



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 04:52 am BST

PDB ID : 2WDV / pdb_00002wdv
Title : E. coli succinate:quinone oxidoreductase (SQR) with an empty quinone- binding pocket
Authors : Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on : 2009-03-26
Resolution : 3.20 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

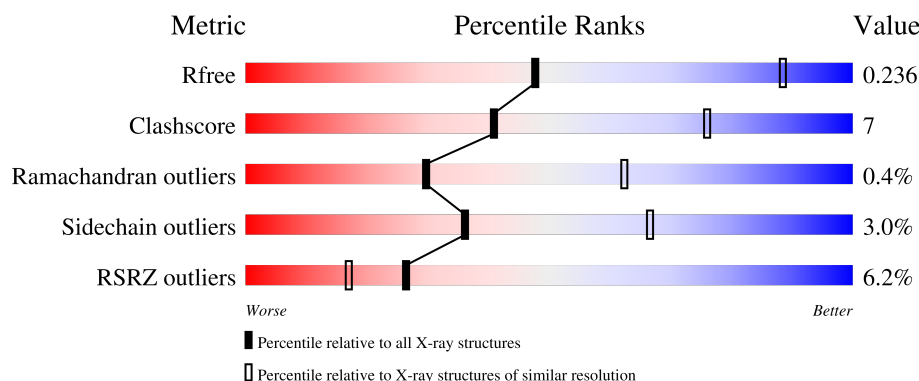
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	<div> <div>18%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	E	588	<div> <div>84%</div> <div>16%</div> <div>.</div> </div>
1	I	588	<div> <div>18%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	B	238	<div> <div>2%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
2	F	238	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>

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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	-
8	FES	J	302	-	-	X	-
9	SF4	F	303	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24855 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			

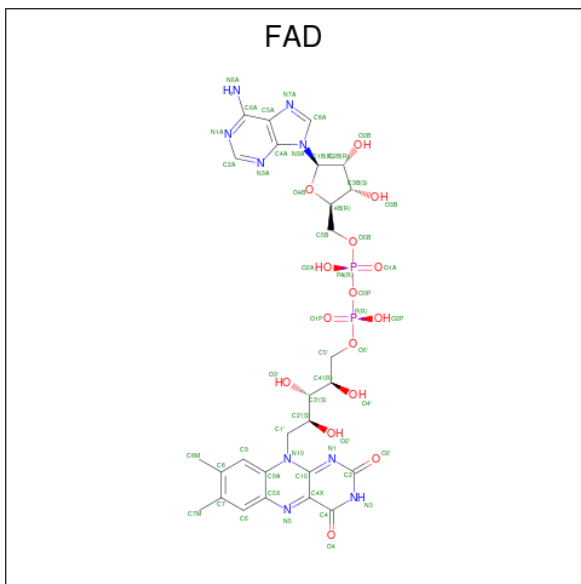
- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT.

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 PROTEIN.

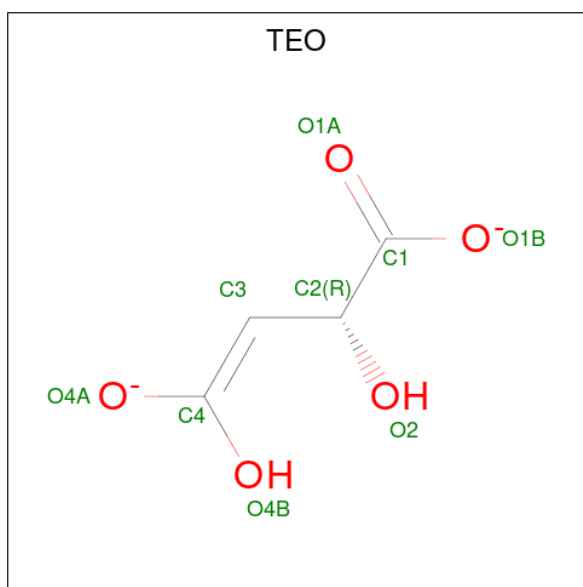
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total 836	C 577	N 123	O 133	S 3	0	0	0
4	H	105	Total 836	C 577	N 123	O 133	S 3	0	0	0
4	L	105	Total 836	C 577	N 123	O 133	S 3	0	0	0

