



wwPDB X-ray Structure Validation Summary Report

Mar 6, 2026 – 02:21 PM UTC

PDB ID : 2WP9 / pdb_00002wp9
Title : Crystal structure of the E. coli succinate:quinone oxidoreductase (SQR) SdhB His207Thr mutant
Authors : Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on : 2009-08-03
Resolution : 2.70 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

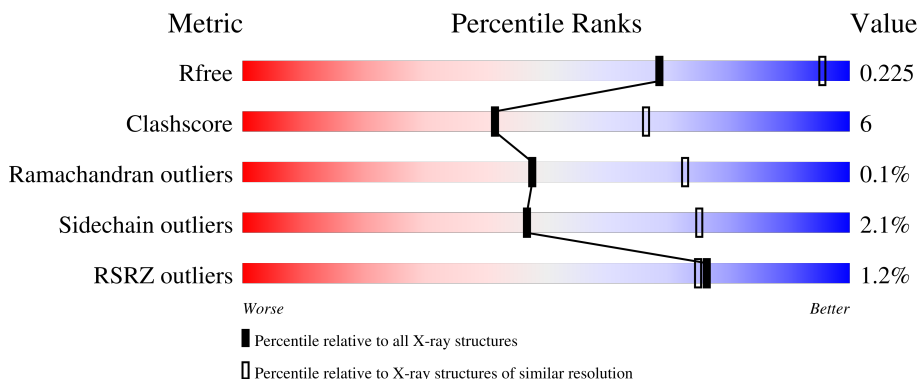
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	588	85% 14% .
1	E	588	86% 14%
1	I	588	2% 87% 13% .
2	B	238	86% 13% .
2	F	238	86% 13% .

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Mol	Chain	Length	Quality of chain
2	J	238	<p>3% 84% 16%</p>
3	C	129	<p>2% 87% 8% 5%</p>
3	G	129	<p>3% 82% 12% 5%</p>
3	K	129	<p>3% 81% 13% 5%</p>
4	D	115	<p>4% 77% 12% 9%</p>
4	H	115	<p>3% 77% 13% 9%</p>
4	L	115	<p>2% 78% 12% 9%</p>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 25058 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	1865	1170	327	348	20	0	0	0
2	F	238	1865	1170	327	348	20	0	0	0
2	J	238	1865	1170	327	348	20	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	207	THR	HIS	engineered mutation	UNP P07014
F	207	THR	HIS	engineered mutation	UNP P07014
J	207	THR	HIS	engineered mutation	UNP P07014

- 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	947	630	153	159	5	0	0	0

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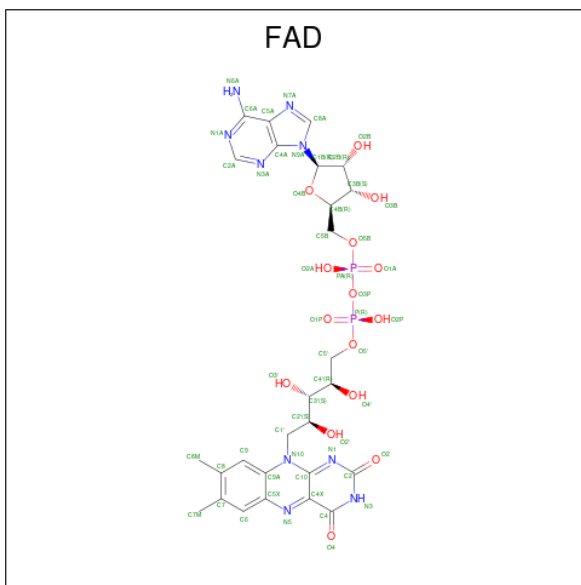
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			947	630	153	159	5			
3	K	122	Total	C	N	O	S	0	0	0
			947	630	153	159	5			

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

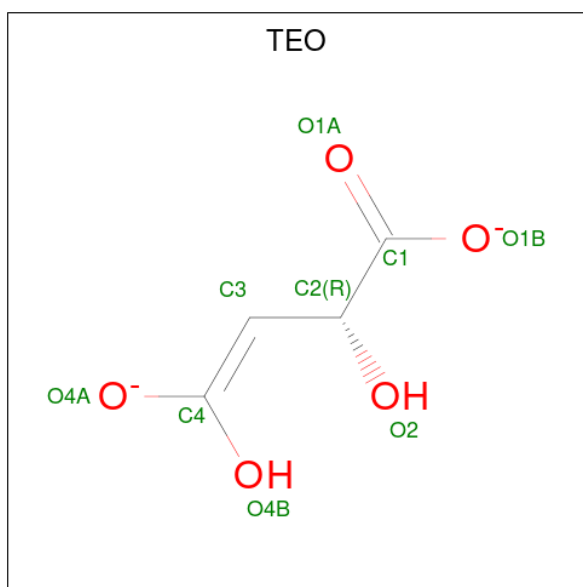
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total	C	N	O	S	0	0	0
			835	577	123	132	3			
4	H	105	Total	C	N	O	S	0	0	0
			835	577	123	132	3			
4	L	105	Total	C	N	O	S	0	0	0
			835	577	123	132	3			

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



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

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

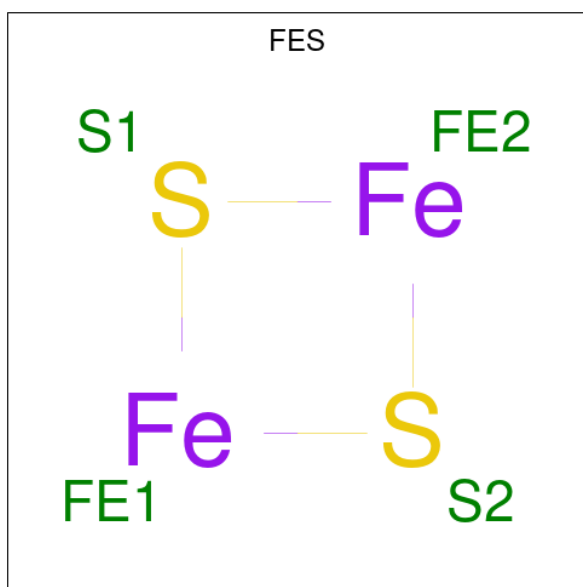


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 4 5	0	0
6	E	1	Total C O 9 4 5	0	0
6	I	1	Total C O 9 4 5	0	0

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

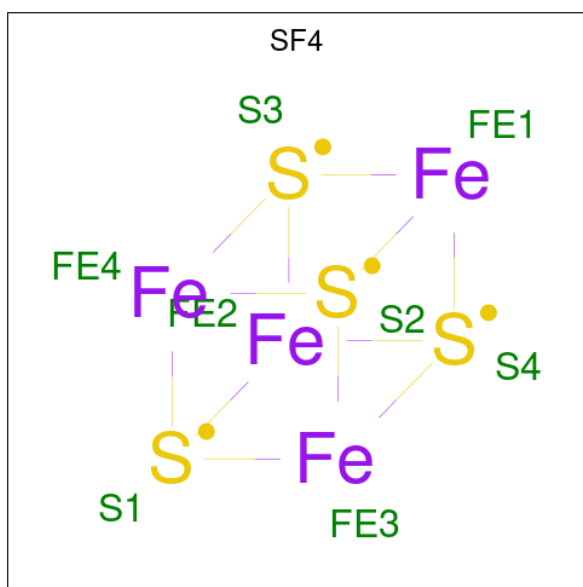
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0
7	I	1	Total Na 1 1	0	0

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



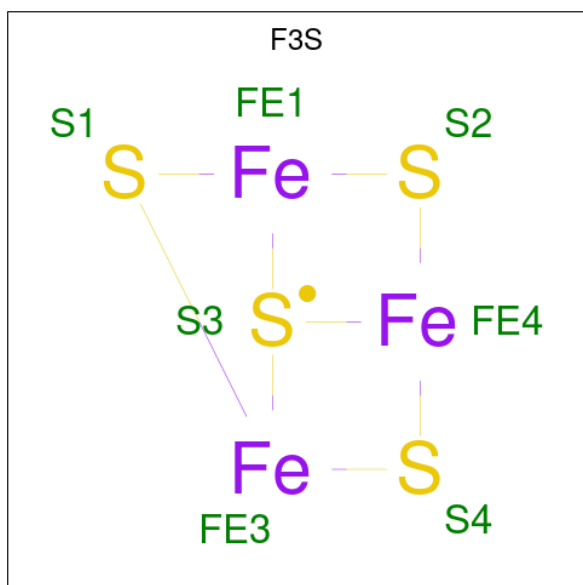
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

