Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:01 AM EDT

PDB ID	:	2WU5
Title	:	Crystal structure of the E. coli succinate:quinone oxidoreductase (SQR) SdhD His71Met mutant
Authors	:	Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on	:	2009-09-29
Resolution	:	2.80 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:

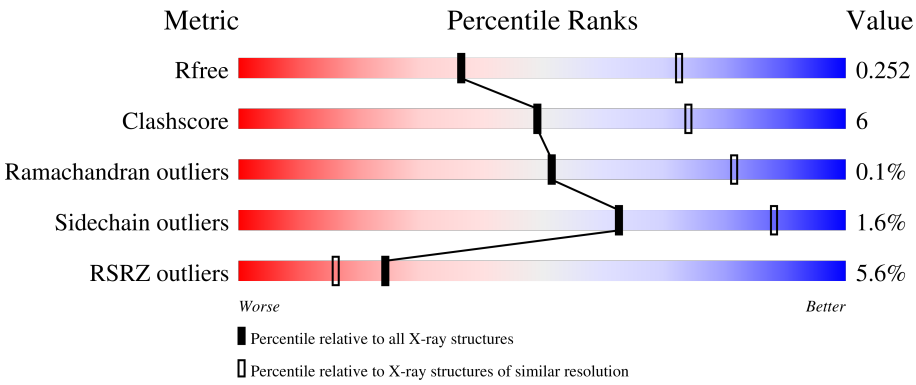
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	588	% 85% 15%
1	E	588	3% 86% 14%
1	I	588	10% 85% 15%
2	B	238	4% 85% 14%
2	F	238	2% 86% 14%

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Mol	Chain	Length	Quality of chain
2	J	238	6% 86% 14%
3	C	129	6% 80% 15% 5%
3	G	129	6% 81% 14% 5%
3	K	129	19% 81% 14% 5%
4	D	115	3% 81% 10% • 9%
4	H	115	9% 83% 8% • 9%
4	L	115	10% 83% 8% • 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	I	1589	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 25164 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	122	948	630	153	160	5	0	0	0
3	G	122	948	630	153	160	5	0	0	0
3	K	122	948	630	153	160	5	0	0	0

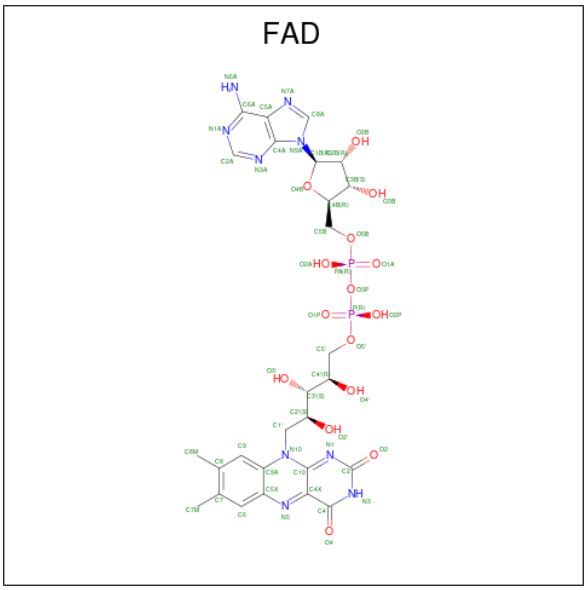
- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	105	834	576	121	133	4	0	0	0
4	H	105	834	576	121	133	4	0	0	0
4	L	105	834	576	121	133	4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

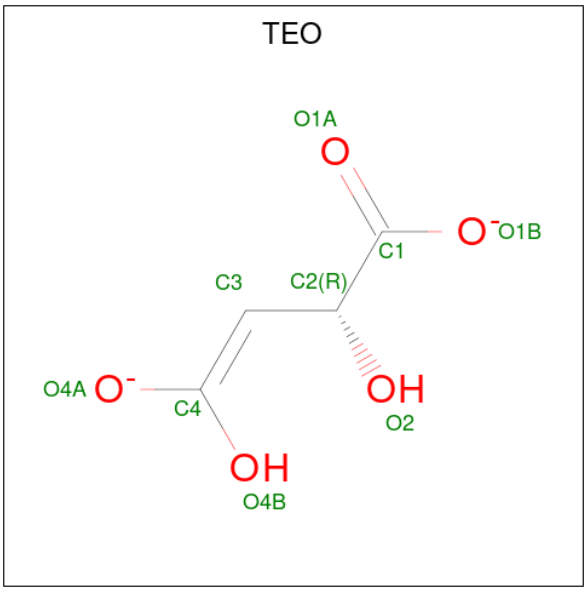
Chain	Residue	Modelled	Actual	Comment	Reference
D	71	MET	HIS	engineered mutation	UNP P0AC44
H	71	MET	HIS	engineered mutation	UNP P0AC44
L	71	MET	HIS	engineered mutation	UNP P0AC44

- 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
5	E	1	53	27	9	15	2	0	0
5	I	1	53	27	9	15	2	0	0

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

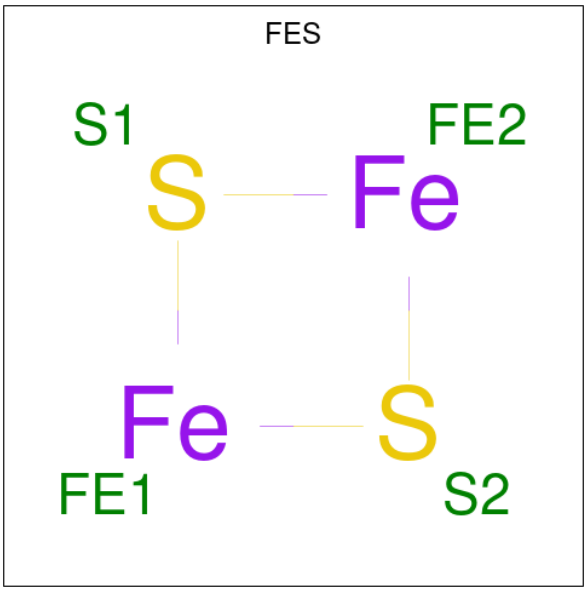


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 4 5	0	0
6	E	1	Total C O 9 4 5	0	0
6	I	1	Total C O 9 4 5	0	0

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

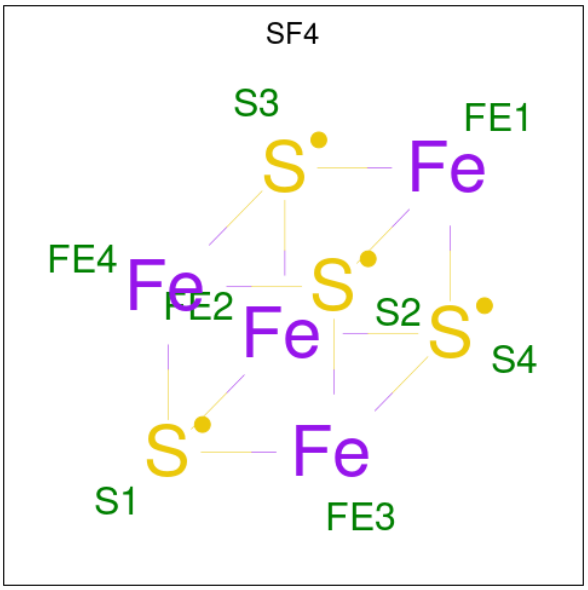
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0
7	I	1	Total Na 1 1	0	0

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	8	4	4	0	0

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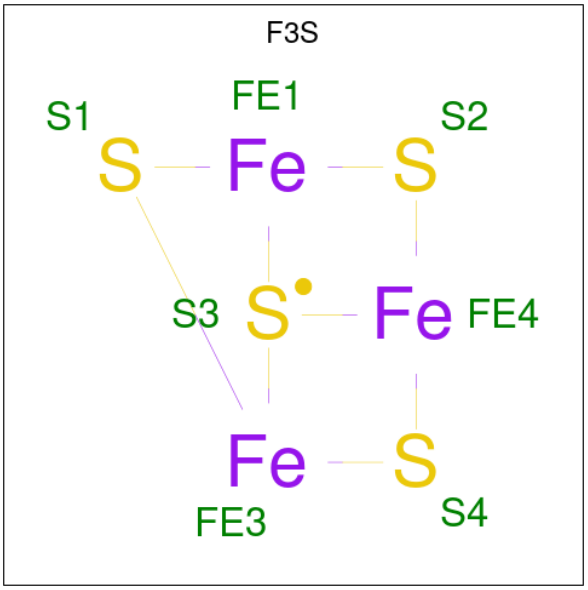
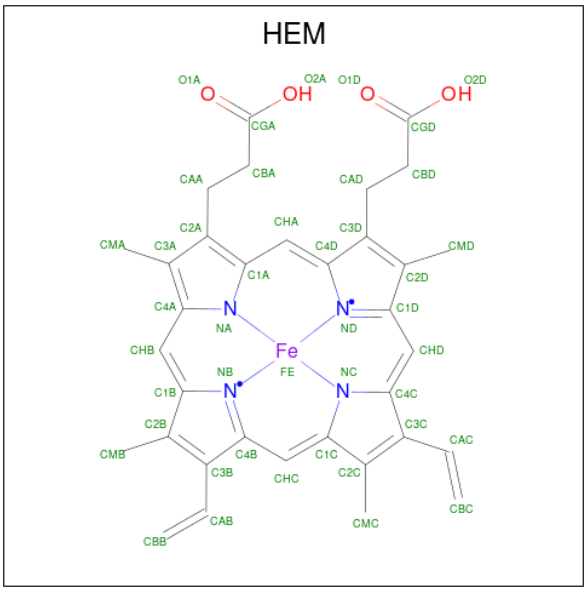
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	F	1	8	4	4	0	0
			Total	Fe	S		
9	J	1	8	4	4	0	0

- Molecule 10 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



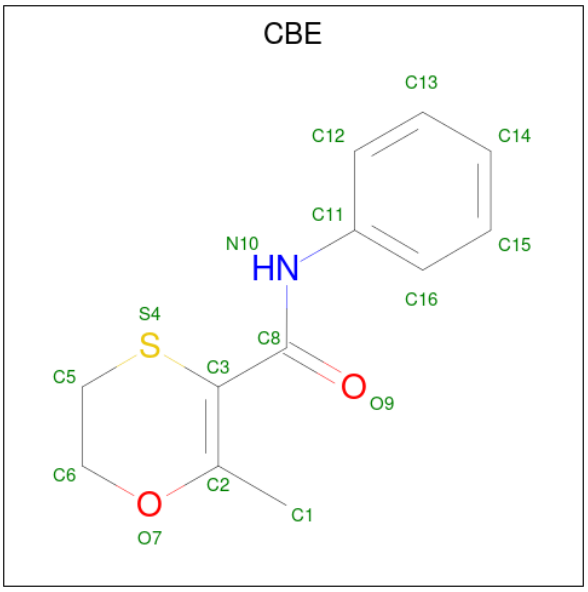
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
10	B	1	7	3	4	0	0
			Total	Fe	S		
10	F	1	7	3	4	0	0
			Total	Fe	S		
10	J	1	7	3	4	0	0

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



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

- Molecule 12 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		
12	C	1	16	12	1	2	1	0	0
			Total	C	N	O	S		
12	G	1	16	12	1	2	1	0	0
			Total	C	N	O	S		
12	K	1	16	12	1	2	1	0	0

- Molecule 13 is water.

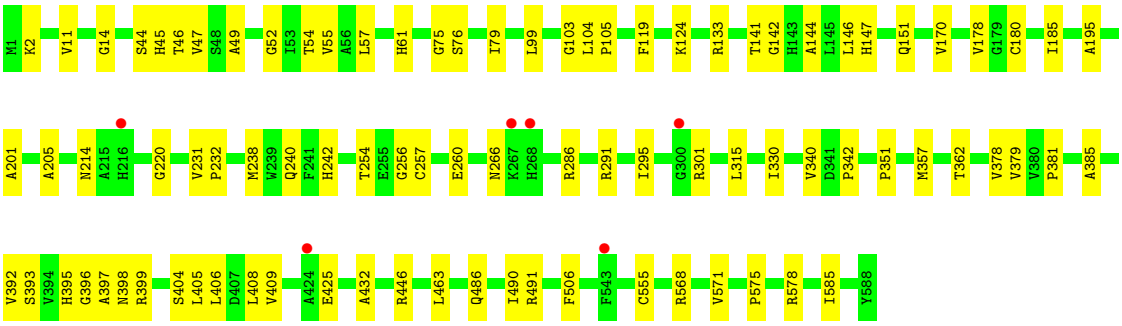
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	66	66	66	0	0
			Total	O		
13	B	33	33	33	0	0
			Total	O		
13	C	6	6	6	0	0
			Total	O		
13	D	2	2	2	0	0
			Total	O		
13	E	36	36	36	0	0
			Total	O		
13	F	28	28	28	0	0
			Total	O		
13	G	8	8	8	0	0
			Total	O		
13	H	2	2	2	0	0
			Total	O		
13	I	23	23	23	0	0
			Total	O		
13	J	15	15	15	0	0
			Total	O		
13	K	2	2	2	0	0
			Total	O		
13	L	1	1	1	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.