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



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

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

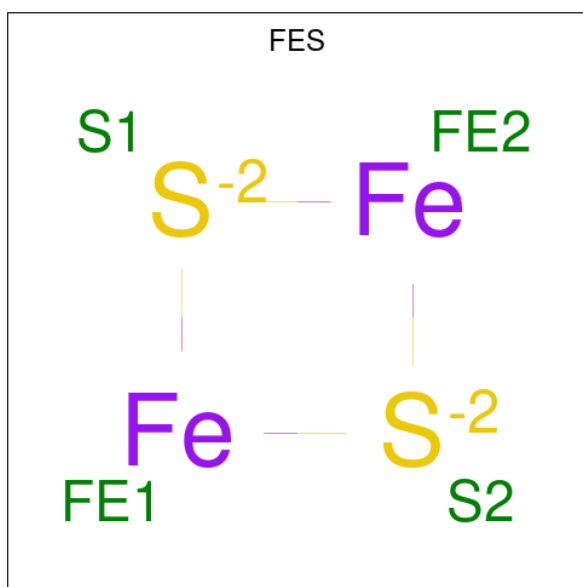


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		
6	E	1	Total	C	O	0	0
			9	4	5		
6	I	1	Total	C	O	0	0
			9	4	5		

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

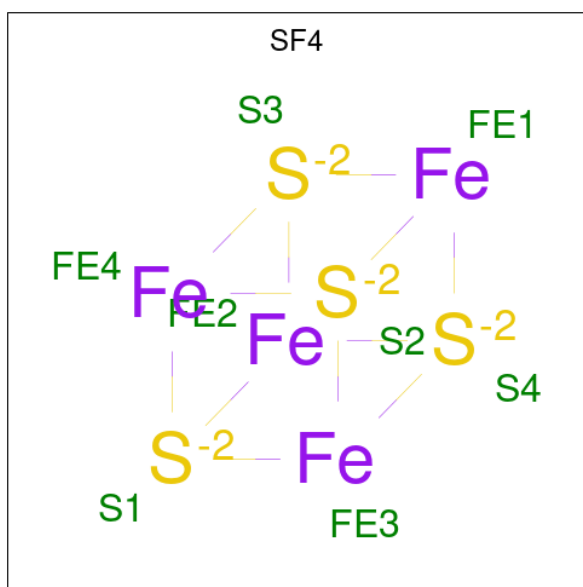
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		
7	E	1	Total	Na	0	0
			1	1		
7	I	1	Total	Na	0	0
			1	1		

- Molecule 8 is 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).



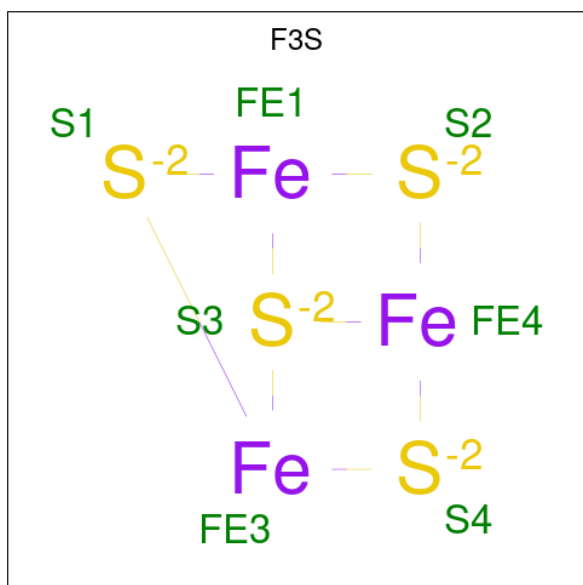
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

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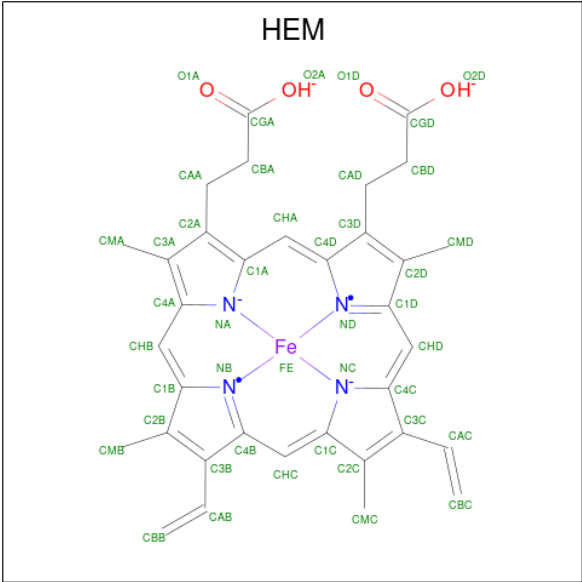
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	Fe	S	0	0
			8	4	4		
9	J	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



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: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).