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

- Molecule 10 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



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

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

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

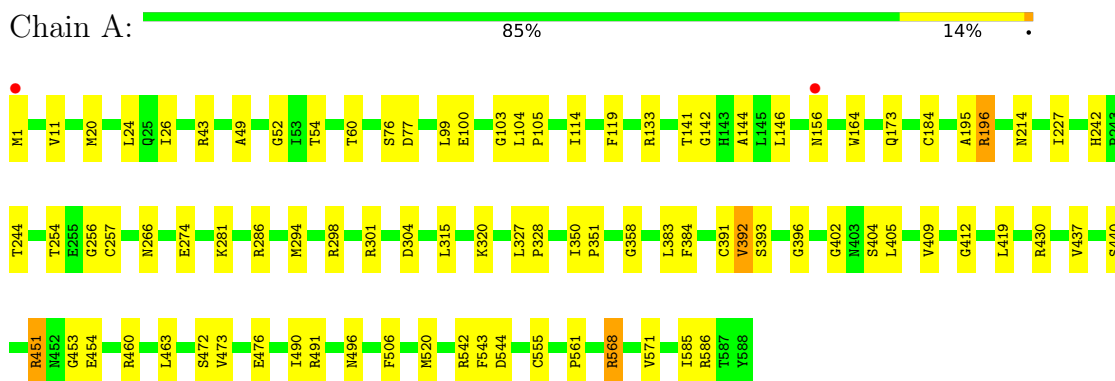
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	53	Total 53	O 53	0	0
13	B	17	Total 17	O 17	0	0
13	C	1	Total 1	O 1	0	0
13	D	1	Total 1	O 1	0	0
13	E	23	Total 23	O 23	0	0
13	F	7	Total 7	O 7	0	0
13	H	1	Total 1	O 1	0	0
13	I	13	Total 13	O 13	0	0
13	J	12	Total 12	O 12	0	0

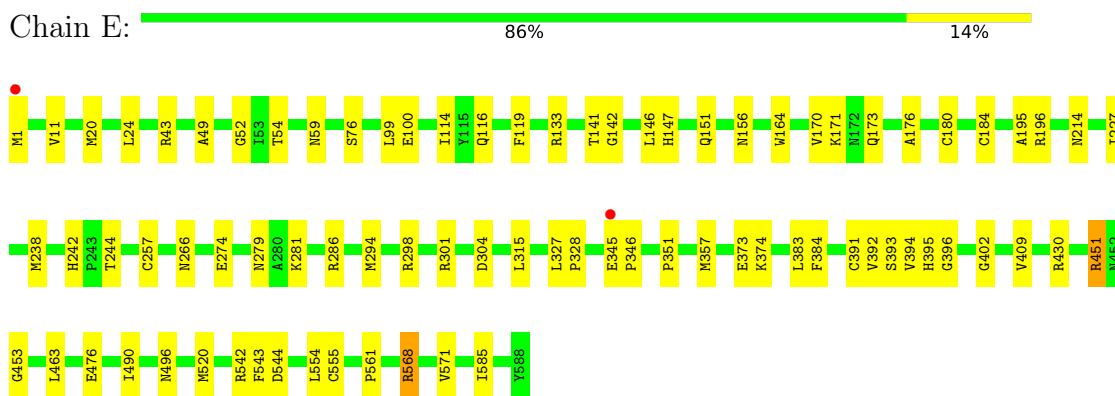
3 Residue-property plots [i](#)

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.

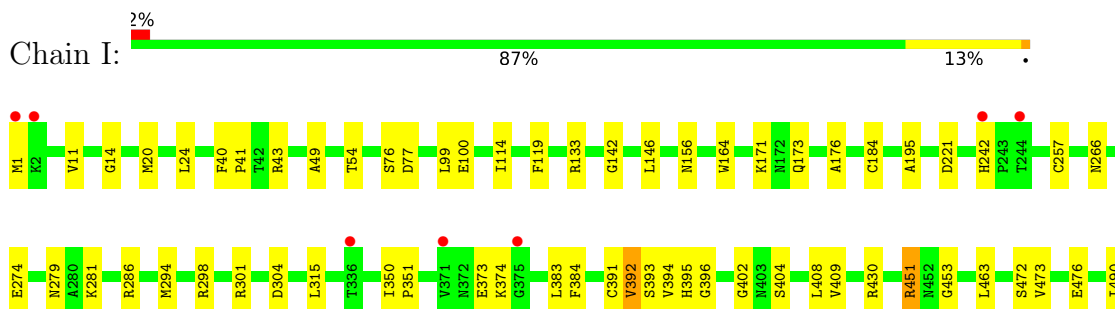
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT



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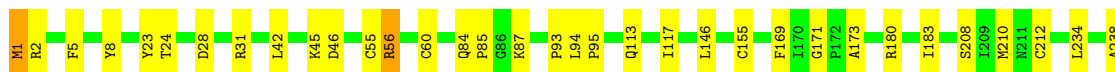
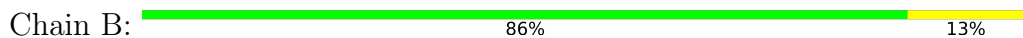


• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

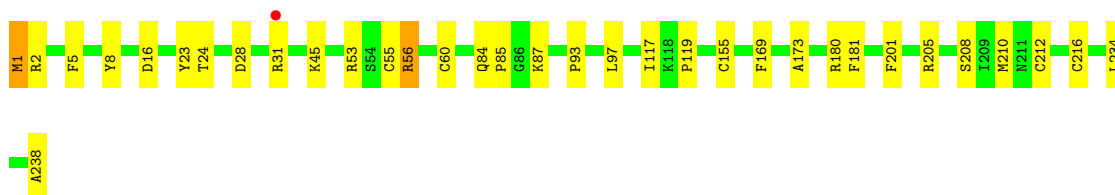
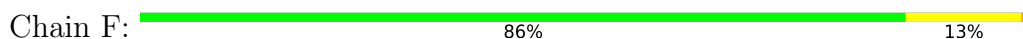




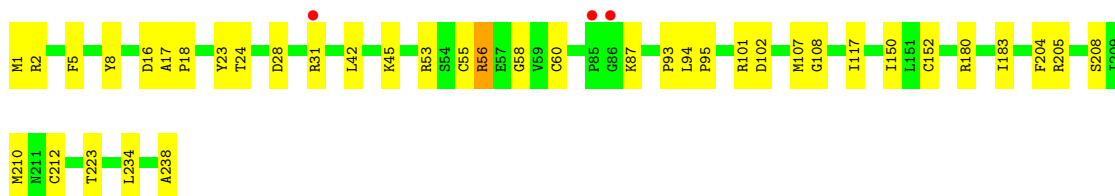
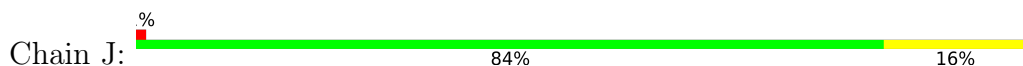
- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



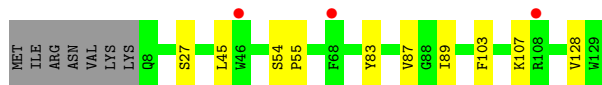
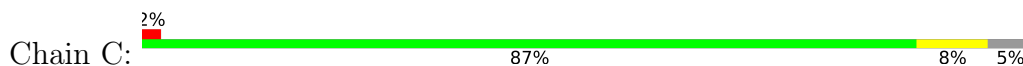
- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



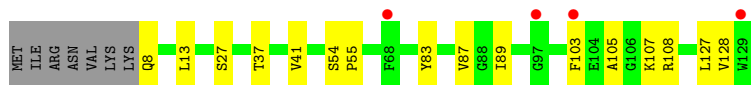
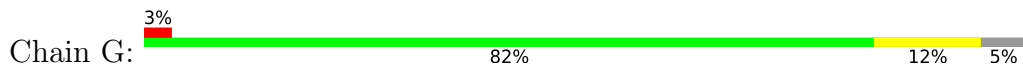
- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



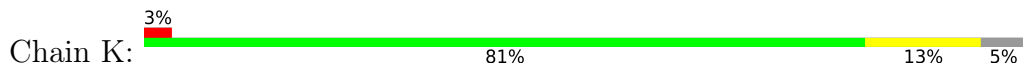
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT



