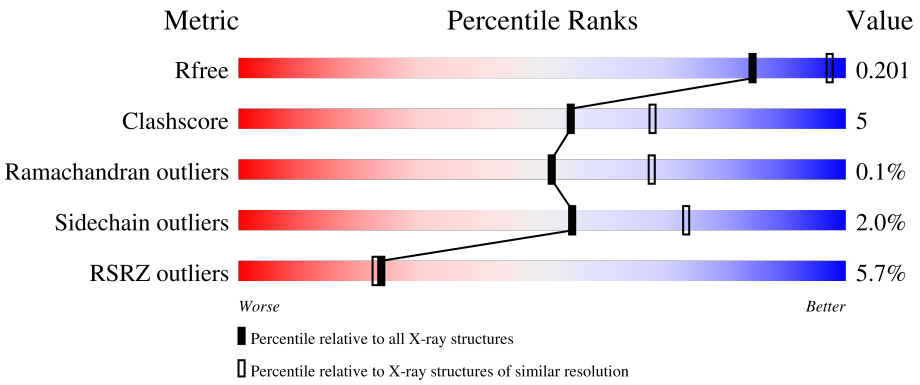
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	3%, 89%, 10%
1	E	588	5%, 90%, 10%
1	I	588	5%, 88%, 11%
2	B	238	6%, 93%, 7%
2	F	238	5%, 95%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	238	5% 90% 9%
3	C	129	12% 85% 9% 6%
3	G	129	9% 84% 10% 6%
3	K	129	12% 84% 9% 6%
4	D	115	5% 79% 10% 9%
4	H	115	10% 79% 10% 9%
4	L	115	7% 81% 9% 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 (i)

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 SUBUNIT.

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

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

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

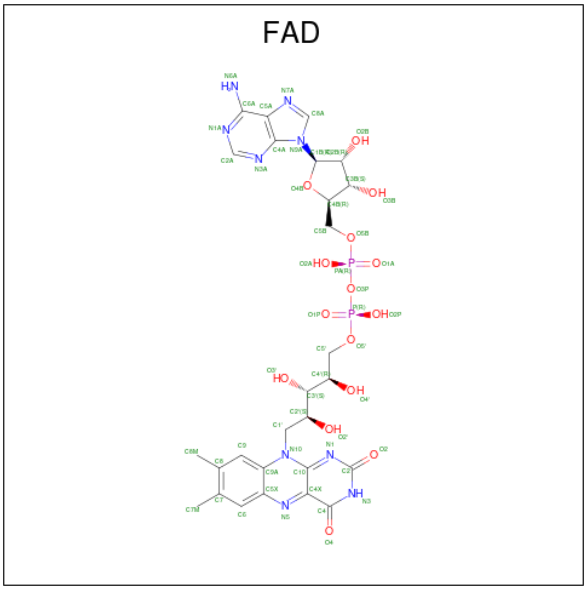
- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT.

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

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

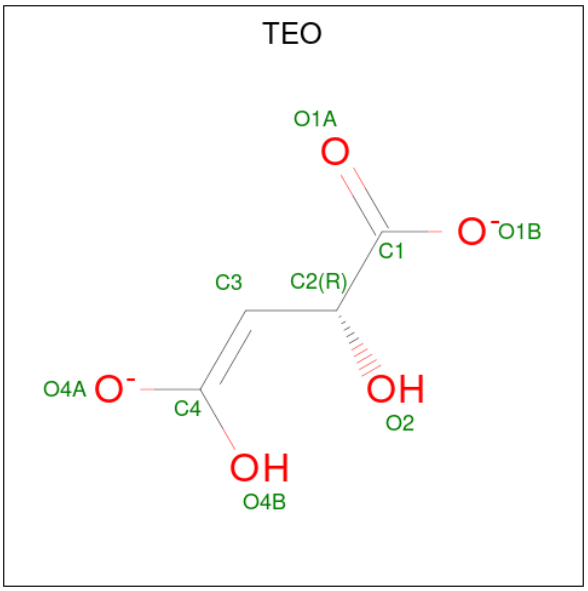
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	105	836	577	123	133	3	0	0	0
			Total	C	N	O	S			
4	H	105	836	577	123	133	3	0	0	0
			Total	C	N	O	S			
4	L	105	836	577	123	133	3	0	0	0

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



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

- Molecule 6 is MALATE LIKE INTERMEDIATE (three-letter code: TEO) (formula: $C_4H_4O_5$).

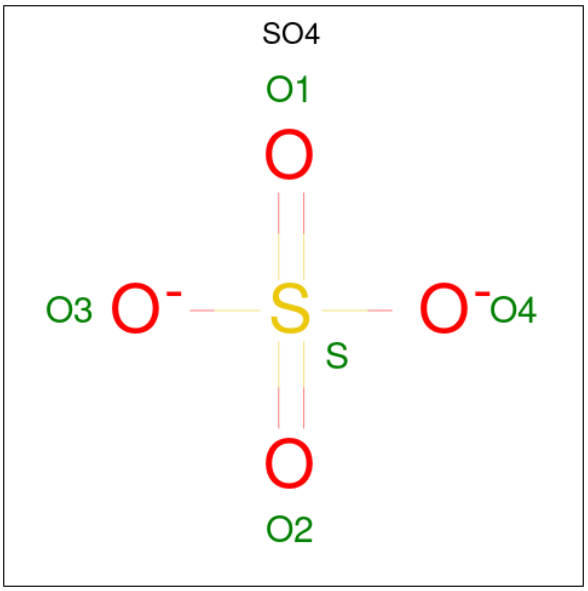


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 4 5	0	0
6	E	1	Total C O 9 4 5	0	0
6	I	1	Total C O 9 4 5	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

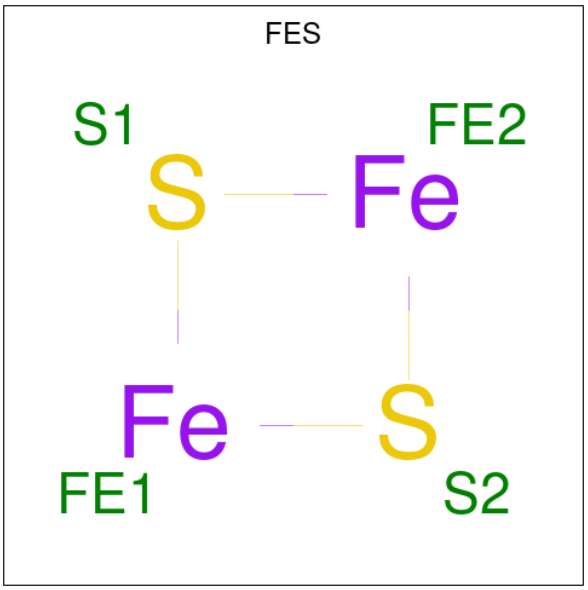
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0
7	I	1	Total Na 1 1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



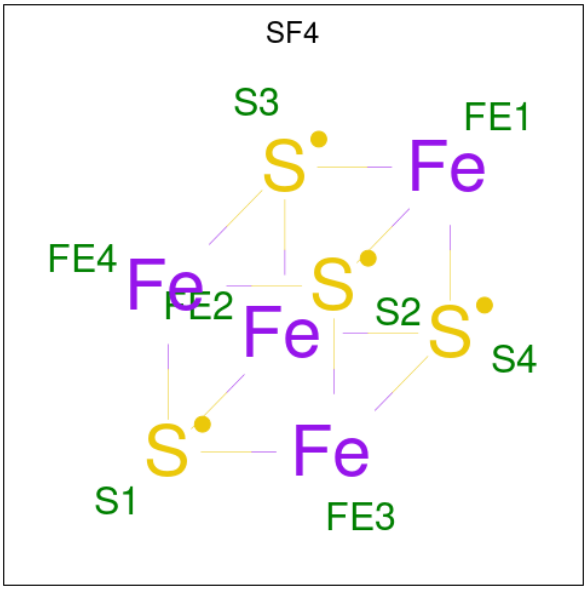
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	4	2	2	0	0

Continued on next page...

Continued from previous page...

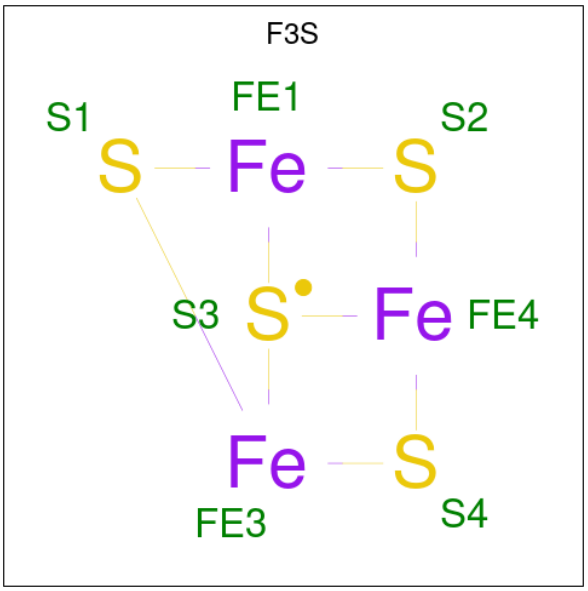
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	F	1	4	2	2	0	0
			Total	Fe	S		
9	J	1	4	2	2	0	0

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



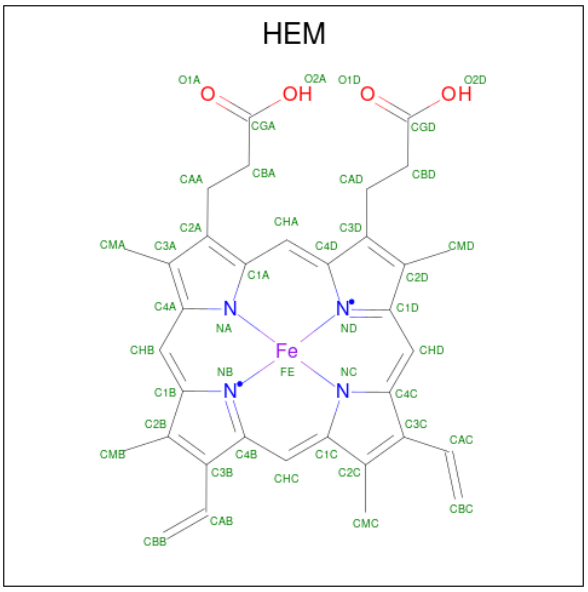
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
10	B	1	8	4	4	0	0
			Total	Fe	S		
10	F	1	8	4	4	0	0
			Total	Fe	S		
10	J	1	8	4	4	0	0

- Molecule 11 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



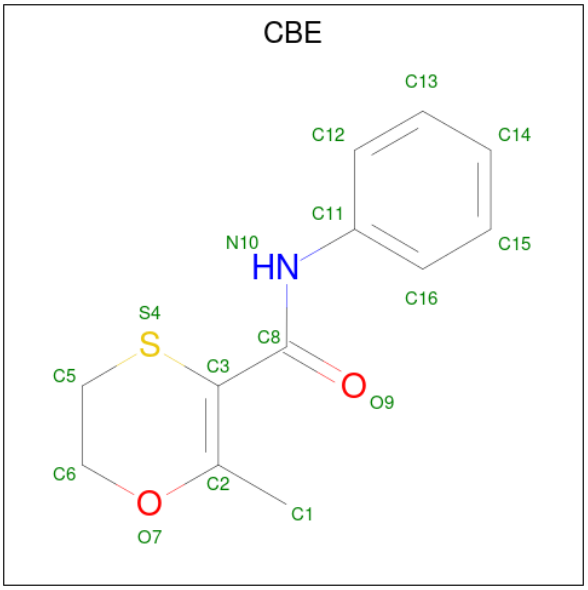
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	B	1	7	3	4	0	0
			Total	Fe	S		
11	F	1	7	3	4	0	0
			Total	Fe	S		
11	J	1	7	3	4	0	0

- Molecule 12 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		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	G	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	K	1	43	34	1	4	4	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
13	C	1	16	12	1	2	1	0	0
			Total	C	N	O	S		
13	G	1	16	12	1	2	1	0	0
			Total	C	N	O	S		
13	K	1	16	12	1	2	1	0	0

- Molecule 14 is water.

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

Continued on next page...

Continued from previous page...

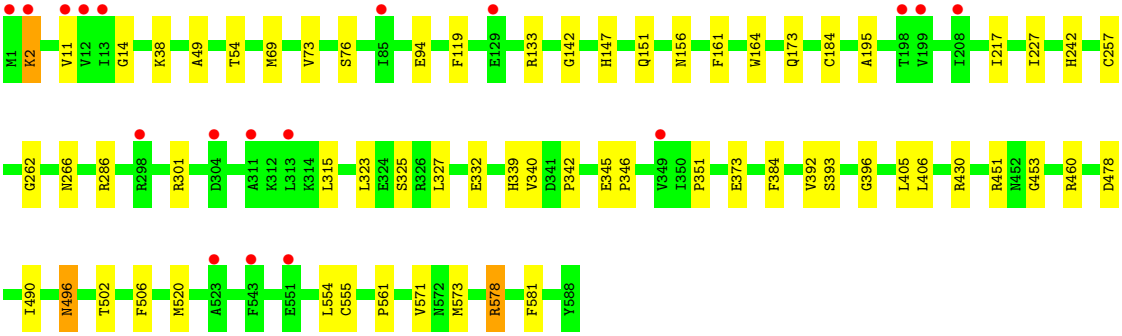
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	D	10	Total O 10 10	0	0
14	E	234	Total O 234 234	0	0
14	F	116	Total O 116 116	0	0
14	G	17	Total O 17 17	0	0
14	H	4	Total O 4 4	0	0
14	I	197	Total O 197 197	0	0
14	J	107	Total O 107 107	0	0
14	K	17	Total O 17 17	0	0
14	L	6	Total O 6 6	0	0

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.