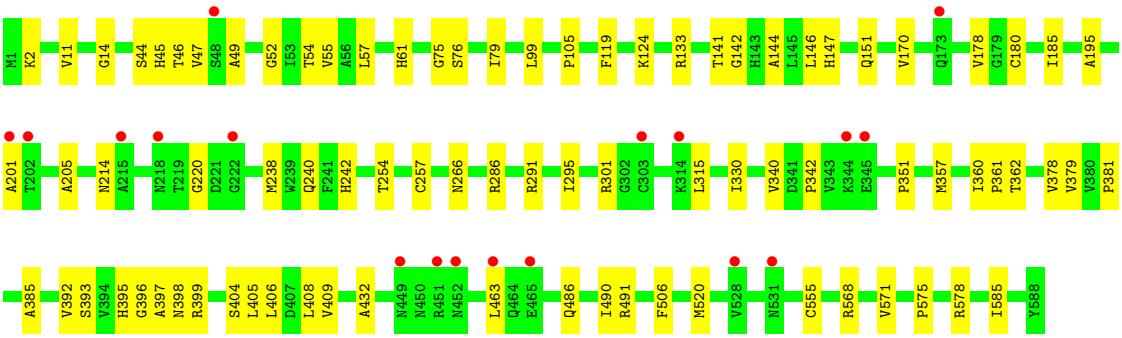
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain A:



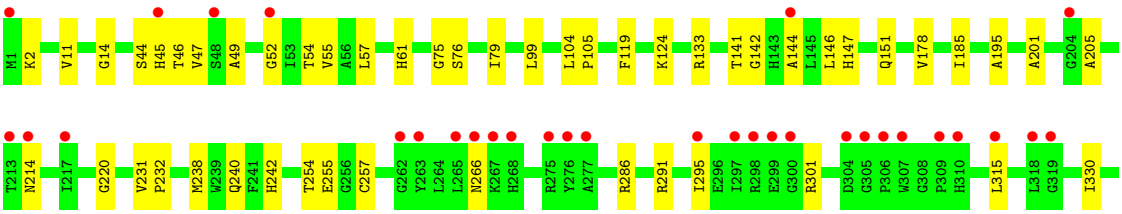
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

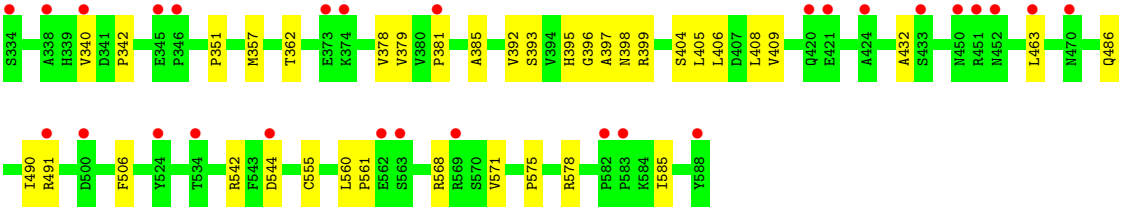
Chain E:



• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

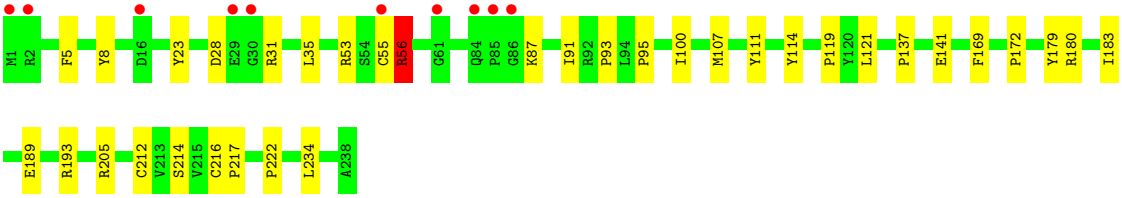
Chain I:





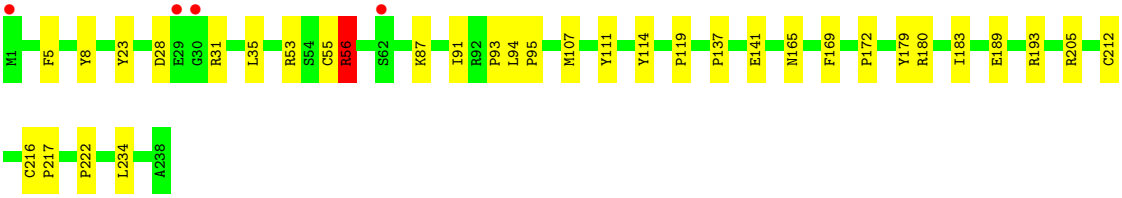
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain B:



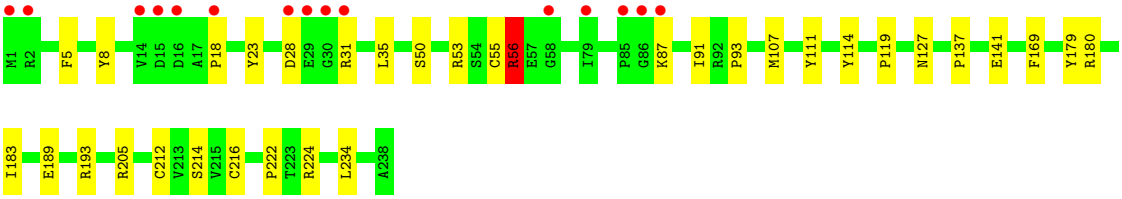
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain F:



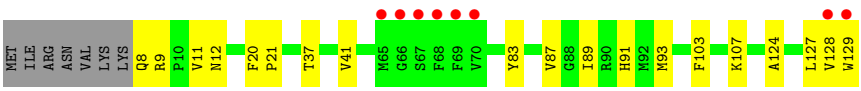
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain J:



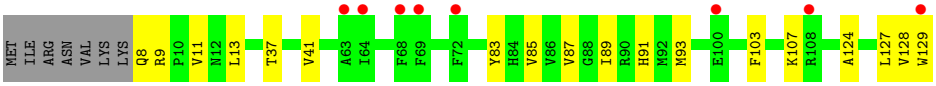
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain C:



• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain G:

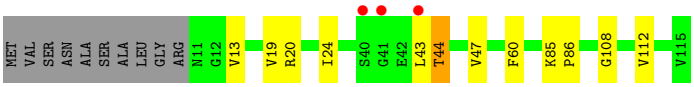


• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain K:

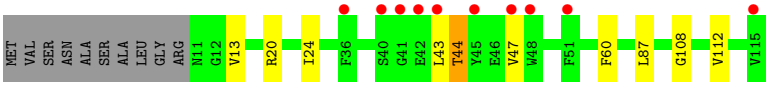
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT

Chain D:



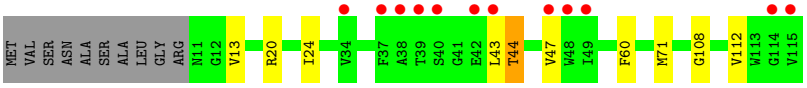
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT

Chain H:



• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN 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	120.06Å 183.82Å 203.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.83 – 2.80 48.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.83-2.80) 99.8 (48.79-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.252 0.215 , 0.252	Depositor DCC
R_{free} test set	5613 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	25164	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: NA, TEO, SF4, HEM, FAD, F3S, FES, CBE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.21	0/4611	0.38	0/6237
1	E	0.21	0/4611	0.38	0/6237
1	I	0.21	0/4611	0.38	0/6237
2	B	0.21	0/1908	0.37	0/2578
2	F	0.21	0/1908	0.37	0/2578
2	J	0.21	0/1908	0.37	0/2578
3	C	0.22	0/970	0.36	0/1316
3	G	0.22	0/970	0.36	0/1316
3	K	0.22	0/970	0.36	0/1316
4	D	0.23	0/856	0.35	0/1170
4	H	0.23	0/856	0.35	0/1170
4	L	0.27	0/856	0.36	0/1170
All	All	0.22	0/25035	0.37	0/33903

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4522	0	4426	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4522	0	4426	54	0
1	I	4522	0	4426	55	0
2	B	1869	0	1850	22	0
2	F	1869	0	1850	19	0
2	J	1869	0	1850	21	0
3	C	948	0	989	12	0
3	G	948	0	989	10	0
3	K	948	0	989	12	0
4	D	834	0	877	6	0
4	H	834	0	877	5	0
4	L	834	0	877	5	0
5	A	53	0	30	8	0
5	E	53	0	29	7	0
5	I	53	0	29	8	0
6	A	9	0	2	3	0
6	E	9	0	3	3	0
6	I	9	0	3	5	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
8	B	4	0	0	0	0
8	F	4	0	0	0	0
8	J	4	0	0	0	0
9	B	8	0	0	0	0
9	F	8	0	0	0	0
9	J	8	0	0	1	0
10	B	7	0	0	1	0
10	F	7	0	0	1	0
10	J	7	0	0	0	0
11	C	43	0	30	6	0
11	G	43	0	30	4	0
11	K	43	0	30	4	0
12	C	16	0	13	2	0
12	G	16	0	13	1	0
12	K	16	0	13	3	0
13	A	66	0	0	3	0
13	B	33	0	0	0	0
13	C	6	0	0	0	0
13	D	2	0	0	0	0
13	E	36	0	0	0	0
13	F	28	0	0	1	0
13	G	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	H	2	0	0	0	0
13	I	23	0	0	1	0
13	J	15	0	0	2	0
13	K	2	0	0	1	0
13	L	1	0	0	0	0
All	All	25164	0	24651	292	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.