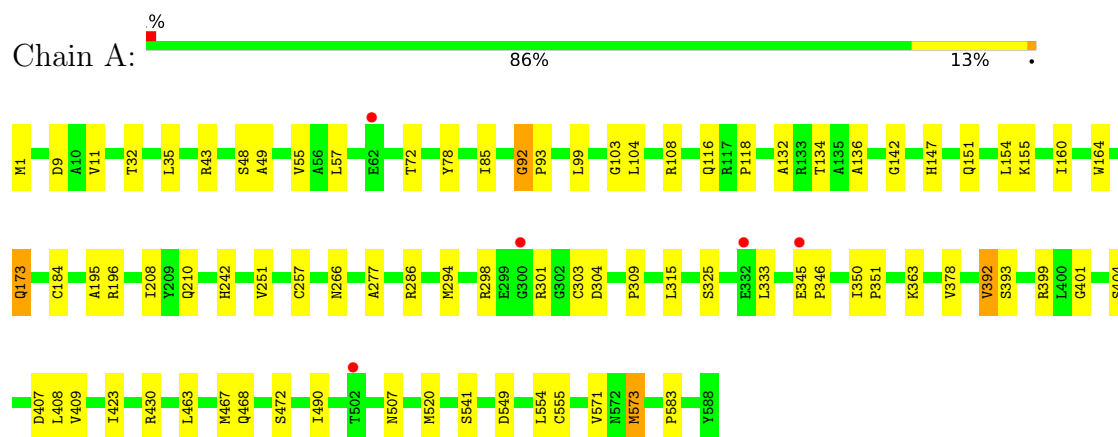


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

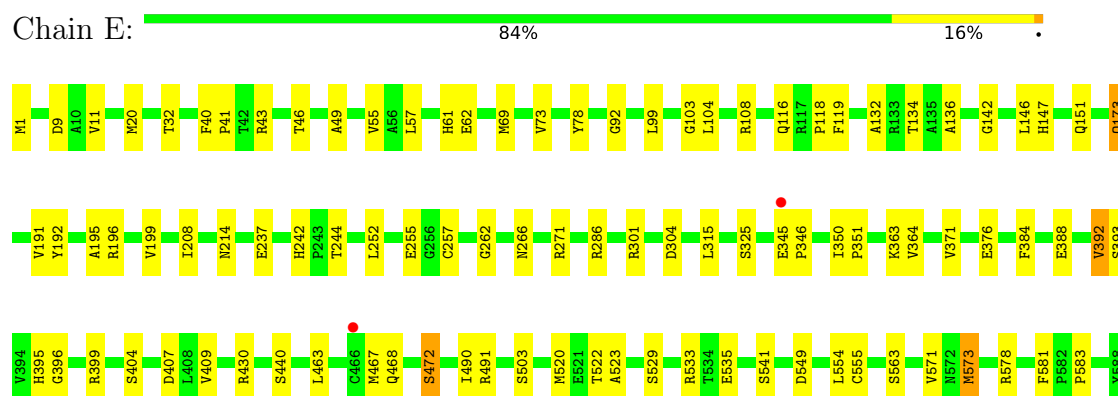
3 Residue-property plots

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.