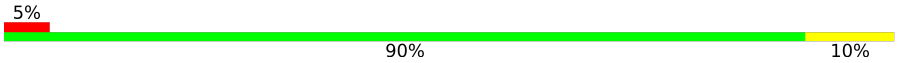
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

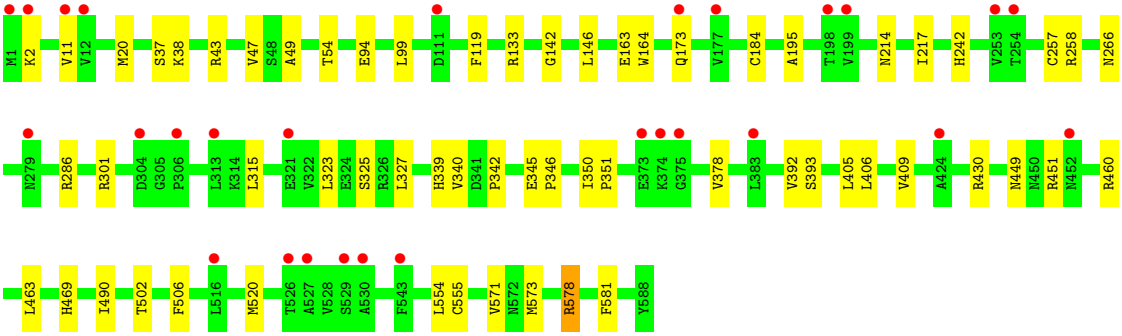
Chain A:



• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

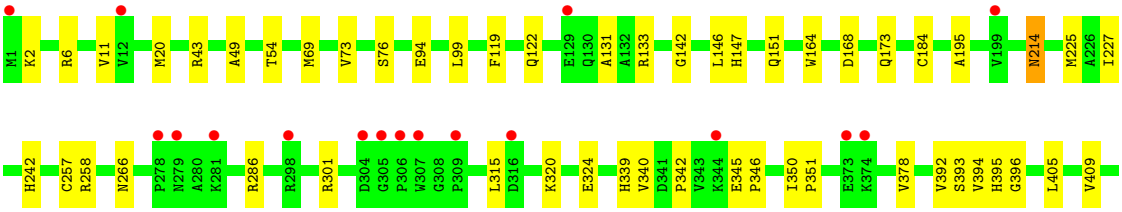
Chain E:

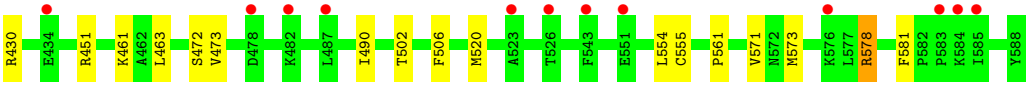




• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

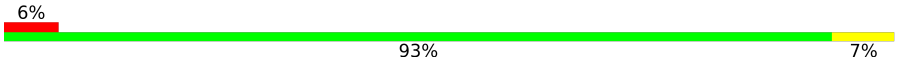
Chain I:

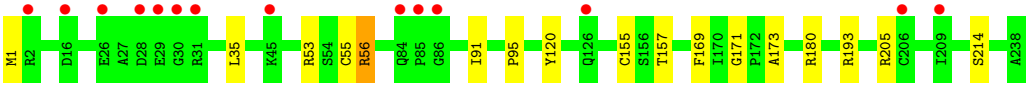




• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

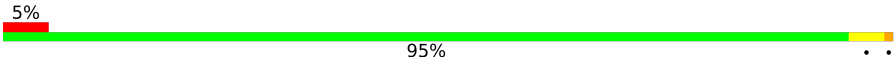
Chain B:

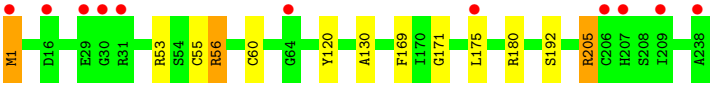




• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

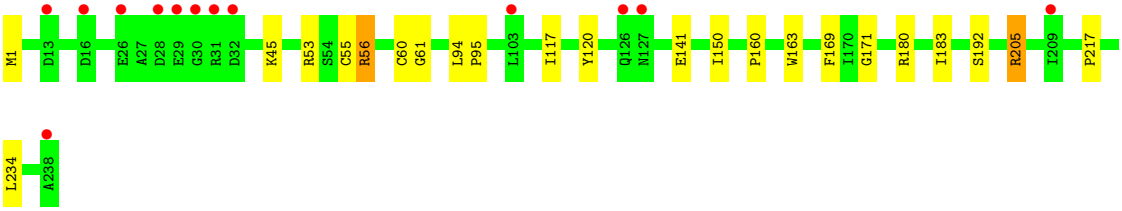
Chain F:





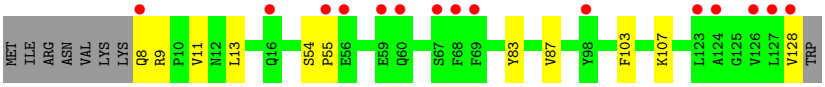
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain J:



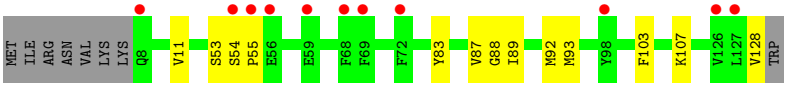
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain C:



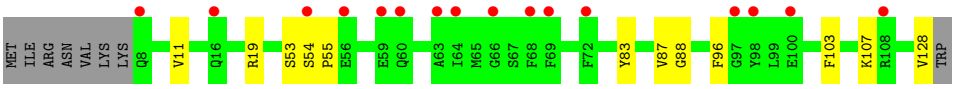
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain G:



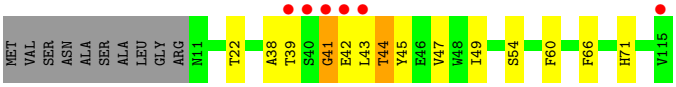
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain K:



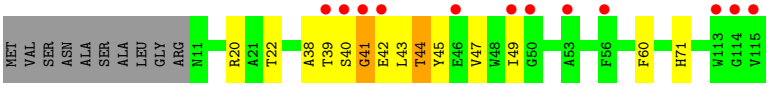
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain D:



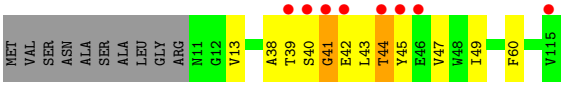
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain H:



• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain L:



4 Data and refinement statistics (i)

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 22.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (133.63-2.40) 99.7 (22.96-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[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: F3S, FAD, NA, SF4, FES, TEO, SO4, CBE, HEM

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	0.74	2/4611 (0.0%)	0.70	1/6237 (0.0%)
1	E	0.69	1/4611 (0.0%)	0.70	1/6237 (0.0%)
1	I	0.64	0/4611	0.66	0/6237
2	B	0.72	0/1908	0.72	1/2578 (0.0%)
2	F	0.66	0/1908	0.71	1/2578 (0.0%)
2	J	0.66	0/1908	0.71	1/2578 (0.0%)
3	C	0.55	0/953	0.55	0/1293
3	G	0.56	0/953	0.56	0/1293
3	K	0.52	0/953	0.57	0/1293
4	D	0.56	0/859	0.56	0/1175
4	H	0.52	0/859	0.57	0/1175
4	L	0.53	0/859	0.55	0/1175
All	All	0.66	3/24993 (0.0%)	0.67	5/33849 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	GLU	CG-CD	5.47	1.60	1.51
1	E	449	ASN	CG-ND2	-5.38	1.19	1.32
1	A	496	ASN	CB-CG	5.08	1.62	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	205	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	460	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	J	205	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	E	460	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	B	193	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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	4522	0	4426	45	0
1	E	4522	0	4426	43	0
1	I	4522	0	4426	50	0
2	B	1869	0	1850	10	0
2	F	1869	0	1850	9	0
2	J	1869	0	1850	15	0
3	C	933	0	979	14	0
3	G	933	0	979	12	0
3	K	933	0	979	11	0
4	D	836	0	875	10	0
4	H	836	0	875	12	0
4	L	836	0	875	9	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

Continued on next page...

Continued from previous page...

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	0	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	4	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	257	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 5.