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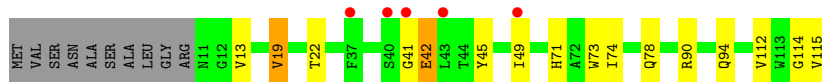
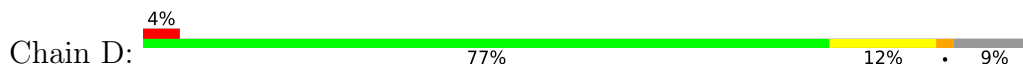


- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

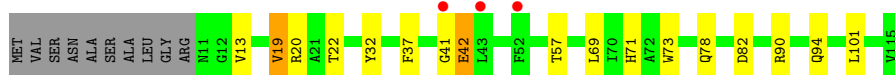
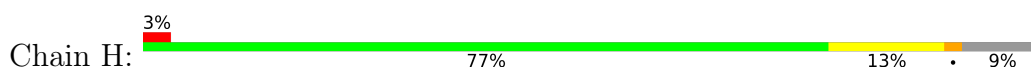




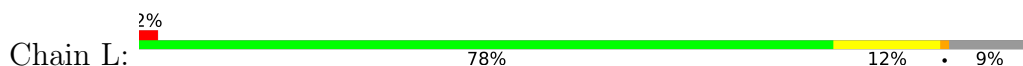
- Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.85Å 183.80Å 202.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.70 48.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.85-2.70) 99.6 (48.85-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.190 , 0.222 0.193 , 0.225	Depositor DCC
R_{free} test set	6188 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtrriage
Anisotropy	0.209	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25058	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, TEO, SF4, CBE, FES, NA, FAD, F3S

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.81	1/4611 (0.0%)	0.92	4/6237 (0.1%)
1	E	0.71	0/4611	0.88	1/6237 (0.0%)
1	I	0.66	0/4611	0.86	1/6237 (0.0%)
2	B	0.84	0/1903	0.98	2/2573 (0.1%)
2	F	0.75	0/1903	0.91	3/2573 (0.1%)
2	J	0.70	0/1903	0.90	1/2573 (0.0%)
3	C	0.74	0/969	0.84	0/1316
3	G	0.68	0/969	0.83	0/1316
3	K	0.62	0/969	0.84	0/1316
4	D	0.76	1/858 (0.1%)	0.86	0/1175
4	H	0.71	1/858 (0.1%)	0.82	0/1175
4	L	0.67	0/858	0.85	0/1175
All	All	0.73	3/25023 (0.0%)	0.89	12/33903 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	78	GLN	CD-OE1	5.38	1.33	1.23
4	H	78	GLN	CD-OE1	5.33	1.33	1.23
1	A	358	GLY	C-O	5.22	1.29	1.23

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	GLY	N-CA-C	-7.79	103.47	112.50
1	A	392	VAL	N-CA-C	7.28	118.08	110.72
1	I	392	VAL	N-CA-C	6.22	117.01	110.72
2	J	204	PHE	N-CA-C	5.46	119.21	112.54
2	F	201	PHE	N-CA-C	5.27	119.70	113.12

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	62	0
1	E	4522	0	4426	61	0
1	I	4522	0	4426	56	0
2	B	1865	0	1850	20	0
2	F	1865	0	1850	24	0
2	J	1865	0	1850	24	0
3	C	947	0	989	8	0
3	G	947	0	989	12	0
3	K	947	0	989	10	0
4	D	835	0	875	10	0
4	H	835	0	875	12	0
4	L	835	0	875	10	0
5	A	53	0	30	7	0
5	E	53	0	29	4	0
5	I	53	0	29	7	0
6	A	9	0	3	2	0
6	E	9	0	3	2	0
6	I	9	0	3	2	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	1	0
9	B	8	0	0	0	0
9	F	8	0	0	1	0
9	J	8	0	0	0	0
10	B	7	0	0	0	0
10	F	7	0	0	0	0
10	J	7	0	0	1	0
11	C	43	0	30	2	0
11	G	43	0	30	7	0
11	K	43	0	30	7	0
12	C	16	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	G	16	0	13	2	0
12	K	16	0	13	2	0
13	A	53	0	0	4	0
13	B	17	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	23	0	0	0	0
13	F	7	0	0	0	0
13	H	1	0	0	1	0
13	I	13	0	0	0	0
13	J	12	0	0	0	0
All	All	25058	0	24646	318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 318 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:451:ARG:HH11	1:A:451:ARG:HG2	1.02	1.17
11:G:1129:HEM:HBC2	11:G:1129:HEM:HHD	1.55	0.88
11:K:1129:HEM:HHC	11:K:1129:HEM:HBB2	1.55	0.88
3:G:103:PHE:CE2	3:G:107:LYS:HE2	2.11	0.85
1:E:490:ILE:HG22	1:E:520:MET:CE	2.08	0.83

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%)	569 (97%)	17 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	586/588 (100%)	569 (97%)	17 (3%)	0	100	100
1	I	586/588 (100%)	571 (97%)	15 (3%)	0	100	100
2	B	236/238 (99%)	227 (96%)	9 (4%)	0	100	100
2	F	236/238 (99%)	223 (94%)	13 (6%)	0	100	100
2	J	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
3	C	120/129 (93%)	116 (97%)	4 (3%)	0	100	100
3	G	120/129 (93%)	117 (98%)	3 (2%)	0	100	100
3	K	120/129 (93%)	119 (99%)	1 (1%)	0	100	100
4	D	103/115 (90%)	97 (94%)	5 (5%)	1 (1%)	12	32
4	H	103/115 (90%)	98 (95%)	4 (4%)	1 (1%)	12	32
4	L	103/115 (90%)	98 (95%)	4 (4%)	1 (1%)	12	32
All	All	3135/3210 (98%)	3029 (97%)	103 (3%)	3 (0%)	48	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	42	GLU
4	L	42	GLU
4	H	42	GLU

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%)	57	81
1	E	473/473 (100%)	464 (98%)	9 (2%)	50	77
1	I	473/473 (100%)	464 (98%)	9 (2%)	50	77
2	B	208/208 (100%)	202 (97%)	6 (3%)	37	67
2	F	208/208 (100%)	201 (97%)	7 (3%)	32	62
2	J	208/208 (100%)	200 (96%)	8 (4%)	29	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	102/109 (94%)	101 (99%)	1 (1%)	68	86
3	G	102/109 (94%)	100 (98%)	2 (2%)	48	76
3	K	102/109 (94%)	100 (98%)	2 (2%)	48	76
4	D	88/96 (92%)	87 (99%)	1 (1%)	65	85
4	H	88/96 (92%)	87 (99%)	1 (1%)	65	85
4	L	88/96 (92%)	87 (99%)	1 (1%)	65	85
All	All	2613/2658 (98%)	2559 (98%)	54 (2%)	47	75

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	87	LYS
1	I	279	ASN
2	J	183	ILE
2	F	180	ARG
3	G	27	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	210	GLN
1	E	216	HIS
2	J	235	GLN
2	F	235	GLN
1	I	531	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
10	F3S	B	304	2	0,9,9	-	-	-		
5	FAD	E	601	1	58,58,58	1.23	5 (8%)	85,89,89	1.71	16 (18%)
6	TEO	A	1589	-	5,8,8	2.30	2 (40%)	4,10,10	3.60	3 (75%)
6	TEO	I	1589	-	5,8,8	1.33	0	4,10,10	1.32	0
8	FES	F	302	2	0,4,4	-	-	-		
12	CBE	K	1130	-	16,17,17	1.21	1 (6%)	17,22,22	2.17	4 (23%)
10	F3S	F	304	2	0,9,9	-	-	-		
12	CBE	G	1130	-	16,17,17	1.28	1 (6%)	17,22,22	1.85	3 (17%)
11	HEM	C	1129	4,3	50,50,50	2.06	8 (16%)	67,82,82	2.03	23 (34%)
11	HEM	G	1129	4,3	50,50,50	1.79	8 (16%)	67,82,82	1.33	7 (10%)
6	TEO	E	1589	-	5,8,8	1.16	0	4,10,10	2.07	1 (25%)
8	FES	B	302	2	0,4,4	-	-	-		
9	SF4	J	303	2	0,12,12	-	-	-		
5	FAD	I	601	1	58,58,58	1.15	5 (8%)	85,89,89	1.77	20 (23%)
5	FAD	A	601	1	58,58,58	1.29	6 (10%)	85,89,89	1.72	17 (20%)
8	FES	J	302	2	0,4,4	-	-	-		
9	SF4	B	303	2	0,12,12	-	-	-		
11	HEM	K	1129	4,3	50,50,50	1.95	10 (20%)	67,82,82	1.49	9 (13%)
10	F3S	J	304	2	0,9,9	-	-	-		
12	CBE	C	1130	-	16,17,17	1.22	1 (6%)	17,22,22	2.12	4 (23%)
9	SF4	F	303	2	0,12,12	-	-	-		

