



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 2WDQ / pdb_00002wdq
Title : E. coli succinate:quinone oxidoreductase (SQR) with carboxin bound
Authors : Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on : 2009-03-25
Resolution : 2.40 Å(reported)

This is a 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

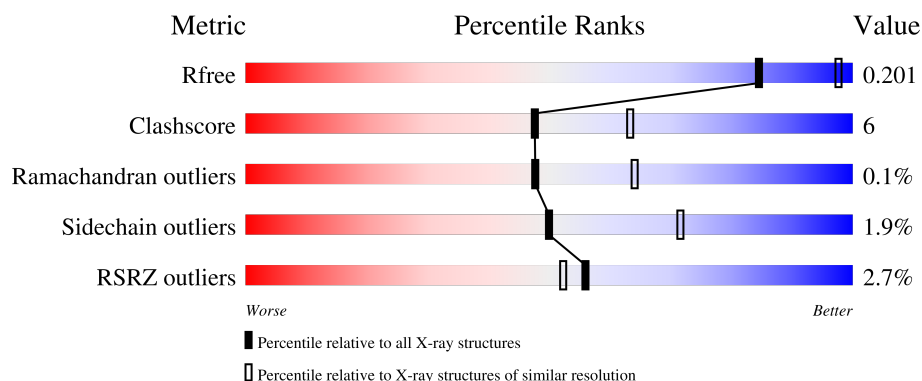
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	588	87% 12% .
1	E	588	90% 10%
1	I	588	88% 12%
2	B	238	92% 6% .
2	F	238	95% 5% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	238	
3	C	129	
3	G	129	
3	K	129	
4	D	115	
4	H	115	
4	L	115	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	TEO	E	1589	-	-	X	-
6	TEO	I	1589	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26034 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUB-UNIT.

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

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

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

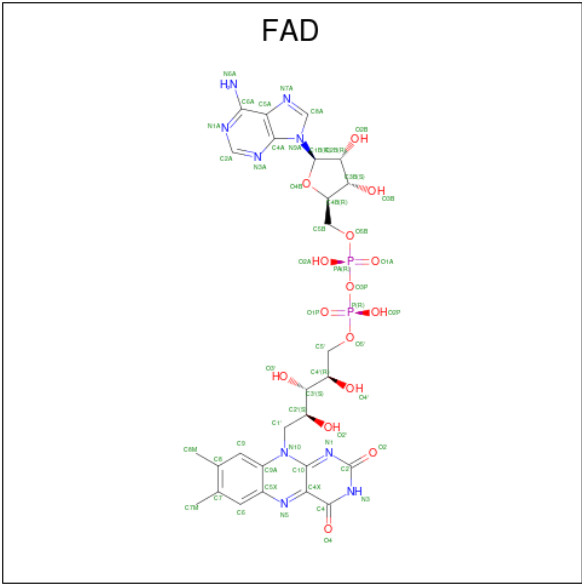
- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT.

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

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

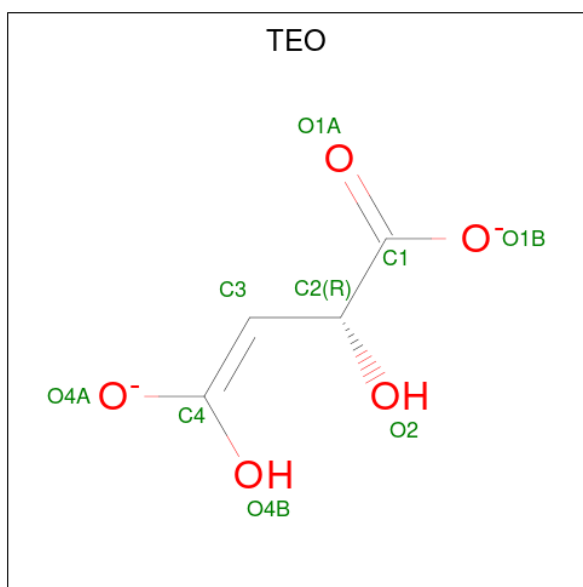
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total	C	N	O	S	0	0	0
			836	577	123	133	3			
4	H	105	Total	C	N	O	S	0	0	0
			836	577	123	133	3			
4	L	105	Total	C	N	O	S	0	0	0
			836	577	123	133	3			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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: C₄H₄O₅).



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

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

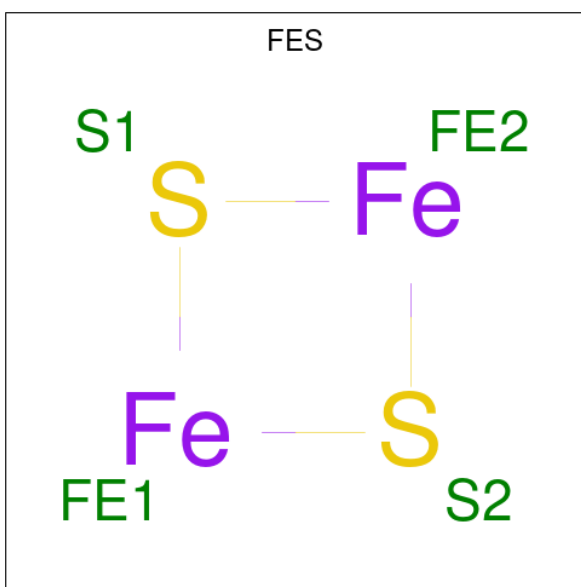
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		
7	E	1	Total	Na	0	0
			1	1		
7	I	1	Total	Na	0	0
			1	1		

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



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

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



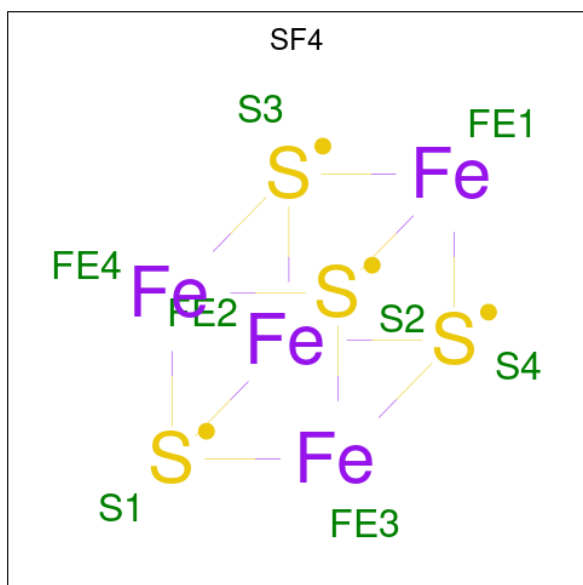
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

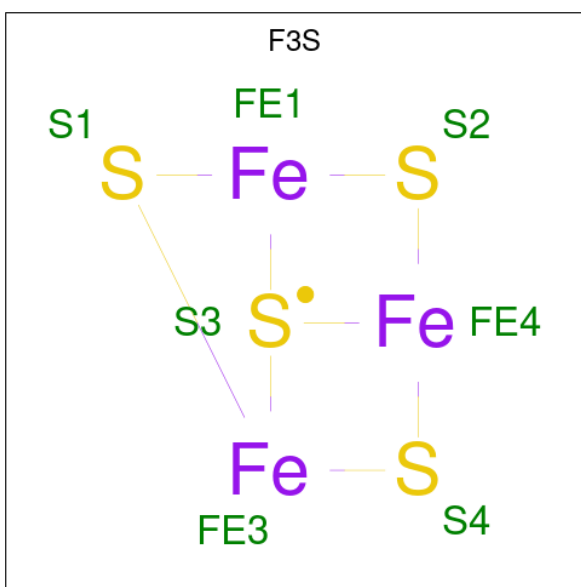
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	Fe	S	0	0
			4	2	2		
9	J	1	Total	Fe	S	0	0
			4	2	2		

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



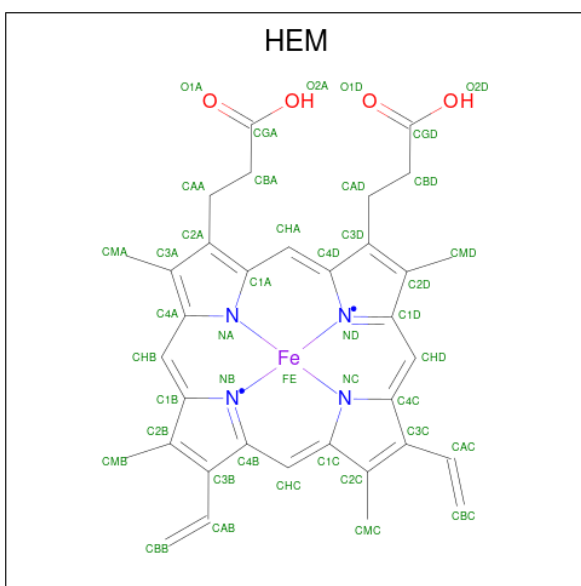
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			8	4	4		
10	F	1	Total	Fe	S	0	0
			8	4	4		
10	J	1	Total	Fe	S	0	0
			8	4	4		

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



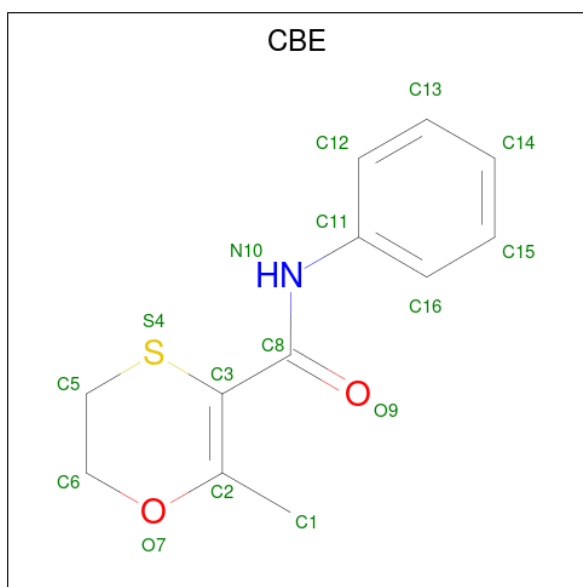
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total 7	Fe 3	S 4	0	0
11	F	1	Total 7	Fe 3	S 4	0	0
11	J	1	Total 7	Fe 3	S 4	0	0

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



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

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



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

- Molecule 14 is water.

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

Continued on next page...

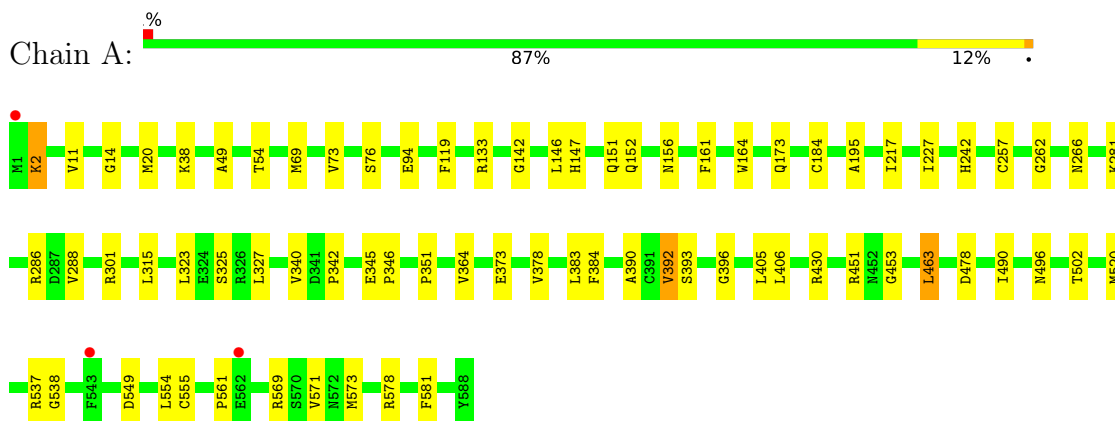
Continued from previous page...