All (257) 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
12:C:1129:HEM:HHD	12:C:1129:HEM:HBC2	1.35	1.09
1:E:502:THR:HG22	14:E:2187:HOH:O	1.70	0.92
1:I:490:ILE:HG22	1:I:520:MET:HE3	1.52	0.89
1:I:490:ILE:HG22	1:I:520:MET:CE	2.02	0.89
12:G:1129:HEM:HHC	12:G:1129:HEM:HBB2	1.58	0.85
1:E:490:ILE:HG22	1:E:520:MET:CE	2.07	0.85
1:I:555:CYS:HA	1:I:571:VAL:HG23	1.59	0.83
1:E:490:ILE:HG22	1:E:520:MET:HE3	1.62	0.79
1:A:490:ILE:HG22	1:A:520:MET:CE	2.18	0.74
1:A:555:CYS:HA	1:A:571:VAL:HG23	1.70	0.73
12:C:1129:HEM:HBC2	12:C:1129:HEM:CHD	2.11	0.73
2:J:45:LYS:HD3	14:J:2012:HOH:O	1.90	0.71
1:E:555:CYS:HA	1:E:571:VAL:HG23	1.74	0.70
1:A:490:ILE:HG22	1:A:520:MET:HE3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:TYR:OH	4:D:49:ILE:HD12	1.92	0.69
12:C:1129:HEM:HHC	12:C:1129:HEM:HBB2	1.73	0.68
1:I:502:THR:HG22	14:I:2167:HOH:O	1.92	0.68
3:C:54:SER:HB2	3:C:55:PRO:HD2	1.75	0.68
13:K:1130:CBE:H16	13:K:1130:CBE:O9	1.94	0.67
1:E:392:VAL:N	1:E:393:SER:HA	2.10	0.67
2:F:55:CYS:O	2:F:56:ARG:HD2	1.95	0.67
3:C:8:GLN:HA	14:C:2001:HOH:O	1.94	0.67
1:E:286:ARG:HH22	6:E:1589:TEO:C3	2.07	0.67
1:A:286:ARG:HH22	6:A:1589:TEO:C3	2.07	0.66
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.75	0.66
1:E:49:ALA:HA	5:E:601:FAD:C6	2.26	0.66
3:C:128:VAL:O	3:C:128:VAL:CG1	2.43	0.65
3:C:103:PHE:CE2	3:C:107:LYS:HE2	2.32	0.65
3:C:128:VAL:O	3:C:128:VAL:HG12	1.96	0.65
1:E:49:ALA:HA	5:E:601:FAD:C5X	2.28	0.64
2:B:55:CYS:O	2:B:56:ARG:HD2	1.98	0.64
3:G:54:SER:HB2	3:G:55:PRO:HD2	1.79	0.64
1:E:490:ILE:HG22	1:E:520:MET:HE1	1.79	0.63
1:I:392:VAL:N	1:I:393:SER:HA	2.13	0.63
1:I:49:ALA:HA	5:I:601:FAD:C5X	2.28	0.63
12:K:1129:HEM:HBC2	12:K:1129:HEM:HHD	1.81	0.63
3:C:103:PHE:CE2	3:C:107:LYS:CE	2.81	0.63
2:J:1:MET:HG3	2:J:1:MET:O	1.99	0.62
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.79	0.62
1:A:49:ALA:HA	5:A:601:FAD:C5X	2.29	0.62
1:I:490:ILE:HG22	1:I:520:MET:HE1	1.82	0.62
4:L:44:THR:HG23	4:L:47:VAL:HG13	1.82	0.62
1:E:578:ARG:NH1	1:E:581:PHE:CZ	2.68	0.61
1:A:578:ARG:NH1	1:A:581:PHE:CZ	2.69	0.61
1:I:54:THR:HG23	1:I:133:ARG:HG3	1.84	0.60
12:G:1129:HEM:HBC2	12:G:1129:HEM:HHD	1.84	0.60
1:I:49:ALA:HA	5:I:601:FAD:C6	2.32	0.60
3:K:54:SER:HB2	3:K:55:PRO:HD2	1.83	0.59
3:G:128:VAL:O	3:G:128:VAL:CG1	2.50	0.59
3:K:103:PHE:CE2	3:K:107:LYS:HE2	2.37	0.59
1:A:392:VAL:N	1:A:393:SER:HA	2.18	0.59
12:K:1129:HEM:HHA	12:K:1129:HEM:HBA2	1.84	0.58
1:A:451:ARG:HD2	14:A:2189:HOH:O	2.03	0.58
5:A:601:FAD:N5	6:A:1589:TEO:H2	2.19	0.58
3:G:103:PHE:CE2	3:G:107:LYS:CE	2.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:103:PHE:CE2	3:G:107:LYS:HE2	2.40	0.57
2:F:1:MET:O	2:F:1:MET:HG3	2.04	0.57
2:J:55:CYS:O	2:J:56:ARG:HD2	2.04	0.57
3:K:103:PHE:CE2	3:K:107:LYS:CE	2.88	0.57
3:K:128:VAL:CG1	3:K:128:VAL:O	2.52	0.57
3:G:128:VAL:O	3:G:128:VAL:HG12	2.04	0.57
4:L:44:THR:CG2	4:L:47:VAL:HG13	2.35	0.56
2:F:56:ARG:O	2:F:56:ARG:HD3	2.05	0.56
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.87	0.56
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.41	0.56
13:C:1130:CBE:H16	13:C:1130:CBE:O9	2.04	0.56
4:D:44:THR:HG23	4:D:47:VAL:HG13	1.88	0.56
1:A:49:ALA:HA	5:A:601:FAD:C6	2.36	0.55
1:E:54:THR:HG23	1:E:133:ARG:HG3	1.89	0.54
3:G:83:TYR:CZ	3:G:87:VAL:HG21	2.41	0.54
1:I:405:LEU:HG	5:I:601:FAD:C2	2.36	0.54
1:A:490:ILE:HG22	1:A:520:MET:HE1	1.87	0.54
1:A:173:GLN:CD	1:A:430:ARG:HH11	2.10	0.54
1:I:257:CYS:HB3	1:I:315:LEU:HD21	1.90	0.54
1:E:99:LEU:HD11	1:E:409:VAL:HG21	1.90	0.54
1:A:76:SER:HB2	1:A:396:GLY:HA3	1.90	0.54
4:H:44:THR:HG23	4:H:47:VAL:HG13	1.90	0.54
2:B:56:ARG:O	2:B:56:ARG:HD3	2.08	0.54
3:G:88:GLY:HA3	12:G:1129:HEM:HBC2	1.90	0.54
1:I:578:ARG:NH1	1:I:581:PHE:CZ	2.76	0.54
2:J:56:ARG:O	2:J:56:ARG:HD3	2.06	0.54
1:I:490:ILE:CG2	1:I:520:MET:HE1	2.37	0.54
5:I:601:FAD:N5	6:I:1589:TEO:H2	2.23	0.54
1:A:266:ASN:HB2	1:A:301:ARG:O	2.08	0.54
1:E:463:LEU:C	1:E:463:LEU:HD23	2.29	0.54
13:K:1130:CBE:O9	13:K:1130:CBE:C16	2.55	0.54
3:K:128:VAL:O	3:K:128:VAL:HG12	2.08	0.53
1:E:578:ARG:NH1	1:E:581:PHE:CE1	2.76	0.53
4:D:44:THR:CG2	4:D:47:VAL:HG13	2.39	0.52
4:D:45:TYR:CZ	4:D:49:ILE:HD12	2.44	0.52
1:E:490:ILE:CG2	1:E:520:MET:HE1	2.39	0.52
4:H:45:TYR:OH	4:H:49:ILE:HD12	2.09	0.52
1:I:99:LEU:HD11	1:I:409:VAL:HG21	1.92	0.52
1:E:257:CYS:HB3	1:E:315:LEU:HD21	1.91	0.51
1:I:286:ARG:HH22	6:I:1589:TEO:C3	2.23	0.51
1:A:156:ASN:HB2	14:A:2054:HOH:O	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:ALA:HA	5:E:601:FAD:N5	2.26	0.51
1:A:257:CYS:HB3	1:A:315:LEU:HD21	1.92	0.51
5:I:601:FAD:C4	6:I:1589:TEO:C3	2.89	0.51
1:A:54:THR:HG23	1:A:133:ARG:HG3	1.92	0.51
1:I:258:ARG:HD3	14:I:2087:HOH:O	2.11	0.50
2:B:1:MET:O	2:B:1:MET:HG3	2.11	0.50
1:A:242:HIS:O	1:A:351:PRO:HA	2.11	0.50
3:G:103:PHE:CE2	3:G:107:LYS:HE3	2.47	0.50
12:K:1129:HEM:HHD	12:K:1129:HEM:CBC	2.41	0.50
12:C:1129:HEM:HHD	12:C:1129:HEM:CBC	2.20	0.50
2:J:169:PHE:CD1	2:J:205:ARG:HB2	2.47	0.49
1:E:20:MET:CE	1:E:146:LEU:CD1	2.91	0.49
13:G:1130:CBE:O9	13:G:1130:CBE:H16	2.12	0.49
4:H:44:THR:CG2	4:H:47:VAL:HG13	2.42	0.49
3:C:103:PHE:CE2	3:C:107:LYS:HE3	2.47	0.49
1:I:173:GLN:CD	1:I:430:ARG:HH11	2.16	0.49
1:I:472:SER:OG	1:I:473:VAL:N	2.46	0.49
1:E:54:THR:O	1:E:406:LEU:HD22	2.12	0.49
4:L:38:ALA:O	4:L:39:THR:CG2	2.61	0.48
1:E:173:GLN:CD	1:E:430:ARG:HH11	2.15	0.48
1:I:49:ALA:HA	5:I:601:FAD:N5	2.29	0.48
4:H:38:ALA:O	4:H:39:THR:CG2	2.61	0.48
1:A:69:MET:O	1:A:73:VAL:HG23	2.14	0.48
1:I:76:SER:HB2	1:I:396:GLY:HA3	1.96	0.48
4:L:41:GLY:O	4:L:42:GLU:C	2.51	0.48
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.48	0.48
1:E:469:HIS:HB3	14:E:2178:HOH:O	2.13	0.48
4:H:41:GLY:O	4:H:42:GLU:C	2.52	0.48
1:I:258:ARG:NH2	14:I:2089:HOH:O	2.45	0.48
1:I:461:LYS:NZ	14:I:2153:HOH:O	2.47	0.48
3:C:54:SER:HB2	3:C:55:PRO:CD	2.43	0.47
4:D:66:PHE:HD1	14:D:2006:HOH:O	1.96	0.47
1:A:405:LEU:HG	5:A:601:FAD:C2	2.44	0.47
5:E:601:FAD:N5	6:E:1589:TEO:H2	2.29	0.47
2:B:155:CYS:SG	2:B:173:ALA:HB2	2.55	0.47
12:G:1129:HEM:HHD	12:G:1129:HEM:CBC	2.43	0.47
1:I:463:LEU:C	1:I:463:LEU:HD23	2.35	0.47
3:G:89:ILE:O	3:G:93:MET:HG3	2.15	0.47
13:C:1130:CBE:O9	13:C:1130:CBE:C16	2.63	0.47
1:I:69:MET:O	1:I:73:VAL:HG23	2.14	0.47
3:G:54:SER:HB2	3:G:55:PRO:CD	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:83:TYR:CZ	3:K:87:VAL:HG21	2.50	0.47
2:J:217:PRO:HD2	10:J:303:SF4:S3	2.55	0.46
4:D:41:GLY:O	4:D:42:GLU:C	2.53	0.46
1:E:242:HIS:O	1:E:351:PRO:HA	2.15	0.46
1:I:554:LEU:HD21	1:I:573:MET:CE	2.45	0.46
1:A:345:GLU:HG2	1:A:346:PRO:HD2	1.98	0.46
1:E:43:ARG:HD3	2:F:60:CYS:O	2.15	0.46
4:H:22:THR:OG1	4:H:71:HIS:HB2	2.16	0.46
12:K:1129:HEM:HBA2	12:K:1129:HEM:CHA	2.44	0.46
1:A:451:ARG:HA	1:A:451:ARG:HD3	1.67	0.46
3:C:103:PHE:CZ	3:C:107:LYS:HE2	2.51	0.46
1:I:578:ARG:NH1	1:I:581:PHE:CE1	2.84	0.46
1:A:161:PHE:HB3	1:A:164:TRP:CD1	2.51	0.46
4:D:44:THR:HG23	4:D:47:VAL:HG22	1.97	0.45
1:A:373:GLU:HG2	14:A:2144:HOH:O	2.15	0.45
1:I:242:HIS:O	1:I:351:PRO:HA	2.15	0.45
1:E:350:ILE:HG13	1:E:351:PRO:HD2	1.99	0.45
1:I:168:ASP:HA	1:I:225:MET:HG2	1.98	0.45
1:I:451:ARG:HD3	1:I:451:ARG:HA	1.67	0.45
1:A:578:ARG:NH1	1:A:581:PHE:CE1	2.84	0.45
3:G:92:MET:HG2	4:H:20:ARG:HG2	1.99	0.45
1:I:350:ILE:HG13	1:I:351:PRO:HD2	1.98	0.45
4:L:45:TYR:OH	4:L:49:ILE:HD12	2.16	0.45
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.52	0.45
1:I:43:ARG:HD3	2:J:60:CYS:O	2.17	0.45
1:E:20:MET:CE	1:E:146:LEU:HD12	2.47	0.45
4:H:44:THR:HG23	4:H:47:VAL:HG22	1.99	0.45
2:B:95:PRO:O	2:B:157:THR:HB	2.16	0.44
1:E:554:LEU:HD21	1:E:573:MET:CE	2.48	0.44
1:I:147:HIS:O	1:I:151:GLN:HG3	2.17	0.44
2:J:117:ILE:C	2:J:117:ILE:HD12	2.38	0.44
1:A:453:GLY:HA3	1:A:496:ASN:O	2.16	0.44
12:C:1129:HEM:HHC	12:C:1129:HEM:CBB	2.46	0.44
1:E:405:LEU:HG	5:E:601:FAD:C2	2.47	0.44
2:F:56:ARG:CD	2:F:56:ARG:C	2.86	0.44
12:C:1129:HEM:HBB2	12:C:1129:HEM:CHC	2.43	0.44
4:D:45:TYR:OH	4:D:49:ILE:CD1	2.63	0.44
1:A:147:HIS:O	1:A:151:GLN:HG3	2.18	0.44
1:A:2:LYS:O	1:A:2:LYS:HD3	2.18	0.44
2:F:169:PHE:CE2	2:F:171:GLY:HA2	2.53	0.44
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:TRP:CH2	1:I:184:CYS:HB2	2.53	0.44
1:I:266:ASN:HB2	1:I:301:ARG:O	2.18	0.44
1:A:286:ARG:HH12	6:A:1589:TEO:C4	2.30	0.44
1:I:122:GLN:HB3	1:I:131:ALA:HB3	2.00	0.44
3:C:13:LEU:HD12	3:C:13:LEU:HA	1.90	0.43
1:A:49:ALA:HB3	1:A:142:GLY:HA3	2.00	0.43
1:I:286:ARG:HH12	6:I:1589:TEO:C4	2.32	0.43
4:D:38:ALA:O	4:D:39:THR:CG2	2.66	0.43
1:I:394:VAL:HG23	1:I:395:HIS:CE1	2.53	0.43
2:B:214:SER:HB3	3:C:103:PHE:CE1	2.52	0.43
2:F:130:ALA:CB	1:I:6:ARG:HG2	2.49	0.43
3:C:8:GLN:HG2	3:C:9:ARG:N	2.32	0.43
1:A:340:VAL:O	1:A:342:PRO:HD3	2.19	0.43
2:F:175:LEU:HD23	2:F:175:LEU:HA	1.91	0.43
1:I:49:ALA:HB3	1:I:142:GLY:HA3	2.01	0.42
1:I:214:ASN:N	1:I:214:ASN:HD22	2.16	0.42
1:I:320:LYS:HE2	1:I:324:GLU:OE2	2.19	0.42
1:I:340:VAL:O	1:I:342:PRO:HD3	2.19	0.42
1:I:345:GLU:HG2	1:I:346:PRO:HD2	2.00	0.42
1:A:49:ALA:HA	5:A:601:FAD:N5	2.33	0.42
2:J:61:GLY:HA2	2:J:150:ILE:HD12	2.00	0.42
3:K:96:PHE:CD1	3:K:96:PHE:N	2.86	0.42
1:E:38:LYS:HE3	1:E:217:ILE:HB	2.00	0.42
2:B:169:PHE:CE2	2:B:171:GLY:HA2	2.54	0.42
2:J:160:PRO:HA	2:J:163:TRP:CE3	2.54	0.42
3:K:88:GLY:HA3	12:K:1129:HEM:HBC2	2.01	0.42
3:K:103:PHE:CE2	3:K:107:LYS:HE3	2.54	0.42
1:A:323:LEU:HD23	1:A:327:LEU:HD12	2.01	0.42
3:G:53:SER:O	3:G:54:SER:HB3	2.20	0.42
1:I:490:ILE:CG2	1:I:520:MET:CE	2.84	0.42
1:E:340:VAL:O	1:E:342:PRO:HD3	2.19	0.42
1:I:227:ILE:HG23	1:I:561:PRO:HB3	2.01	0.42
1:A:38:LYS:HE3	1:A:217:ILE:HB	2.01	0.42
1:E:286:ARG:HH22	6:E:1589:TEO:C4	2.32	0.42
1:E:451:ARG:HA	1:E:451:ARG:HD3	1.75	0.42
12:G:1129:HEM:HBA2	12:G:1129:HEM:HHA	2.02	0.42
1:A:173:GLN:CG	1:A:430:ARG:HH11	2.33	0.41
2:B:35:LEU:HD11	2:B:91:ILE:HD11	2.02	0.41
2:J:234:LEU:HD23	4:L:13:VAL:HG13	2.02	0.41
12:K:1129:HEM:HBC2	12:K:1129:HEM:CHD	2.50	0.41
1:E:323:LEU:HD23	1:E:327:LEU:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:38:ALA:C	4:L:39:THR:HG23	2.40	0.41
1:E:286:ARG:HH12	6:E:1589:TEO:C4	2.32	0.41
2:J:183:ILE:C	2:J:183:ILE:HD12	2.41	0.41
3:K:53:SER:O	3:K:54:SER:HB3	2.20	0.41
1:A:227:ILE:HG23	1:A:561:PRO:HB3	2.03	0.41
1:A:262:GLY:HA3	1:A:315:LEU:HD23	2.02	0.41
1:E:164:TRP:CH2	1:E:184:CYS:HB2	2.55	0.41
1:E:37:SER:O	1:E:163:GLU:N	2.53	0.41
4:H:40:SER:O	4:H:41:GLY:C	2.57	0.41
1:I:49:ALA:HB1	5:I:601:FAD:C4X	2.51	0.41
1:I:350:ILE:CG1	1:I:351:PRO:HD2	2.50	0.41
1:A:384:PHE:CD2	1:A:384:PHE:N	2.89	0.41
4:H:38:ALA:O	4:H:39:THR:HG22	2.19	0.41
1:A:54:THR:O	1:A:406:LEU:HD22	2.21	0.41
2:B:214:SER:HB3	3:C:103:PHE:CZ	2.55	0.41
1:A:490:ILE:CG2	1:A:520:MET:HE1	2.51	0.41
1:E:258:ARG:HD3	14:E:2094:HOH:O	2.20	0.41
1:E:345:GLU:HG2	1:E:346:PRO:HD2	2.03	0.41
1:I:20:MET:CE	1:I:146:LEU:CD1	2.99	0.41
2:J:94:LEU:HA	2:J:95:PRO:HD3	1.92	0.41
2:J:169:PHE:CE2	2:J:171:GLY:HA2	2.55	0.41
3:K:19:ARG:NH1	14:K:2008:HOH:O	2.53	0.41
1:A:14:GLY:HA2	5:A:601:FAD:H1B	2.03	0.41
1:E:49:ALA:HB3	1:E:142:GLY:HA3	2.03	0.41
1:E:266:ASN:HB2	1:E:301:ARG:O	2.20	0.41
5:E:601:FAD:H1'1	5:E:601:FAD:H9	1.84	0.41
4:H:45:TYR:CZ	4:H:49:ILE:HD12	2.55	0.41
4:D:22:THR:OG1	4:D:71:HIS:HB2	2.21	0.40
1:A:554:LEU:HD21	1:A:573:MET:CE	2.51	0.40
1:E:49:ALA:HB1	5:E:601:FAD:C4X	2.52	0.40
2:J:234:LEU:CD2	4:L:13:VAL:HG13	2.51	0.40
1:E:20:MET:HE2	1:E:146:LEU:CD1	2.50	0.40
1:A:478:ASP:HB2	14:A:2202:HOH:O	2.22	0.40
1:I:554:LEU:HD21	1:I:573:MET:HE1	2.01	0.40
1:E:214:ASN:N	1:E:214:ASN:HD22	2.19	0.40
4:H:38:ALA:C	4:H:39:THR:HG23	2.41	0.40
4:L:40:SER:O	4:L:41:GLY:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	15	23
4	H	103/115 (90%)	96 (93%)	6 (6%)	1 (1%)	15	23
4	L	103/115 (90%)	97 (94%)	5 (5%)	1 (1%)	15	23
All	All	3132/3210 (98%)	3033 (97%)	96 (3%)	3 (0%)	51	68