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
10	F3S	B	304	2	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	E	601	1	-	5/34/50/50	0/6/6/6
6	TEO	A	1589	-	-	4/6/8/8	-
6	TEO	I	1589	-	-	2/6/8/8	-
8	FES	F	302	2	-	-	0/1/1/1
12	CBE	K	1130	-	-	1/6/19/19	0/2/2/2
10	F3S	F	304	2	-	-	0/3/3/3
12	CBE	G	1130	-	-	1/6/19/19	0/2/2/2
11	HEM	C	1129	4,3	-	6/14/54/54	-
11	HEM	G	1129	4,3	-	7/14/54/54	-
6	TEO	E	1589	-	-	3/6/8/8	-
8	FES	B	302	2	-	-	0/1/1/1
9	SF4	J	303	2	-	-	0/6/5/5
5	FAD	I	601	1	-	5/34/50/50	0/6/6/6
5	FAD	A	601	1	-	7/34/50/50	0/6/6/6
8	FES	J	302	2	-	-	0/1/1/1
9	SF4	B	303	2	-	-	0/6/5/5
11	HEM	K	1129	4,3	-	9/14/54/54	-
10	F3S	J	304	2	-	-	0/3/3/3
12	CBE	C	1130	-	-	0/6/19/19	0/2/2/2
9	SF4	F	303	2	-	-	0/6/5/5

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	1129	HEM	C3D-C2D	7.94	1.53	1.36
11	G	1129	HEM	C3D-C2D	7.83	1.53	1.36
11	C	1129	HEM	C3D-C2D	7.04	1.52	1.36
11	C	1129	HEM	FE-NB	7.01	2.16	1.94
11	C	1129	HEM	FE-ND	6.32	2.14	1.94

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	1130	CBE	O7-C2-C1	7.36	118.00	109.30
5	E	601	FAD	N3A-C2A-N1A	-6.45	118.82	128.58
12	C	1130	CBE	O7-C2-C1	6.38	116.84	109.30
11	C	1129	HEM	C4D-ND-C1D	6.08	112.41	105.21
6	A	1589	TEO	O1A-C1-C2	-5.56	109.20	122.52

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

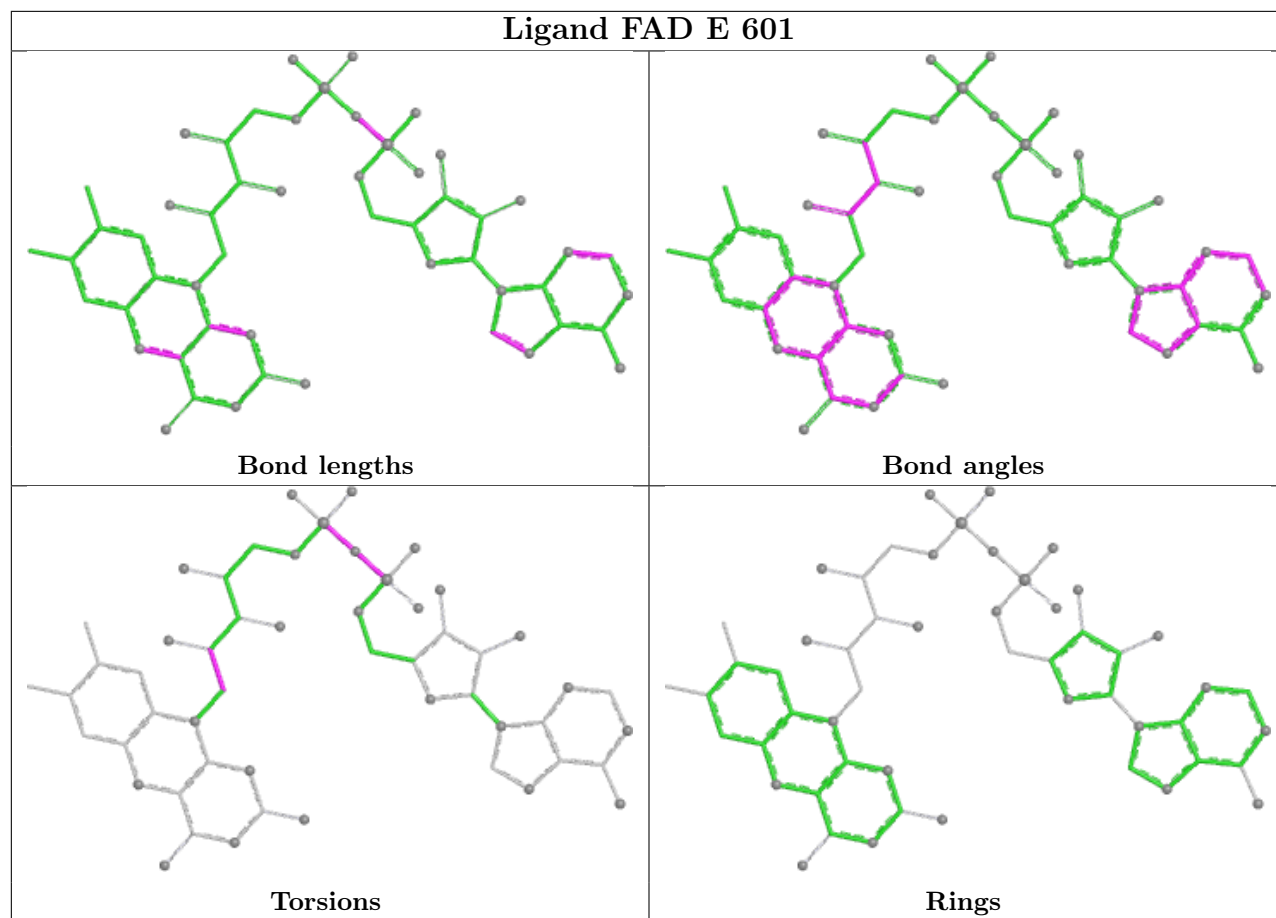
Mol	Chain	Res	Type	Atoms
5	A	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	PA-O3P-P-O5'
5	E	601	FAD	N10-C1'-C2'-O2'
5	I	601	FAD	C5B-O5B-PA-O1A

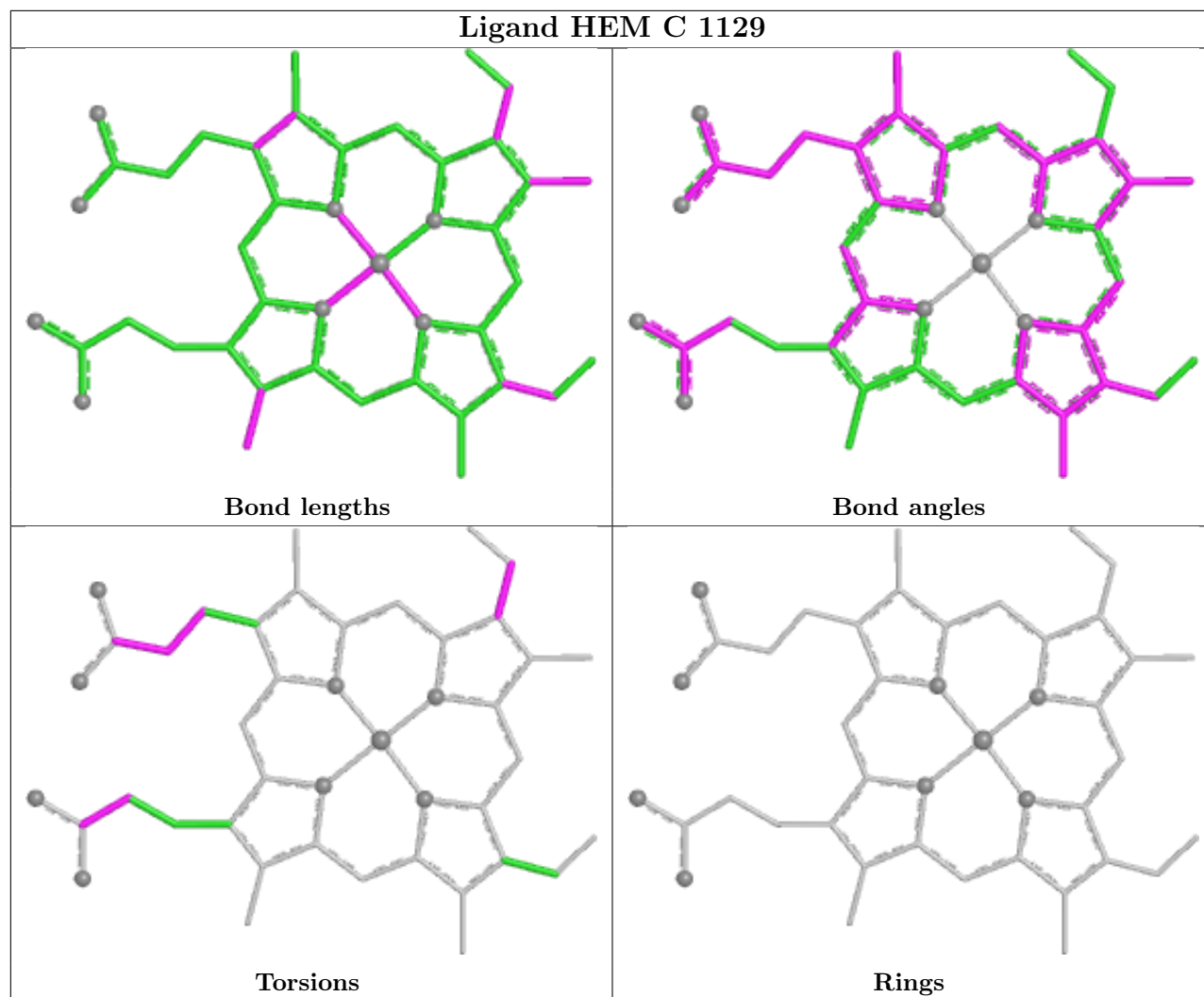
There are no ring outliers.