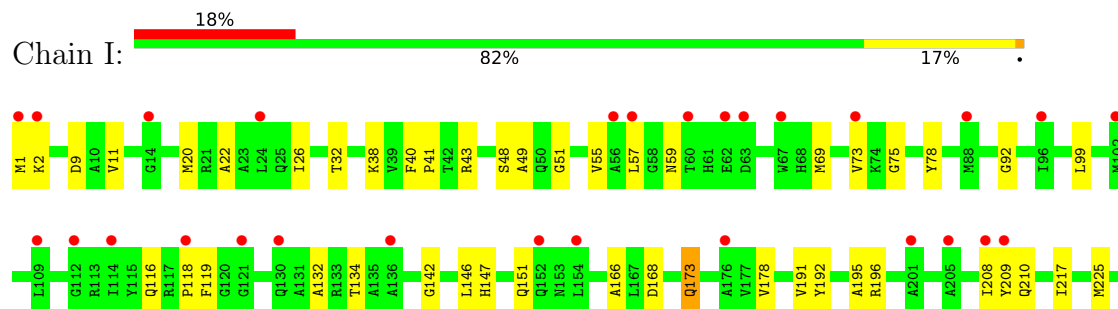
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

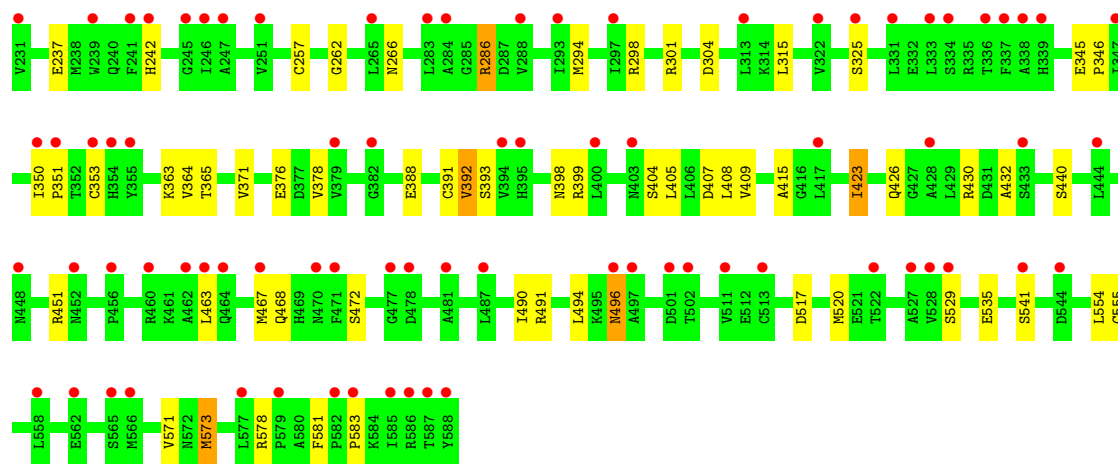


• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

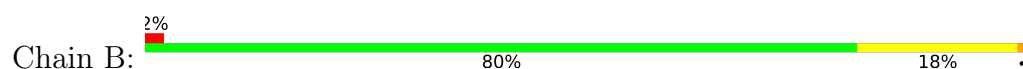
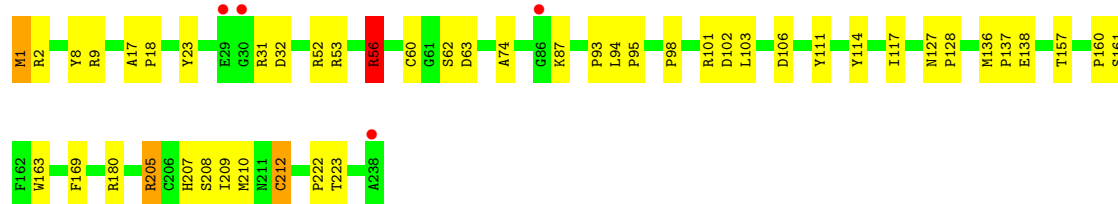


• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

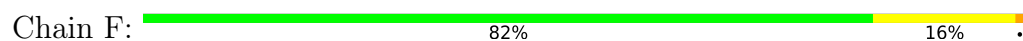
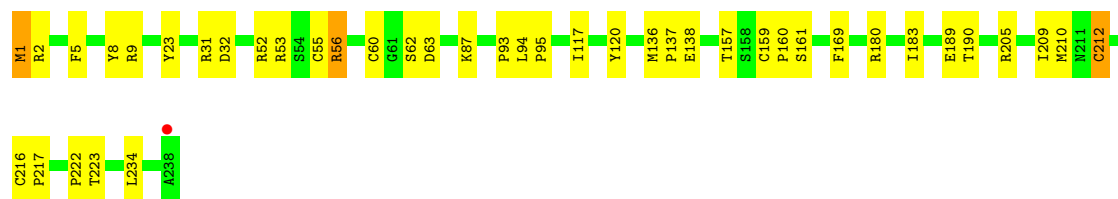