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 (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	473/473 (100%)	466 (98%)	7 (2%)	65	80
1	E	473/473 (100%)	464 (98%)	9 (2%)	57	75
1	I	473/473 (100%)	465 (98%)	8 (2%)	60	78
2	B	208/208 (100%)	204 (98%)	4 (2%)	57	75
2	F	208/208 (100%)	202 (97%)	6 (3%)	42	62
2	J	208/208 (100%)	202 (97%)	6 (3%)	42	62
3	C	101/109 (93%)	100 (99%)	1 (1%)	76	88
3	G	101/109 (93%)	100 (99%)	1 (1%)	76	88
3	K	101/109 (93%)	100 (99%)	1 (1%)	76	88
4	D	88/96 (92%)	84 (96%)	4 (4%)	27	44
4	H	88/96 (92%)	85 (97%)	3 (3%)	37	56
4	L	88/96 (92%)	85 (97%)	3 (3%)	37	56
All	All	2610/2658 (98%)	2557 (98%)	53 (2%)	55	74

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	94	GLU
1	A	119	PHE
1	A	325	SER
1	A	339	HIS
1	A	506	PHE
1	A	578	ARG
2	B	53	ARG
2	B	56	ARG
2	B	120	TYR
2	B	180	ARG
3	C	11	VAL
4	D	43	LEU
4	D	44	THR
4	D	54	SER
4	D	60	PHE
1	E	2	LYS
1	E	47	VAL
1	E	94	GLU
1	E	119	PHE
1	E	325	SER
1	E	339	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	378	VAL
1	E	506	PHE
1	E	578	ARG
2	F	1	MET
2	F	53	ARG
2	F	56	ARG
2	F	120	TYR
2	F	180	ARG
2	F	192	SER
3	G	11	VAL
4	H	43	LEU
4	H	44	THR
4	H	60	PHE
1	I	2	LYS
1	I	94	GLU
1	I	119	PHE
1	I	214	ASN
1	I	339	HIS
1	I	378	VAL
1	I	506	PHE
1	I	578	ARG
2	J	53	ARG
2	J	56	ARG
2	J	120	TYR
2	J	141	GLU
2	J	180	ARG
2	J	192	SER
3	K	11	VAL
4	L	43	LEU
4	L	44	THR
4	L	60	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	I	1589	-	6,8,8	0.98	0	4,10,10	1.44	1 (25%)
12	HEM	K	1129	3,4	41,50,50	1.95	8 (19%)	45,82,82	1.79	9 (20%)
9	FES	B	302	2	0,4,4	-	-	-		
12	HEM	G	1129	3,4	41,50,50	1.86	7 (17%)	45,82,82	1.82	11 (24%)
12	HEM	C	1129	3,4	41,50,50	1.98	7 (17%)	45,82,82	1.67	9 (20%)
8	SO4	A	1591	-	4,4,4	0.22	0	6,6,6	0.18	0
8	SO4	I	1591	-	4,4,4	0.15	0	6,6,6	0.47	0
10	SF4	F	303	2	0,12,12	-	-	-		
9	FES	J	302	2	0,4,4	-	-	-		
10	SF4	B	303	2	0,12,12	-	-	-		
6	TEO	E	1589	-	6,8,8	1.04	0	4,10,10	2.38	3 (75%)
11	F3S	B	304	2	0,9,9	-	-	-		
5	FAD	A	601	1	53,58,58	1.20	3 (5%)	68,89,89	1.54	13 (19%)
6	TEO	A	1589	-	6,8,8	1.30	1 (16%)	4,10,10	2.14	1 (25%)
9	FES	F	302	2	0,4,4	-	-	-		
5	FAD	E	601	1	53,58,58	1.06	2 (3%)	68,89,89	1.63	17 (25%)
11	F3S	F	304	2	0,9,9	-	-	-		
8	SO4	E	1591	-	4,4,4	0.24	0	6,6,6	0.36	0
13	CBE	C	1130	-	16,17,17	1.06	1 (6%)	16,22,22	1.85	2 (12%)
5	FAD	I	601	1	53,58,58	1.31	6 (11%)	68,89,89	1.44	14 (20%)
11	F3S	J	304	2	0,9,9	-	-	-		
13	CBE	K	1130	-	16,17,17	1.19	2 (12%)	16,22,22	1.56	2 (12%)
10	SF4	J	303	2	0,12,12	-	-	-		
13	CBE	G	1130	-	16,17,17	1.14	1 (6%)	16,22,22	1.89	2 (12%)