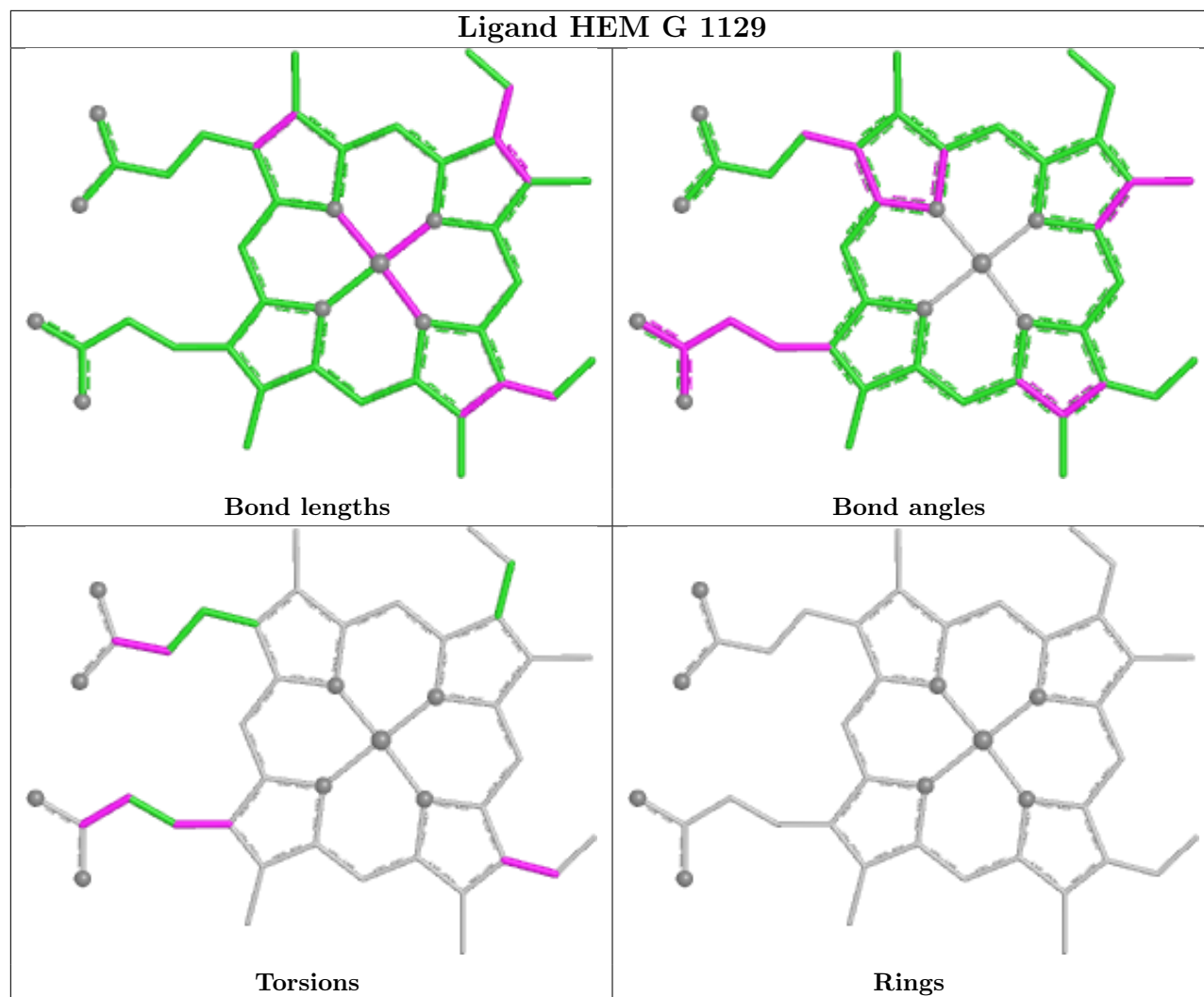
15 monomers are involved in 48 short contacts:

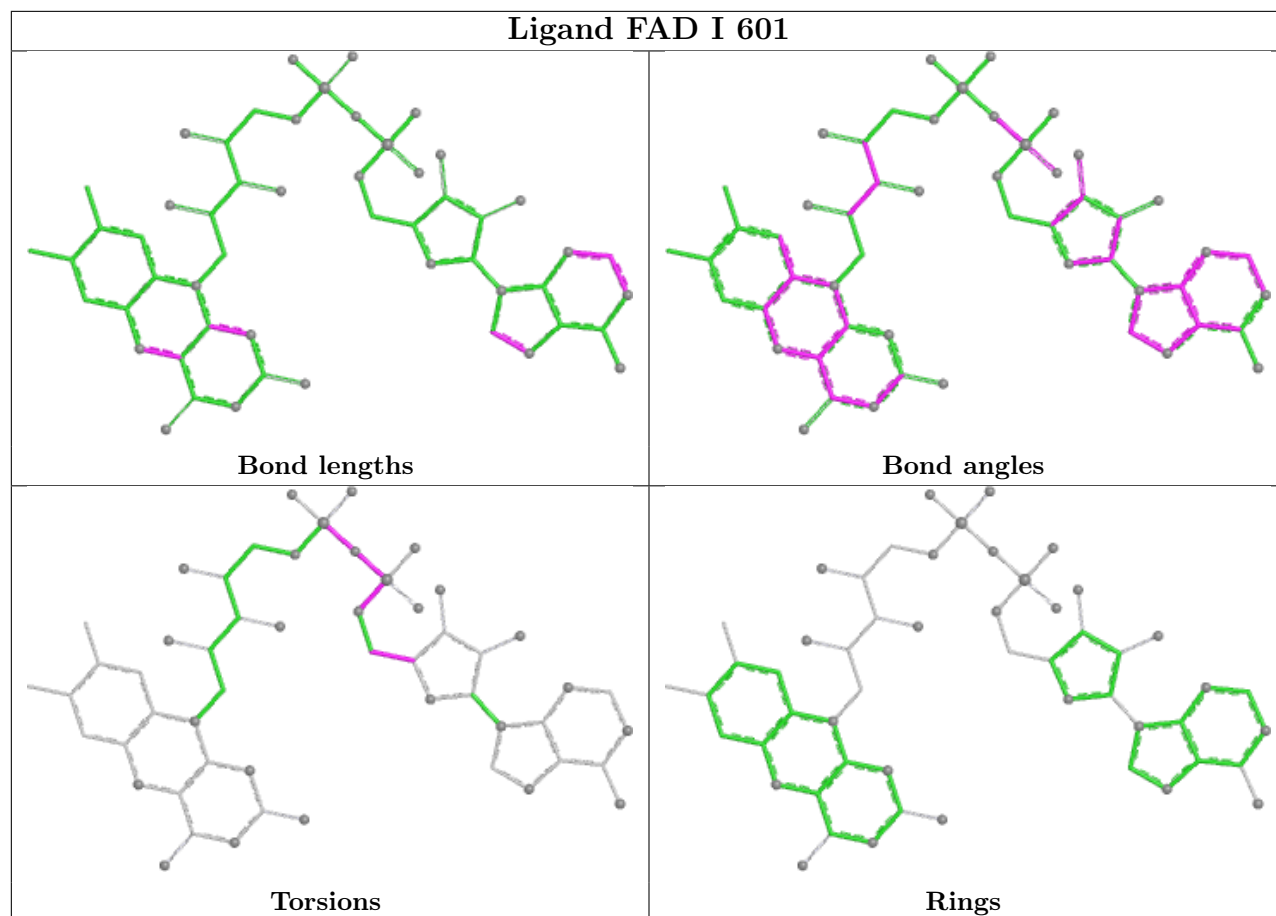
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	601	FAD	4	0
6	A	1589	TEO	2	0
6	I	1589	TEO	2	0
12	K	1130	CBE	2	0
12	G	1130	CBE	2	0
11	C	1129	HEM	2	0
11	G	1129	HEM	7	0
6	E	1589	TEO	2	0
5	I	601	FAD	7	0
5	A	601	FAD	7	0
8	J	302	FES	1	0
11	K	1129	HEM	7	0
10	J	304	F3S	1	0
12	C	1130	CBE	2	0
9	F	303	SF4	1	0