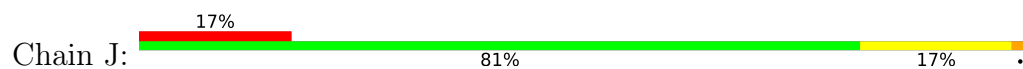
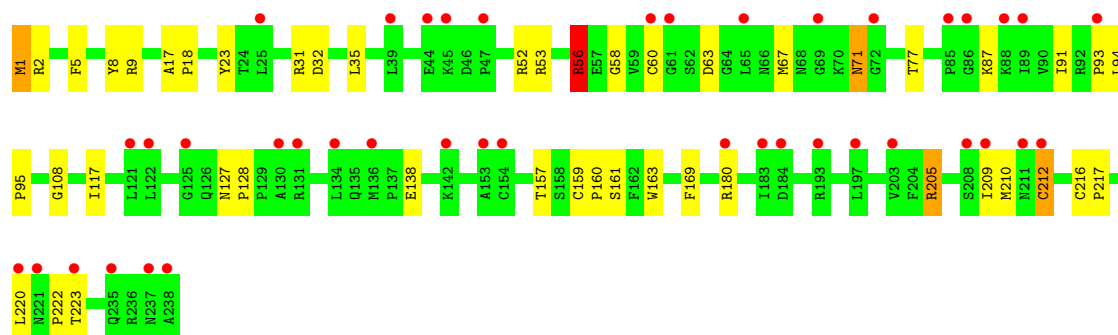
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



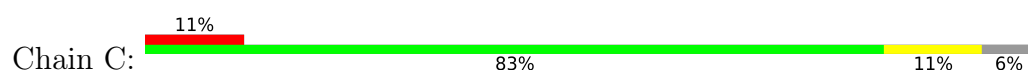
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



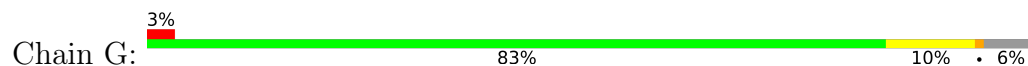
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



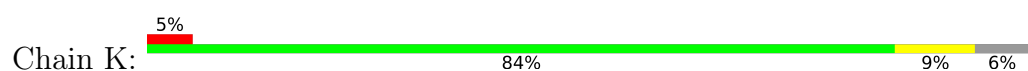
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT



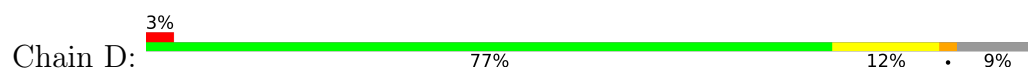
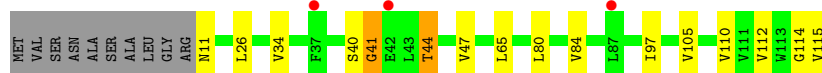
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT



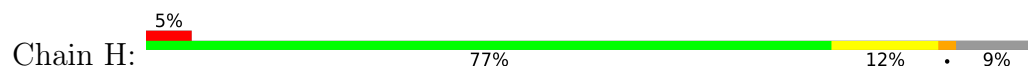
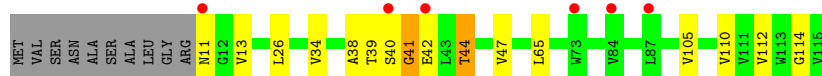
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT



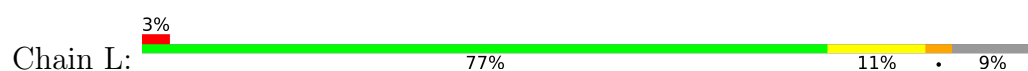
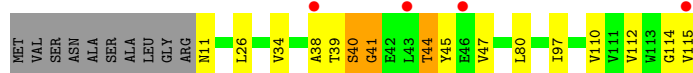
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN



• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN



• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.34Å 184.85Å 204.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.85 – 3.20 51.85 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.85-3.20) 99.7 (51.85-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.205 , 0.233 0.207 , 0.236	Depositor DCC
R_{free} test set	3844 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 97.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	24855	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: FES, TEO, FAD, NA, SF4, HEM, 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	0.77	2/4611 (0.0%)	0.92	6/6237 (0.1%)
1	E	0.68	1/4611 (0.0%)	0.90	7/6237 (0.1%)
1	I	0.56	2/4611 (0.0%)	0.87	3/6237 (0.0%)
2	B	0.80	0/1908	0.96	1/2578 (0.0%)
2	F	0.71	0/1908	0.95	1/2578 (0.0%)
2	J	0.60	1/1908 (0.1%)	0.91	0/2578
3	C	0.67	0/953	0.84	1/1293 (0.1%)
3	G	0.64	0/953	0.86	1/1293 (0.1%)
3	K	0.56	0/953	0.85	1/1293 (0.1%)
4	D	0.61	0/859	0.80	1/1175 (0.1%)
4	H	0.62	0/859	0.80	0/1175
4	L	0.57	0/859	0.81	0/1175
All	All	0.67	6/24993 (0.0%)	0.89	22/33849 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	173	GLN	CD-NE2	-7.02	1.18	1.33
1	E	173	GLN	CD-NE2	-7.01	1.18	1.33
2	J	71	ASN	CG-ND2	-6.68	1.19	1.33
1	A	173	GLN	CD-NE2	-6.48	1.19	1.33
1	A	210	GLN	CD-OE1	5.32	1.33	1.23
1	I	210	GLN	CD-OE1	5.13	1.33	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	9	ARG	N-CA-C	8.89	121.12	109.83
3	C	9	ARG	N-CA-C	8.38	120.32	109.93
3	G	9	ARG	N-CA-C	8.08	121.23	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	392	VAL	N-CA-C	7.47	117.55	110.53
1	I	392	VAL	N-CA-C	6.61	116.74	110.53
2	F	62	SER	N-CA-C	6.26	117.77	111.07
2	B	62	SER	N-CA-C	6.06	117.55	111.07
1	A	392	VAL	N-CA-C	6.05	116.83	110.72
1	E	196	ARG	N-CA-C	-5.79	106.22	113.28
1	I	286	ARG	N-CA-C	5.63	117.09	111.07
1	E	503	SER	N-CA-C	5.58	117.52	110.33
1	A	196	ARG	N-CA-C	-5.57	106.48	113.28
1	A	136	ALA	N-CA-C	5.50	117.43	109.07
1	E	244	THR	N-CA-C	5.47	116.26	108.54
4	D	84	VAL	N-CA-C	5.29	114.92	106.88
1	I	196	ARG	N-CA-C	-5.26	106.86	113.28
1	E	255	GLU	N-CA-C	-5.25	106.57	112.87
1	E	136	ALA	N-CA-C	5.12	117.03	108.99
1	A	277	ALA	CA-C-N	5.12	125.41	119.47
1	A	277	ALA	C-N-CA	5.12	125.41	119.47
1	A	108	ARG	N-CA-C	5.05	117.68	109.24
1	E	108	ARG	N-CA-C	5.01	117.61	109.24

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	58	0
1	I	4522	0	4426	67	0
2	B	1869	0	1850	27	0
2	F	1869	0	1850	25	0
2	J	1869	0	1850	28	0
3	C	933	0	979	8	0
3	G	933	0	979	11	0
3	K	933	0	979	10	0
4	D	836	0	875	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	836	0	875	11	0
4	L	836	0	875	11	0
5	A	53	0	30	6	0
5	E	53	0	30	5	0
5	I	53	0	29	8	0
6	A	9	0	3	2	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	B	4	0	0	0	0
8	F	4	0	0	0	0
8	J	4	0	0	2	0
9	B	8	0	0	0	0
9	F	8	0	0	2	0
9	J	8	0	0	1	0
10	B	7	0	0	0	0
10	F	7	0	0	1	0
10	J	7	0	0	1	0
11	C	43	0	30	4	0
11	G	43	0	30	5	0
11	K	43	0	30	8	0
All	All	24855	0	24578	322	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 7.