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	I	1589	-	-	1/6/8/8	-
12	HEM	K	1129	3,4	-	7/12/54/54	-
9	FES	B	302	2	-	-	0/1/1/1
12	HEM	G	1129	3,4	-	3/12/54/54	-
12	HEM	C	1129	3,4	-	2/12/54/54	-
10	SF4	F	303	2	-	-	0/6/5/5
9	FES	J	302	2	-	-	0/1/1/1
10	SF4	B	303	2	-	-	0/6/5/5
6	TEO	E	1589	-	-	4/6/8/8	-
11	F3S	B	304	2	-	-	0/3/3/3
5	FAD	A	601	1	-	5/30/50/50	0/6/6/6
6	TEO	A	1589	-	-	3/6/8/8	-
9	FES	F	302	2	-	-	0/1/1/1
5	FAD	E	601	1	-	5/30/50/50	0/6/6/6
11	F3S	F	304	2	-	-	0/3/3/3
13	CBE	C	1130	-	-	2/6/19/19	0/1/2/2
5	FAD	I	601	1	-	3/30/50/50	0/6/6/6
11	F3S	J	304	2	-	-	0/3/3/3
13	CBE	K	1130	-	-	2/6/19/19	0/1/2/2
10	SF4	J	303	2	-	-	0/6/5/5
13	CBE	G	1130	-	-	2/6/19/19	0/1/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1129	HEM	C3D-C2D	7.60	1.52	1.36
12	K	1129	HEM	C3D-C2D	7.10	1.51	1.36
12	G	1129	HEM	C3D-C2D	6.98	1.51	1.36
12	C	1129	HEM	C3C-C2C	-5.66	1.32	1.40
12	G	1129	HEM	C3C-C2C	-5.49	1.32	1.40
12	K	1129	HEM	C3C-C2C	-5.39	1.32	1.40
5	I	601	FAD	C2A-N3A	4.85	1.39	1.32
5	A	601	FAD	C4X-N5	4.39	1.39	1.30
5	I	601	FAD	C4X-N5	4.38	1.39	1.30
5	E	601	FAD	C4X-N5	4.20	1.38	1.30
13	G	1130	CBE	C11-N10	-3.47	1.34	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	C2A-N3A	3.41	1.37	1.32
13	K	1130	CBE	C11-N10	-3.18	1.35	1.41
12	G	1129	HEM	C3C-CAC	3.03	1.54	1.47
12	C	1129	HEM	CAA-C2A	2.91	1.56	1.52
13	C	1130	CBE	C11-N10	-2.79	1.36	1.41
12	K	1129	HEM	C3B-C2B	-2.74	1.31	1.37
12	K	1129	HEM	C3C-CAC	2.67	1.53	1.47
12	K	1129	HEM	FE-NB	2.61	2.09	1.96
5	I	601	FAD	C2A-N1A	2.50	1.38	1.33
12	C	1129	HEM	C3C-CAC	2.46	1.52	1.47
5	I	601	FAD	C2B-C1B	-2.45	1.50	1.53
12	C	1129	HEM	CAB-C3B	2.43	1.54	1.47
5	A	601	FAD	C10-N1	2.43	1.38	1.33
12	G	1129	HEM	CAB-C3B	2.40	1.54	1.47
12	C	1129	HEM	C3B-C2B	-2.35	1.32	1.37
13	K	1130	CBE	C1-C2	2.32	1.54	1.49
12	G	1129	HEM	C3B-C2B	-2.32	1.32	1.37
5	E	601	FAD	C2A-N3A	2.31	1.35	1.32
12	K	1129	HEM	CAB-C3B	2.29	1.53	1.47
12	G	1129	HEM	FE-NB	2.28	2.08	1.96
5	I	601	FAD	C10-N1	2.28	1.37	1.33
12	K	1129	HEM	CAA-C2A	2.24	1.55	1.52
5	I	601	FAD	C2'-C3'	-2.17	1.49	1.53
12	C	1129	HEM	CMD-C2D	2.12	1.55	1.50
12	K	1129	HEM	CMB-C2B	2.04	1.55	1.50
6	A	1589	TEO	C2-C1	-2.02	1.50	1.54
12	G	1129	HEM	CAA-C2A	2.01	1.55	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1130	CBE	O7-C2-C1	6.29	116.88	109.32
5	A	601	FAD	N3A-C2A-N1A	-6.19	119.00	128.68
5	E	601	FAD	N3A-C2A-N1A	-6.07	119.19	128.68
12	K	1129	HEM	C4D-ND-C1D	5.75	111.02	105.07
13	C	1130	CBE	O7-C2-C1	5.59	116.05	109.32
12	G	1129	HEM	C4D-ND-C1D	5.20	110.45	105.07
12	C	1129	HEM	C4D-ND-C1D	5.08	110.32	105.07
13	K	1130	CBE	O7-C2-C1	4.66	114.93	109.32
5	I	601	FAD	N3A-C2A-N1A	-4.41	121.78	128.68
12	K	1129	HEM	CAD-CBD-CGD	-4.00	105.00	113.60
13	K	1130	CBE	C11-N10-C8	-3.85	120.85	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	1129	HEM	C2C-C3C-C4C	3.76	109.52	106.90
5	E	601	FAD	C4X-C10-N10	3.70	121.89	116.48
5	I	601	FAD	C4X-C10-N10	3.59	121.73	116.48
12	G	1129	HEM	CMD-C2D-C1D	3.45	130.30	125.04
5	A	601	FAD	C4X-C10-N10	3.44	121.51	116.48
12	C	1129	HEM	CMD-C2D-C1D	3.40	130.22	125.04
6	E	1589	TEO	O1A-C1-C2	-3.32	114.41	122.42
12	K	1129	HEM	C4B-CHC-C1C	3.32	126.94	122.56
6	A	1589	TEO	O1A-C1-C2	-3.28	114.50	122.42
13	C	1130	CBE	C11-N10-C8	-3.28	121.83	127.53
5	A	601	FAD	O2'-C2'-C3'	-3.20	101.31	109.10
12	G	1129	HEM	C2C-C3C-C4C	3.09	109.05	106.90
5	E	601	FAD	C4-N3-C2	-3.08	119.95	125.64
12	G	1129	HEM	CMB-C2B-C1B	2.91	129.46	125.04
12	C	1129	HEM	C1D-C2D-C3D	-2.88	103.93	106.96
12	G	1129	HEM	O2A-CGA-CBA	2.83	123.13	114.03
5	I	601	FAD	C4-C4X-N5	2.81	122.23	118.23
12	G	1129	HEM	C4B-CHC-C1C	2.80	126.25	122.56
12	K	1129	HEM	CAD-C3D-C4D	2.78	129.51	124.66
5	I	601	FAD	O2'-C2'-C3'	-2.73	102.45	109.10
5	A	601	FAD	O4'-C4'-C3'	2.71	115.70	109.10
5	I	601	FAD	C10-N1-C2	2.69	122.29	116.90
5	A	601	FAD	C5X-C9A-N10	2.69	120.73	117.95
12	K	1129	HEM	C2C-C3C-C4C	2.68	108.77	106.90
5	E	601	FAD	C4X-C4-N3	2.67	119.97	113.19
12	G	1129	HEM	CAD-C3D-C4D	2.65	129.29	124.66
12	K	1129	HEM	CMA-C3A-C4A	-2.65	124.39	128.46
5	E	601	FAD	C10-C4X-N5	-2.62	119.29	124.86
12	G	1129	HEM	CAD-CBD-CGD	-2.59	108.03	113.60
5	I	601	FAD	C10-C4X-N5	-2.59	119.37	124.86
5	I	601	FAD	C4X-C4-N3	2.56	119.69	113.19
5	A	601	FAD	C4X-C4-N3	2.55	119.66	113.19
5	E	601	FAD	C4A-C5A-N7A	-2.52	106.78	109.40
5	A	601	FAD	C10-N1-C2	2.50	121.90	116.90
12	K	1129	HEM	CMB-C2B-C1B	2.47	128.81	125.04
5	E	601	FAD	C9A-C5X-N5	-2.47	119.75	122.43
5	E	601	FAD	C5A-C6A-N6A	2.47	124.11	120.35
6	E	1589	TEO	O1B-C1-C2	2.46	118.85	113.07
5	I	601	FAD	C4-N3-C2	-2.43	121.14	125.64
5	A	601	FAD	C9A-C5X-N5	-2.39	119.84	122.43
5	I	601	FAD	O5'-C5'-C4'	-2.36	103.05	109.36
12	C	1129	HEM	CAD-CBD-CGD	-2.36	108.53	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	1129	HEM	CBA-CAA-C2A	-2.35	108.61	112.62
5	E	601	FAD	C10-N1-C2	2.33	121.55	116.90
5	E	601	FAD	O5'-C5'-C4'	-2.31	103.20	109.36
12	G	1129	HEM	C4B-C3B-C2B	2.29	108.93	107.11
5	E	601	FAD	C4-C4X-N5	2.28	121.47	118.23
12	K	1129	HEM	O1D-CGD-CBD	-2.27	115.78	123.08
12	C	1129	HEM	CHA-C4D-ND	2.27	127.19	124.38
5	I	601	FAD	C4A-C5A-N7A	-2.27	107.03	109.40
5	E	601	FAD	O4-C4-C4X	-2.25	120.63	126.60
5	E	601	FAD	C9-C9A-N10	-2.25	118.80	121.84
5	A	601	FAD	C4-N3-C2	-2.22	121.55	125.64
5	A	601	FAD	C4X-C10-N1	-2.21	119.59	124.73
5	A	601	FAD	C10-C4X-N5	-2.19	120.22	124.86
5	E	601	FAD	C2A-N1A-C6A	2.18	122.48	118.75
5	A	601	FAD	C4'-C3'-C2'	-2.17	108.85	113.36
5	I	601	FAD	O4-C4-C4X	-2.16	120.87	126.60
5	E	601	FAD	O2'-C2'-C3'	-2.11	103.97	109.10
5	I	601	FAD	O4'-C4'-C5'	-2.09	105.21	109.92
12	K	1129	HEM	O2D-CGD-CBD	2.09	120.75	114.03
12	G	1129	HEM	CAB-C3B-C2B	-2.09	121.73	128.60
12	C	1129	HEM	O2D-CGD-CBD	2.08	120.73	114.03
5	I	601	FAD	O2-C2-N3	2.08	122.70	118.65
6	E	1589	TEO	O2-C2-C1	2.07	114.98	109.61
6	I	1589	TEO	O1A-C1-C2	-2.05	117.48	122.42
5	E	601	FAD	C4X-C10-N1	-2.05	119.98	124.73
5	E	601	FAD	C4'-C3'-C2'	-2.03	109.13	113.36
12	C	1129	HEM	O1A-CGA-CBA	-2.03	116.57	123.08
5	A	601	FAD	C4-C4X-N5	2.02	121.11	118.23
5	I	601	FAD	C1B-N9A-C4A	-2.02	123.10	126.64
13	G	1130	CBE	C3-C8-N10	-2.01	112.34	115.91
12	C	1129	HEM	CHB-C1B-NB	2.01	126.86	124.38

There are no chirality outliers.

All (39) 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
6	E	1589	TEO	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	I	1589	TEO	O2-C2-C3-C4
12	K	1129	HEM	C1A-C2A-CAA-CBA
12	K	1129	HEM	C3A-C2A-CAA-CBA
13	K	1130	CBE	C2-C3-C8-O9
6	A	1589	TEO	O1A-C1-C2-O2
6	A	1589	TEO	O1B-C1-C2-O2
12	K	1129	HEM	C2B-C3B-CAB-CBB
12	K	1129	HEM	C4B-C3B-CAB-CBB
13	C	1130	CBE	C2-C3-C8-O9
13	C	1130	CBE	C2-C3-C8-N10
13	G	1130	CBE	C2-C3-C8-N10
13	K	1130	CBE	C2-C3-C8-N10
5	A	601	FAD	PA-O3P-P-O5'
12	G	1129	HEM	C4B-C3B-CAB-CBB
13	G	1130	CBE	C2-C3-C8-O9
5	E	601	FAD	N10-C1'-C2'-O2'
5	E	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	P-O3P-PA-O2A
5	E	601	FAD	P-O3P-PA-O2A
6	E	1589	TEO	O2-C2-C3-C4
12	C	1129	HEM	CAD-CBD-CGD-O2D
12	G	1129	HEM	CAD-CBD-CGD-O1D
12	C	1129	HEM	CAD-CBD-CGD-O1D
6	E	1589	TEO	O1A-C1-C2-O2
6	E	1589	TEO	O1B-C1-C2-O2
12	G	1129	HEM	CAD-CBD-CGD-O2D
12	K	1129	HEM	CAA-CBA-CGA-O1A
12	K	1129	HEM	CAA-CBA-CGA-O2A
5	A	601	FAD	O4B-C4B-C5B-O5B
5	E	601	FAD	O4B-C4B-C5B-O5B
5	I	601	FAD	P-O3P-PA-O2A
5	I	601	FAD	O4B-C4B-C5B-O5B
12	K	1129	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

13 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1589	TEO	4	0
12	K	1129	HEM	6	0
12	G	1129	HEM	5	0
12	C	1129	HEM	6	0

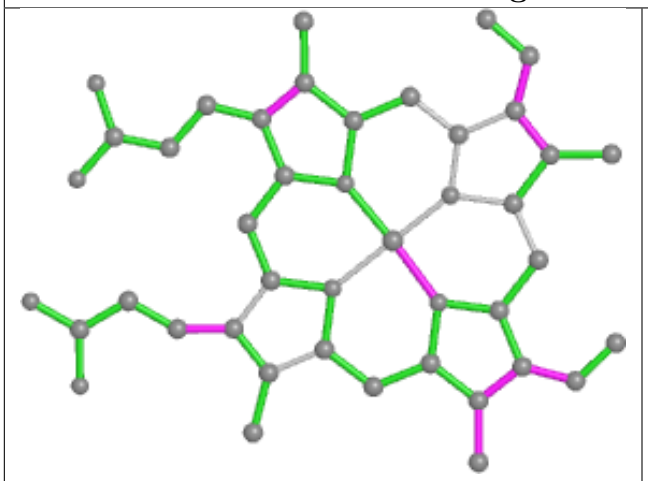
Continued on next page...

Continued from previous page...

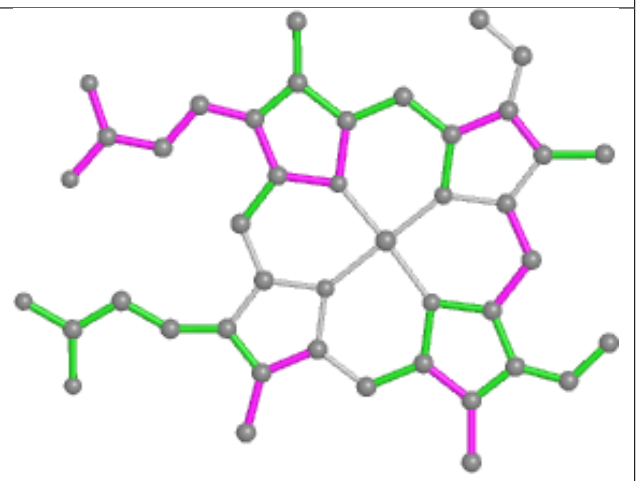
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1589	TEO	4	0
5	A	601	FAD	6	0
6	A	1589	TEO	3	0
5	E	601	FAD	7	0
13	C	1130	CBE	2	0
5	I	601	FAD	7	0
13	K	1130	CBE	2	0
10	J	303	SF4	1	0
13	G	1130	CBE	1	0

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.