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

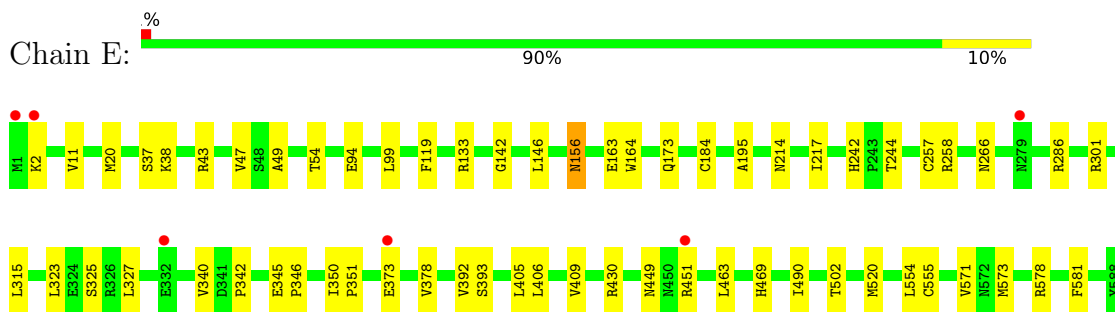
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

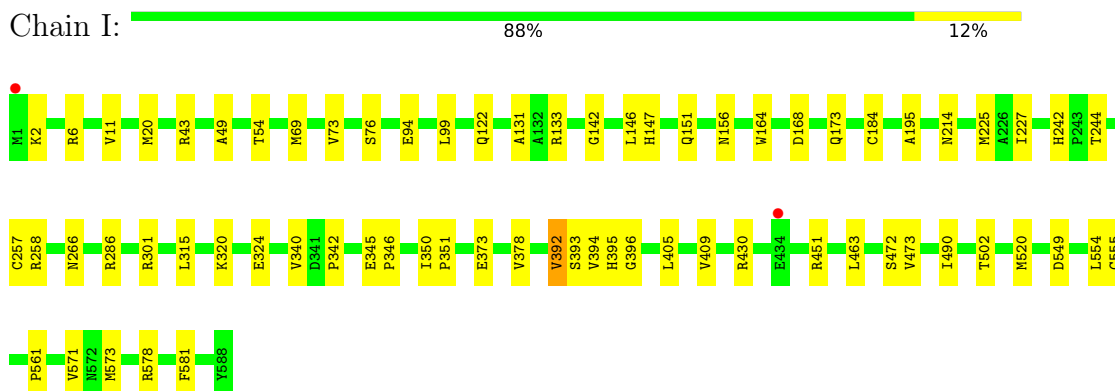
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT



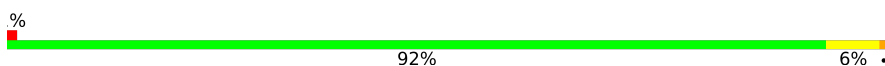
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT



• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

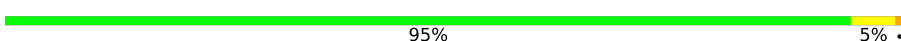


- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain B: 



- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain F: 



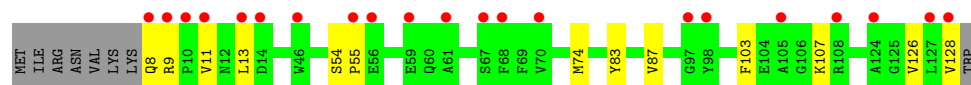
- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain J: 



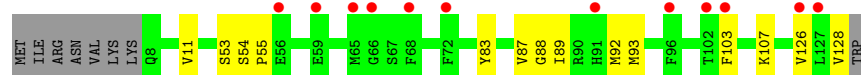
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain C: 



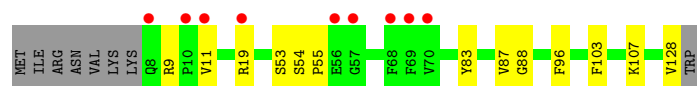
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain G: 



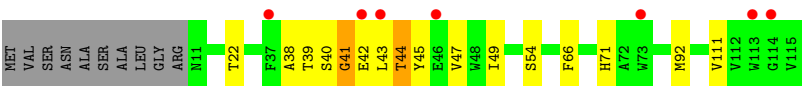
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain K: 

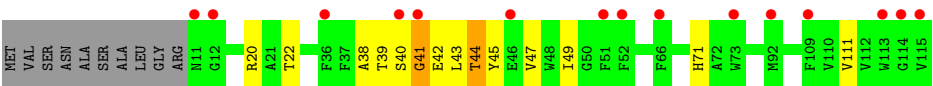
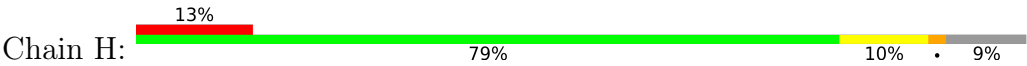


- Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

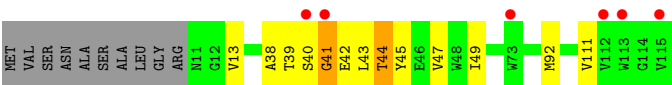
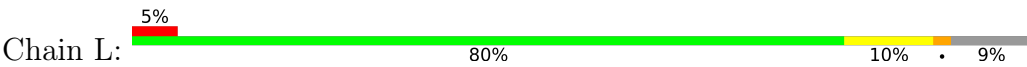
Chain D: 



● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT



● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT



4 Data and refinement statistics

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

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, HEM, SO4, SF4, FES, CBE, TEO, NA, F3S

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	3/4611 (0.1%)	0.94	2/6237 (0.0%)
1	E	0.84	2/4611 (0.0%)	0.92	1/6237 (0.0%)
1	I	0.77	0/4611	0.88	2/6237 (0.0%)
2	B	0.86	1/1908 (0.1%)	0.93	1/2578 (0.0%)
2	F	0.82	0/1908	0.91	0/2578
2	J	0.82	0/1908	0.90	1/2578 (0.0%)
3	C	0.68	0/953	0.78	0/1293
3	G	0.67	0/953	0.79	0/1293
3	K	0.66	0/953	0.81	1/1293 (0.1%)
4	D	0.72	0/859	0.80	0/1175
4	H	0.65	0/859	0.80	1/1175 (0.1%)
4	L	0.66	0/859	0.77	0/1175
All	All	0.80	6/24993 (0.0%)	0.89	9/33849 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	449	ASN	CG-ND2	-6.60	1.19	1.33
1	E	156	ASN	CG-ND2	-6.07	1.20	1.33
1	A	152	GLN	CD-NE2	-5.76	1.21	1.33
1	A	288	VAL	CA-CB	5.39	1.60	1.54
1	A	390	ALA	CA-CB	-5.32	1.45	1.53
2	B	215	VAL	C-O	-5.02	1.19	1.24

All (9) bond angle outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	244	THR	N-CA-C	5.64	117.27	109.54
1	I	392	VAL	N-CA-C	5.57	116.35	110.72
2	J	213	VAL	CB-CA-C	-5.38	104.87	112.14
4	H	111	VAL	N-CA-C	5.20	115.41	110.53
1	A	281	LYS	CB-CA-C	-5.14	110.63	116.54
1	A	392	VAL	N-CA-C	5.03	115.80	110.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4522	0	4426	49	0
1	E	4522	0	4426	44	0
1	I	4522	0	4426	50	0
2	B	1869	0	1850	13	0
2	F	1869	0	1850	9	0
2	J	1869	0	1850	18	0
3	C	933	0	979	16	0
3	G	933	0	979	14	0
3	K	933	0	979	11	0
4	D	836	0	875	13	0
4	H	836	0	875	13	0
4	L	836	0	875	11	0
5	A	53	0	29	6	0
5	E	53	0	30	7	0
5	I	53	0	29	7	0
6	A	9	0	3	3	0
6	E	9	0	3	4	0
6	I	9	0	3	4	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
8	A	5	0	0	0	0
8	E	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	5	0	0	0	0
9	B	4	0	0	0	0
9	F	4	0	0	0	0
9	J	4	0	0	0	0
10	B	8	0	0	0	0
10	F	8	0	0	0	0
10	J	8	0	0	1	0
11	B	7	0	0	0	0
11	F	7	0	0	0	0
11	J	7	0	0	0	0
12	C	43	0	30	6	0
12	G	43	0	30	5	0
12	K	43	0	30	6	0
13	C	16	0	13	2	0
13	G	16	0	13	1	0
13	K	16	0	13	2	0
14	A	258	0	0	5	0
14	B	128	0	0	1	0
14	C	22	0	0	1	0
14	D	10	0	0	1	0
14	E	234	0	0	3	0
14	F	116	0	0	0	0
14	G	17	0	0	0	0
14	H	4	0	0	0	0
14	I	197	0	0	3	0
14	J	107	0	0	1	0
14	K	17	0	0	1	0
14	L	6	0	0	0	0
All	All	26034	0	24616	278	0