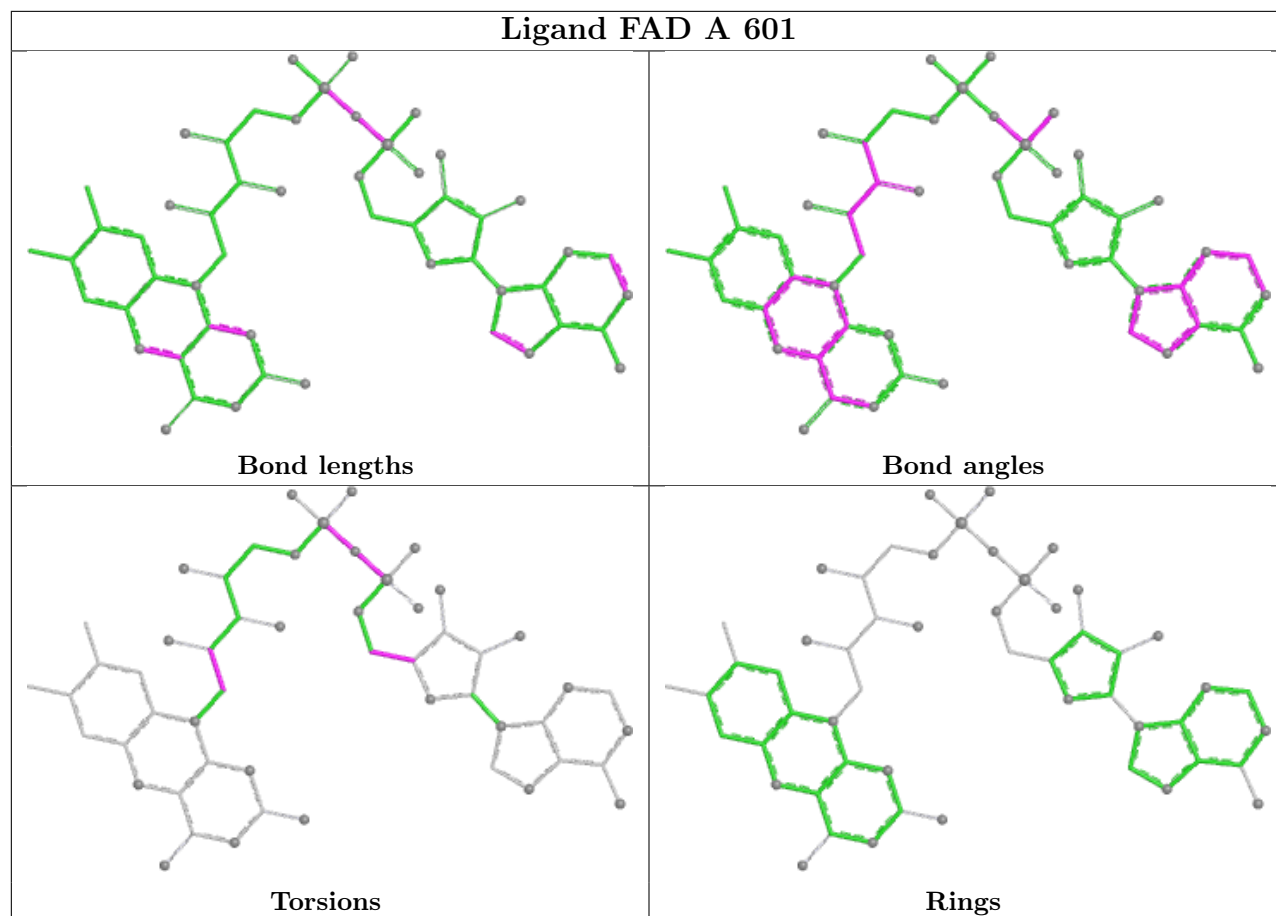
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