All (292) 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)
11:G:305:HEM:HBC2	11:G:305:HEM:HHD	1.49	0.93
11:C:305:HEM:HHD	11:C:305:HEM:HBC2	1.52	0.90
11:K:305:HEM:HBC2	11:K:305:HEM:HHD	1.53	0.89
11:K:305:HEM:HHC	11:K:305:HEM:HBB2	1.54	0.89
11:G:305:HEM:HHC	11:G:305:HEM:HBB2	1.53	0.88
11:C:305:HEM:HHC	11:C:305:HEM:HBB2	1.53	0.87
1:A:555:CYS:HA	1:A:571:VAL:HG23	1.63	0.81
1:E:555:CYS:HA	1:E:571:VAL:HG23	1.63	0.80
1:I:555:CYS:HA	1:I:571:VAL:HG23	1.63	0.80
1:E:49:ALA:HB3	1:E:142:GLY:HA3	1.69	0.75
1:I:49:ALA:HB3	1:I:142:GLY:HA3	1.69	0.74
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.69	0.73
2:J:50:SER:HA	13:J:2002:HOH:O	1.92	0.69
2:B:55:CYS:O	2:B:56:ARG:HD3	1.94	0.68
2:F:55:CYS:O	2:F:56:ARG:HD3	1.94	0.67
12:K:1130:CBE:H16	12:K:1130:CBE:O9	1.94	0.67
1:I:392:VAL:N	1:I:393:SER:HA	2.10	0.67
2:J:55:CYS:O	2:J:56:ARG:HD3	1.94	0.67
1:E:392:VAL:N	1:E:393:SER:HA	2.10	0.66
1:E:76:SER:HB2	1:E:396:GLY:HA3	1.77	0.66
1:E:555:CYS:SG	1:E:568:ARG:HD2	2.36	0.66
1:A:76:SER:HB2	1:A:396:GLY:HA3	1.78	0.66
1:E:286:ARG:HH22	6:E:1589:TEO:C3	2.09	0.66
1:A:555:CYS:SG	1:A:568:ARG:HD2	2.36	0.65
1:I:76:SER:HB2	1:I:396:GLY:HA3	1.77	0.65
1:I:408:LEU:HD11	5:I:601:FAD:H4'	1.78	0.65
1:I:555:CYS:SG	1:I:568:ARG:HD2	2.36	0.65
1:A:392:VAL:N	1:A:393:SER:HA	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:PRO:HD2	1:E:144:ALA:HB1	1.80	0.64
1:I:105:PRO:HD2	1:I:144:ALA:HB1	1.80	0.64
2:J:114:TYR:O	2:J:119:PRO:HG3	1.99	0.63
1:A:105:PRO:HD2	1:A:144:ALA:HB1	1.80	0.63
2:B:114:TYR:O	2:B:119:PRO:HG3	1.99	0.62
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.35	0.62
2:J:169:PHE:CD1	2:J:205:ARG:HB2	2.35	0.62
1:I:99:LEU:HD11	1:I:409:VAL:HG21	1.81	0.62
2:F:114:TYR:O	2:F:119:PRO:HG3	1.99	0.61
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.35	0.61
1:A:99:LEU:HD11	1:A:409:VAL:HG21	1.81	0.61
1:E:99:LEU:HD11	1:E:409:VAL:HG21	1.81	0.61
3:K:127:LEU:O	3:K:127:LEU:HD23	2.01	0.60
2:F:234:LEU:HD23	4:H:13:VAL:HG13	1.82	0.60
3:G:127:LEU:HD23	3:G:127:LEU:O	2.01	0.60
1:E:408:LEU:HD11	5:E:601:FAD:H4'	1.82	0.60
1:I:49:ALA:HA	5:I:601:FAD:C5X	2.31	0.60
1:A:2:LYS:O	1:A:2:LYS:HD3	2.02	0.60
3:C:127:LEU:HD23	3:C:127:LEU:O	2.01	0.59
1:E:2:LYS:O	1:E:2:LYS:HD3	2.02	0.59
1:I:2:LYS:O	1:I:2:LYS:HD3	2.03	0.59
2:F:56:ARG:HG2	2:F:56:ARG:O	2.03	0.59
2:J:56:ARG:O	2:J:56:ARG:HG2	2.02	0.59
1:I:286:ARG:HH22	6:I:1589:TEO:C3	2.16	0.59
2:B:56:ARG:O	2:B:56:ARG:HG2	2.02	0.59
5:I:601:FAD:N5	6:I:1589:TEO:H2	2.18	0.59
2:B:172:PRO:HG3	10:B:304:F3S:S3	2.43	0.58
1:A:405:LEU:HG	5:A:601:FAD:C2	2.34	0.57
12:C:1130:CBE:H16	12:C:1130:CBE:O9	2.04	0.57
2:J:127:ASN:HA	13:J:2007:HOH:O	2.04	0.57
2:F:172:PRO:HG3	10:F:304:F3S:S3	2.45	0.56
1:I:49:ALA:HA	5:I:601:FAD:N5	2.21	0.56
1:A:286:ARG:HH22	6:A:1589:TEO:C3	2.18	0.56
1:I:49:ALA:HB3	1:I:142:GLY:CA	2.36	0.56
2:J:28:ASP:HB3	2:J:31:ARG:HB3	1.88	0.56
1:A:408:LEU:HD11	5:A:601:FAD:H4'	1.88	0.55
2:F:28:ASP:HB3	2:F:31:ARG:HB3	1.88	0.55
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.89	0.55
2:B:28:ASP:HB3	2:B:31:ARG:HB3	1.88	0.54
5:I:601:FAD:C4	6:I:1589:TEO:C3	2.86	0.54
1:A:49:ALA:HB3	1:A:142:GLY:CA	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HD11	2:B:91:ILE:HD11	1.89	0.54
1:E:575:PRO:HB2	1:E:578:ARG:O	2.08	0.54
1:A:425:GLU:HG2	13:A:2049:HOH:O	2.06	0.54
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.89	0.54
1:A:379:VAL:O	1:A:381:PRO:HD3	2.08	0.54
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.89	0.54
5:A:601:FAD:N5	6:A:1589:TEO:H2	2.23	0.54
1:E:49:ALA:HB3	1:E:142:GLY:CA	2.36	0.54
1:I:379:VAL:O	1:I:381:PRO:HD3	2.08	0.54
1:E:286:ARG:HH22	6:E:1589:TEO:C4	2.21	0.54
1:E:49:ALA:HA	5:E:601:FAD:N5	2.24	0.53
1:A:575:PRO:HB2	1:A:578:ARG:O	2.08	0.53
1:E:379:VAL:O	1:E:381:PRO:HD3	2.08	0.53
2:F:35:LEU:HD11	2:F:91:ILE:HD11	1.90	0.53
2:J:35:LEU:HD11	2:J:91:ILE:HD11	1.90	0.53
1:I:575:PRO:HB2	1:I:578:ARG:O	2.08	0.53
1:E:486:GLN:O	1:E:490:ILE:HG13	2.10	0.52
1:I:486:GLN:O	1:I:490:ILE:HG13	2.10	0.52
2:J:5:PHE:HB2	2:J:23:TYR:HB2	1.91	0.52
1:I:405:LEU:HG	5:I:601:FAD:C2	2.40	0.51
2:B:5:PHE:HB2	2:B:23:TYR:HB2	1.91	0.51
2:F:5:PHE:HB2	2:F:23:TYR:HB2	1.91	0.51
1:E:49:ALA:HA	5:E:601:FAD:C5X	2.40	0.51
1:A:49:ALA:HA	5:A:601:FAD:C5X	2.40	0.51
1:A:178:VAL:HG21	1:A:432:ALA:HB2	1.93	0.50
1:A:486:GLN:O	1:A:490:ILE:HG13	2.10	0.50
4:D:44:THR:HG23	4:D:47:VAL:HG22	1.93	0.50
2:F:212:CYS:HB2	2:F:222:PRO:HG2	1.94	0.50
1:I:178:VAL:HG21	1:I:432:ALA:HB2	1.93	0.50
1:A:238:MET:O	1:A:357:MET:HB2	2.12	0.50
2:B:212:CYS:HB2	2:B:222:PRO:HG2	1.94	0.50
11:C:305:HEM:HBB2	11:C:305:HEM:CHC	2.30	0.50
1:E:238:MET:O	1:E:357:MET:HB2	2.12	0.50
1:E:178:VAL:HG21	1:E:432:ALA:HB2	1.93	0.50
2:B:100:ILE:HG12	3:C:9:ARG:NH1	2.26	0.49
4:L:44:THR:HG23	4:L:47:VAL:HG22	1.94	0.49
3:C:103:PHE:CE2	3:C:107:LYS:HE3	2.47	0.49
4:H:44:THR:HG23	4:H:47:VAL:HG22	1.93	0.49
1:I:45:HIS:CE1	1:I:214:ASN:HA	2.47	0.49
2:J:212:CYS:HB2	2:J:222:PRO:HG2	1.93	0.49
2:B:95:PRO:HA	3:C:12:ASN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:HA	5:A:601:FAD:N5	2.27	0.49
1:E:240:GLN:HB2	1:E:357:MET:SD	2.53	0.49
1:I:147:HIS:O	1:I:151:GLN:HG3	2.13	0.49
11:K:305:HEM:HBB2	11:K:305:HEM:CHC	2.32	0.49
1:E:45:HIS:CE1	1:E:214:ASN:HA	2.47	0.49
1:A:240:GLN:HB2	1:A:357:MET:SD	2.53	0.49
3:C:128:VAL:HG12	3:C:128:VAL:O	2.12	0.49
1:E:79:ILE:HD11	1:E:397:ALA:HB2	1.95	0.49
1:E:242:HIS:O	1:E:351:PRO:HA	2.13	0.49
5:E:601:FAD:C4	6:E:1589:TEO:C3	2.91	0.49
1:A:45:HIS:CE1	1:A:214:ASN:HA	2.47	0.48
1:A:147:HIS:O	1:A:151:GLN:HG3	2.12	0.48
1:A:242:HIS:O	1:A:351:PRO:HA	2.13	0.48
1:I:238:MET:O	1:I:357:MET:HB2	2.12	0.48
1:E:185:ILE:O	1:E:506:PHE:HA	2.14	0.48
3:K:37:THR:O	3:K:41:VAL:HG23	2.13	0.48
1:A:46:THR:HB	1:A:146:LEU:HD13	1.96	0.48
1:A:185:ILE:O	1:A:506:PHE:HA	2.13	0.48
3:G:103:PHE:CE2	3:G:107:LYS:HE3	2.48	0.48
12:G:1130:CBE:O9	12:G:1130:CBE:H16	2.12	0.48
1:I:242:HIS:O	1:I:351:PRO:HA	2.13	0.48
2:J:234:LEU:HD23	4:L:13:VAL:HG13	1.95	0.48
3:K:103:PHE:CE2	3:K:107:LYS:HE3	2.47	0.48
3:K:128:VAL:HG12	3:K:128:VAL:O	2.12	0.48
3:C:37:THR:O	3:C:41:VAL:HG23	2.13	0.48
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.48	0.48
1:A:79:ILE:HD11	1:A:397:ALA:HB2	1.96	0.48
3:G:85:VAL:HG22	11:G:305:HEM:HMC3	1.94	0.48
1:A:446:ARG:NE	13:A:2053:HOH:O	2.46	0.48
2:F:179:TYR:O	2:F:183:ILE:HG13	2.14	0.48
1:I:240:GLN:HB2	1:I:357:MET:SD	2.53	0.48
12:K:1130:CBE:O9	12:K:1130:CBE:C16	2.55	0.48
3:G:37:THR:O	3:G:41:VAL:HG23	2.13	0.48
1:I:185:ILE:O	1:I:506:PHE:HA	2.13	0.48
3:G:128:VAL:HG12	3:G:128:VAL:O	2.12	0.48
2:J:179:TYR:O	2:J:183:ILE:HG13	2.14	0.48
3:K:83:TYR:CZ	3:K:87:VAL:HG21	2.48	0.48
3:G:83:TYR:CZ	3:G:87:VAL:HG21	2.48	0.48
1:I:52:GLY:HA2	1:I:141:THR:HG21	1.96	0.48
2:B:179:TYR:O	2:B:183:ILE:HG13	2.14	0.47
1:E:147:HIS:O	1:E:151:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:SER:HB3	5:A:601:FAD:N1	2.29	0.47
1:E:405:LEU:HG	5:E:601:FAD:C2	2.44	0.47
1:A:446:ARG:NH2	13:A:2053:HOH:O	2.48	0.47
1:I:46:THR:HB	1:I:146:LEU:HD13	1.97	0.47
1:I:79:ILE:HD11	1:I:397:ALA:HB2	1.95	0.47
1:E:52:GLY:HA2	1:E:141:THR:HG21	1.96	0.47
1:A:395:HIS:ND1	1:A:399:ARG:HG3	2.30	0.46
1:E:46:THR:HB	1:E:146:LEU:HD13	1.96	0.46
5:A:601:FAD:C4	6:A:1589:TEO:C3	2.93	0.46
1:E:395:HIS:ND1	1:E:399:ARG:HG3	2.30	0.46
12:C:1130:CBE:O9	12:C:1130:CBE:C16	2.63	0.46
1:E:14:GLY:HA3	1:E:201:ALA:O	2.16	0.46
6:I:1589:TEO:O4B	6:I:1589:TEO:O2	2.28	0.46
1:A:14:GLY:HA3	1:A:201:ALA:O	2.16	0.46
11:G:305:HEM:HBB2	11:G:305:HEM:CHC	2.32	0.46
5:A:601:FAD:H9	5:A:601:FAD:H1'1	1.76	0.46
1:A:52:GLY:HA2	1:A:141:THR:HG21	1.96	0.46
11:C:305:HEM:HBC2	11:C:305:HEM:CHD	2.31	0.46
1:E:14:GLY:HA2	5:E:601:FAD:H1B	1.98	0.46
1:I:14:GLY:HA3	1:I:201:ALA:O	2.16	0.46
4:L:108:GLY:O	4:L:112:VAL:HG22	2.17	0.45
1:I:395:HIS:ND1	1:I:399:ARG:HG3	2.30	0.45
3:K:107:LYS:HD2	13:K:2001:HOH:O	2.16	0.45
3:C:8:GLN:HG2	3:C:9:ARG:N	2.32	0.45
1:A:54:THR:HG23	1:A:133:ARG:HG3	1.98	0.45
4:D:108:GLY:O	4:D:112:VAL:HG22	2.16	0.45
3:G:8:GLN:HG2	3:G:9:ARG:N	2.32	0.45
1:E:54:THR:HG23	1:E:133:ARG:HG3	1.98	0.45
1:E:214:ASN:N	1:E:214:ASN:HD22	2.14	0.45
3:G:13:LEU:HD12	3:G:13:LEU:HA	1.87	0.45
1:I:254:THR:HG22	1:I:330:ILE:HG21	1.99	0.45
2:B:234:LEU:HB3	4:H:87:LEU:HD21	1.99	0.45
4:H:108:GLY:O	4:H:112:VAL:HG22	2.16	0.45
1:A:214:ASN:HD22	1:A:214:ASN:N	2.14	0.44
1:I:231:VAL:HA	1:I:232:PRO:HD3	1.84	0.44
2:J:216:CYS:HA	9:J:303:SF4:S4	2.57	0.44
3:K:28:ILE:HA	12:K:1130:CBE:S4	2.57	0.44
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.99	0.44
2:B:107:MET:HB2	2:B:111:TYR:CE2	2.52	0.44
1:I:54:THR:HG23	1:I:133:ARG:HG3	1.98	0.44
1:E:266:ASN:HB2	1:E:301:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:SER:O	1:A:408:LEU:HG	2.18	0.44
2:J:107:MET:HB2	2:J:111:TYR:CE2	2.53	0.44
2:J:214:SER:HB3	3:K:103:PHE:CZ	2.52	0.44
1:A:254:THR:HG22	1:A:330:ILE:HG21	2.00	0.43
1:I:266:ASN:HB2	1:I:301:ARG:O	2.18	0.43
2:J:8:TYR:CG	2:J:93:PRO:HD3	2.53	0.43
3:K:8:GLN:HG2	3:K:9:ARG:N	2.32	0.43
1:E:55:VAL:HG13	1:E:57:LEU:HG	1.99	0.43
1:I:404:SER:O	1:I:408:LEU:HG	2.18	0.43
1:A:104:LEU:HA	1:A:105:PRO:HD3	1.78	0.43
1:I:214:ASN:N	1:I:214:ASN:HD22	2.14	0.43
1:E:61:HIS:CE1	1:E:124:LYS:HE2	2.54	0.43
1:E:404:SER:O	1:E:408:LEU:HG	2.18	0.43
1:I:55:VAL:HG13	1:I:57:LEU:HG	1.99	0.43
1:I:340:VAL:O	1:I:342:PRO:HD3	2.19	0.43
2:B:216:CYS:HA	2:B:217:PRO:HD2	1.91	0.43
1:E:254:THR:HG22	1:E:330:ILE:HG21	1.99	0.43
2:F:107:MET:HB2	2:F:111:TYR:CE2	2.53	0.43
2:B:214:SER:HB3	3:C:103:PHE:CZ	2.52	0.43
1:E:340:VAL:O	1:E:342:PRO:HD3	2.19	0.43
2:F:8:TYR:CG	2:F:93:PRO:HD3	2.54	0.43
1:I:286:ARG:HH22	6:I:1589:TEO:C4	2.31	0.43
1:A:257:CYS:HB3	1:A:315:LEU:HD21	2.01	0.43
1:A:340:VAL:O	1:A:342:PRO:HD3	2.18	0.43
1:E:75:GLY:O	1:E:398:ASN:HB3	2.19	0.43
1:I:75:GLY:O	1:I:398:ASN:HB3	2.18	0.43
1:A:54:THR:O	1:A:406:LEU:HD22	2.19	0.43
1:A:61:HIS:CE1	1:A:124:LYS:HE2	2.54	0.43
1:A:362:THR:HG21	1:A:385:ALA:HB3	2.01	0.43
2:B:189:GLU:O	2:B:193:ARG:HG3	2.19	0.43
11:C:305:HEM:HAD1	4:D:19:VAL:HG11	2.01	0.43
1:A:103:GLY:HA2	2:B:121:LEU:HD22	2.00	0.43
1:I:61:HIS:CE1	1:I:124:LYS:HE2	2.54	0.43
1:I:463:LEU:C	1:I:463:LEU:HD23	2.40	0.43
1:A:266:ASN:HB2	1:A:301:ARG:O	2.18	0.42
2:B:8:TYR:CG	2:B:93:PRO:HD3	2.54	0.42
1:E:257:CYS:HB3	1:E:315:LEU:HD21	2.01	0.42
3:G:89:ILE:O	3:G:93:MET:HG3	2.19	0.42
1:A:75:GLY:O	1:A:398:ASN:HB3	2.19	0.42
1:I:54:THR:O	1:I:406:LEU:HD22	2.19	0.42
1:I:255:GLU:HA	13:I:2015:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:362:THR:HG21	1:I:385:ALA:HB3	2.00	0.42
2:J:189:GLU:O	2:J:193:ARG:HG3	2.19	0.42
1:A:205:ALA:HB2	1:A:220:GLY:CA	2.49	0.42
1:A:231:VAL:HA	1:A:232:PRO:HD3	1.84	0.42
1:E:463:LEU:C	1:E:463:LEU:HD23	2.39	0.42
1:I:291:ARG:O	1:I:295:ILE:HG13	2.19	0.42
3:K:89:ILE:O	3:K:93:MET:HG3	2.19	0.42
1:E:205:ALA:HB2	1:E:220:GLY:HA3	2.02	0.42
2:F:189:GLU:O	2:F:193:ARG:HG3	2.19	0.42
1:I:104:LEU:HA	1:I:105:PRO:HD3	1.77	0.42
3:K:124:ALA:O	3:K:128:VAL:HG23	2.19	0.42
1:E:54:THR:O	1:E:406:LEU:HD22	2.19	0.42
4:H:20:ARG:O	4:H:24:ILE:HG13	2.20	0.42
1:I:205:ALA:HB2	1:I:220:GLY:CA	2.49	0.42
1:I:399:ARG:CZ	1:I:404:SER:HB2	2.50	0.42
1:E:205:ALA:HB2	1:E:220:GLY:CA	2.49	0.42
3:G:124:ALA:O	3:G:128:VAL:HG23	2.20	0.42
1:I:205:ALA:HB2	1:I:220:GLY:HA3	2.02	0.42
1:I:257:CYS:HB3	1:I:315:LEU:HD21	2.01	0.42
4:D:20:ARG:O	4:D:24:ILE:HG13	2.19	0.42
2:F:94:LEU:HA	2:F:95:PRO:HD3	1.85	0.42
1:A:463:LEU:HD23	1:A:463:LEU:C	2.39	0.42
1:I:44:SER:O	1:I:47:VAL:HG12	2.20	0.42
2:B:234:LEU:HD23	4:D:13:VAL:HG13	2.02	0.41
2:F:55:CYS:O	2:F:56:ARG:CD	2.66	0.41
4:L:20:ARG:O	4:L:24:ILE:HG13	2.20	0.41
1:E:520:MET:HB2	1:E:520:MET:HE2	1.94	0.41
11:K:305:HEM:C4B	4:L:71:MET:HG2	2.55	0.41
2:B:55:CYS:O	2:B:56:ARG:CD	2.66	0.41
1:E:408:LEU:HD11	5:E:601:FAD:C4'	2.49	0.41
11:C:305:HEM:HHD	11:C:305:HEM:CBC	2.38	0.41
1:E:362:THR:HG21	1:E:385:ALA:HB3	2.01	0.41
1:A:205:ALA:HB2	1:A:220:GLY:HA3	2.02	0.41
1:E:291:ARG:O	1:E:295:ILE:HG13	2.20	0.41
5:I:601:FAD:H1'1	5:I:601:FAD:H9	1.78	0.41
1:A:399:ARG:CZ	1:A:404:SER:HB2	2.50	0.41
3:C:89:ILE:O	3:C:93:MET:HG3	2.19	0.41
1:E:399:ARG:CZ	1:E:404:SER:HB2	2.50	0.41
2:F:165:ASN:HB2	13:F:2022:HOH:O	2.20	0.41
1:I:49:ALA:HA	5:I:601:FAD:C6	2.50	0.41
1:A:291:ARG:O	1:A:295:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:55:CYS:O	2:J:56:ARG:CD	2.66	0.41
3:C:124:ALA:O	3:C:128:VAL:HG23	2.20	0.41
1:E:44:SER:O	1:E:47:VAL:HG12	2.21	0.41
2:J:224:ARG:NH2	3:K:102:THR:HG22	2.36	0.41
1:A:44:SER:O	1:A:47:VAL:HG12	2.20	0.41
1:A:170:VAL:HG23	1:A:180:CYS:HA	2.03	0.41
2:J:137:PRO:O	2:J:141:GLU:HG3	2.21	0.41
1:A:256:GLY:O	1:A:260:GLU:HG2	2.21	0.40
1:E:360:ILE:HA	1:E:361:PRO:HD2	1.90	0.40
2:F:137:PRO:O	2:F:141:GLU:HG3	2.21	0.40
4:D:85:LYS:HB2	4:D:86:PRO:HD3	2.03	0.40
3:C:20:PHE:HA	3:C:21:PRO:HD3	1.90	0.40
1:I:542:ARG:HB3	1:I:544:ASP:OD1	2.22	0.40
1:I:560:LEU:HA	1:I:561:PRO:HD3	1.85	0.40
1:E:170:VAL:HG23	1:E:180:CYS:HA	2.03	0.40
2:J:8:TYR:CZ	2:J:18:PRO:HB3	2.56	0.40
2:B:137:PRO:O	2:B:141:GLU:HG3	2.21	0.40
2:F:216:CYS:HA	2:F:217:PRO:HD2	1.91	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%)	565 (96%)	21 (4%)	0	100	100
1	E	586/588 (100%)	565 (96%)	21 (4%)	0	100	100
1	I	586/588 (100%)	566 (97%)	20 (3%)	0	100	100
2	B	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	34	66
2	F	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	34	66
2	J	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	120/129 (93%)	120 (100%)	0	0	100	100
3	G	120/129 (93%)	120 (100%)	0	0	100	100
3	K	120/129 (93%)	120 (100%)	0	0	100	100
4	D	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
4	H	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
4	L	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
All	All	3135/3210 (98%)	3025 (96%)	107 (3%)	3 (0%)	51	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	ARG
2	F	56	ARG
2	J	56	ARG