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

All (278) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:THR:HG22	14:A:2215:HOH:O	1.41	1.17
1:I:490:ILE:HG22	1:I:520:MET:HE1	1.34	1.10
12:C:1129:HEM:HHD	12:C:1129:HEM:HBC2	1.35	1.09
1:E:490:ILE:HG22	1:E:520:MET:HE1	1.38	0.99
1:I:490:ILE:CG2	1:I:520:MET:HE1	1.99	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ILE:HG22	1:A:520:MET:HE1	1.49	0.92
1:E:502:THR:HG22	14:E:2187:HOH:O	1.70	0.92
1:I:490:ILE:HG22	1:I:520:MET:CE	2.02	0.89
12:G:1129:HEM:HHC	12:G:1129:HEM:HBB2	1.58	0.85
1:E:490:ILE:CG2	1:E:520:MET:HE1	2.07	0.84
1:E:490:ILE:HG22	1:E:520:MET:CE	2.07	0.84
1:I:555:CYS:HA	1:I:571:VAL:HG23	1.59	0.83
1:A:490:ILE:HG22	1:A:520:MET:CE	2.18	0.74
1:A:555:CYS:HA	1:A:571:VAL:HG23	1.70	0.73
12:C:1129:HEM:HBC2	12:C:1129:HEM:CHD	2.11	0.73
1:I:554:LEU:HD21	1:I:573:MET:HE1	1.72	0.71
2:J:45:LYS:HD3	14:J:2012:HOH:O	1.90	0.71
1:A:490:ILE:CG2	1:A:520:MET:HE1	2.20	0.71
1:E:555:CYS:HA	1:E:571:VAL:HG23	1.74	0.70
4:D:45:TYR:OH	4:D:49:ILE:HD12	1.92	0.69
12:C:1129:HEM:HHC	12:C:1129:HEM:HBB2	1.73	0.68
1:I:502:THR:HG22	14:I:2167:HOH:O	1.92	0.68
3:C:54:SER:HB2	3:C:55:PRO:HD2	1.75	0.68
13:K:1130:CBE:H16	13:K:1130:CBE:O9	1.94	0.67
1:E:392:VAL:N	1:E:393:SER:HA	2.10	0.67
2:F:55:CYS:O	2:F:56:ARG:HD2	1.95	0.67
3:C:8:GLN:HA	14:C:2001:HOH:O	1.94	0.67
1:E:286:ARG:HH22	6:E:1589:TEO:C3	2.07	0.67
1:A:286:ARG:HH22	6:A:1589:TEO:C3	2.07	0.66
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.75	0.66
1:E:49:ALA:HA	5:E:601:FAD:C6	2.26	0.66
3:C:128:VAL:O	3:C:128:VAL:CG1	2.43	0.65
1:E:554:LEU:HD21	1:E:573:MET:HE1	1.76	0.65
3:C:103:PHE:CE2	3:C:107:LYS:HE2	2.32	0.65
3:C:128:VAL:O	3:C:128:VAL:HG12	1.96	0.65
1:A:554:LEU:HD21	1:A:573:MET:HE1	1.79	0.64
1:E:49:ALA:HA	5:E:601:FAD:C5X	2.28	0.64
2:B:55:CYS:O	2:B:56:ARG:HD2	1.98	0.64
3:G:54:SER:HB2	3:G:55:PRO:HD2	1.79	0.64
1:I:392:VAL:N	1:I:393:SER:HA	2.13	0.63
1:I:49:ALA:HA	5:I:601:FAD:C5X	2.28	0.63
12:K:1129:HEM:HBC2	12:K:1129:HEM:HHD	1.81	0.63
3:C:103:PHE:CE2	3:C:107:LYS:CE	2.81	0.63
2:J:1:MET:HG3	2:J:1:MET:O	1.99	0.62
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.79	0.62
1:A:49:ALA:HA	5:A:601:FAD:C5X	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:44:THR:HG23	4:L:47:VAL:HG13	1.82	0.62
1:E:578:ARG:NH1	1:E:581:PHE:CZ	2.68	0.61
1:A:578:ARG:NH1	1:A:581:PHE:CZ	2.69	0.61
1:I:54:THR:HG23	1:I:133:ARG:HG3	1.84	0.60
12:G:1129:HEM:HBC2	12:G:1129:HEM:HHD	1.84	0.60
1:I:49:ALA:HA	5:I:601:FAD:C6	2.32	0.60
3:K:54:SER:HB2	3:K:55:PRO:HD2	1.83	0.59
3:G:128:VAL:O	3:G:128:VAL:CG1	2.50	0.59
1:A:173:GLN:CD	1:A:430:ARG:HH11	2.10	0.59
3:K:103:PHE:CE2	3:K:107:LYS:HE2	2.37	0.59
1:A:392:VAL:N	1:A:393:SER:HA	2.18	0.59
12:K:1129:HEM:HHHA	12:K:1129:HEM:HBA2	1.84	0.58
1:A:451:ARG:HD2	14:A:2189:HOH:O	2.03	0.58
1:E:463:LEU:C	1:E:463:LEU:HD23	2.29	0.58
5:A:601:FAD:N5	6:A:1589:TEO:H2	2.19	0.58
3:G:103:PHE:CE2	3:G:107:LYS:CE	2.86	0.58
3:G:103:PHE:CE2	3:G:107:LYS:HE2	2.40	0.57
2:F:1:MET:O	2:F:1:MET:HG3	2.04	0.57
2:J:55:CYS:O	2:J:56:ARG:HD2	2.04	0.57
3:K:103:PHE:CE2	3:K:107:LYS:CE	2.88	0.57
3:K:128:VAL:CG1	3:K:128:VAL:O	2.52	0.57
3:G:128:VAL:O	3:G:128:VAL:HG12	2.04	0.57
4:L:44:THR:CG2	4:L:47:VAL:HG13	2.35	0.56
2:F:56:ARG:O	2:F:56:ARG:HD3	2.05	0.56
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.87	0.56
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.41	0.56
13:C:1130:CBE:H16	13:C:1130:CBE:O9	2.04	0.56
4:D:44:THR:HG23	4:D:47:VAL:HG13	1.88	0.56
1:A:49:ALA:HA	5:A:601:FAD:C6	2.36	0.55
1:E:20:MET:HE2	1:E:146:LEU:HD11	1.89	0.55
1:E:54:THR:HG23	1:E:133:ARG:HG3	1.89	0.54
3:G:83:TYR:CZ	3:G:87:VAL:HG21	2.41	0.54
1:I:405:LEU:HG	5:I:601:FAD:C2	2.36	0.54
1:I:257:CYS:HB3	1:I:315:LEU:HD21	1.90	0.54
1:E:99:LEU:HD11	1:E:409:VAL:HG21	1.90	0.54
1:A:76:SER:HB2	1:A:396:GLY:HA3	1.90	0.54
4:H:44:THR:HG23	4:H:47:VAL:HG13	1.90	0.54
2:B:56:ARG:O	2:B:56:ARG:HD3	2.08	0.54
3:G:88:GLY:HA3	12:G:1129:HEM:HBC2	1.90	0.54
1:I:578:ARG:NH1	1:I:581:PHE:CZ	2.76	0.54
2:J:56:ARG:O	2:J:56:ARG:HD3	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:173:GLN:CD	1:I:430:ARG:HH11	2.16	0.54
5:I:601:FAD:N5	6:I:1589:TEO:H2	2.23	0.54
1:A:266:ASN:HB2	1:A:301:ARG:O	2.08	0.54
13:K:1130:CBE:O9	13:K:1130:CBE:C16	2.55	0.54
3:K:128:VAL:O	3:K:128:VAL:HG12	2.08	0.53
1:E:173:GLN:CD	1:E:430:ARG:HH11	2.15	0.53
1:E:578:ARG:NH1	1:E:581:PHE:CE1	2.76	0.53
4:L:41:GLY:O	4:L:42:GLU:C	2.51	0.53
4:D:44:THR:CG2	4:D:47:VAL:HG13	2.39	0.52
4:D:45:TYR:CZ	4:D:49:ILE:HD12	2.44	0.52
4:H:41:GLY:O	4:H:42:GLU:C	2.52	0.52
4:H:45:TYR:OH	4:H:49:ILE:HD12	2.09	0.52
1:I:99:LEU:HD11	1:I:409:VAL:HG21	1.92	0.52
1:I:463:LEU:C	1:I:463:LEU:HD23	2.35	0.52
1:E:257:CYS:HB3	1:E:315:LEU:HD21	1.91	0.51
1:I:286:ARG:HH22	6:I:1589:TEO:C3	2.23	0.51
1:A:156:ASN:HB2	14:A:2054:HOH:O	2.09	0.51
1:E:49:ALA:HA	5:E:601:FAD:N5	2.26	0.51
4:D:41:GLY:O	4:D:42:GLU:C	2.53	0.51
1:A:257:CYS:HB3	1:A:315:LEU:HD21	1.92	0.51
5:I:601:FAD:C4	6:I:1589:TEO:C3	2.89	0.51
1:A:54:THR:HG23	1:A:133:ARG:HG3	1.92	0.51
1:I:258:ARG:HD3	14:I:2087:HOH:O	2.11	0.50
2:B:1:MET:O	2:B:1:MET:HG3	2.11	0.50
1:A:242:HIS:O	1:A:351:PRO:HA	2.11	0.50
3:G:103:PHE:CE2	3:G:107:LYS:HE3	2.47	0.50
12:K:1129:HEM:HHD	12:K:1129:HEM:CBC	2.41	0.50
12:C:1129:HEM:HHD	12:C:1129:HEM:CBC	2.20	0.50
2:J:169:PHE:CD1	2:J:205:ARG:HB2	2.47	0.49
1:E:20:MET:CE	1:E:146:LEU:CD1	2.91	0.49
13:G:1130:CBE:O9	13:G:1130:CBE:H16	2.12	0.49
4:H:44:THR:CG2	4:H:47:VAL:HG13	2.42	0.49
2:J:117:ILE:C	2:J:117:ILE:HD12	2.38	0.49
3:C:103:PHE:CE2	3:C:107:LYS:HE3	2.47	0.49
2:F:56:ARG:CD	2:F:56:ARG:C	2.86	0.49
1:I:472:SER:OG	1:I:473:VAL:N	2.46	0.49
1:E:54:THR:O	1:E:406:LEU:HD22	2.12	0.49
4:L:38:ALA:O	4:L:39:THR:CG2	2.61	0.48
1:I:49:ALA:HA	5:I:601:FAD:N5	2.29	0.48
4:H:38:ALA:O	4:H:39:THR:CG2	2.61	0.48
1:A:69:MET:O	1:A:73:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:76:SER:HB2	1:I:396:GLY:HA3	1.96	0.48
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.48	0.48
1:E:469:HIS:HB3	14:E:2178:HOH:O	2.13	0.48
1:I:258:ARG:NH2	14:I:2089:HOH:O	2.45	0.48
3:C:54:SER:HB2	3:C:55:PRO:CD	2.43	0.47
4:D:66:PHE:HD1	14:D:2006:HOH:O	1.96	0.47
1:A:405:LEU:HG	5:A:601:FAD:C2	2.44	0.47
5:E:601:FAD:N5	6:E:1589:TEO:H2	2.29	0.47
2:B:155:CYS:SG	2:B:173:ALA:HB2	2.55	0.47
12:G:1129:HEM:HHD	12:G:1129:HEM:CBC	2.43	0.47
3:G:89:ILE:O	3:G:93:MET:HG3	2.15	0.47
13:C:1130:CBE:O9	13:C:1130:CBE:C16	2.63	0.47
1:I:69:MET:O	1:I:73:VAL:HG23	2.14	0.47
3:G:54:SER:HB2	3:G:55:PRO:CD	2.45	0.47
3:K:83:TYR:CZ	3:K:87:VAL:HG21	2.50	0.47
2:J:217:PRO:HD2	10:J:303:SF4:S3	2.55	0.46
4:L:38:ALA:C	4:L:39:THR:HG23	2.40	0.46
1:E:242:HIS:O	1:E:351:PRO:HA	2.15	0.46
2:J:183:ILE:C	2:J:183:ILE:HD12	2.41	0.46
1:A:345:GLU:HG2	1:A:346:PRO:HD2	1.98	0.46
1:E:43:ARG:HD3	2:F:60:CYS:O	2.15	0.46
4:H:22:THR:OG1	4:H:71:HIS:HB2	2.16	0.46
12:K:1129:HEM:HBA2	12:K:1129:HEM:CHA	2.44	0.46
1:A:451:ARG:HA	1:A:451:ARG:HD3	1.67	0.46
3:C:103:PHE:CZ	3:C:107:LYS:HE2	2.51	0.46
1:I:578:ARG:NH1	1:I:581:PHE:CE1	2.84	0.46
1:A:161:PHE:HB3	1:A:164:TRP:CD1	2.51	0.46
4:D:44:THR:HG23	4:D:47:VAL:HG22	1.97	0.45
1:A:373:GLU:HG2	14:A:2144:HOH:O	2.15	0.45
4:H:40:SER:O	4:H:41:GLY:C	2.57	0.45
1:I:242:HIS:O	1:I:351:PRO:HA	2.15	0.45
1:E:350:ILE:HG13	1:E:351:PRO:HD2	1.99	0.45
1:I:168:ASP:HA	1:I:225:MET:HG2	1.98	0.45
1:I:451:ARG:HD3	1:I:451:ARG:HA	1.67	0.45
1:A:578:ARG:NH1	1:A:581:PHE:CE1	2.84	0.45
3:G:92:MET:HG2	4:H:20:ARG:HG2	1.99	0.45
1:I:20:MET:HE2	1:I:146:LEU:HD11	1.99	0.45
1:I:350:ILE:HG13	1:I:351:PRO:HD2	1.98	0.45
4:L:45:TYR:OH	4:L:49:ILE:HD12	2.16	0.45
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.52	0.45
4:H:38:ALA:C	4:H:39:THR:HG23	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:43:ARG:HD3	2:J:60:CYS:O	2.17	0.45
1:E:20:MET:CE	1:E:146:LEU:HD12	2.47	0.45
4:H:44:THR:HG23	4:H:47:VAL:HG22	1.99	0.45
2:B:95:PRO:O	2:B:157:THR:HB	2.16	0.44
1:I:147:HIS:O	1:I:151:GLN:HG3	2.17	0.44
1:A:453:GLY:HA3	1:A:496:ASN:O	2.16	0.44
12:C:1129:HEM:HH3	12:C:1129:HEM:CBB	2.46	0.44
1:E:405:LEU:HG	5:E:601:FAD:C2	2.47	0.44
12:C:1129:HEM:HBB2	12:C:1129:HEM:CHC	2.43	0.44
4:D:45:TYR:OH	4:D:49:ILE:CD1	2.63	0.44
1:A:147:HIS:O	1:A:151:GLN:HG3	2.18	0.44
2:B:117:ILE:C	2:B:117:ILE:HD12	2.42	0.44
1:A:2:LYS:O	1:A:2:LYS:HD3	2.18	0.44
2:F:169:PHE:CE2	2:F:171:GLY:HA2	2.53	0.44
1:I:554:LEU:HD21	1:I:573:MET:CE	2.45	0.44
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.53	0.44
1:I:164:TRP:CH2	1:I:184:CYS:HB2	2.53	0.44
1:I:266:ASN:HB2	1:I:301:ARG:O	2.18	0.44
2:J:56:ARG:C	2:J:56:ARG:CD	2.91	0.44
1:A:286:ARG:HH12	6:A:1589:TEO:C4	2.30	0.44
1:I:122:GLN:HB3	1:I:131:ALA:HB3	2.00	0.44
4:L:40:SER:O	4:L:41:GLY:C	2.59	0.44
3:C:13:LEU:HD12	3:C:13:LEU:HA	1.90	0.43
4:D:92:MET:N	4:D:92:MET:HE2	2.33	0.43
1:A:49:ALA:HB3	1:A:142:GLY:HA3	2.00	0.43
1:I:286:ARG:HH12	6:I:1589:TEO:C4	2.32	0.43
4:D:38:ALA:O	4:D:39:THR:CG2	2.66	0.43
1:I:394:VAL:HG23	1:I:395:HIS:CE1	2.53	0.43
2:B:1:MET:HE2	14:B:2055:HOH:O	2.18	0.43
2:B:214:SER:HB3	3:C:103:PHE:CE1	2.52	0.43
2:F:130:ALA:CB	1:I:6:ARG:HG2	2.49	0.43
3:C:8:GLN:HG2	3:C:9:ARG:N	2.32	0.43
1:A:340:VAL:O	1:A:342:PRO:HD3	2.19	0.43
2:F:175:LEU:HD23	2:F:175:LEU:HA	1.91	0.43
1:I:49:ALA:HB3	1:I:142:GLY:HA3	2.01	0.42
1:I:214:ASN:N	1:I:214:ASN:HD22	2.16	0.42
1:I:320:LYS:HE2	1:I:324:GLU:OE2	2.19	0.42
1:I:340:VAL:O	1:I:342:PRO:HD3	2.19	0.42
1:I:345:GLU:HG2	1:I:346:PRO:HD2	2.00	0.42
1:I:549:ASP:OD1	1:I:549:ASP:C	2.62	0.42
1:A:49:ALA:HA	5:A:601:FAD:N5	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:61:GLY:HA2	2:J:150:ILE:HD12	2.00	0.42
3:K:96:PHE:CD1	3:K:96:PHE:N	2.86	0.42
1:E:38:LYS:HE3	1:E:217:ILE:HB	2.00	0.42
2:J:1:MET:HE3	2:J:1:MET:HB2	1.81	0.42
2:B:169:PHE:CE2	2:B:171:GLY:HA2	2.54	0.42
2:J:160:PRO:HA	2:J:163:TRP:CE3	2.54	0.42
3:K:88:GLY:HA3	12:K:1129:HEM:HBC2	2.01	0.42
3:K:103:PHE:CE2	3:K:107:LYS:HE3	2.54	0.42
1:A:323:LEU:HD23	1:A:327:LEU:HD12	2.01	0.42
2:B:56:ARG:C	2:B:56:ARG:CD	2.93	0.42
3:G:53:SER:O	3:G:54:SER:HB3	2.20	0.42
4:L:38:ALA:C	4:L:39:THR:CG2	2.93	0.42
1:A:463:LEU:HD23	1:A:463:LEU:C	2.44	0.42
1:E:156:ASN:CG	1:E:156:ASN:O	2.63	0.42
1:E:340:VAL:O	1:E:342:PRO:HD3	2.19	0.42
1:I:227:ILE:HG23	1:I:561:PRO:HB3	2.01	0.42
1:A:38:LYS:HE3	1:A:217:ILE:HB	2.01	0.42
1:E:286:ARG:HH22	6:E:1589:TEO:C4	2.32	0.42
1:E:451:ARG:HA	1:E:451:ARG:HD3	1.75	0.42
12:G:1129:HEM:HBA2	12:G:1129:HEM:HHA	2.02	0.42
1:A:173:GLN:CG	1:A:430:ARG:HH11	2.33	0.41
2:B:35:LEU:HD11	2:B:91:ILE:HD11	2.02	0.41
2:J:234:LEU:HD23	4:L:13:VAL:HG13	2.02	0.41
12:K:1129:HEM:HBC2	12:K:1129:HEM:CHD	2.50	0.41
1:E:323:LEU:HD23	1:E:327:LEU:HD12	2.01	0.41
1:E:286:ARG:HH12	6:E:1589:TEO:C4	2.32	0.41
3:K:53:SER:O	3:K:54:SER:HB3	2.20	0.41
1:A:227:ILE:HG23	1:A:561:PRO:HB3	2.03	0.41
3:C:74:MET:HE2	3:C:74:MET:HB2	1.91	0.41
4:H:38:ALA:C	4:H:39:THR:CG2	2.92	0.41
2:J:11:ASN:OD1	2:J:11:ASN:C	2.63	0.41
1:A:262:GLY:HA3	1:A:315:LEU:HD23	2.02	0.41
1:E:164:TRP:CH2	1:E:184:CYS:HB2	2.55	0.41
1:E:37:SER:O	1:E:163:GLU:N	2.53	0.41
1:I:49:ALA:HB1	5:I:601:FAD:C4X	2.51	0.41
1:I:350:ILE:CG1	1:I:351:PRO:HD2	2.50	0.41
1:A:383:LEU:C	1:A:384:PHE:CD2	2.99	0.41
1:A:384:PHE:CD2	1:A:384:PHE:N	2.89	0.41
3:G:126:VAL:C	3:G:128:VAL:H	2.28	0.41
4:H:38:ALA:O	4:H:39:THR:HG22	2.19	0.41
1:I:156:ASN:O	1:I:156:ASN:CG	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:MET:HE2	1:A:146:LEU:HD11	2.03	0.41
1:A:54:THR:O	1:A:406:LEU:HD22	2.21	0.41
2:B:214:SER:HB3	3:C:103:PHE:CZ	2.55	0.41
3:G:126:VAL:C	3:G:128:VAL:N	2.79	0.41
1:E:258:ARG:HD3	14:E:2094:HOH:O	2.20	0.41
1:E:345:GLU:HG2	1:E:346:PRO:HD2	2.03	0.41
1:I:20:MET:CE	1:I:146:LEU:CD1	2.99	0.41
2:J:94:LEU:HA	2:J:95:PRO:HD3	1.92	0.41
2:J:169:PHE:CE2	2:J:171:GLY:HA2	2.55	0.41
3:K:19:ARG:NH1	14:K:2008:HOH:O	2.53	0.41
1:A:14:GLY:HA2	5:A:601:FAD:H1B	2.03	0.41
1:A:537:ARG:O	1:A:538:GLY:C	2.64	0.41
4:D:38:ALA:C	4:D:39:THR:HG23	2.46	0.41
1:E:49:ALA:HB3	1:E:142:GLY:HA3	2.03	0.41
1:E:266:ASN:HB2	1:E:301:ARG:O	2.20	0.41
5:E:601:FAD:H1'1	5:E:601:FAD:H9	1.84	0.41
4:H:45:TYR:CZ	4:H:49:ILE:HD12	2.55	0.41
4:D:22:THR:OG1	4:D:71:HIS:HB2	2.21	0.40
3:C:126:VAL:C	3:C:128:VAL:H	2.29	0.40
1:E:49:ALA:HB1	5:E:601:FAD:C4X	2.52	0.40
2:J:234:LEU:CD2	4:L:13:VAL:HG13	2.51	0.40
4:L:92:MET:HE2	4:L:92:MET:N	2.37	0.40
1:A:478:ASP:HB2	14:A:2202:HOH:O	2.22	0.40
4:D:40:SER:O	4:D:41:GLY:C	2.64	0.40
1:E:20:MET:HE3	1:E:146:LEU:HD12	2.04	0.40
1:A:549:ASP:C	1:A:549:ASP:OD1	2.64	0.40
1:E:214:ASN:N	1:E:214:ASN:HD22	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	473/473 (100%)	465 (98%)	8 (2%)	53	74
1	E	473/473 (100%)	466 (98%)	7 (2%)	57	77
1	I	473/473 (100%)	469 (99%)	4 (1%)	73	86
2	B	208/208 (100%)	203 (98%)	5 (2%)	43	65
2	F	208/208 (100%)	202 (97%)	6 (3%)	37	60
2	J	208/208 (100%)	201 (97%)	7 (3%)	32	54