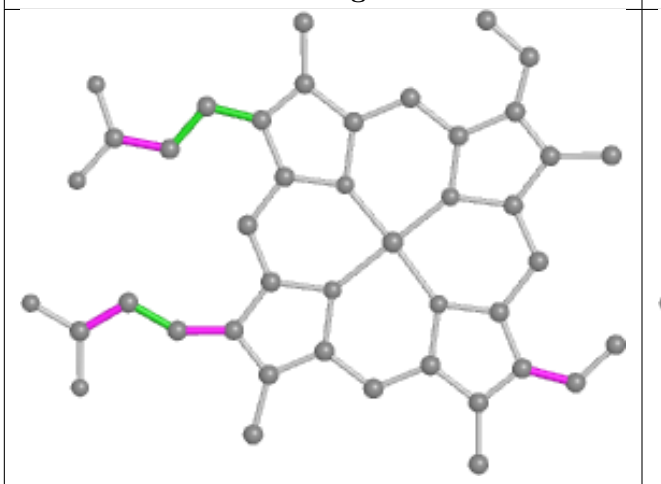
Ligand HEM K 1129



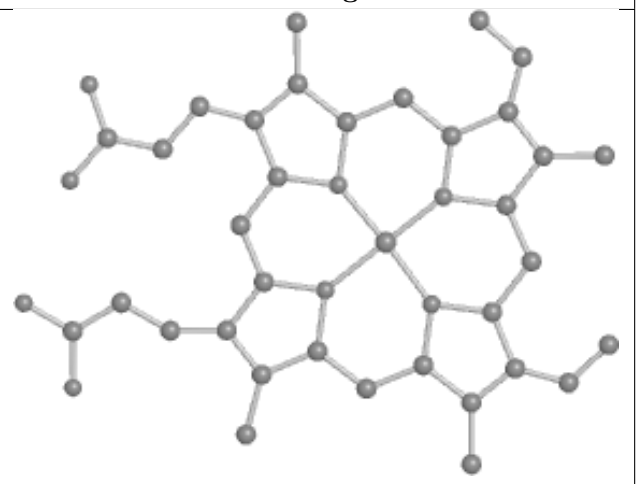
Bond lengths



Bond angles

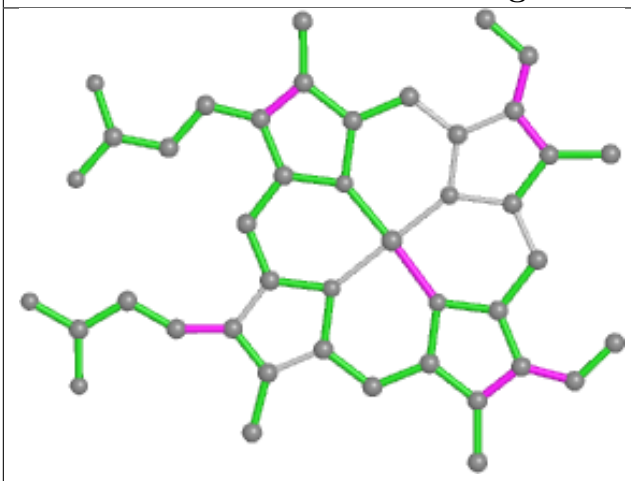


Torsions

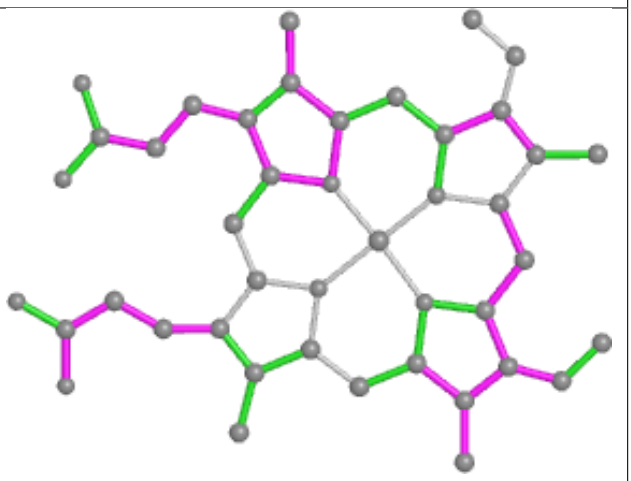


Rings

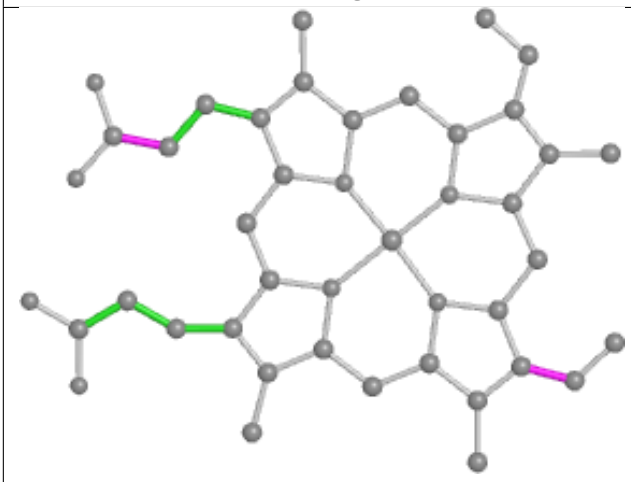
Ligand HEM G 1129



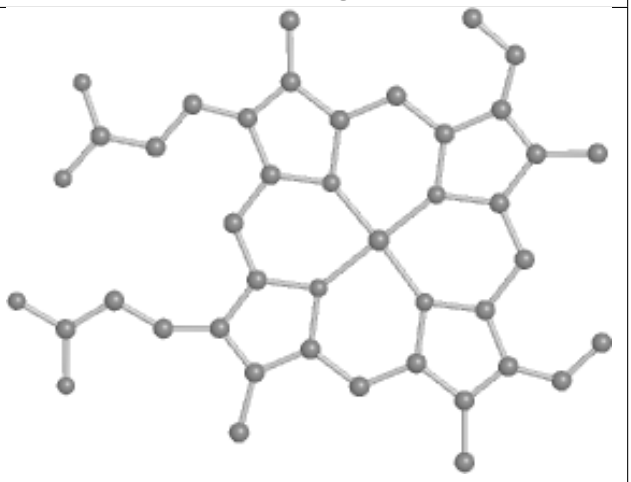
Bond lengths



Bond angles

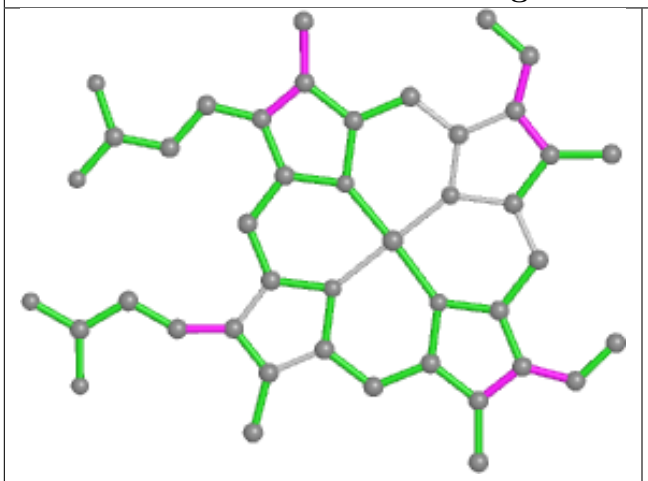


Torsions

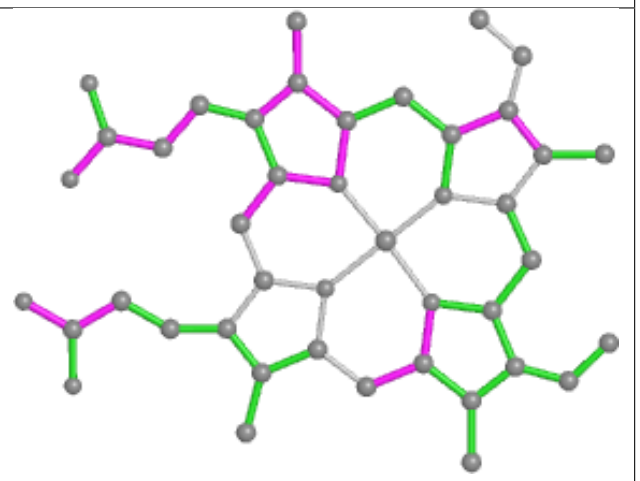


Rings

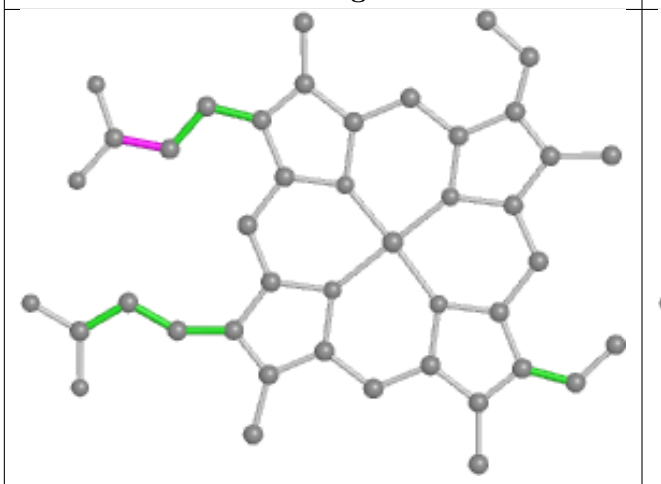
Ligand HEM C 1129



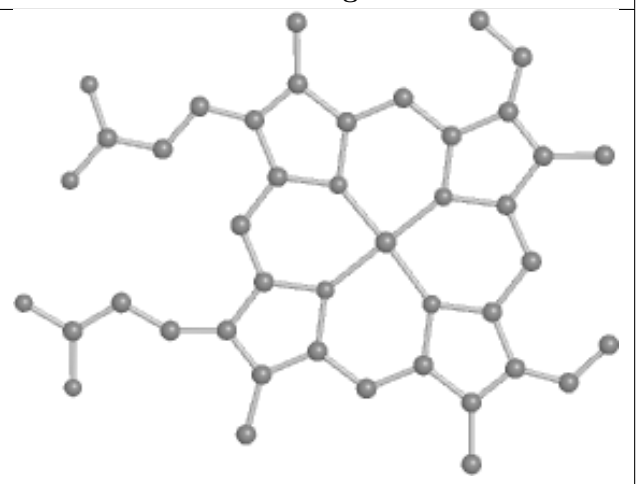
Bond lengths



Bond angles

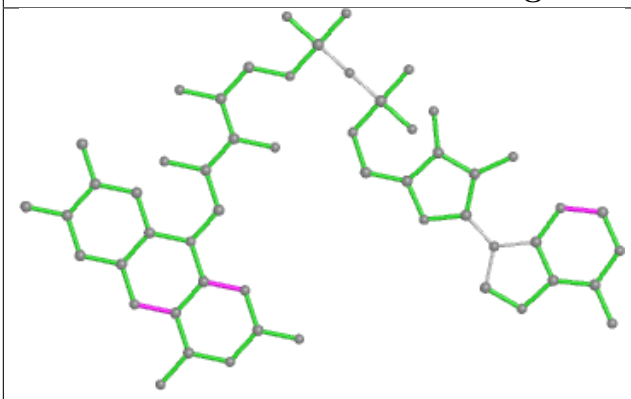


Torsions

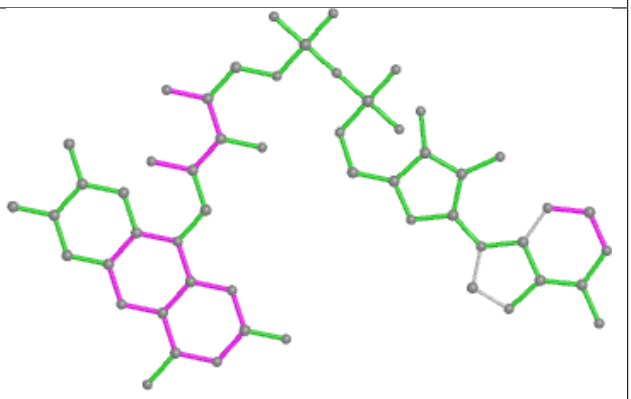


Rings

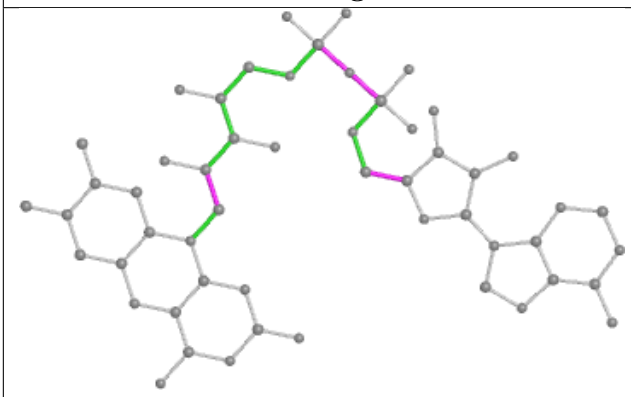
Ligand FAD A 601



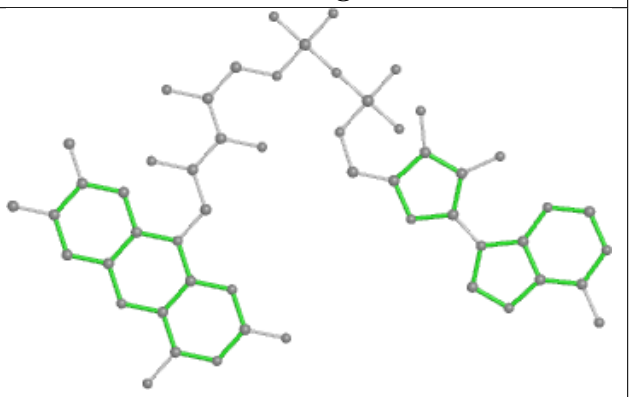
Bond lengths



Bond angles

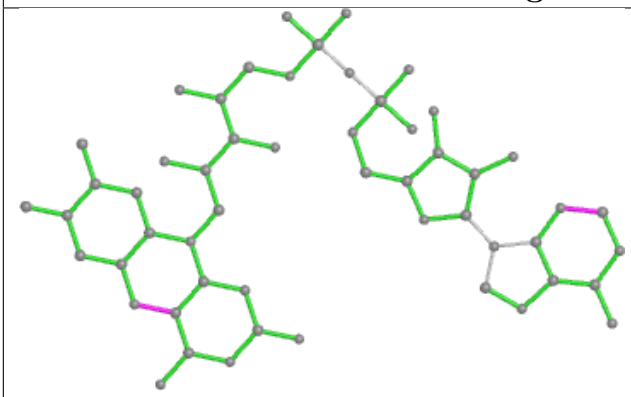


Torsions

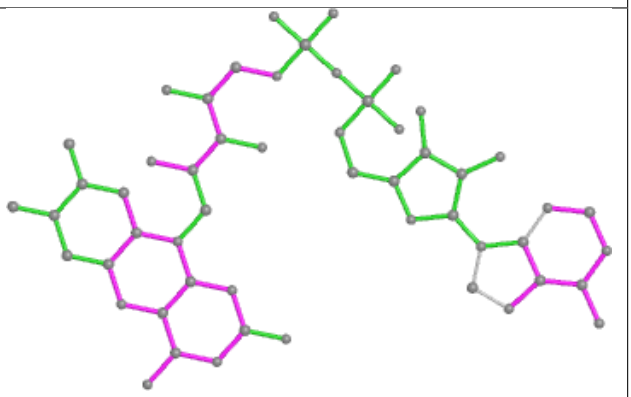


Rings

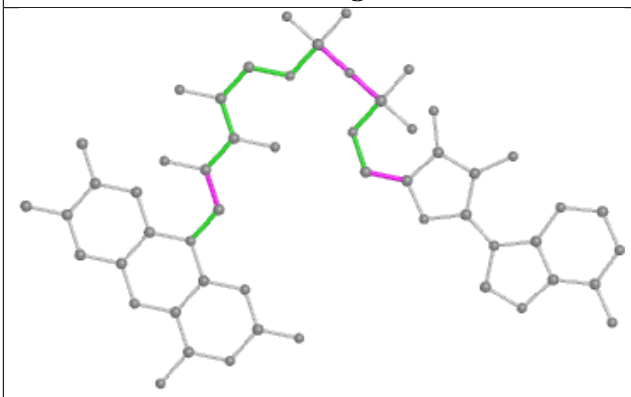
Ligand FAD E 601



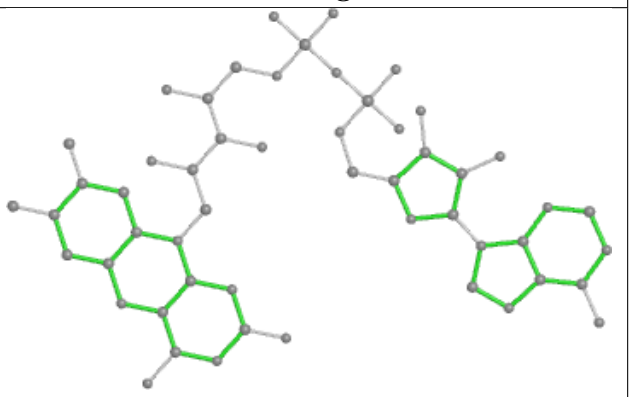
Bond lengths



Bond angles

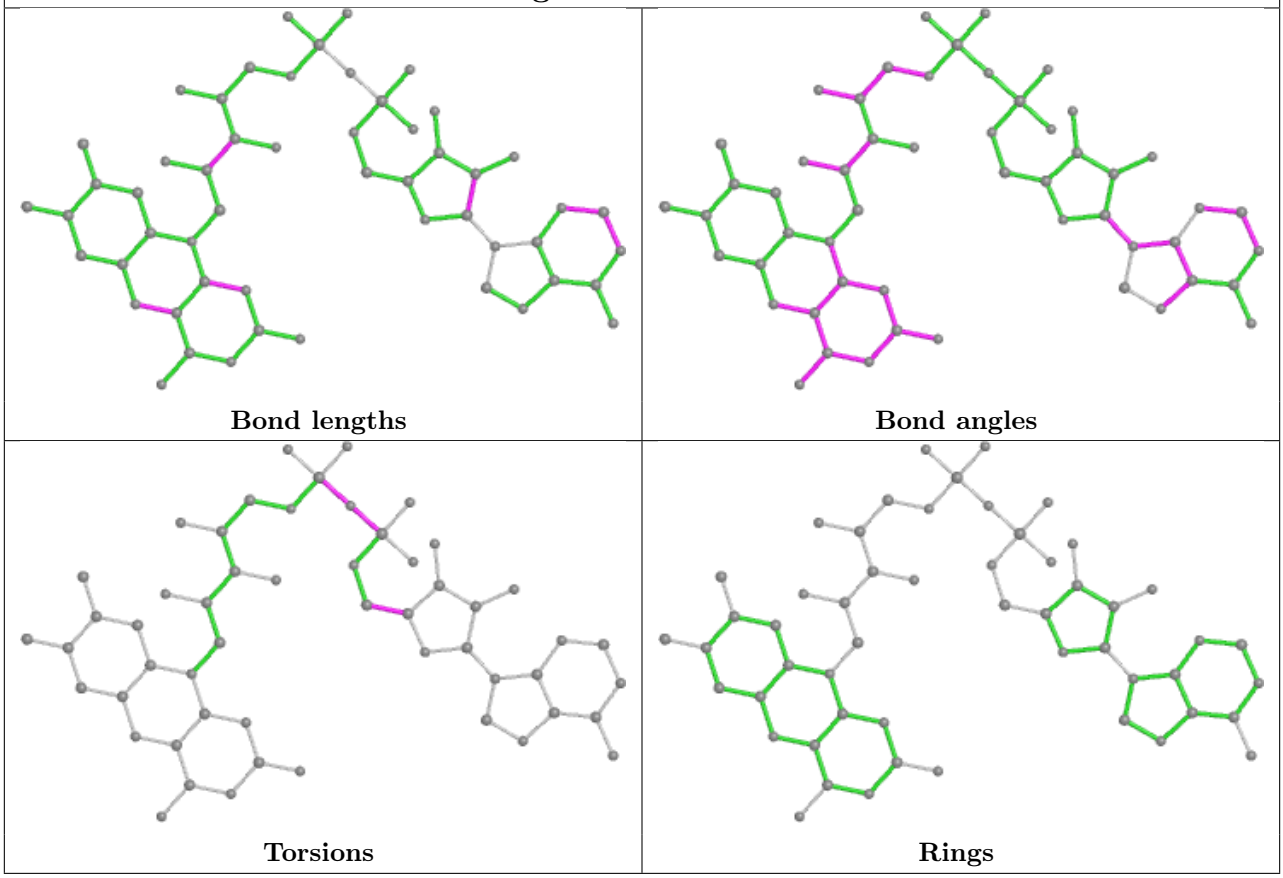


Torsions



Rings

Ligand FAD I 601



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%)	0.19	18 (3%)	49	47	33, 39, 52, 72	0
1	E	588/588 (100%)	0.23	28 (4%)	30	29	33, 39, 52, 72	0
1	I	588/588 (100%)	0.31	29 (4%)	29	28	33, 39, 52, 72	0
2	B	238/238 (100%)	0.25	14 (5%)	22	21	28, 35, 49, 69	0
2	F	238/238 (100%)	0.22	11 (4%)	32	31	28, 34, 49, 69	0
2	J	238/238 (100%)	0.22	13 (5%)	25	24	28, 35, 49, 69	0
3	C	121/129 (93%)	0.31	15 (12%)	4	3	45, 54, 67, 73	0
3	G	121/129 (93%)	0.20	11 (9%)	9	8	45, 54, 67, 73	0
3	K	121/129 (93%)	0.45	16 (13%)	3	3	45, 54, 67, 73	0
4	D	105/115 (91%)	0.15	6 (5%)	23	22	44, 49, 69, 72	0
4	H	105/115 (91%)	0.44	12 (11%)	5	4	44, 50, 69, 72	0
4	L	105/115 (91%)	0.32	8 (7%)	13	12	44, 49, 69, 72	0
All	All	3156/3210 (98%)	0.26	181 (5%)	23	22	28, 40, 61, 73	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	115	VAL	6.3
3	G	68	PHE	6.0
4	L	40	SER	5.9
2	F	29	GLU	5.9
3	K	68	PHE	5.8
4	L	42	GLU	5.7
1	I	1	MET	5.6
4	H	42	GLU	5.5
2	B	85	PRO	5.1
4	D	42	GLU	5.1
4	H	46	GLU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	69	PHE	5.0
3	G	69	PHE	5.0
2	F	30	GLY	5.0
4	H	40	SER	4.9
4	H	114	GLY	4.9
1	I	306	PRO	4.9
2	B	16	ASP	4.9
4	L	41	GLY	4.7
3	K	98	TYR	4.4
1	E	1	MET	4.4
3	K	56	GLU	4.4
4	H	41	GLY	4.3
2	J	31	ARG	4.3
3	C	68	PHE	4.3
4	L	115	VAL	4.3
1	A	543	PHE	4.3
1	I	304	ASP	4.2
1	I	585	ILE	4.2
4	L	46	GLU	4.2
3	C	98	TYR	4.2
2	B	31	ARG	4.0
1	E	2	LYS	4.0
1	A	1	MET	4.0
1	E	374	LYS	4.0
4	D	40	SER	3.8
1	I	478	ASP	3.8
1	I	305	GLY	3.8
3	G	56	GLU	3.8
4	H	56	PHE	3.8
2	F	31	ARG	3.8
3	G	127	LEU	3.8
2	B	29	GLU	3.7
3	C	56	GLU	3.7
2	J	16	ASP	3.6
2	J	30	GLY	3.6
1	A	304	ASP	3.6
1	I	434	GLU	3.6
3	K	72	PHE	3.6
4	D	39	THR	3.6
2	F	1	MET	3.6
2	B	209	ILE	3.5
4	H	113	TRP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	576	LYS	3.4
1	I	298	ARG	3.4
1	E	198	THR	3.4
1	I	584	LYS	3.4
4	D	41	GLY	3.4
1	E	530	ALA	3.4
1	I	523	ALA	3.4