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%)	469 (99%)	4 (1%)	81	94
1	E	473/473 (100%)	469 (99%)	4 (1%)	81	94
1	I	473/473 (100%)	469 (99%)	4 (1%)	81	94
2	B	208/208 (100%)	204 (98%)	4 (2%)	57	85
2	F	208/208 (100%)	204 (98%)	4 (2%)	57	85
2	J	208/208 (100%)	204 (98%)	4 (2%)	57	85
3	C	102/109 (94%)	99 (97%)	3 (3%)	42	76
3	G	102/109 (94%)	99 (97%)	3 (3%)	42	76
3	K	102/109 (94%)	99 (97%)	3 (3%)	42	76
4	D	88/96 (92%)	85 (97%)	3 (3%)	37	71
4	H	88/96 (92%)	85 (97%)	3 (3%)	37	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	88/96 (92%)	85 (97%)	3 (3%)	37	71
All	All	2613/2658 (98%)	2571 (98%)	42 (2%)	62	88

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	PHE
1	A	378	VAL
1	A	491	ARG
1	A	585	ILE
2	B	53	ARG
2	B	56	ARG
2	B	87	LYS
2	B	180	ARG
3	C	11	VAL
3	C	91	HIS
3	C	129	TRP
4	D	43	LEU
4	D	44	THR
4	D	60	PHE
1	E	119	PHE
1	E	378	VAL
1	E	491	ARG
1	E	585	ILE
2	F	53	ARG
2	F	56	ARG
2	F	87	LYS
2	F	180	ARG
3	G	11	VAL
3	G	91	HIS
3	G	129	TRP
4	H	43	LEU
4	H	44	THR
4	H	60	PHE
1	I	119	PHE
1	I	378	VAL
1	I	491	ARG
1	I	585	ILE
2	J	53	ARG
2	J	56	ARG
2	J	87	LYS
2	J	180	ARG

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Mol	Chain	Res	Type
3	K	11	VAL
3	K	91	HIS
3	K	129	TRP
4	L	43	LEU
4	L	44	THR
4	L	60	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	78	GLN
3	G	30	HIS
4	H	78	GLN
4	L	78	GLN

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 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
11	HEM	G	305	4,3	42,50,50	1.96	6 (14%)	46,82,82	1.63	6 (13%)
6	TEO	A	1589	-	5,8,8	3.43	2 (40%)	4,10,10	3.61	3 (75%)
6	TEO	E	1589	-	5,8,8	1.45	0	4,10,10	2.11	2 (50%)
5	FAD	I	601	1	54,58,58	1.20	5 (9%)	71,89,89	1.37	9 (12%)
11	HEM	K	305	4,3	42,50,50	1.99	7 (16%)	46,82,82	1.59	6 (13%)
8	FES	J	302	2	0,4,4	-	-	-		
9	SF4	F	303	2	0,12,12	-	-	-		
8	FES	F	302	2	0,4,4	-	-	-		
12	CBE	C	1130	-	16,17,17	1.11	1 (6%)	17,22,22	1.83	2 (11%)
12	CBE	K	1130	-	16,17,17	1.22	2 (12%)	17,22,22	1.57	2 (11%)
5	FAD	A	601	-	54,58,58	1.19	4 (7%)	71,89,89	1.40	8 (11%)
11	HEM	C	305	4,3	42,50,50	1.99	7 (16%)	46,82,82	1.59	6 (13%)
9	SF4	B	303	2	0,12,12	-	-	-		
10	F3S	B	304	2	0,9,9	-	-	-		
6	TEO	I	1589	-	5,8,8	1.02	0	4,10,10	2.06	1 (25%)
5	FAD	E	601	1	54,58,58	1.19	5 (9%)	71,89,89	1.41	10 (14%)
8	FES	B	302	2	0,4,4	-	-	-		
12	CBE	G	1130	-	16,17,17	1.18	1 (6%)	17,22,22	1.96	3 (17%)
9	SF4	J	303	2	0,12,12	-	-	-		
10	F3S	F	304	2	0,9,9	-	-	-		
10	F3S	J	304	2	0,9,9	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEM	G	305	4,3	-	3/12/54/54	-
6	TEO	A	1589	-	-	4/6/8/8	-
6	TEO	E	1589	-	-	2/6/8/8	-
5	FAD	I	601	1	-	4/30/50/50	0/6/6/6
11	HEM	K	305	4,3	-	4/12/54/54	-
9	SF4	F	303	2	-	-	0/6/5/5
8	FES	F	302	2	-	-	0/1/1/1
12	CBE	C	1130	-	-	1/6/19/19	0/2/2/2
12	CBE	K	1130	-	-	2/6/19/19	0/2/2/2
5	FAD	A	601	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEM	C	305	4,3	-	3/12/54/54	-
9	SF4	B	303	2	-	-	0/6/5/5
10	F3S	B	304	2	-	-	0/3/3/3
6	TEO	I	1589	-	-	3/6/8/8	-
5	FAD	E	601	1	-	2/30/50/50	0/6/6/6
8	FES	B	302	2	-	-	0/1/1/1
12	CBE	G	1130	-	-	1/6/19/19	0/2/2/2
9	SF4	J	303	2	-	-	0/6/5/5
8	FES	J	302	2	-	-	0/1/1/1
10	F3S	J	304	2	-	-	0/3/3/3
10	F3S	F	304	2	-	-	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	305	HEM	C3D-C2D	8.08	1.54	1.36
11	C	305	HEM	C3D-C2D	8.02	1.54	1.36
11	G	305	HEM	C3D-C2D	7.96	1.53	1.36
6	A	1589	TEO	O2-C2	-5.30	1.36	1.43
6	A	1589	TEO	C2-C1	-5.29	1.43	1.54
11	C	305	HEM	C3C-C2C	-4.87	1.33	1.40
11	K	305	HEM	C3C-C2C	-4.81	1.33	1.40
11	G	305	HEM	C3C-C2C	-4.78	1.33	1.40
5	I	601	FAD	C2A-N3A	4.15	1.38	1.32
5	A	601	FAD	C2A-N3A	4.05	1.38	1.32
5	E	601	FAD	C2A-N3A	3.97	1.38	1.32
5	A	601	FAD	C4X-N5	3.67	1.38	1.30
5	E	601	FAD	C4X-N5	3.64	1.38	1.30
5	I	601	FAD	C4X-N5	3.56	1.38	1.30
11	C	305	HEM	C3C-CAC	3.50	1.55	1.47
12	G	1130	CBE	C11-N10	-3.45	1.34	1.41
11	K	305	HEM	C3C-CAC	3.44	1.55	1.47
11	G	305	HEM	C3C-CAC	3.41	1.55	1.47
12	K	1130	CBE	C11-N10	-3.21	1.35	1.41
11	K	305	HEM	C3C-C4C	3.01	1.45	1.41
11	G	305	HEM	C3C-C4C	2.95	1.45	1.41
11	C	305	HEM	C3C-C4C	2.89	1.45	1.41
11	G	305	HEM	CAB-C3B	2.81	1.54	1.47
11	C	305	HEM	CAB-C3B	2.79	1.54	1.47
12	C	1130	CBE	C11-N10	-2.77	1.36	1.41
5	A	601	FAD	C2A-N1A	2.75	1.38	1.33
11	K	305	HEM	CAB-C3B	2.72	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	601	FAD	C10-N1	2.64	1.38	1.33
5	I	601	FAD	C10-N1	2.61	1.38	1.33
5	I	601	FAD	C2A-N1A	2.60	1.38	1.33
5	E	601	FAD	C2A-N1A	2.54	1.38	1.33
5	A	601	FAD	C10-N1	2.52	1.38	1.33
12	K	1130	CBE	C1-C2	2.25	1.54	1.49
11	K	305	HEM	CMD-C2D	2.19	1.55	1.50
11	C	305	HEM	CMD-C2D	2.16	1.55	1.50
11	C	305	HEM	FE-ND	2.14	2.09	1.98
11	G	305	HEM	CMD-C2D	2.06	1.55	1.50
5	E	601	FAD	P-O3P	2.06	1.61	1.59
11	K	305	HEM	FE-ND	2.02	2.09	1.98
5	I	601	FAD	P-O3P	2.01	1.61	1.59