Continued on next page...

Continued from previous page...

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

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	94	GLU
1	A	119	PHE
1	A	325	SER
1	A	364	VAL
1	A	378	VAL
1	A	463	LEU
1	A	569	ARG
2	B	1	MET
2	B	56	ARG
2	B	141	GLU
2	B	180	ARG
2	B	213	VAL
3	C	11	VAL
4	D	43	LEU
4	D	44	THR
4	D	54	SER
4	D	111	VAL
1	E	2	LYS
1	E	47	VAL
1	E	94	GLU
1	E	119	PHE
1	E	325	SER
1	E	373	GLU
1	E	378	VAL
2	F	1	MET
2	F	56	ARG
2	F	141	GLU
2	F	180	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	192	SER
2	F	234	LEU
3	G	11	VAL
4	H	43	LEU
4	H	44	THR
1	I	2	LYS
1	I	94	GLU
1	I	373	GLU
1	I	378	VAL
2	J	1	MET
2	J	24	THR
2	J	56	ARG
2	J	141	GLU
2	J	180	ARG
2	J	192	SER
2	J	213	VAL
3	K	11	VAL
4	L	43	LEU
4	L	44	THR
4	L	111	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	214	ASN
1	A	218	ASN
1	A	469	HIS
2	B	109	GLN
2	B	135	GLN
2	B	235	GLN
2	B	237	ASN
1	E	125	ASN
1	E	156	ASN
1	E	173	GLN
1	E	218	ASN
1	E	398	ASN
2	F	41	GLN
2	F	109	GLN
2	F	135	GLN
2	F	235	GLN
2	F	237	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	210	GLN
1	I	214	ASN
1	I	218	ASN
2	J	41	GLN
2	J	109	GLN
2	J	133	HIS
2	J	135	GLN
2	J	235	GLN
2	J	237	ASN
3	K	30	HIS
3	K	91	HIS

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 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	TEO	E	1589	-	5,8,8	1.15	0	4,10,10	2.43	3 (75%)
8	SO4	I	1591	-	4,4,4	0.22	0	6,6,6	0.39	0
8	SO4	E	1591	-	4,4,4	0.34	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CBE	G	1130	-	16,17,17	1.18	1 (6%)	17,22,22	1.97	3 (17%)
10	SF4	F	303	2	0,12,12	-	-	-		
9	FES	B	302	2	0,4,4	-	-	-		
10	SF4	B	303	2	0,12,12	-	-	-		
5	FAD	I	601	1	58,58,58	1.19	6 (10%)	85,89,89	1.75	21 (24%)
11	F3S	J	304	2	0,9,9	-	-	-		
12	HEM	C	1129	4,3	50,50,50	1.71	10 (20%)	67,82,82	1.38	10 (14%)
8	SO4	A	1591	-	4,4,4	0.33	0	6,6,6	0.16	0
6	TEO	I	1589	-	5,8,8	1.05	0	4,10,10	1.48	1 (25%)
12	HEM	K	1129	4,3	50,50,50	1.75	11 (22%)	67,82,82	1.45	10 (14%)
10	SF4	J	303	2	0,12,12	-	-	-		
11	F3S	B	304	2	0,9,9	-	-	-		
11	F3S	F	304	2	0,9,9	-	-	-		
5	FAD	A	601	1	58,58,58	1.13	5 (8%)	85,89,89	1.81	23 (27%)
9	FES	J	302	2	0,4,4	-	-	-		
12	HEM	G	1129	4,3	50,50,50	1.68	9 (18%)	67,82,82	1.46	11 (16%)
13	CBE	C	1130	-	16,17,17	1.12	1 (6%)	17,22,22	1.82	2 (11%)
5	FAD	E	601	1	58,58,58	1.05	3 (5%)	85,89,89	1.87	23 (27%)
9	FES	F	302	2	0,4,4	-	-	-		
13	CBE	K	1130	-	16,17,17	1.21	2 (12%)	17,22,22	1.57	2 (11%)
6	TEO	A	1589	-	5,8,8	1.38	0	4,10,10	2.18	1 (25%)

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

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

Continued on next page...

Continued from previous page...

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

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1129	HEM	C3D-C2D	7.48	1.52	1.36
12	K	1129	HEM	C3D-C2D	6.98	1.51	1.36
12	G	1129	HEM	C3D-C2D	6.86	1.51	1.36
12	K	1129	HEM	FE-NB	4.83	2.09	1.94
12	G	1129	HEM	FE-NB	4.30	2.08	1.94
5	A	601	FAD	C4X-N5	3.95	1.39	1.30
5	I	601	FAD	C4X-N5	3.94	1.39	1.30
5	E	601	FAD	C4X-N5	3.78	1.38	1.30
12	G	1129	HEM	FE-ND	3.67	2.06	1.94
13	G	1130	CBE	C11-N10	-3.48	1.34	1.41
12	K	1129	HEM	FE-ND	3.45	2.05	1.94
12	C	1129	HEM	FE-NB	3.39	2.05	1.94
5	I	601	FAD	C2A-N3A	3.37	1.39	1.33
13	K	1130	CBE	C11-N10	-3.19	1.35	1.41
13	C	1130	CBE	C11-N10	-2.79	1.36	1.41
5	A	601	FAD	C8A-N7A	2.70	1.36	1.31
12	K	1129	HEM	C3B-C2B	-2.67	1.31	1.37
12	C	1129	HEM	CMC-C2C	2.63	1.56	1.50
5	I	601	FAD	C2A-N1A	2.60	1.38	1.33
12	C	1129	HEM	CAB-C3B	2.50	1.54	1.47
12	G	1129	HEM	CAC-C3C	2.48	1.54	1.47
12	G	1129	HEM	CAB-C3B	2.47	1.54	1.47
5	A	601	FAD	C10-N1	2.45	1.38	1.33
5	E	601	FAD	P-O3P	2.45	1.62	1.59
12	G	1129	HEM	C2A-C3A	-2.41	1.32	1.38
12	K	1129	HEM	CMA-C3A	2.37	1.55	1.50
12	K	1129	HEM	CAB-C3B	2.36	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	601	FAD	C2'-C3'	-2.31	1.49	1.53
12	K	1129	HEM	CMC-C2C	2.30	1.55	1.50
5	I	601	FAD	C10-N1	2.30	1.37	1.33
12	C	1129	HEM	C3C-C2C	-2.29	1.32	1.37
12	C	1129	HEM	C3B-C2B	-2.29	1.32	1.37
12	G	1129	HEM	C3B-C2B	-2.25	1.32	1.37
13	K	1130	CBE	C1-C2	2.25	1.54	1.49
12	G	1129	HEM	CMC-C2C	2.23	1.55	1.50
12	K	1129	HEM	CAC-C3C	2.21	1.53	1.47
12	C	1129	HEM	CMD-C2D	2.20	1.55	1.50
12	G	1129	HEM	C3C-C2C	-2.17	1.32	1.37
5	A	601	FAD	P-O3P	2.17	1.61	1.59
12	K	1129	HEM	FE-NA	2.17	2.02	1.95
12	K	1129	HEM	CMB-C2B	2.12	1.55	1.50
12	K	1129	HEM	C3C-C2C	-2.10	1.32	1.37
12	C	1129	HEM	CMA-C3A	2.09	1.55	1.50
5	I	601	FAD	C8A-N7A	2.07	1.35	1.31
5	A	601	FAD	C2A-N3A	2.06	1.37	1.33
12	C	1129	HEM	CAC-C3C	2.04	1.52	1.47
5	E	601	FAD	C4X-C10	-2.01	1.38	1.44
12	C	1129	HEM	C2A-C3A	-2.01	1.33	1.38