3	C	59	GLU	3.3
3	G	98	TYR	3.3
2	J	29	GLU	3.3
1	I	482	LYS	3.3
4	H	50	GLY	3.3
1	I	543	PHE	3.3
3	K	8	GLN	3.3
2	J	103	LEU	3.2
2	B	30	GLY	3.2
3	K	59	GLU	3.2
2	J	127	ASN	3.2
1	A	313	LEU	3.2
1	A	551	GLU	3.2
4	L	44	THR	3.1
1	E	313	LEU	3.1
4	D	115	VAL	3.1
3	C	69	PHE	3.1
2	J	28	ASP	3.1
3	C	127	LEU	3.1
1	E	253	VAL	3.1
3	K	108	ARG	3.0
4	H	39	THR	3.0
1	A	199	VAL	3.0
3	K	54	SER	3.0
2	F	238	ALA	3.0
1	I	279	ASN	3.0
3	G	72	PHE	2.9
1	E	375	GLY	2.9
4	H	53	ALA	2.9
1	A	12	VAL	2.9
3	C	126	VAL	2.9
2	B	86	GLY	2.9
1	I	316	ASP	2.9
1	I	374	LYS	2.9
4	L	45	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	306	PRO	2.8
2	J	238	ALA	2.8
3	C	123	LEU	2.8
2	B	206	CYS	2.8
1	E	527	ALA	2.7
3	K	100	GLU	2.7
3	K	66	GLY	2.7
3	C	124	ALA	2.7
1	I	583	PRO	2.7
1	E	279	ASN	2.7
1	A	349	VAL	2.7
3	C	128	VAL	2.7
1	I	129	GLU	2.6
1	E	373	GLU	2.6
1	A	198	THR	2.6
3	K	63	ALA	2.6
3	G	54	SER	2.6
4	L	39	THR	2.6
3	K	60	GLN	2.6
1	E	254	THR	2.6
1	I	12	VAL	2.6
3	G	55	PRO	2.6
1	I	307	TRP	2.6
3	C	8	GLN	2.6
3	G	59	GLU	2.6
1	A	2	LYS	2.5
1	I	526	THR	2.5
1	E	11	VAL	2.5
2	F	16	ASP	2.5
3	C	67	SER	2.5
1	I	199	VAL	2.5
1	A	129	GLU	2.5
3	G	126	VAL	2.5
1	E	173	GLN	2.4
1	E	543	PHE	2.4
1	A	13	ILE	2.4
3	C	16	GLN	2.4
1	I	487	LEU	2.4
2	B	28	ASP	2.4
2	F	209	ILE	2.4
3	K	64	ILE	2.4
2	J	26	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	16	GLN	2.4
1	A	11	VAL	2.4
2	J	126	GLN	2.4
1	E	529	SER	2.3
1	E	304	ASP	2.3
4	H	49	ILE	2.3
1	I	373	GLU	2.3
1	A	298	ARG	2.3
3	C	55	PRO	2.3
1	E	199	VAL	2.3
2	B	26	GLU	2.3
1	I	344	LYS	2.3
2	J	13	ASP	2.3
1	A	208	ILE	2.2
3	C	60	GLN	2.2
1	E	177	VAL	2.2
1	E	383	LEU	2.2
2	J	32	ASP	2.2
1	E	12	VAL	2.2
1	E	321	GLU	2.2
1	I	551	GLU	2.2
1	A	311	ALA	2.2
1	A	85	ILE	2.2
2	F	206	CYS	2.2
3	G	8	GLN	2.2
1	E	452	ASN	2.2
2	F	175	LEU	2.2
2	B	126	GLN	2.1
1	E	424	ALA	2.1
2	J	209	ILE	2.1
1	I	309	PRO	2.1
2	B	2	ARG	2.1
1	E	526	THR	2.1
2	F	207	HIS	2.1
1	A	523	ALA	2.1
2	B	45	LYS	2.1
1	E	516	LEU	2.1
4	D	43	LEU	2.1
3	K	97	GLY	2.1
1	I	278	PRO	2.0
2	B	84	GLN	2.0
2	F	64	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	111	ASP	2.0
1	I	281	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
6	TEO	I	1589	9/9	0.94	0.12	45,46,49,51	0
6	TEO	A	1589	9/9	0.95	0.10	36,40,42,46	0
13	CBE	G	1130	16/16	0.95	0.12	34,38,41,41	0
7	NA	I	1590	1/1	0.96	0.05	29,29,29,29	0
11	F3S	F	304	7/7	0.96	0.07	32,34,35,36	0
13	CBE	C	1130	16/16	0.96	0.14	37,39,42,43	0
6	TEO	E	1589	9/9	0.96	0.12	32,35,37,40	0
13	CBE	K	1130	16/16	0.96	0.13	39,44,47,47	0
8	SO4	I	1591	5/5	0.97	0.23	58,59,60,62	0
11	F3S	B	304	7/7	0.97	0.07	31,32,34,37	0
7	NA	E	1590	1/1	0.97	0.05	24,24,24,24	0
11	F3S	J	304	7/7	0.97	0.07	32,35,37,38	0
12	HEM	C	1129	43/43	0.97	0.14	36,40,53,57	0
12	HEM	G	1129	43/43	0.97	0.12	36,41,52,57	0
12	HEM	K	1129	43/43	0.97	0.11	42,46,57,63	0
5	FAD	I	601	53/53	0.97	0.09	29,33,41,43	0
8	SO4	A	1591	5/5	0.97	0.22	70,70,71,71	0
8	SO4	E	1591	5/5	0.97	0.24	66,66,68,69	0
5	FAD	A	601	53/53	0.98	0.09	21,29,34,37	0
5	FAD	E	601	53/53	0.98	0.10	25,30,38,40	0
9	FES	B	302	4/4	0.98	0.05	29,29,31,31	0

Continued on next page...