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	FAD	N3A-C2A-N1A	-6.56	119.77	128.67
5	E	601	FAD	N3A-C2A-N1A	-6.44	119.94	128.67
5	I	601	FAD	N3A-C2A-N1A	-6.42	119.96	128.67
12	G	1130	CBE	O7-C2-C1	6.39	116.85	109.30
12	C	1130	CBE	O7-C2-C1	5.75	116.09	109.30
6	A	1589	TEO	O1A-C1-C2	-5.67	108.92	122.52
11	K	305	HEM	C4D-ND-C1D	5.62	111.86	105.21
11	G	305	HEM	C4D-ND-C1D	5.58	111.82	105.21
11	C	305	HEM	C4D-ND-C1D	5.43	111.64	105.21
12	K	1130	CBE	O7-C2-C1	4.77	114.93	109.30
6	A	1589	TEO	O1B-C1-C2	3.88	122.08	113.00
12	K	1130	CBE	C11-N10-C8	-3.71	120.87	127.45
5	A	601	FAD	C4'-C3'-C2'	-3.40	107.92	113.57
12	C	1130	CBE	C11-N10-C8	-3.17	121.82	127.45
11	G	305	HEM	C4C-CHD-C1D	3.16	126.73	122.56
6	I	1589	TEO	O1A-C1-C2	-3.13	115.01	122.52
5	I	601	FAD	C4-N3-C2	-3.09	120.15	125.64
5	E	601	FAD	C4'-C3'-C2'	-3.06	108.48	113.57
5	E	601	FAD	C4-N3-C2	-3.05	120.23	125.64
5	A	601	FAD	C4-N3-C2	-3.05	120.23	125.64
5	I	601	FAD	C4'-C3'-C2'	-2.90	108.74	113.57
11	K	305	HEM	C3B-C2B-C1B	2.76	108.48	106.41
11	C	305	HEM	C4B-CHC-C1C	2.73	126.17	122.56
6	E	1589	TEO	O1A-C1-C2	-2.73	115.97	122.52
5	E	601	FAD	C4X-C4-N3	2.66	120.02	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	305	HEM	C3B-C2B-C1B	2.65	108.40	106.41
11	G	305	HEM	C3B-C2B-C1B	2.64	108.40	106.41
5	I	601	FAD	C4X-C4-N3	2.63	119.96	113.25
5	A	601	FAD	C4X-C4-N3	2.62	119.93	113.25
6	E	1589	TEO	O1B-C1-O1A	2.59	129.95	124.08
5	E	601	FAD	O4-C4-C4X	-2.52	119.89	126.53
5	E	601	FAD	C9A-C5X-N5	-2.49	119.81	122.45
5	E	601	FAD	C10-C4X-N5	-2.45	119.80	124.81
11	K	305	HEM	C4B-CHC-C1C	2.44	125.78	122.56
5	A	601	FAD	C10-C4X-N5	-2.40	119.90	124.81
5	A	601	FAD	O4-C4-C4X	-2.39	120.22	126.53
5	I	601	FAD	O4-C4-C4X	-2.39	120.22	126.53
5	I	601	FAD	C10-C4X-N5	-2.38	119.95	124.81
5	A	601	FAD	C9A-C5X-N5	-2.37	119.94	122.45
11	G	305	HEM	C4B-CHC-C1C	2.35	125.66	122.56
5	I	601	FAD	C4X-C10-N10	2.35	119.84	116.48
5	E	601	FAD	C4X-C10-N10	2.35	119.84	116.48
5	I	601	FAD	C9A-C5X-N5	-2.33	119.98	122.45
12	G	1130	CBE	C1-C2-C3	-2.30	119.06	124.36
5	E	601	FAD	O4B-C1B-N9A	2.28	111.76	108.75
11	K	305	HEM	C1B-NB-C4B	2.26	107.89	105.21
11	K	305	HEM	C4C-CHD-C1D	2.23	125.51	122.56
11	C	305	HEM	C1B-NB-C4B	2.21	107.82	105.21
11	C	305	HEM	C3B-C4B-NB	-2.20	107.89	109.47
11	C	305	HEM	C4C-CHD-C1D	2.20	125.47	122.56
5	A	601	FAD	C4X-C10-N10	2.19	119.62	116.48
11	G	305	HEM	C1B-NB-C4B	2.17	107.78	105.21
6	A	1589	TEO	O1B-C1-O1A	2.17	129.00	124.08
11	K	305	HEM	C3B-C4B-NB	-2.15	107.93	109.47
12	G	1130	CBE	C3-C8-N10	-2.13	112.35	115.97
5	E	601	FAD	C5X-C9A-N10	2.07	119.84	117.97
5	I	601	FAD	C5X-C9A-N10	2.03	119.80	117.97
11	G	305	HEM	C3B-C4B-NB	-2.01	108.02	109.47

There are no chirality outliers.

All (32) 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	N10-C1'-C2'-O2'
5	E	601	FAD	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
5	I	601	FAD	N10-C1'-C2'-O2'
6	I	1589	TEO	O2-C2-C3-C4
11	K	305	HEM	C1A-C2A-CAA-CBA
11	K	305	HEM	C3A-C2A-CAA-CBA
11	C	305	HEM	C4B-C3B-CAB-CBB
11	G	305	HEM	C4B-C3B-CAB-CBB
11	K	305	HEM	C4B-C3B-CAB-CBB
12	K	1130	CBE	C2-C3-C8-O9
5	I	601	FAD	N10-C1'-C2'-C3'
6	A	1589	TEO	O2-C2-C3-C4
6	E	1589	TEO	O2-C2-C3-C4
6	A	1589	TEO	O1B-C1-C2-C3
11	G	305	HEM	C4D-C3D-CAD-CBD
5	I	601	FAD	O4B-C4B-C5B-O5B
6	A	1589	TEO	O1B-C1-C2-O2
6	I	1589	TEO	O1A-C1-C2-O2
6	A	1589	TEO	O1A-C1-C2-O2
6	I	1589	TEO	O1B-C1-C2-O2
12	C	1130	CBE	C2-C3-C8-N10
12	G	1130	CBE	C2-C3-C8-N10
12	K	1130	CBE	C2-C3-C8-N10
11	G	305	HEM	C2D-C3D-CAD-CBD
5	A	601	FAD	O4B-C4B-C5B-O5B
11	C	305	HEM	CAA-CBA-CGA-O2A
6	E	1589	TEO	O1B-C1-C2-O2
11	K	305	HEM	CAD-CBD-CGD-O1D
11	C	305	HEM	CAA-CBA-CGA-O1A
5	I	601	FAD	C3B-C4B-C5B-O5B

There are no ring outliers.

15 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	305	HEM	4	0
6	A	1589	TEO	3	0
6	E	1589	TEO	3	0
5	I	601	FAD	8	0
11	K	305	HEM	4	0
12	C	1130	CBE	2	0
12	K	1130	CBE	3	0
5	A	601	FAD	8	0
11	C	305	HEM	6	0

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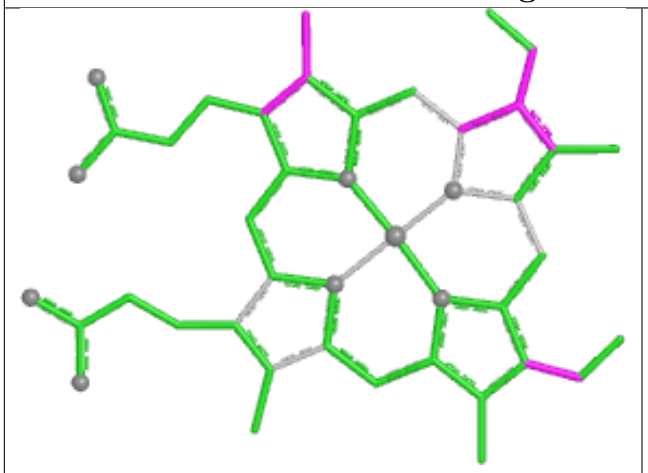
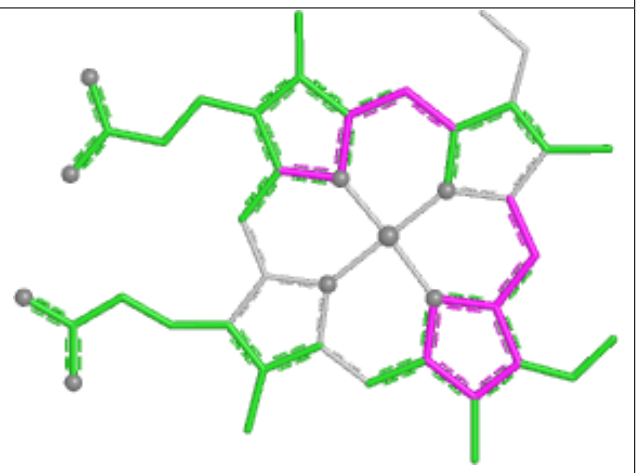
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	304	F3S	1	0
6	I	1589	TEO	5	0
5	E	601	FAD	7	0
12	G	1130	CBE	1	0
9	J	303	SF4	1	0
10	F	304	F3S	1	0

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.