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	1130	CBE	O7-C2-C1	6.42	116.88	109.30
5	A	601	FAD	N3A-C2A-N1A	-6.33	119.00	128.58
5	E	601	FAD	N3A-C2A-N1A	-6.20	119.19	128.58
13	C	1130	CBE	O7-C2-C1	5.71	116.05	109.30
12	K	1129	HEM	C4D-ND-C1D	4.90	111.02	105.21
13	K	1130	CBE	O7-C2-C1	4.76	114.93	109.30
5	E	601	FAD	N9A-C8A-N7A	-4.68	107.29	113.94
5	E	601	FAD	O2A-PA-O3P	4.60	119.71	107.27
5	I	601	FAD	N3A-C2A-N1A	-4.49	121.78	128.58
12	G	1129	HEM	C4D-ND-C1D	4.43	110.45	105.21
5	E	601	FAD	C5A-N7A-C8A	4.37	110.32	103.45
5	I	601	FAD	O2A-PA-O3P	4.34	119.01	107.27
12	C	1129	HEM	C4D-ND-C1D	4.32	110.32	105.21
5	I	601	FAD	N9A-C8A-N7A	-4.32	107.81	113.94
5	A	601	FAD	C5A-C4A-N3A	-4.31	120.78	126.72
5	A	601	FAD	N9A-C8A-N7A	-3.98	108.28	113.94
5	A	601	FAD	O2A-PA-O3P	3.95	117.95	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	C2A-N3A-C4A	3.93	121.42	111.83
5	I	601	FAD	C5A-C4A-N3A	-3.85	121.42	126.72
5	I	601	FAD	C5A-N7A-C8A	3.83	109.48	103.45
5	E	601	FAD	C5A-C4A-N3A	-3.82	121.46	126.72
5	E	601	FAD	C4X-C10-N10	3.78	121.89	116.48
13	K	1130	CBE	C11-N10-C8	-3.72	120.85	127.45
5	I	601	FAD	O3P-PA-O1A	-3.67	99.65	110.70
5	I	601	FAD	C4X-C10-N10	3.67	121.73	116.48
5	A	601	FAD	C4X-C10-N10	3.51	121.51	116.48
5	E	601	FAD	C2A-N3A-C4A	3.49	120.35	111.83
5	A	601	FAD	O2'-C2'-C3'	-3.39	101.31	109.25
6	E	1589	TEO	O1A-C1-C2	-3.38	114.41	122.52
12	G	1129	HEM	CMD-C2D-C1D	3.37	130.30	125.03
6	A	1589	TEO	O1A-C1-C2	-3.34	114.50	122.52
5	E	601	FAD	C4A-C5A-N7A	-3.33	106.78	110.58
5	A	601	FAD	O3P-P-O1P	-3.32	100.72	110.70
12	C	1129	HEM	CMD-C2D-C1D	3.32	130.22	125.03
12	K	1129	HEM	CAD-CBD-CGD	-3.27	105.00	113.67
5	A	601	FAD	C5A-N7A-C8A	3.21	108.50	103.45
5	E	601	FAD	C4-N3-C2	-3.21	119.95	125.64
13	C	1130	CBE	C11-N10-C8	-3.16	121.83	127.45
12	C	1129	HEM	C4C-C3C-C2C	3.13	109.52	106.81
5	I	601	FAD	C4A-C5A-N7A	-3.10	107.03	110.58
5	A	601	FAD	C5X-C9A-N10	3.05	120.73	117.97
5	I	601	FAD	C2A-N3A-C4A	3.02	119.21	111.83
5	I	601	FAD	C4-C4X-N5	2.91	122.23	118.21
12	C	1129	HEM	C1D-C2D-C3D	-2.90	103.93	106.98
5	I	601	FAD	O2'-C2'-C3'	-2.90	102.45	109.25
12	G	1129	HEM	O2A-CGA-CBA	2.89	123.13	114.00
5	A	601	FAD	C4'-C3'-C2'	-2.84	108.85	113.57
12	G	1129	HEM	CMB-C2B-C1B	2.83	129.46	125.03
5	A	601	FAD	O3P-PA-O1A	-2.77	102.36	110.70
12	K	1129	HEM	CAD-C3D-C4D	2.76	129.51	124.70
5	A	601	FAD	O4'-C4'-C3'	2.76	115.70	109.25
5	E	601	FAD	C10-C4X-N5	-2.70	119.29	124.81
5	E	601	FAD	C4'-C3'-C2'	-2.67	109.13	113.57
5	I	601	FAD	C10-C4X-N5	-2.66	119.37	124.81
12	G	1129	HEM	CAD-C3D-C4D	2.64	129.29	124.70
5	E	601	FAD	C4X-C4-N3	2.64	119.97	113.25
12	G	1129	HEM	C4C-C3C-C2C	2.58	109.05	106.81
5	I	601	FAD	C4'-C3'-C2'	-2.58	109.28	113.57
5	E	601	FAD	C9A-C5X-N5	-2.55	119.75	122.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	601	FAD	C4-N3-C2	-2.53	121.14	125.64
5	I	601	FAD	C4X-C4-N3	2.53	119.69	113.25
5	A	601	FAD	C4X-C4-N3	2.52	119.66	113.25
5	I	601	FAD	C10-N1-C2	2.51	122.29	116.85
6	E	1589	TEO	O1B-C1-C2	2.50	118.85	113.00
5	A	601	FAD	C9A-C5X-N5	-2.47	119.84	122.45
12	K	1129	HEM	CMB-C2B-C1B	2.41	128.81	125.03
5	I	601	FAD	O5'-C5'-C4'	-2.36	103.05	109.36
5	E	601	FAD	C4-C4X-N5	2.36	121.47	118.21
5	A	601	FAD	C10-N1-C2	2.33	121.90	116.85
12	K	1129	HEM	CHC-C1C-NC	2.33	126.99	124.45
5	A	601	FAD	N3A-C4A-N9A	2.31	131.10	127.17
13	G	1130	CBE	C1-C2-C3	-2.31	119.03	124.36
5	E	601	FAD	O5'-C5'-C4'	-2.31	103.20	109.36
12	K	1129	HEM	O1D-CGD-CBD	-2.31	115.78	123.09
5	A	601	FAD	C4-N3-C2	-2.31	121.55	125.64
5	E	601	FAD	C2A-N1A-C6A	2.28	122.48	118.73
12	C	1129	HEM	CHA-C4D-ND	2.28	127.19	124.37
5	E	601	FAD	C9-C9A-N10	-2.27	118.80	121.85
5	E	601	FAD	O2'-C2'-C3'	-2.25	103.97	109.25
12	K	1129	HEM	C4C-C3C-C2C	2.25	108.77	106.81
5	A	601	FAD	C10-C4X-N5	-2.25	120.22	124.81
5	E	601	FAD	O4-C4-C4X	-2.24	120.63	126.53
5	A	601	FAD	C4A-C5A-N7A	-2.19	108.08	110.58
5	E	601	FAD	C10-N1-C2	2.17	121.55	116.85
5	I	601	FAD	O4'-C4'-C5'	-2.16	105.21	109.99
12	G	1129	HEM	C3B-C4B-NB	-2.15	107.92	109.47
5	I	601	FAD	O2-C2-N3	2.14	122.70	118.58
5	I	601	FAD	O4-C4-C4X	-2.14	120.87	126.53
12	C	1129	HEM	CHD-C4C-NC	2.14	126.78	124.45
12	K	1129	HEM	O2D-CGD-CBD	2.14	120.75	114.00
13	G	1130	CBE	C3-C8-N10	-2.13	112.34	115.97
12	C	1129	HEM	O2D-CGD-CBD	2.13	120.73	114.00
6	E	1589	TEO	O2-C2-C1	2.13	114.98	109.54
12	G	1129	HEM	CAD-CBD-CGD	-2.12	108.03	113.67
12	K	1129	HEM	CHA-C1A-NA	2.12	127.70	123.86
12	G	1129	HEM	CHC-C1C-NC	2.12	126.76	124.45
5	A	601	FAD	C5A-C4A-N9A	2.11	108.12	105.81
5	A	601	FAD	C4-C4X-N5	2.10	121.11	118.21
6	I	1589	TEO	O1A-C1-C2	-2.10	117.48	122.52
5	E	601	FAD	N3A-C4A-N9A	2.10	130.74	127.17
5	E	601	FAD	C5X-C9A-N10	2.08	119.85	117.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	1129	HEM	CMC-C2C-C1C	2.06	128.36	124.73
12	G	1129	HEM	CAB-C3B-C2B	-2.06	121.73	128.43
12	C	1129	HEM	O1A-CGA-CBA	-2.06	116.57	123.09
5	I	601	FAD	N3A-C4A-N9A	2.04	130.64	127.17
12	G	1129	HEM	CMB-C2B-C3B	-2.04	123.49	128.43
5	A	601	FAD	C4X-C10-N1	-2.04	119.59	124.59
12	C	1129	HEM	CHB-C1B-NB	2.02	126.86	124.37
5	E	601	FAD	C4A-N9A-C8A	2.01	107.85	105.74
12	C	1129	HEM	O2A-CGA-CBA	2.00	120.33	114.00

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	N10-C1'-C2'-C3'
5	E	601	FAD	PA-O3P-P-O5'
5	I	601	FAD	PA-O3P-P-O5'
6	A	1589	TEO	O2-C2-C3-C4
6	E	1589	TEO	C1-C2-C3-C4
6	I	1589	TEO	O2-C2-C3-C4
12	K	1129	HEM	C1A-C2A-CAA-CBA
6	A	1589	TEO	O1A-C1-C2-O2
6	A	1589	TEO	O1B-C1-C2-O2
5	A	601	FAD	PA-O3P-P-O5'
13	K	1130	CBE	C2-C3-C8-O9
12	K	1129	HEM	C2B-C3B-CAB-CBB
12	C	1129	HEM	C4C-C3C-CAC-CBC
12	G	1129	HEM	C4B-C3B-CAB-CBB
12	K	1129	HEM	C4B-C3B-CAB-CBB
12	K	1129	HEM	C3A-C2A-CAA-CBA
5	E	601	FAD	N10-C1'-C2'-O2'
5	E	601	FAD	N10-C1'-C2'-C3'
6	E	1589	TEO	O2-C2-C3-C4
5	A	601	FAD	P-O3P-PA-O2A
5	E	601	FAD	P-O3P-PA-O2A
12	G	1129	HEM	C1A-C2A-CAA-CBA
12	C	1129	HEM	CAD-CBD-CGD-O2D
6	E	1589	TEO	O1A-C1-C2-O2
6	E	1589	TEO	O1B-C1-C2-O2
13	C	1130	CBE	C2-C3-C8-N10
13	G	1130	CBE	C2-C3-C8-N10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	K	1130	CBE	C2-C3-C8-N10
12	C	1129	HEM	CAD-CBD-CGD-O1D
12	G	1129	HEM	CAD-CBD-CGD-O1D
5	I	601	FAD	P-O3P-PA-O2A
12	G	1129	HEM	CAD-CBD-CGD-O2D
12	K	1129	HEM	CAA-CBA-CGA-O2A
12	K	1129	HEM	CAA-CBA-CGA-O1A
5	A	601	FAD	P-O3P-PA-O1A
5	E	601	FAD	P-O3P-PA-O1A
5	I	601	FAD	P-O3P-PA-O1A