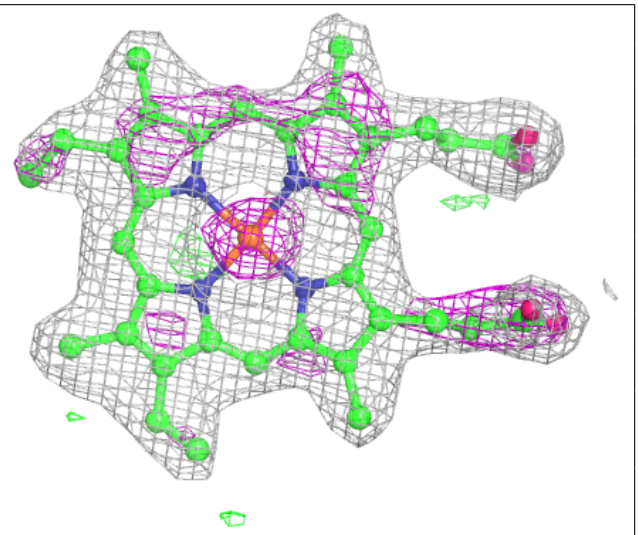
Continued from previous page...

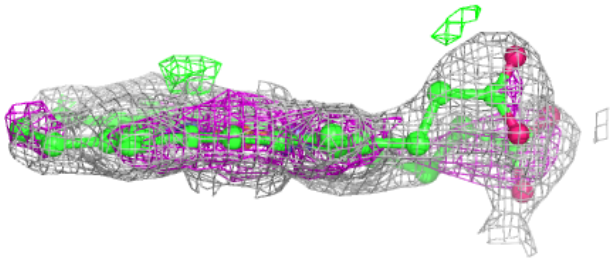
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	FES	F	302	4/4	0.98	0.06	28,28,29,31	0
9	FES	J	302	4/4	0.98	0.07	30,32,32,33	0
10	SF4	B	303	8/8	0.98	0.06	28,29,33,33	0
10	SF4	J	303	8/8	0.98	0.06	30,32,34,36	0
7	NA	A	1590	1/1	0.98	0.06	22,22,22,22	0
10	SF4	F	303	8/8	0.99	0.05	30,31,32,33	0

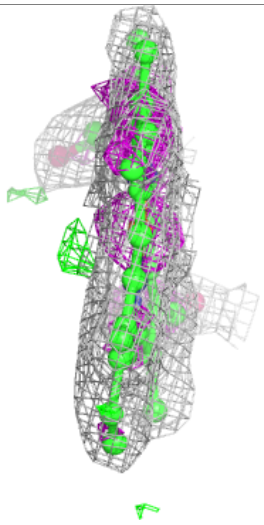
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

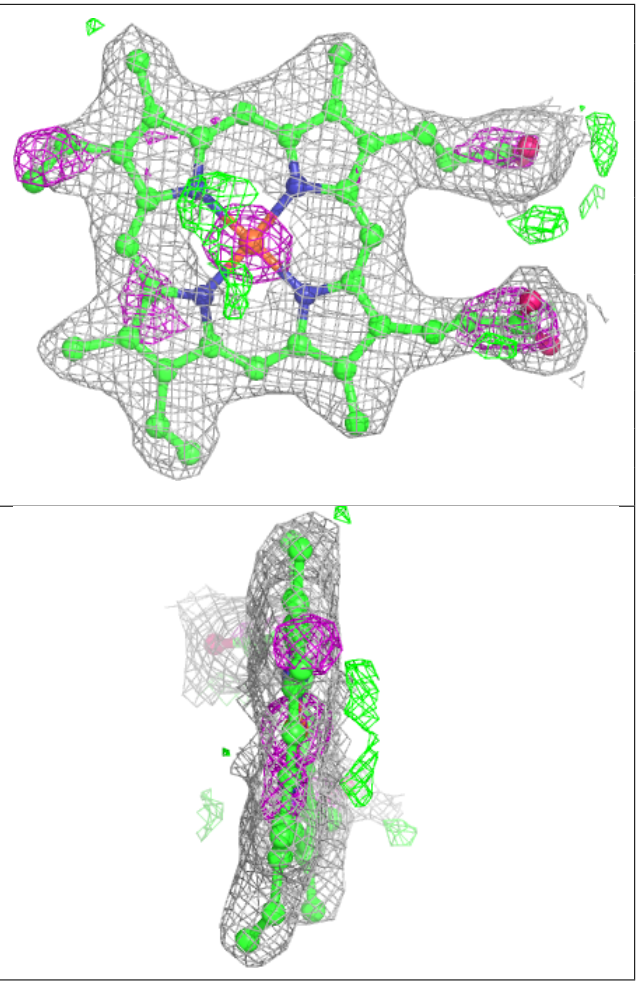






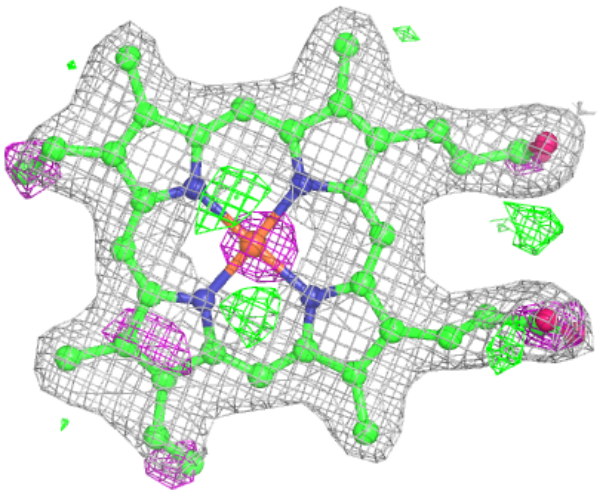
Electron density around HEM G 1129:

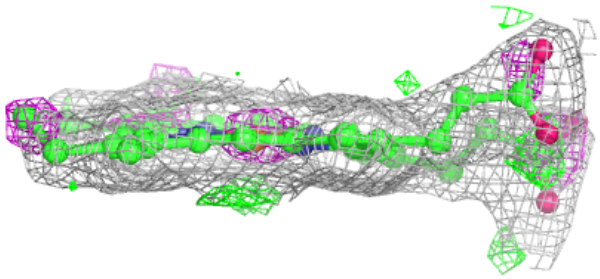
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

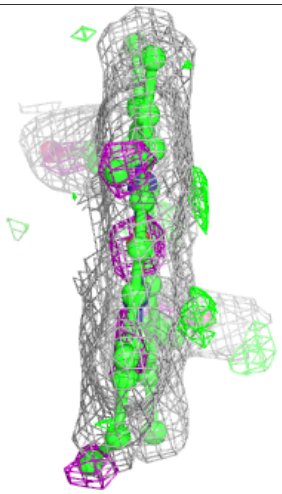


Electron density around HEM K 1129:

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

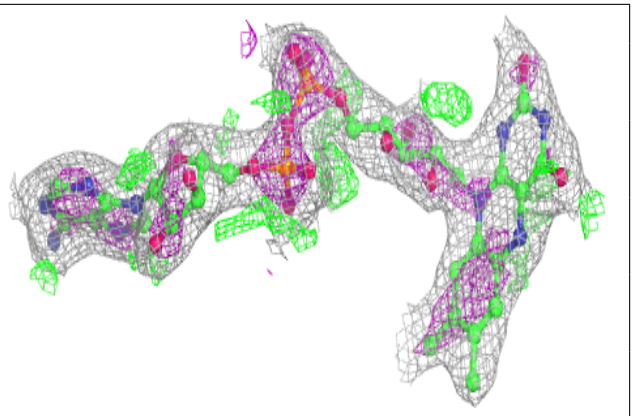


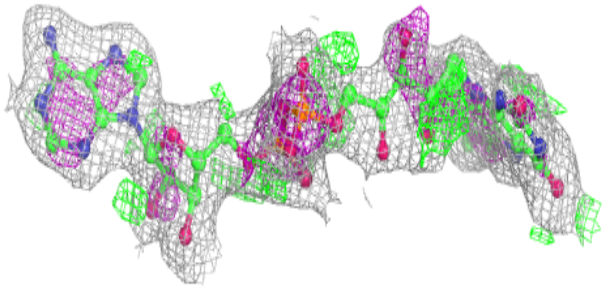


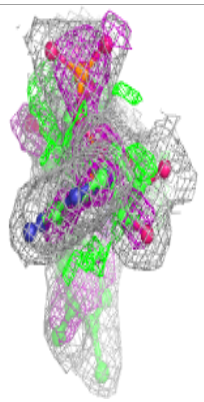


Electron density around FAD I 601:

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

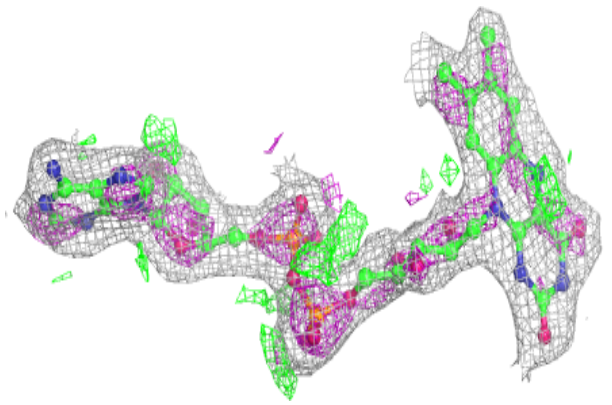


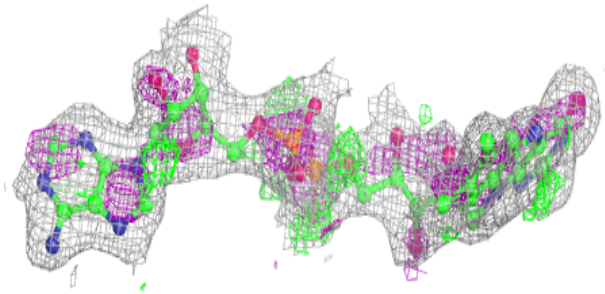


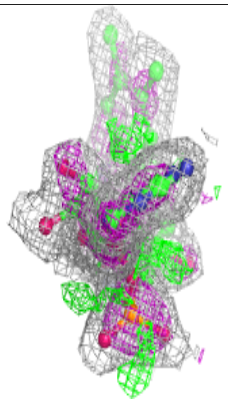


Electron density around FAD A 601:

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

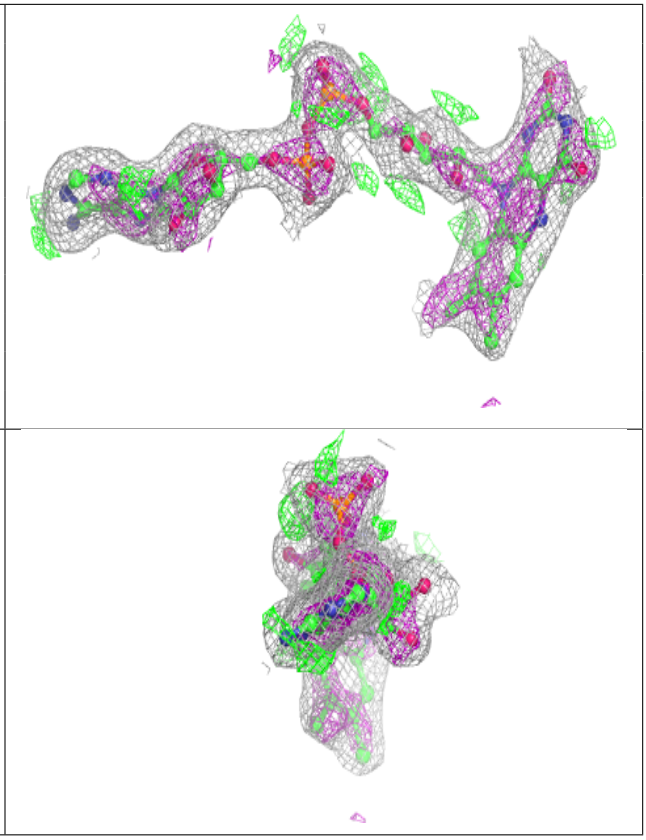






Electron density around FAD E 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.