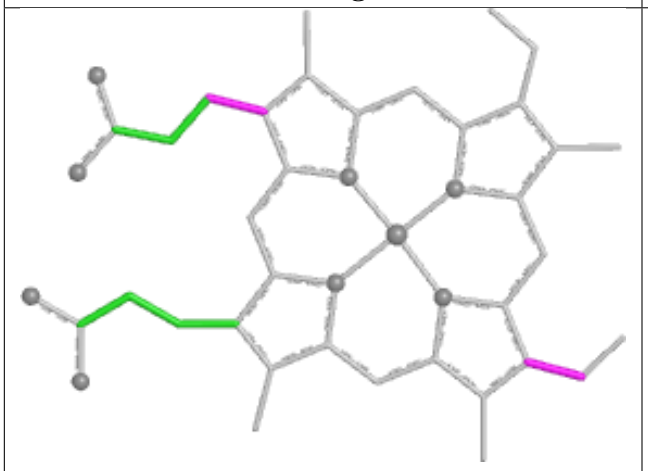
Ligand HEM G 305



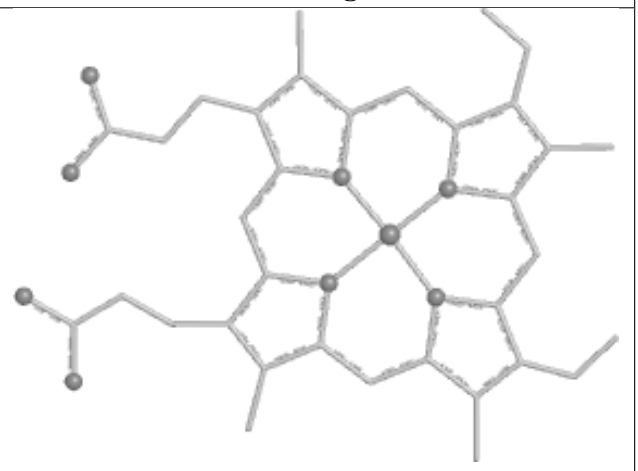
Bond lengths



Bond angles

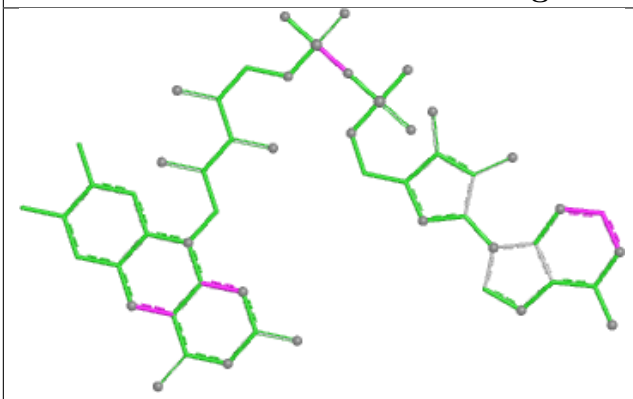


Torsions

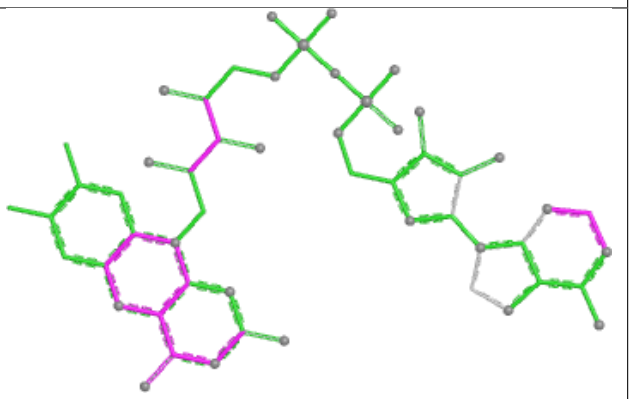


Rings

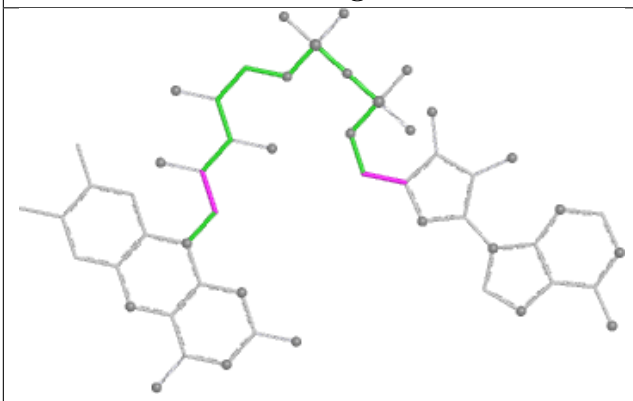
Ligand FAD I 601



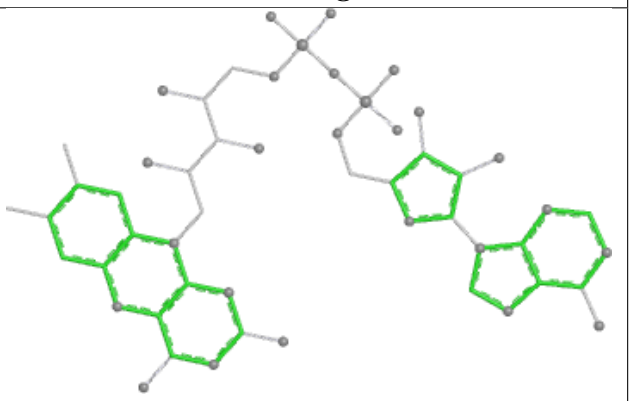
Bond lengths



Bond angles

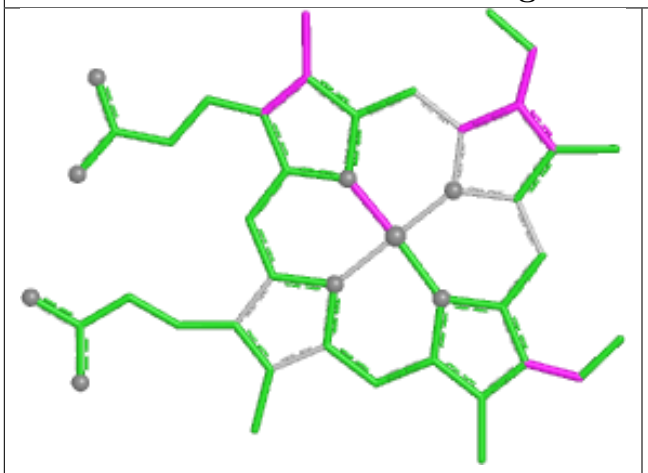


Torsions

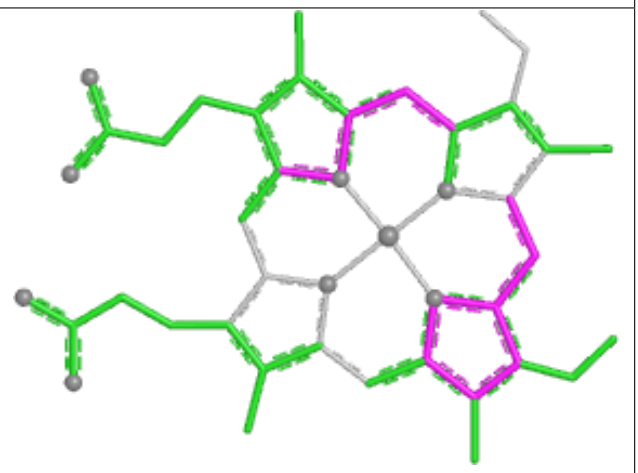


Rings

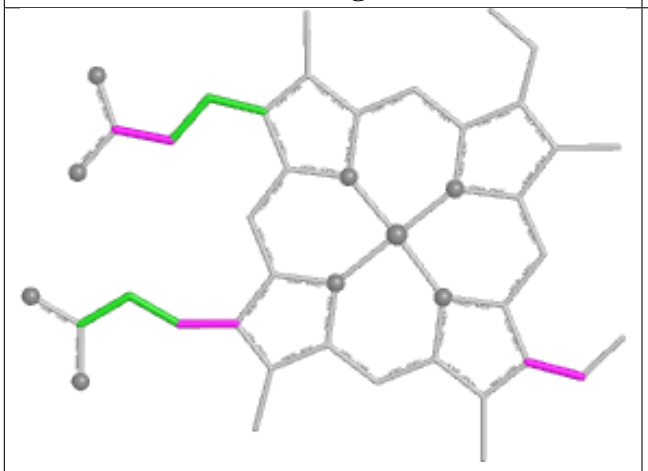
Ligand HEM K 305



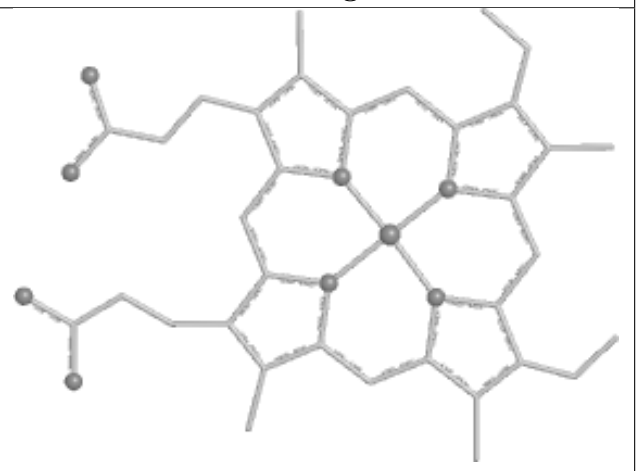
Bond lengths



Bond angles

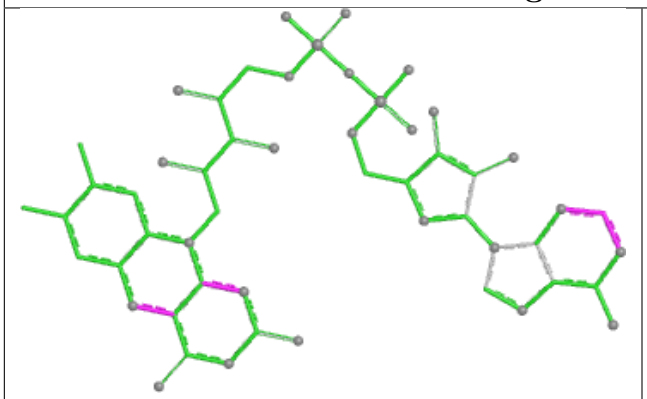


Torsions

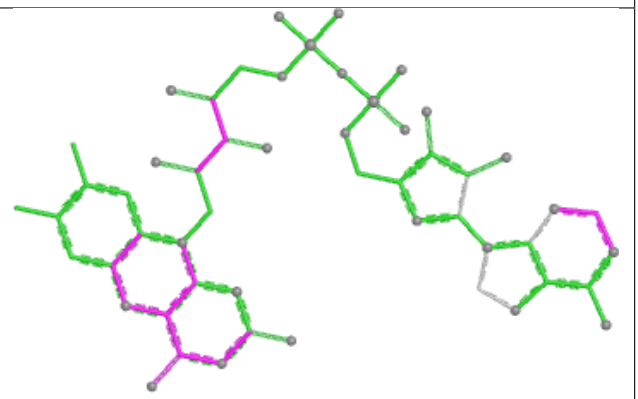


Rings

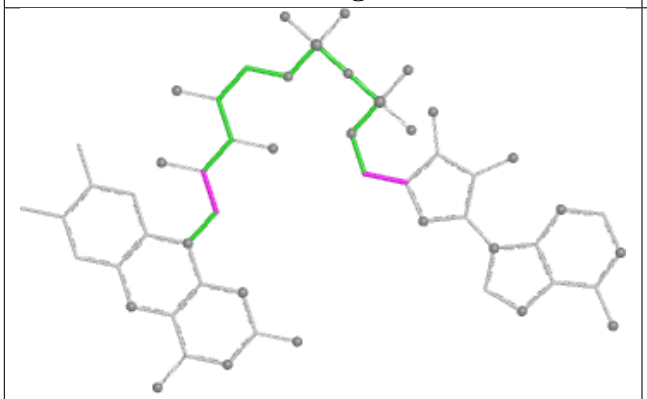
Ligand FAD A 601



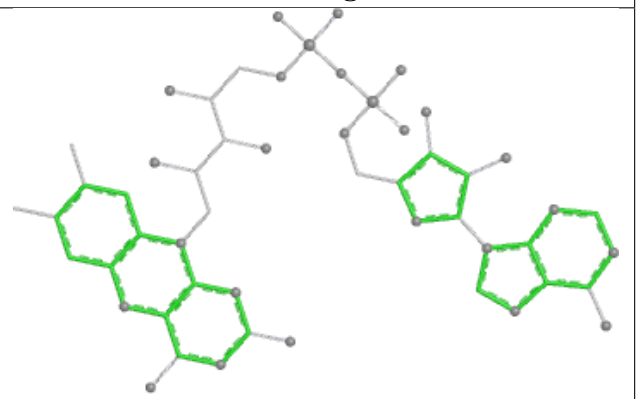
Bond lengths



Bond angles

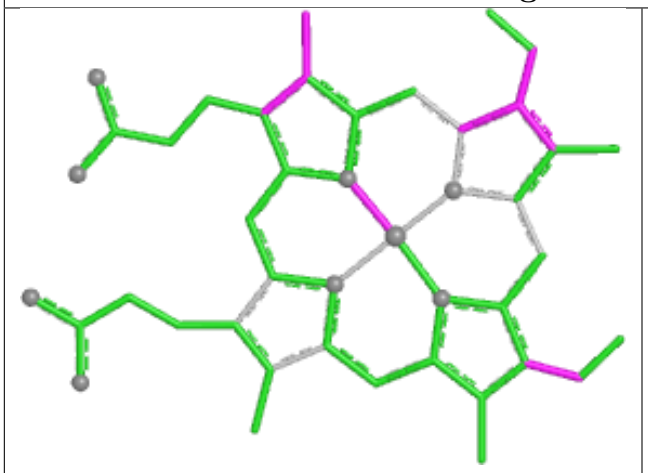


Torsions

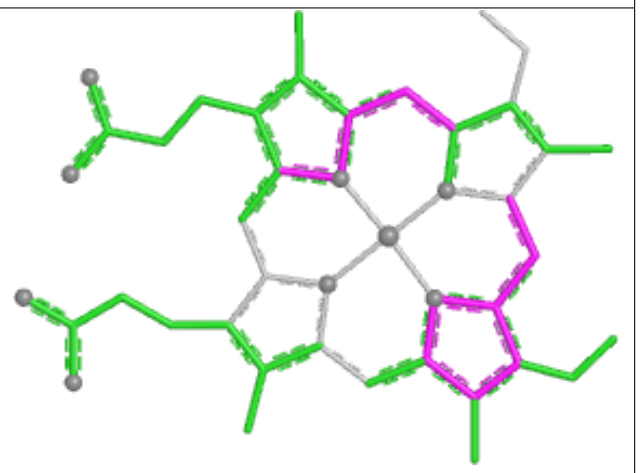


Rings

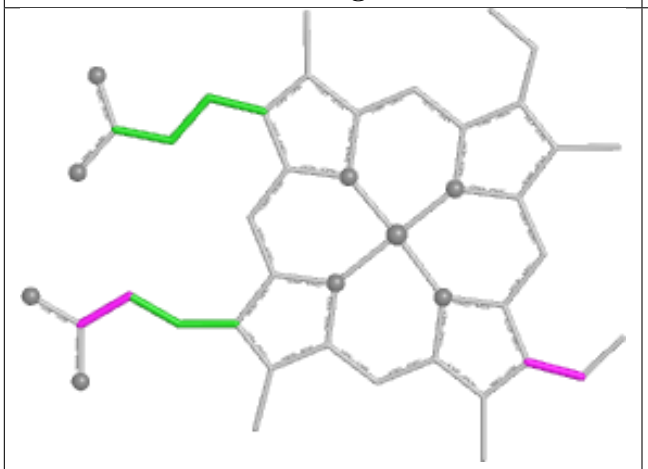
Ligand HEM C 305



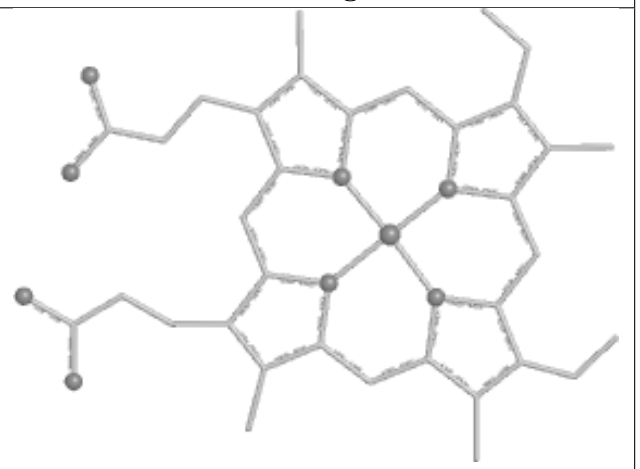
Bond lengths



Bond angles

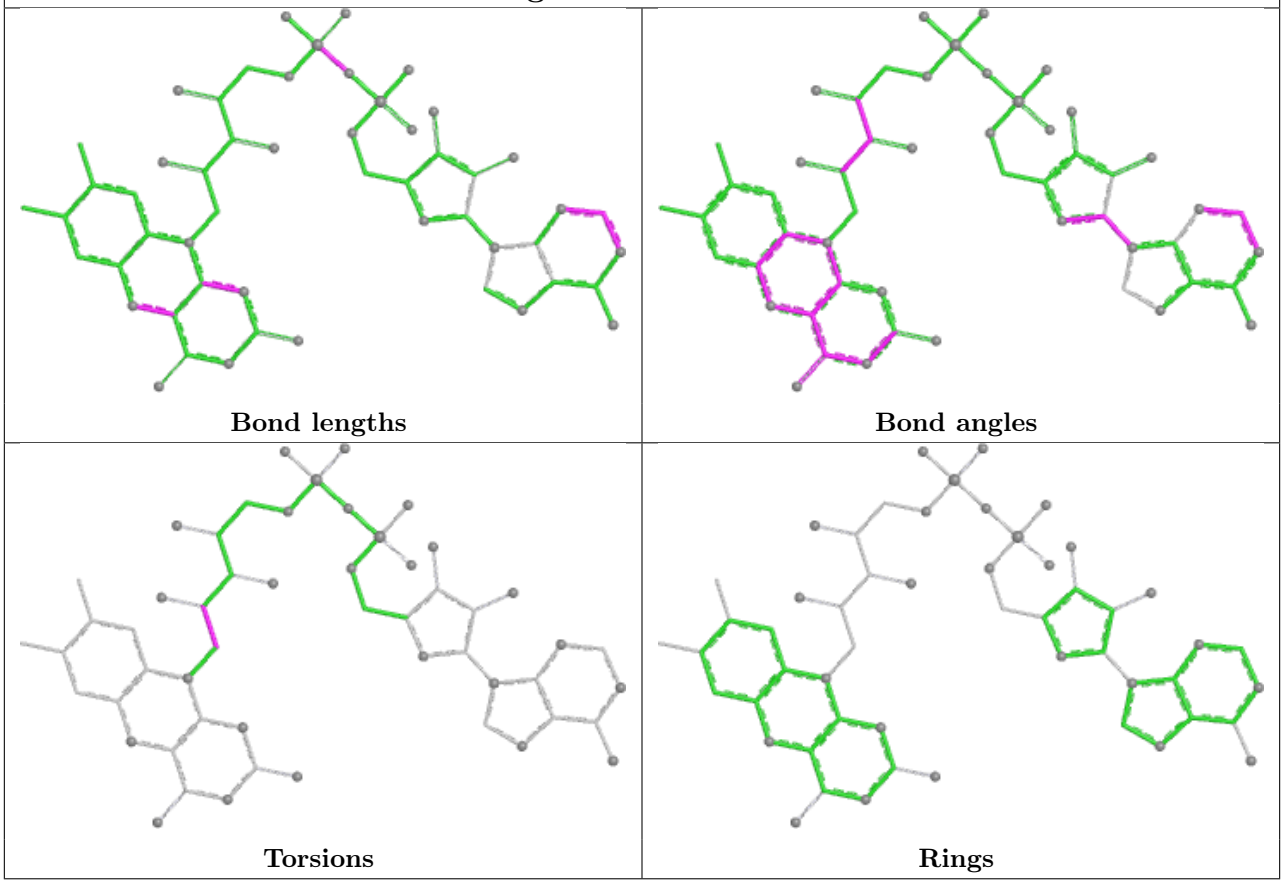


Torsions



Rings

Ligand FAD E 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%)	0.03	6 (1%)	82	77	36, 60, 102, 151	0
1	E	588/588 (100%)	0.14	18 (3%)	49	39	41, 67, 107, 155	0
1	I	588/588 (100%)	0.51	60 (10%)	6	3	53, 77, 117, 170	0
2	B	238/238 (100%)	0.00	10 (4%)	36	26	36, 58, 108, 157	0
2	F	238/238 (100%)	-0.09	4 (1%)	70	63	44, 62, 110, 158	0
2	J	238/238 (100%)	0.19	15 (6%)	20	12	56, 71, 116, 159	0
3	C	122/129 (94%)	0.13	8 (6%)	18	11	54, 82, 120, 171	0
3	G	122/129 (94%)	0.30	8 (6%)	18	11	54, 87, 121, 173	0
3	K	122/129 (94%)	0.98	24 (19%)	1	0	69, 93, 124, 170	0
4	D	105/115 (91%)	0.03	3 (2%)	51	41	52, 74, 125, 186	0
4	H	105/115 (91%)	0.20	10 (9%)	8	4	52, 74, 125, 184	0
4	L	105/115 (91%)	0.32	12 (11%)	5	3	61, 80, 126, 182	0
All	All	3159/3210 (98%)	0.21	178 (5%)	24	16	36, 70, 117, 186	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	129	TRP	12.3
3	G	129	TRP	8.1
3	G	68	PHE	7.4
3	C	129	TRP	6.8
1	I	1	MET	6.6
4	D	41	GLY	5.7
3	K	101	GLU	5.6
4	L	115	VAL	5.4
3	C	68	PHE	5.2
1	I	338	ALA	5.1
3	K	68	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
3	K	69	PHE	5.0
1	I	346	PRO	4.9
4	L	38	ALA	4.9
1	I	266	ASN	4.8
1	I	268	HIS	4.6
1	E	449	ASN	4.6
1	I	298	ARG	4.5
4	H	41	GLY	4.4
2	F	29	GLU	4.3
1	I	276	TYR	4.3
4	L	37	PHE	4.2
1	I	267	LYS	4.1
2	J	29	GLU	4.1
2	J	2	ARG	4.0
4	H	42	GLU	4.0
3	C	69	PHE	4.0
2	J	28	ASP	4.0
1	I	340	VAL	4.0
1	I	452	ASN	3.9