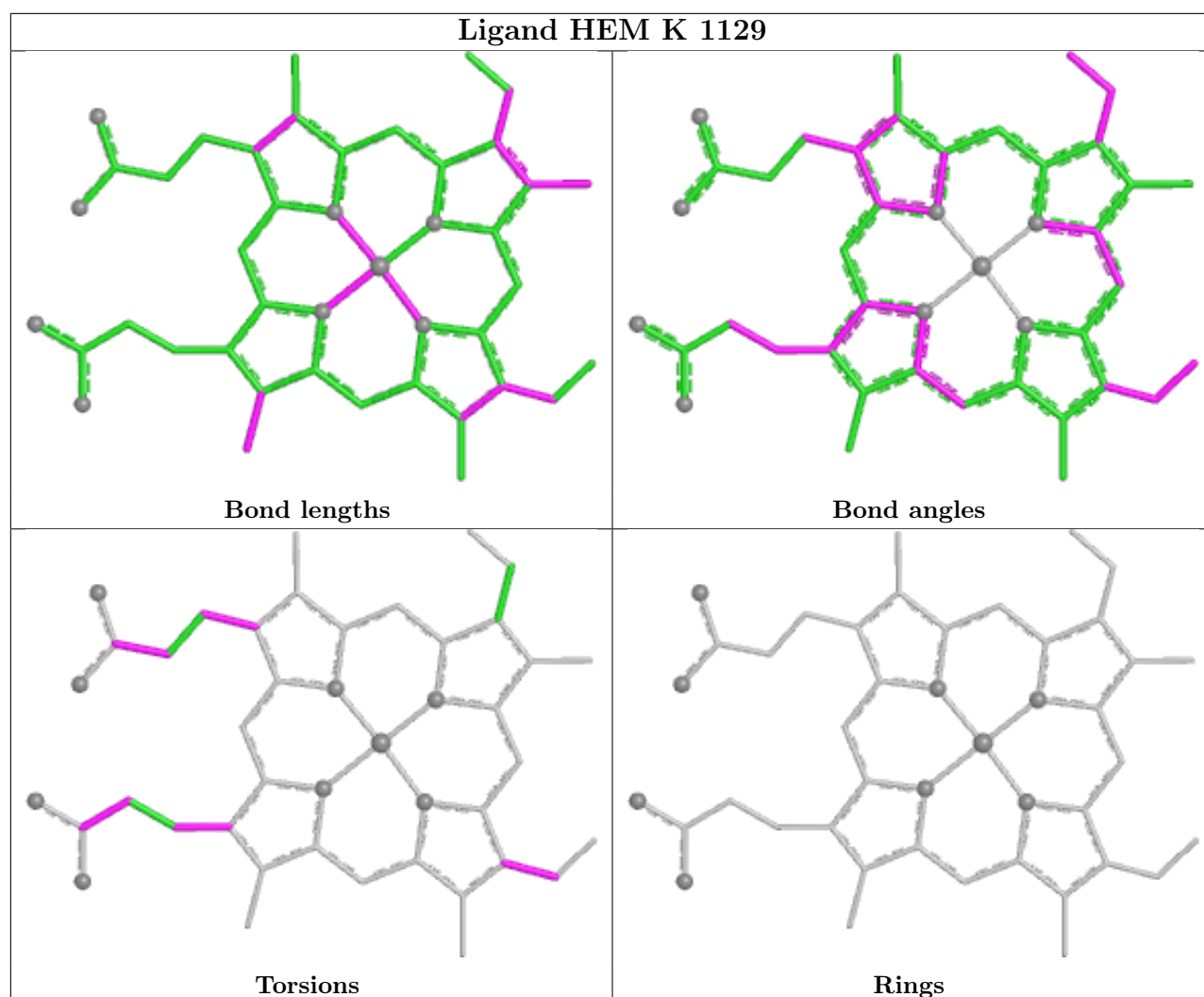












5.7 Other polymers [i](#)

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%)	-0.53	2 (0%) 90 89	35, 50, 67, 78	0
1	E	588/588 (100%)	-0.28	2 (0%) 90 89	42, 60, 85, 94	0
1	I	588/588 (100%)	0.11	10 (1%) 69 67	47, 72, 101, 120	0
2	B	238/238 (100%)	-0.53	0 100 100	36, 47, 67, 82	0
2	F	238/238 (100%)	-0.25	1 (0%) 88 87	45, 56, 88, 104	0
2	J	238/238 (100%)	-0.15	3 (1%) 75 73	48, 61, 101, 120	0
3	C	122/129 (94%)	0.13	3 (2%) 58 55	51, 68, 106, 119	0
3	G	122/129 (94%)	0.35	4 (3%) 49 45	59, 81, 118, 129	0
3	K	122/129 (94%)	0.47	4 (3%) 49 45	70, 86, 125, 134	0
4	D	105/115 (91%)	0.23	5 (4%) 35 32	47, 66, 106, 125	0
4	H	105/115 (91%)	0.16	3 (2%) 53 50	53, 71, 138, 161	0
4	L	105/115 (91%)	0.23	2 (1%) 66 63	60, 77, 137, 159	0
All	All	3159/3210 (98%)	-0.14	39 (1%) 76 75	35, 61, 104, 161	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	MET	4.3
1	E	1	MET	3.9
1	I	336	THR	3.8
2	J	85	PRO	3.7
3	G	68	PHE	3.7

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

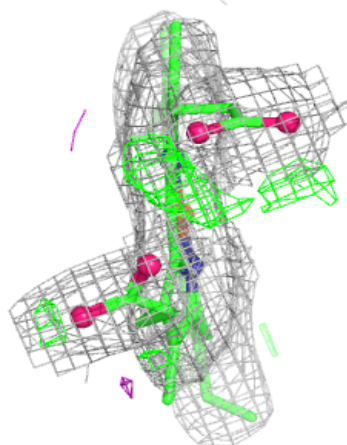
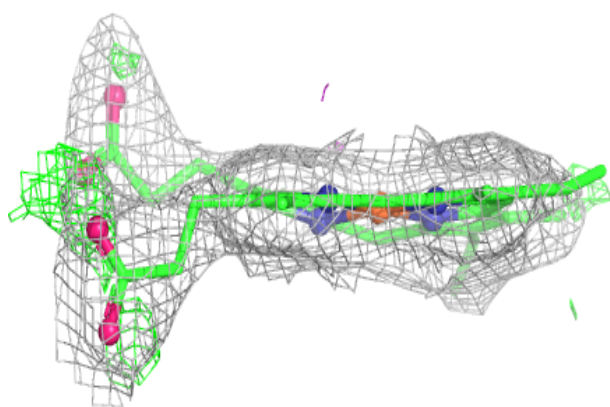
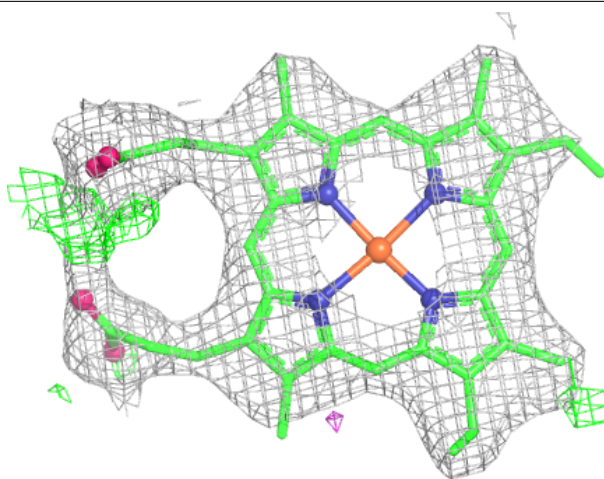
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	TEO	I	1589	9/9	0.90	0.10	68,70,72,74	0
6	TEO	E	1589	9/9	0.93	0.10	45,47,49,53	0
7	NA	A	1590	1/1	0.94	0.05	31,31,31,31	0
7	NA	I	1590	1/1	0.94	0.11	49,49,49,49	0
12	CBE	K	1130	16/16	0.94	0.12	72,73,76,76	0
11	HEM	C	1129	43/43	0.95	0.11	52,55,59,63	0
12	CBE	C	1130	16/16	0.96	0.08	46,49,53,53	0
5	FAD	E	601	53/53	0.97	0.07	40,52,60,62	0
5	FAD	I	601	53/53	0.97	0.07	47,55,62,63	0
11	HEM	G	1129	43/43	0.97	0.10	62,65,67,72	0
6	TEO	A	1589	9/9	0.97	0.06	46,48,52,55	0
12	CBE	G	1130	16/16	0.97	0.07	53,55,58,58	0
7	NA	E	1590	1/1	0.97	0.05	37,37,37,37	0
11	HEM	K	1129	43/43	0.98	0.07	51,57,63,65	0
5	FAD	A	601	53/53	0.98	0.06	30,39,50,55	0
10	F3S	F	304	7/7	0.99	0.04	50,51,53,54	0
10	F3S	J	304	7/7	0.99	0.04	53,55,59,61	0
8	FES	F	302	4/4	0.99	0.04	49,50,51,54	0
8	FES	J	302	4/4	0.99	0.03	56,58,59,60	0
9	SF4	B	303	8/8	0.99	0.04	38,39,41,41	0
9	SF4	F	303	8/8	0.99	0.04	45,46,49,50	0
9	SF4	J	303	8/8	0.99	0.04	47,51,52,52	0
10	F3S	B	304	7/7	0.99	0.03	41,43,47,49	0
8	FES	B	302	4/4	1.00	0.04	37,43,45,47	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.

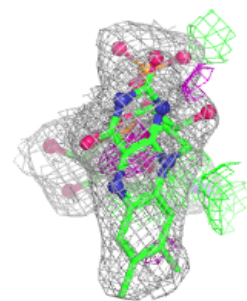
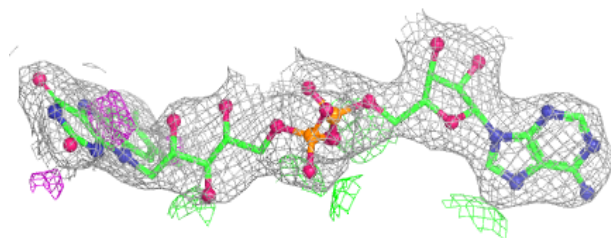
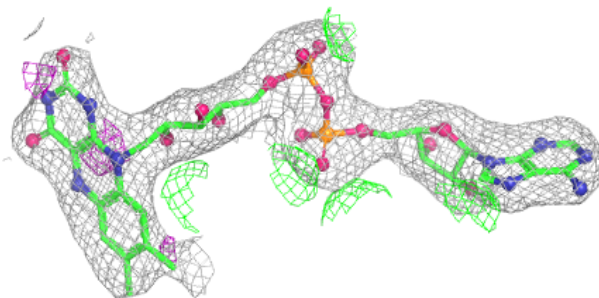
Electron density around HEM C 1129:

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

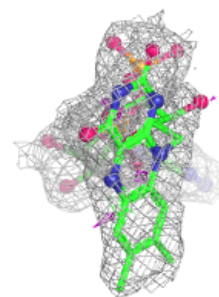
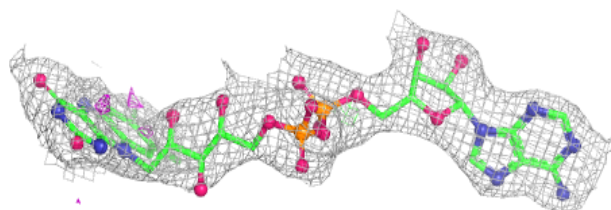
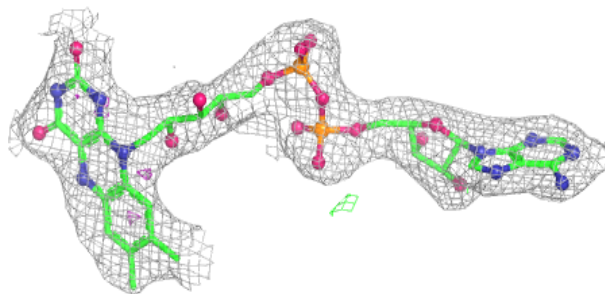