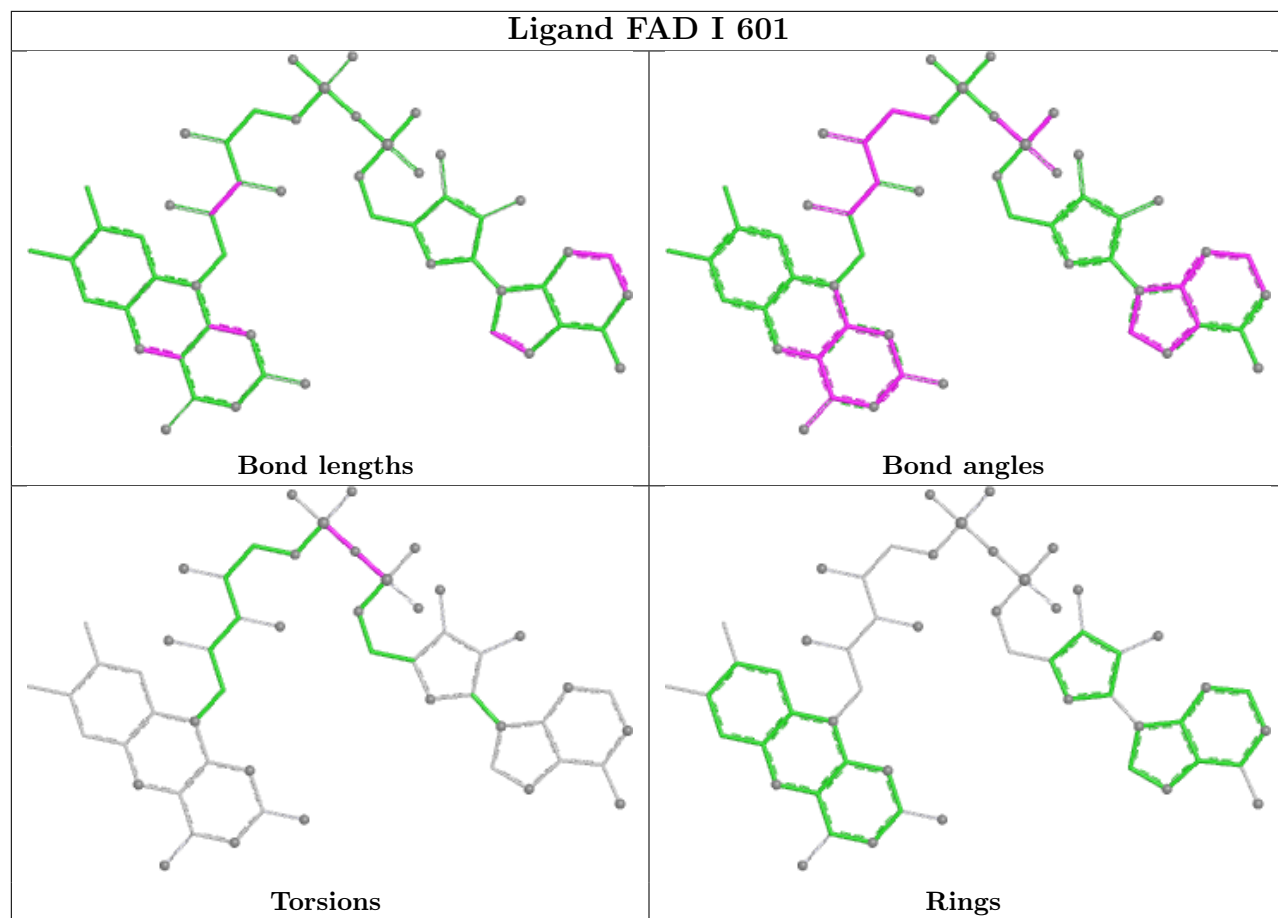
There are no ring outliers.

13 monomers are involved in 50 short contacts:

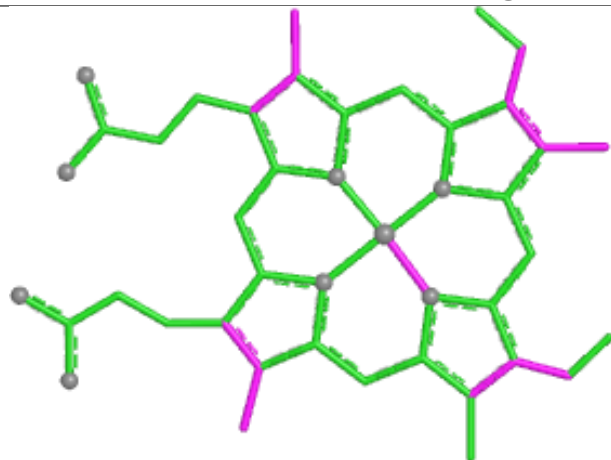
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1589	TEO	4	0
13	G	1130	CBE	1	0
5	I	601	FAD	7	0
12	C	1129	HEM	6	0
6	I	1589	TEO	4	0
12	K	1129	HEM	6	0
10	J	303	SF4	1	0
5	A	601	FAD	6	0
12	G	1129	HEM	5	0
13	C	1130	CBE	2	0
5	E	601	FAD	7	0
13	K	1130	CBE	2	0
6	A	1589	TEO	3	0