1	I	204	GLY	3.8
1	E	202	THR	3.8
2	J	16	ASP	3.7
2	J	58	GLY	3.7
1	I	381	PRO	3.6
4	H	47	VAL	3.6
3	K	8	GLN	3.6
1	I	213	THR	3.6
1	I	297	ILE	3.5
2	J	31	ARG	3.5
3	K	126	VAL	3.5
1	E	452	ASN	3.5
3	K	108	ARG	3.5
1	E	528	VAL	3.5
3	K	103	PHE	3.5
1	I	534	THR	3.4
2	B	1	MET	3.4
3	K	98	TYR	3.4
1	I	500	ASP	3.4
3	K	67	SER	3.4
4	H	115	VAL	3.4
1	I	588	TYR	3.4
2	B	86	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
3	K	102	THR	3.2
2	B	2	ARG	3.2
3	K	128	VAL	3.2
1	I	582	PRO	3.2
3	K	65	MET	3.2
1	E	463	LEU	3.1
1	E	451	ARG	3.1
2	B	84	GLN	3.1
1	I	334	SER	3.1
1	I	463	LEU	3.1
1	I	307	TRP	3.1
3	G	64	ILE	3.1
1	I	374	LYS	3.0
1	I	345	GLU	3.0
1	E	344	LYS	3.0
1	A	300	GLY	3.0
1	I	562	GLU	3.0
2	J	15	ASP	3.0
3	G	69	PHE	2.9
4	H	51	PHE	2.9
1	I	306	PRO	2.9
1	I	262	GLY	2.9
1	I	421	GLU	2.9
3	G	63	ALA	2.9
1	I	563	SER	2.9
1	I	295	ILE	2.8
2	J	86	GLY	2.8
1	I	315	LEU	2.8
1	I	420	GLN	2.8
3	C	70	VAL	2.8
4	L	39	THR	2.8
2	B	30	GLY	2.8
3	K	110	ALA	2.8
1	I	544	ASP	2.7
3	C	66	GLY	2.7
2	J	14	VAL	2.7
3	K	111	LYS	2.7
1	E	48	SER	2.6
4	D	40	SER	2.6
4	H	40	SER	2.6
4	L	49	ILE	2.6
4	H	43	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	345	GLU	2.6
1	I	373	GLU	2.6
2	J	79	ILE	2.6
4	H	48	TRP	2.6
2	F	30	GLY	2.6
1	I	424	ALA	2.6
3	K	107	LYS	2.6
1	I	309	PRO	2.6
1	I	304	ASP	2.5
1	I	277	ALA	2.5
2	B	29	GLU	2.5
4	L	114	GLY	2.5
1	I	310	HIS	2.5
1	I	451	ARG	2.5
3	K	79	THR	2.5
1	A	424	ALA	2.5
1	I	275	ARG	2.5
2	B	55	CYS	2.5
4	L	43	LEU	2.5
1	I	265	LEU	2.4
3	K	66	GLY	2.4
3	C	128	VAL	2.4
1	I	48	SER	2.4
1	I	433	SER	2.4
1	A	543	PHE	2.4
2	B	85	PRO	2.4
3	G	72	PHE	2.4
1	I	305	GLY	2.4
3	G	108	ARG	2.4
3	K	87	VAL	2.3
3	G	100	GLU	2.3
3	K	61	ALA	2.3
3	K	122	LEU	2.3
4	L	42	GLU	2.3
4	L	34	VAL	2.3
1	A	268	HIS	2.3
1	E	215	ALA	2.3
2	F	1	MET	2.3
4	H	36	PHE	2.3
1	E	531	ASN	2.3
1	I	470	ASN	2.3
1	E	222	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	218	ASN	2.2
1	I	491	ARG	2.2
3	C	67	SER	2.2
4	D	43	LEU	2.2
2	J	18	PRO	2.2
3	K	91	HIS	2.2
1	E	303	CYS	2.2
1	I	299	GLU	2.2
1	E	201	ALA	2.2
1	I	263	TYR	2.2
2	J	87	LYS	2.2
4	L	40	SER	2.2
2	J	85	PRO	2.2
4	L	48	TRP	2.2
3	K	109	SER	2.2
1	I	300	GLY	2.1
1	I	583	PRO	2.1
1	I	569	ARG	2.1
1	A	216	HIS	2.1
1	I	52	GLY	2.1
4	L	47	VAL	2.1
1	I	318	LEU	2.1
3	K	22	ILE	2.1
1	I	319	GLY	2.1
2	B	16	ASP	2.1
1	E	465	GLU	2.1
2	B	61	GLY	2.1
2	J	1	MET	2.1
1	I	217	ILE	2.0
1	E	314	LYS	2.0
4	H	45	TYR	2.0
1	I	214	ASN	2.0
1	I	45	HIS	2.0
1	I	144	ALA	2.0
2	F	62	SER	2.0
1	I	524	TYR	2.0
1	E	173	GLN	2.0
1	I	450	ASN	2.0
1	A	267	LYS	2.0
2	J	30	GLY	2.0
3	C	65	MET	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.