Electron density around FAD E 601:

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

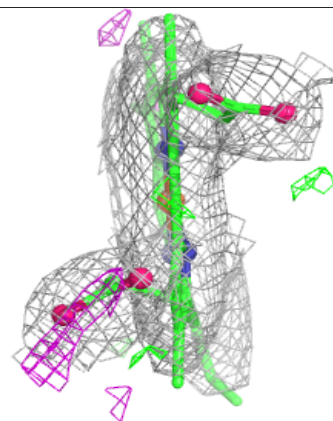
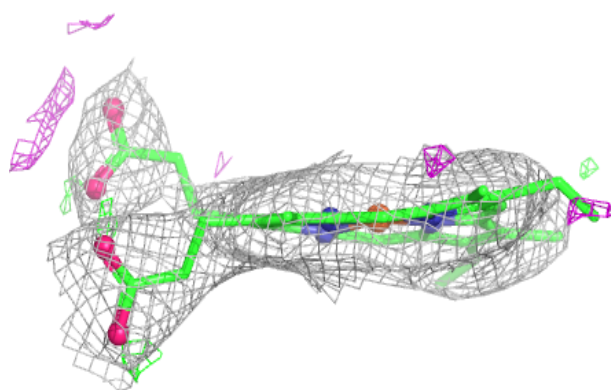
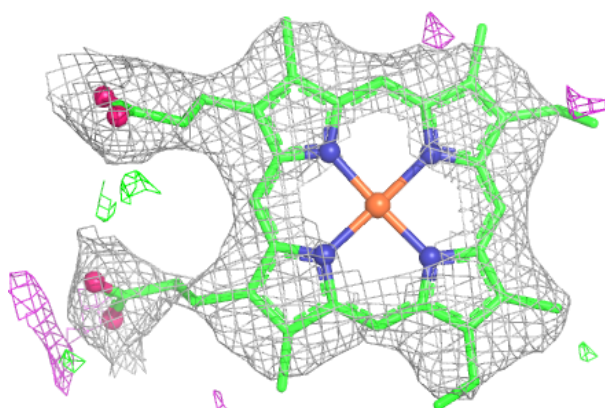
**Electron density around FAD I 601:**

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



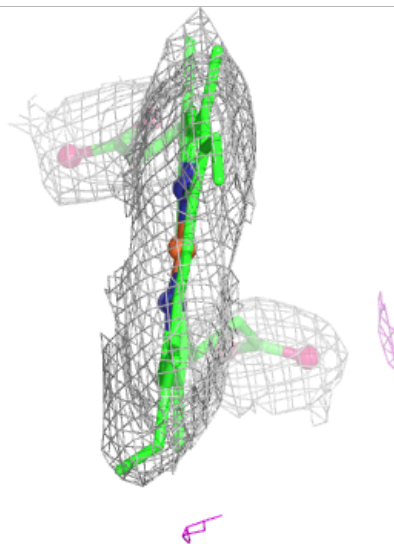
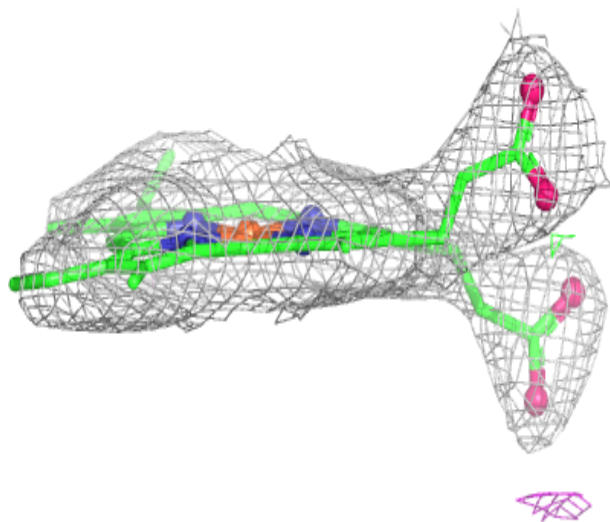
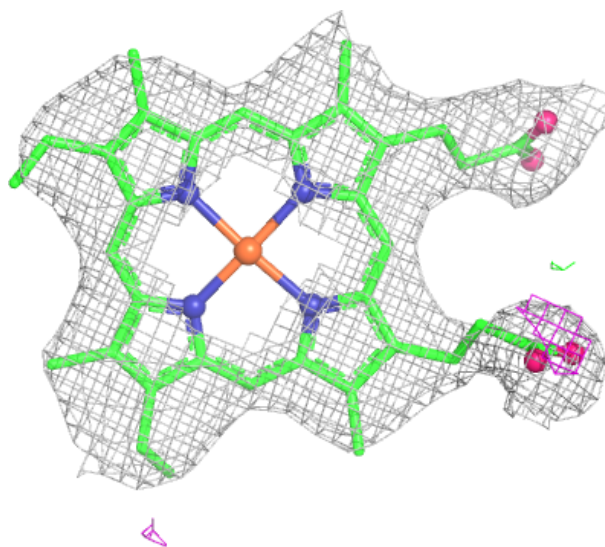
Electron density around HEM G 1129:

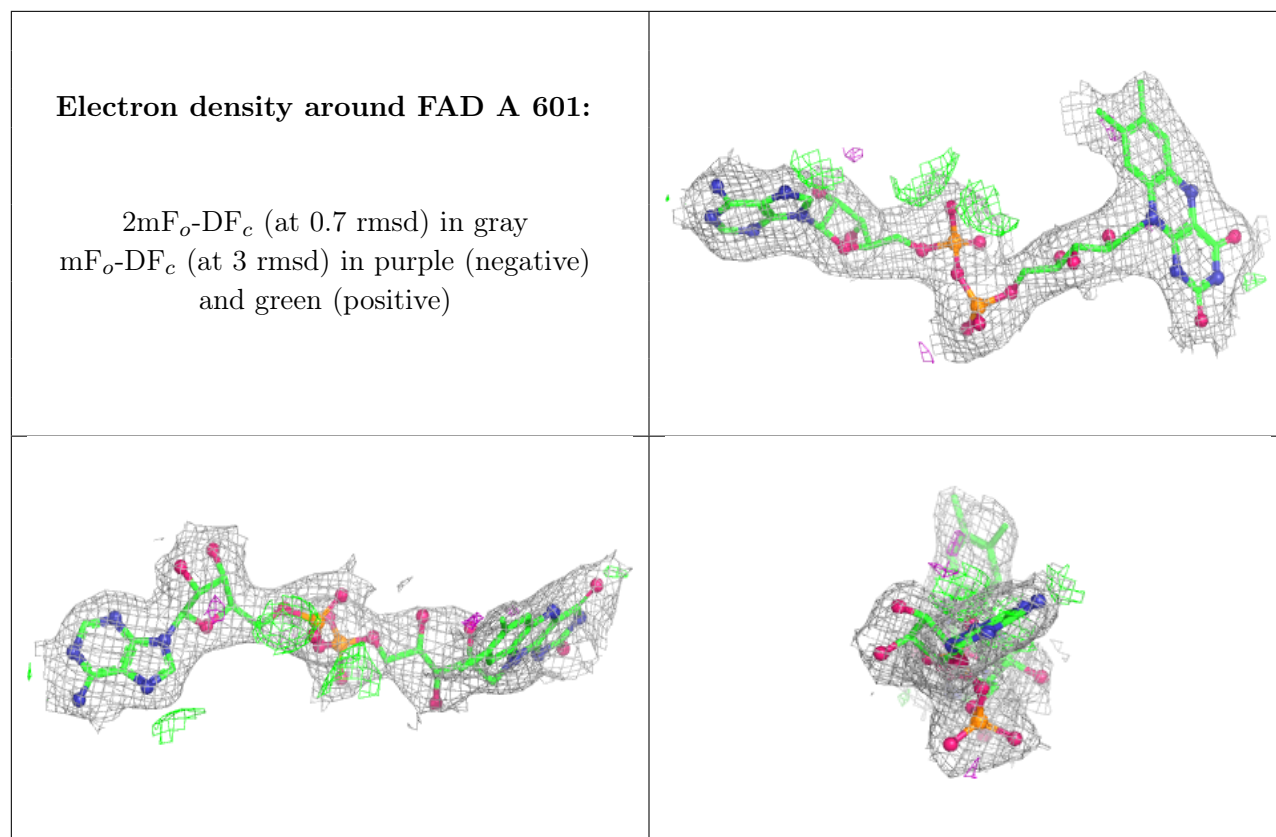
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.