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

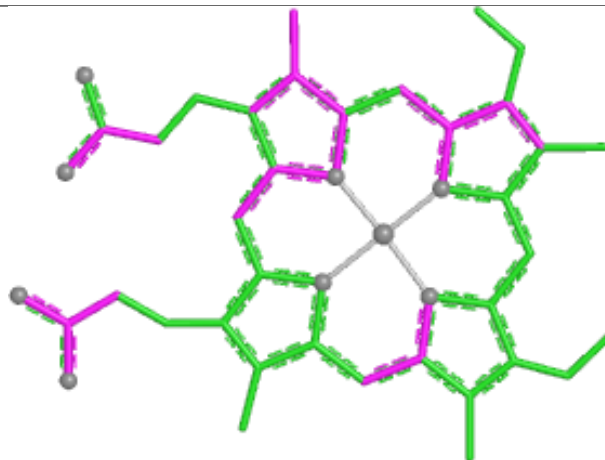
Ligand FAD I 601



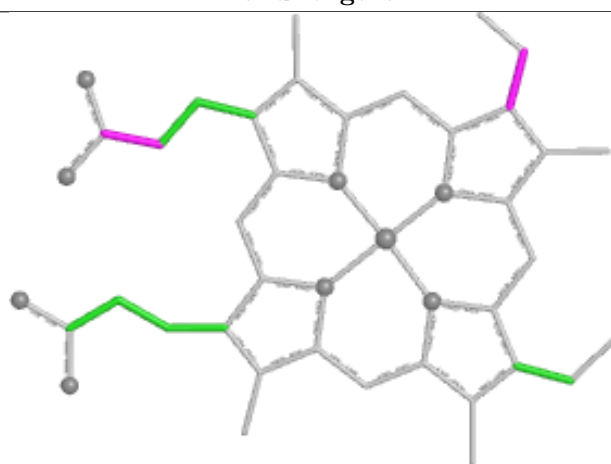
Ligand HEM C 1129



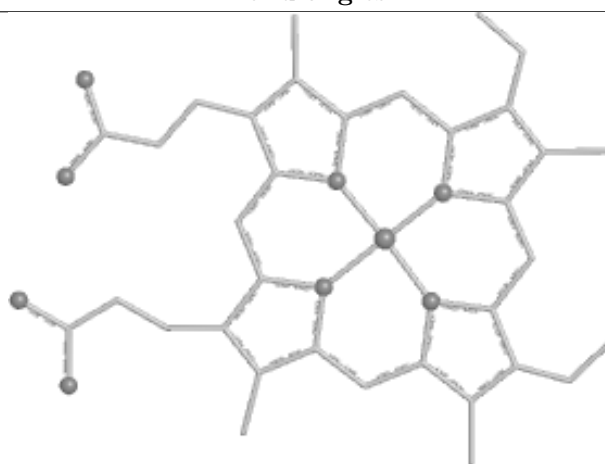
Bond lengths



Bond angles

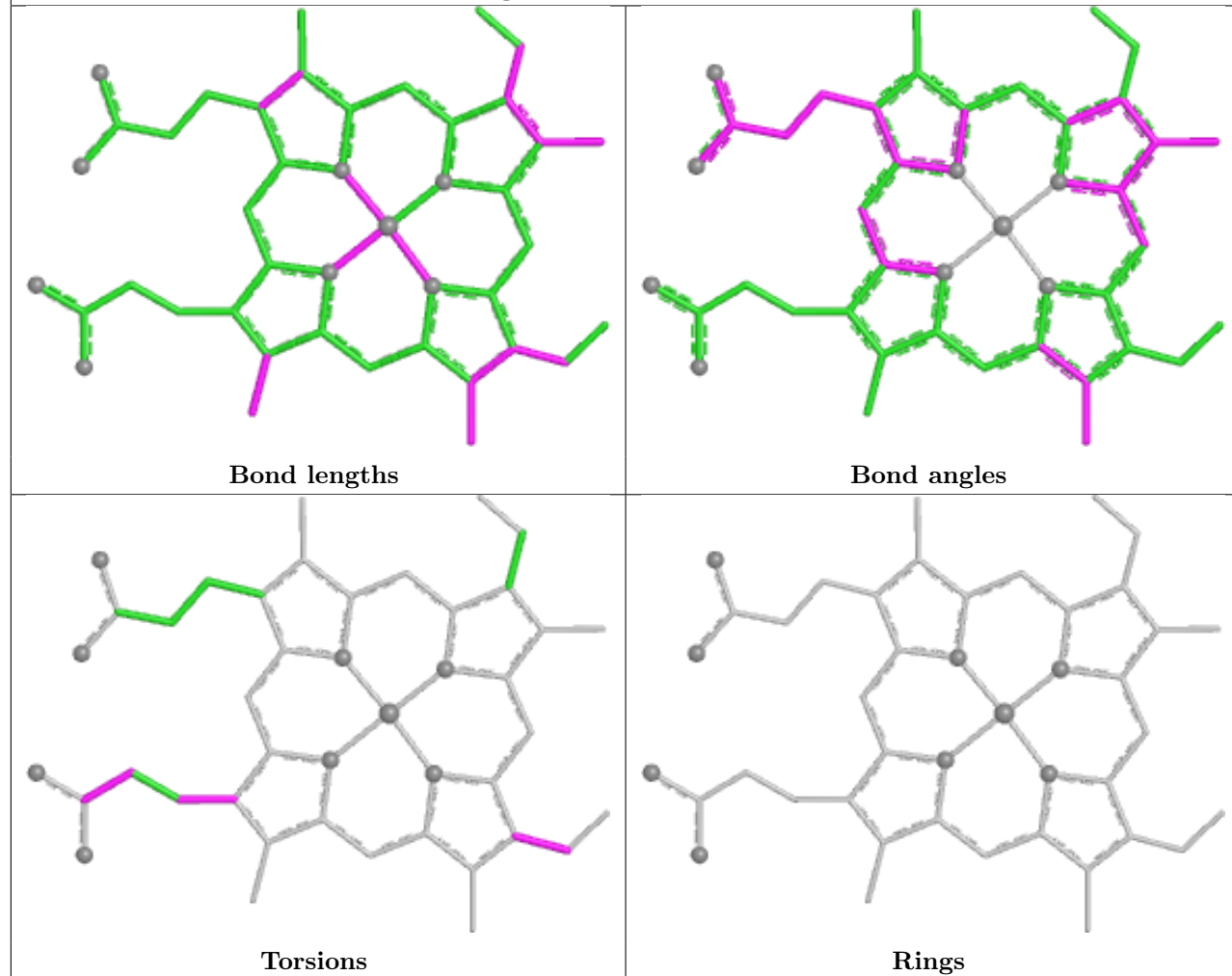


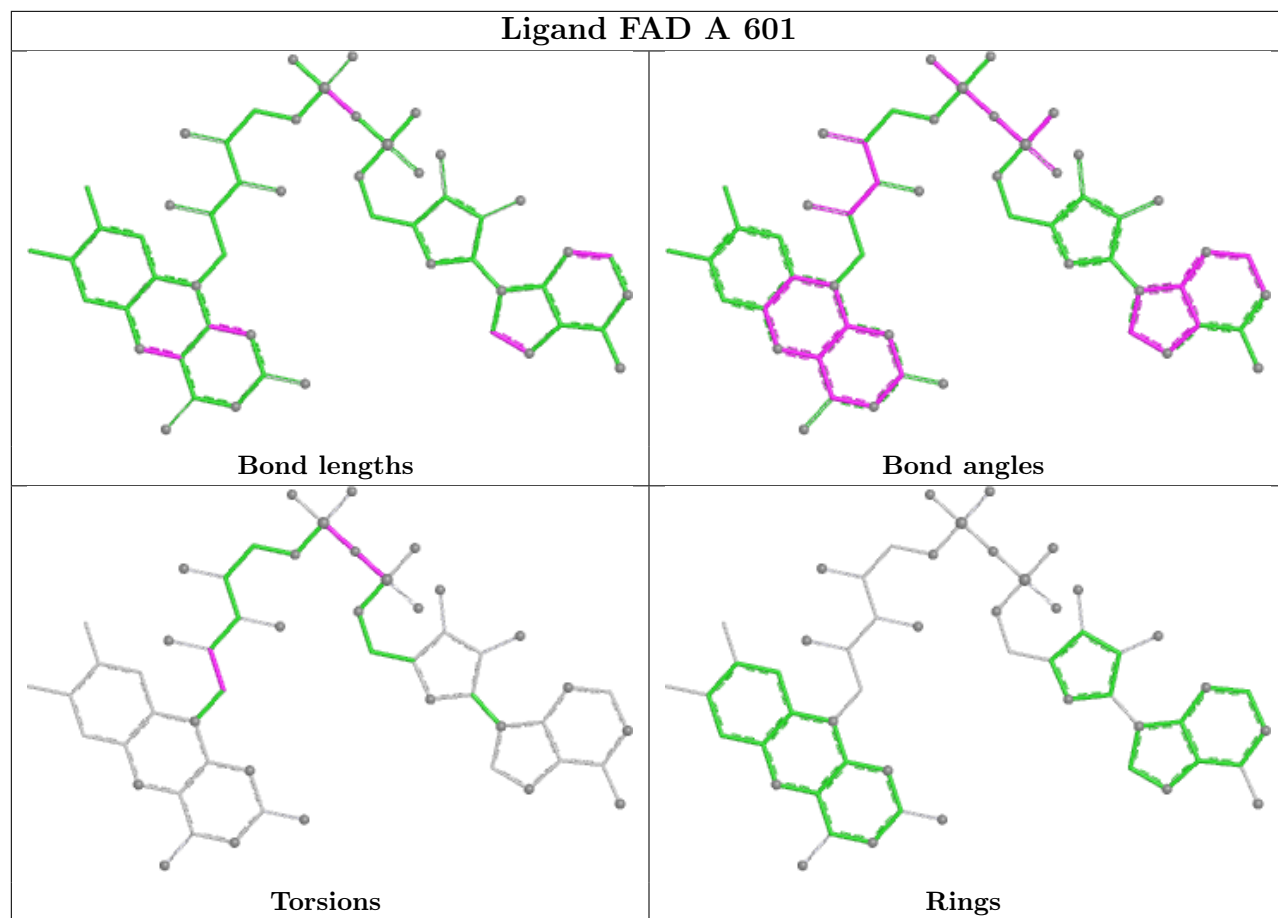
Torsions



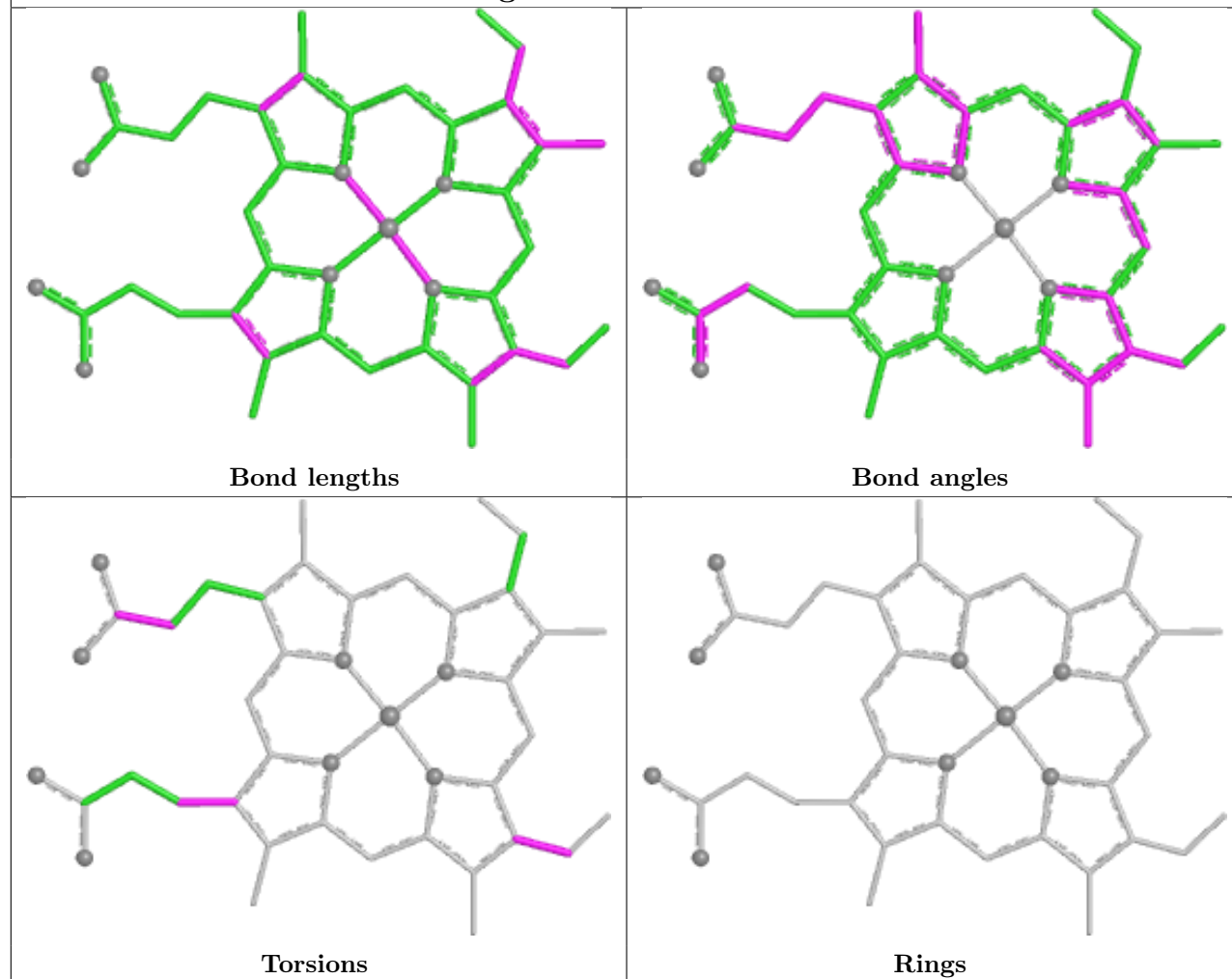
Rings

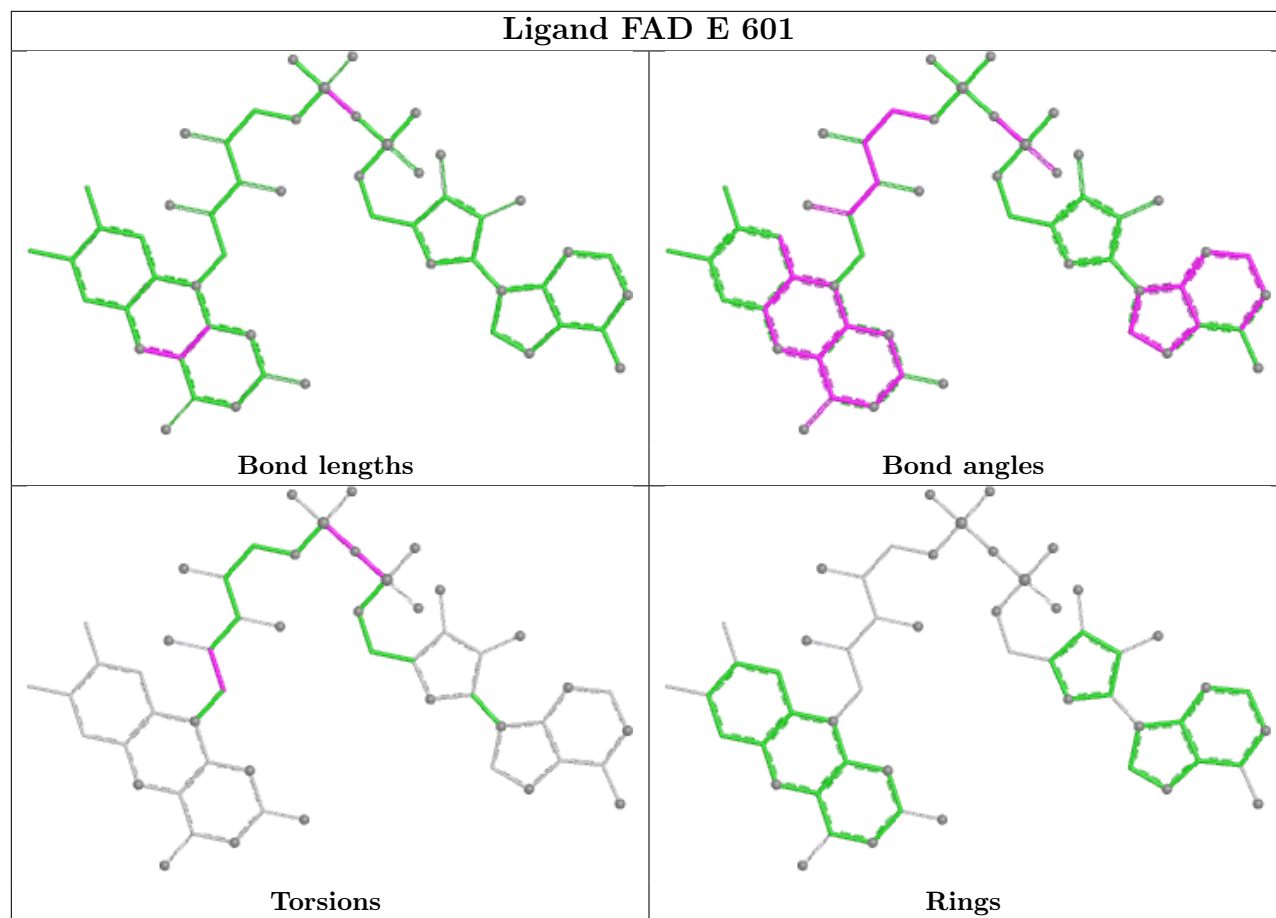
Ligand HEM K 1129





Ligand HEM G 1129





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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	588/588 (100%)	-0.17	3 (0%) 87 85	33, 39, 52, 72	0
1	E	588/588 (100%)	-0.04	6 (1%) 79 76	33, 39, 52, 72	0
1	I	588/588 (100%)	0.17	2 (0%) 90 88	33, 39, 52, 72	0
2	B	238/238 (100%)	-0.11	3 (1%) 75 71	28, 35, 49, 69	0
2	F	238/238 (100%)	-0.13	1 (0%) 88 86	28, 34, 49, 69	0
2	J	238/238 (100%)	-0.15	0 100 100	28, 35, 49, 69	0
3	C	121/129 (93%)	1.28	21 (17%) 4 3	45, 54, 67, 73	0
3	G	121/129 (93%)	0.95	12 (9%) 13 9	45, 54, 67, 73	0
3	K	121/129 (93%)	1.08	9 (7%) 20 17	45, 54, 67, 73	0
4	D	105/115 (91%)	0.64	7 (6%) 24 20	44, 49, 69, 72	0
4	H	105/115 (91%)	1.12	15 (14%) 6 5	44, 50, 69, 72	0
4	L	105/115 (91%)	0.72	6 (5%) 29 25	44, 49, 69, 72	0
All	All	3156/3210 (98%)	0.17	85 (2%) 56 52	28, 40, 61, 73	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	113	TRP	4.6
3	K	56	GLU	4.4
4	H	115	VAL	4.1
3	K	68	PHE	3.9
3	C	10	PRO	3.8
3	G	96	PHE	3.7
4	H	114	GLY	3.7
3	K	10	PRO	3.7
1	I	434	GLU	3.6
3	C	68	PHE	3.6
1	I	1	MET	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	85	PRO	3.5
3	K	57	GLY	3.5
3	G	68	PHE	3.2
2	B	86	GLY	3.2
3	C	11	VAL	3.2
4	H	66	PHE	3.2
3	C	55	PRO	3.1
4	H	73	TRP	3.1
3	K	8	GLN	3.1
1	E	2	LYS	3.1
3	C	127	LEU	3.1
3	C	8	GLN	3.0
3	C	128	VAL	3.0
3	C	9	ARG	3.0
3	G	127	LEU	2.9
3	C	59	GLU	2.9
4	L	113	TRP	2.9
3	C	97	GLY	2.9
3	C	70	VAL	2.8
1	E	1	MET	2.8
4	L	112	VAL	2.8
3	G	59	GLU	2.8
3	G	66	GLY	2.7
4	H	52	PHE	2.7
3	C	56	GLU	2.7
3	G	126	VAL	2.7
3	C	98	TYR	2.7
4	H	92	MET	2.7
3	C	124	ALA	2.7
1	E	279	ASN	2.6
2	B	238	ALA	2.6
4	L	73	TRP	2.6
4	D	114	GLY	2.6
3	C	13	LEU	2.6
4	H	40	SER	2.6
4	L	115	VAL	2.5