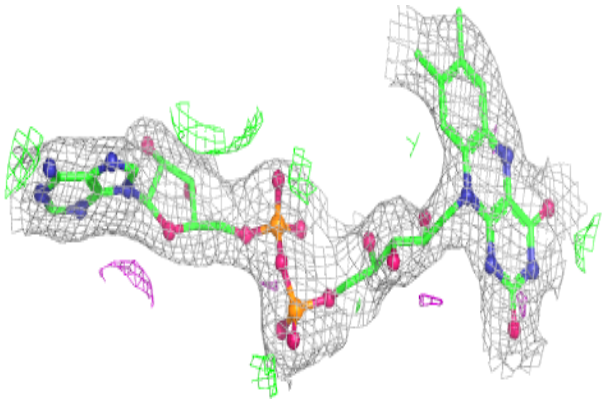
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NA	E	1590	1/1	0.85	0.47	39,39,39,39	0
6	TEO	I	1589	9/9	0.87	0.31	66,86,104,126	0
7	NA	I	1590	1/1	0.89	0.68	64,64,64,64	0
5	FAD	I	601	53/53	0.95	0.28	53,83,120,218	0
7	NA	A	1590	1/1	0.95	0.40	35,35,35,35	0
12	CBE	K	1130	16/16	0.95	0.23	46,84,107,110	0
6	TEO	E	1589	9/9	0.96	0.17	44,53,63,81	0
5	FAD	E	601	53/53	0.96	0.26	30,59,90,95	0
11	HEM	C	305	43/43	0.97	0.20	40,71,82,87	0
11	HEM	G	305	43/43	0.97	0.19	22,78,110,118	0
12	CBE	C	1130	16/16	0.97	0.15	26,42,64,67	0
5	FAD	A	601	53/53	0.97	0.23	22,50,74,93	0
8	FES	J	302	4/4	0.98	0.21	90,91,92,92	0
11	HEM	K	305	43/43	0.98	0.18	58,89,128,156	0
9	SF4	J	303	8/8	0.98	0.14	65,72,76,80	0
6	TEO	A	1589	9/9	0.98	0.25	31,44,56,57	0
10	F3S	J	304	7/7	0.99	0.11	64,70,84,87	0
8	FES	B	302	4/4	0.99	0.21	35,38,43,52	0
9	SF4	B	303	8/8	0.99	0.18	40,46,51,52	0
9	SF4	F	303	8/8	0.99	0.15	47,51,53,53	0
8	FES	F	302	4/4	0.99	0.22	44,51,54,58	0
12	CBE	G	1130	16/16	0.99	0.18	33,54,81,87	0
10	F3S	B	304	7/7	0.99	0.13	42,45,53,57	0
10	F3S	F	304	7/7	1.00	0.11	54,56,60,60	0

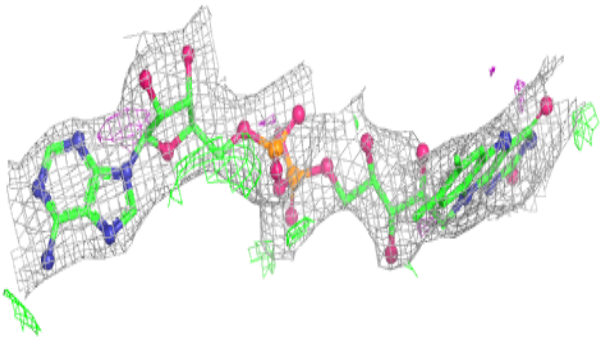
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

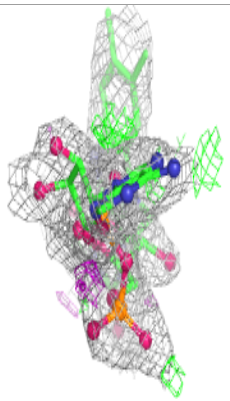
orientation to approximate a three-dimensional view.

Electron density around FAD 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)

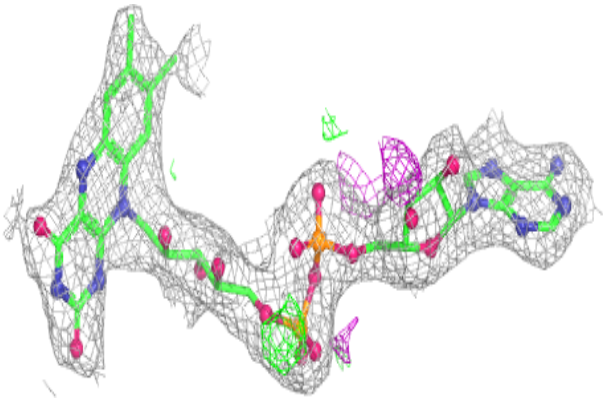


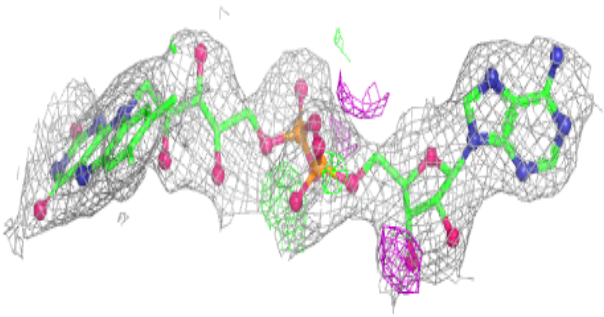


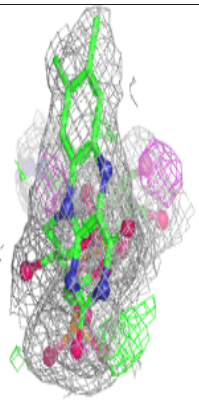


Electron density around FAD E 601:

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

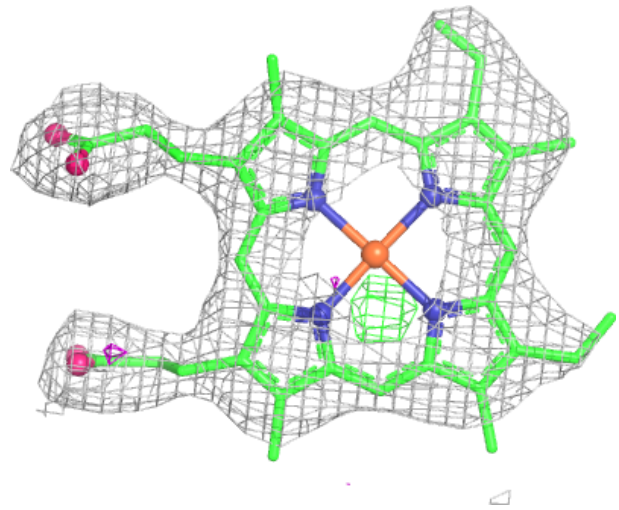


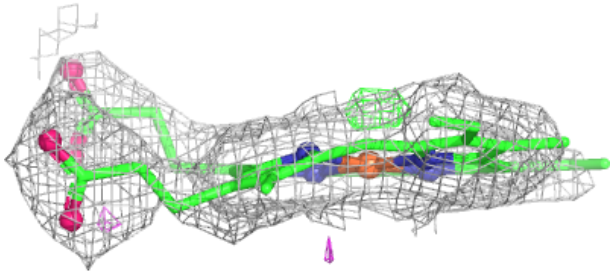


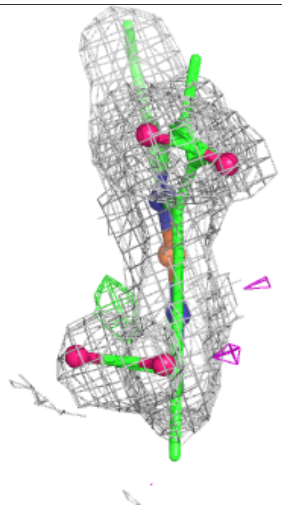


Electron density around HEM C 305:

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

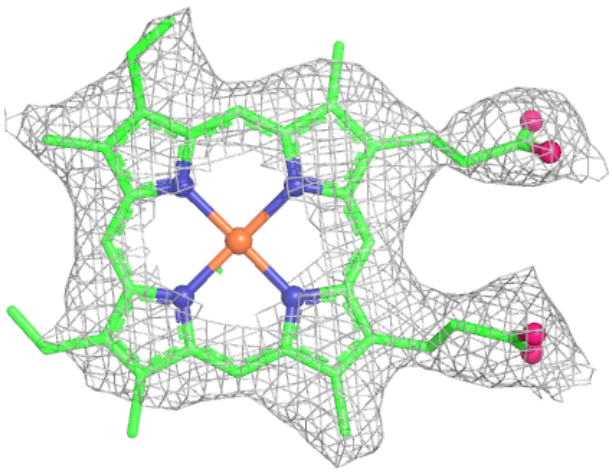


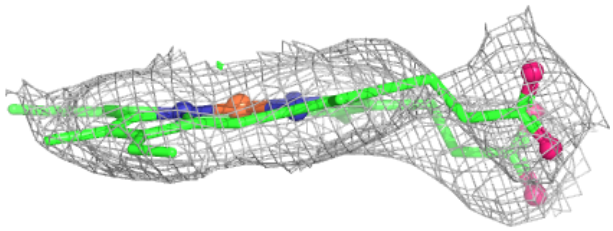


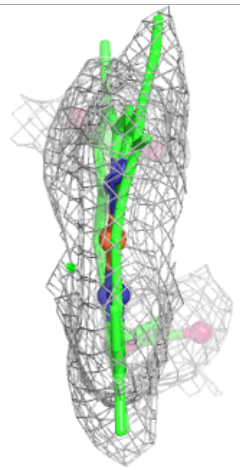


Electron density around HEM G 305:

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

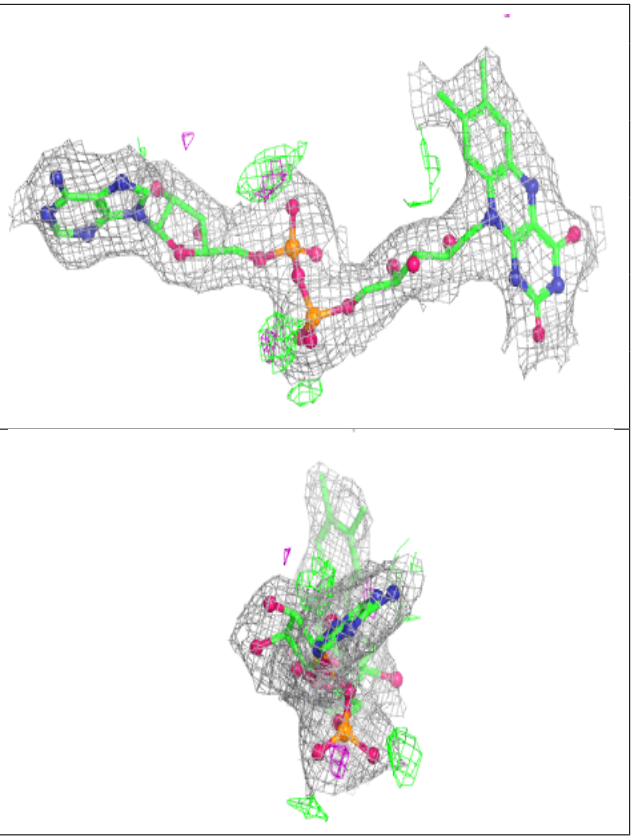






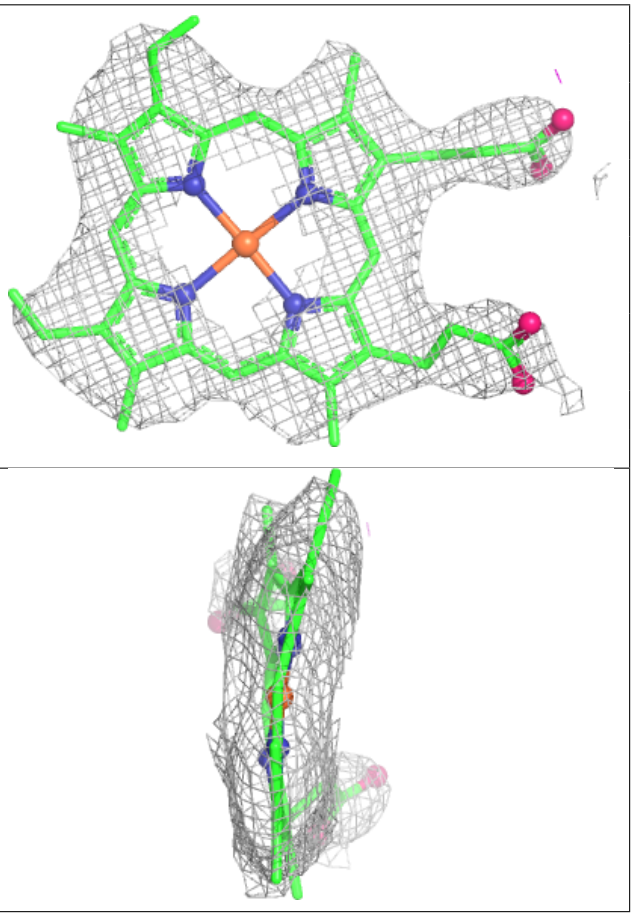
Electron density around FAD A 601:

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



Electron density around HEM K 305:

$2mF_o$-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.