4	D	43	LEU	2.4
3	K	69	PHE	2.4
3	C	46	TRP	2.4
4	D	73	TRP	2.4
3	C	61	ALA	2.4
3	G	56	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	103	PHE	2.4
3	C	105	ALA	2.4
4	H	46	GLU	2.4
3	G	102	THR	2.3
4	H	41	GLY	2.3
4	L	41	GLY	2.3
1	A	1	MET	2.3
3	K	19	ARG	2.3
3	C	67	SER	2.3
4	L	40	SER	2.3
4	D	113	TRP	2.3
4	D	42	GLU	2.2
4	H	36	PHE	2.2
4	H	11	ASN	2.2
3	C	14	ASP	2.2
3	G	91	HIS	2.1
1	E	451	ARG	2.1
4	H	109	PHE	2.1
4	H	12	GLY	2.1
1	E	373	GLU	2.1
1	A	543	PHE	2.1
3	G	72	PHE	2.1
1	A	562	GLU	2.1
4	D	46	GLU	2.1
3	K	70	VAL	2.0
4	D	37	PHE	2.0
2	F	238	ALA	2.0
1	E	332	GLU	2.0
3	G	65	MET	2.0
3	C	108	ARG	2.0
3	K	11	VAL	2.0
4	H	51	PHE	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

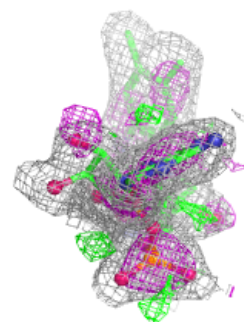
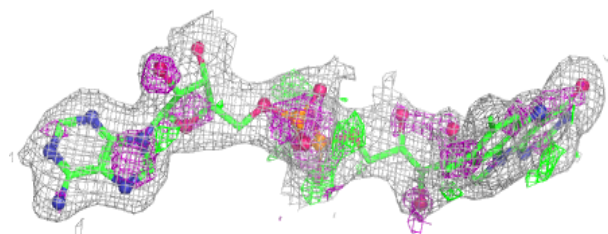
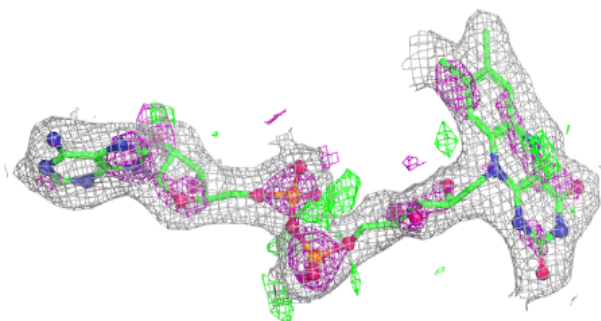
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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

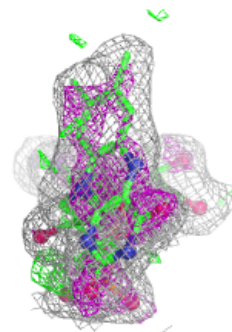
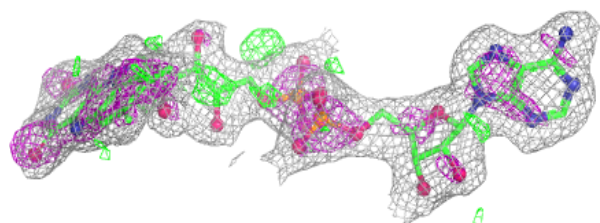
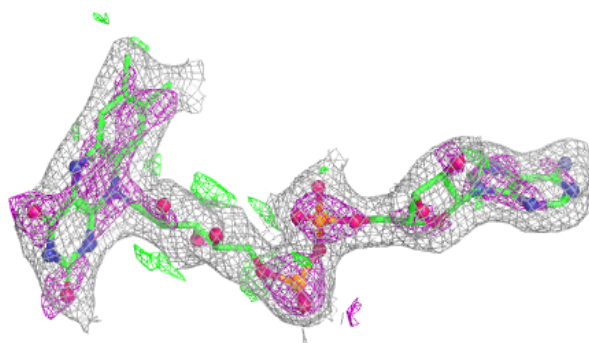
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 601:

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

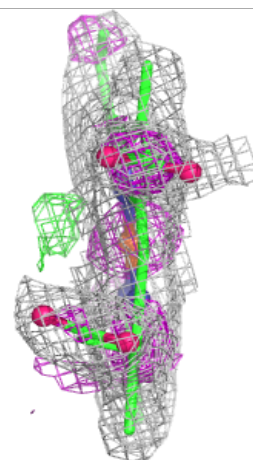
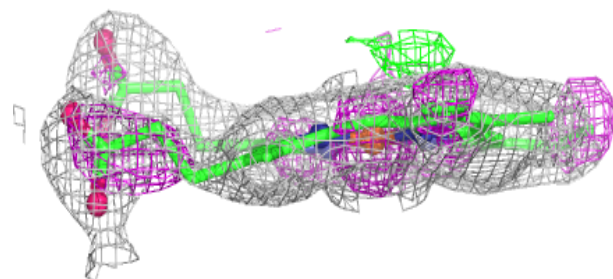
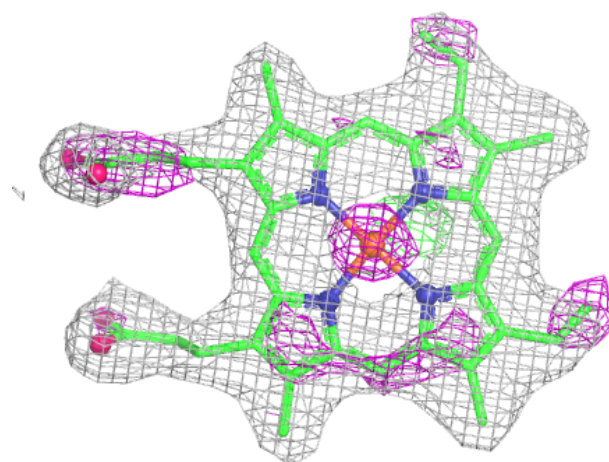
**Electron density around FAD E 601:**

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



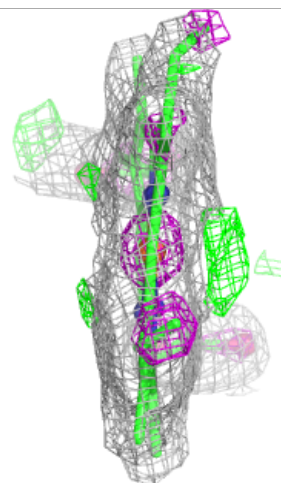
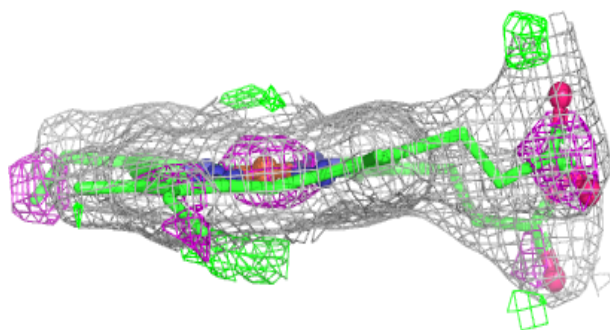
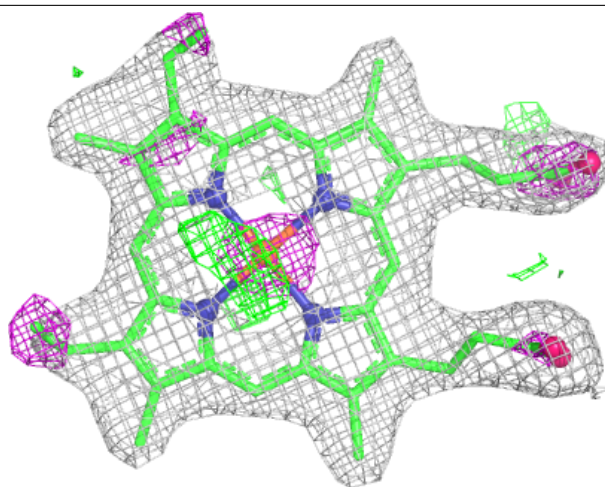
Electron density around HEM C 1129:

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



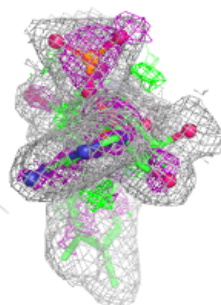
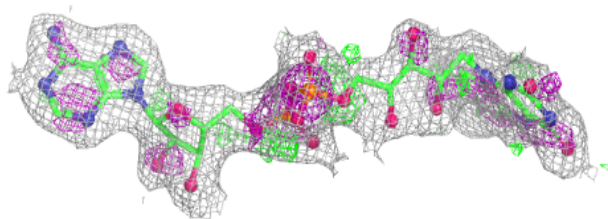
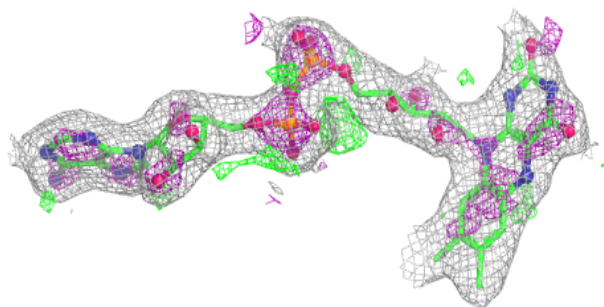
Electron density around HEM K 1129:

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

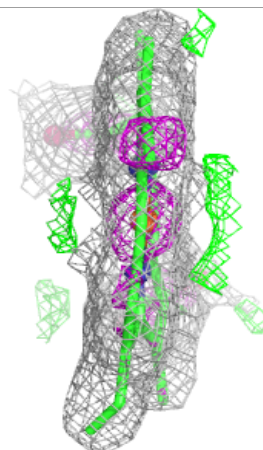
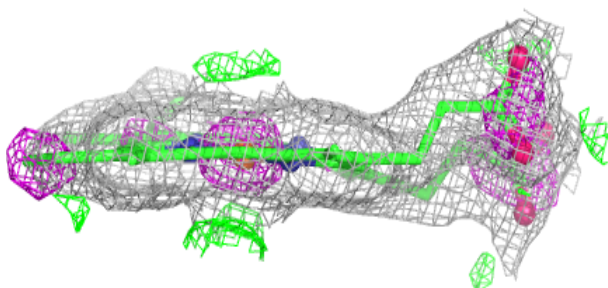
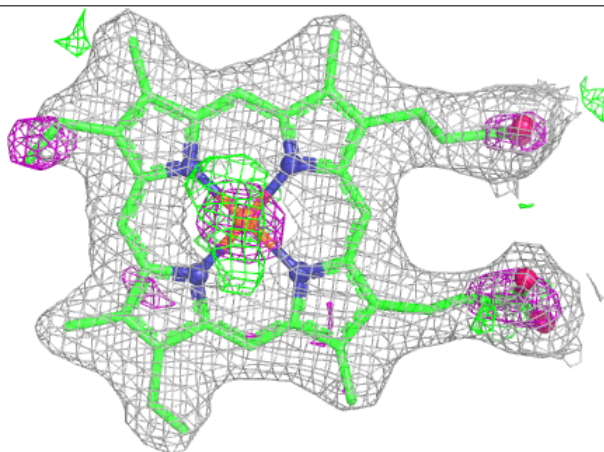


Electron density around FAD I 601:

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

**Electron density around HEM G 1129:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.