All (322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:1129:HEM:HHD	11:C:1129:HEM:HBC2	1.39	1.04
11:K:1129:HEM:HHB	11:K:1129:HEM:HBA2	1.39	1.02
1:E:555:CYS:HA	1:E:571:VAL:HG23	1.50	0.94
1:I:490:ILE:HG22	1:I:520:MET:HE1	1.48	0.93
11:K:1129:HEM:HBB2	4:L:26:LEU:HD13	1.51	0.90
1:A:490:ILE:HG22	1:A:520:MET:HE1	1.54	0.90
1:E:490:ILE:HG22	1:E:520:MET:HE1	1.52	0.88
1:I:555:CYS:HA	1:I:571:VAL:HG23	1.52	0.88
1:A:555:CYS:HA	1:A:571:VAL:HG23	1.58	0.84
11:G:1129:HEM:HBC2	11:G:1129:HEM:HHD	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:GLU:HG2	1:E:346:PRO:HD2	1.61	0.83
1:I:51:GLY:HA3	6:I:1589:TEO:O1A	1.83	0.78
2:J:58:GLY:HA2	8:J:302:FES:S1	2.26	0.76
1:I:345:GLU:HG2	1:I:346:PRO:HD2	1.68	0.76
11:K:1129:HEM:HBC2	11:K:1129:HEM:HHD	1.66	0.75
1:A:147:HIS:O	1:A:151:GLN:HG3	1.88	0.74
1:E:388:GLU:OE1	5:E:601:FAD:O3'	2.03	0.74
1:I:490:ILE:HG22	1:I:520:MET:CE	2.16	0.73
2:B:1:MET:O	2:B:1:MET:HG3	1.88	0.72
1:A:345:GLU:HG2	1:A:346:PRO:HD2	1.69	0.72
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.70	0.72
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.70	0.72
1:A:554:LEU:HD21	1:A:573:MET:HE1	1.72	0.71
1:E:490:ILE:HG22	1:E:520:MET:CE	2.21	0.71
1:I:490:ILE:CG2	1:I:520:MET:HE1	2.21	0.71
1:I:147:HIS:O	1:I:151:GLN:HG3	1.91	0.71
1:A:408:LEU:HD21	5:A:601:FAD:H5'2	1.73	0.69
1:E:490:ILE:CG2	1:E:520:MET:HE1	2.24	0.68
1:I:392:VAL:N	1:I:393:SER:HA	2.09	0.67
1:A:490:ILE:HG22	1:A:520:MET:CE	2.25	0.66
11:G:1129:HEM:HHC	11:G:1129:HEM:HBB2	1.77	0.66
1:A:49:ALA:HA	5:A:601:FAD:N5	2.12	0.65
1:E:554:LEU:HD21	1:E:573:MET:HE1	1.79	0.65
2:J:169:PHE:CD1	2:J:205:ARG:HB2	2.32	0.65
2:J:160:PRO:HG2	2:J:209:ILE:HD13	1.77	0.65
1:I:49:ALA:HB3	1:I:142:GLY:HA3	1.79	0.64
1:A:350:ILE:HG13	1:A:351:PRO:HD2	1.80	0.63
1:A:490:ILE:CG2	1:A:520:MET:HE1	2.26	0.63
11:C:1129:HEM:HBC2	11:C:1129:HEM:CHD	2.17	0.63
1:E:392:VAL:N	1:E:393:SER:HA	2.12	0.63
1:A:286:ARG:HH22	6:A:1589:TEO:C3	2.13	0.62
3:G:31:ARG:NE	11:G:1129:HEM:O1A	2.32	0.62
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.35	0.62
1:I:554:LEU:HD21	1:I:573:MET:HE1	1.80	0.62
1:A:392:VAL:N	1:A:393:SER:HA	2.13	0.62
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.35	0.62
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.81	0.61
1:E:173:GLN:CD	1:E:430:ARG:HH11	2.09	0.60
1:E:147:HIS:O	1:E:151:GLN:HG3	2.01	0.60
2:F:160:PRO:HG2	2:F:209:ILE:HD13	1.83	0.60
1:I:173:GLN:CD	1:I:430:ARG:HH11	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:128:VAL:HG12	3:K:128:VAL:O	2.02	0.60
1:E:286:ARG:HH12	6:E:1589:TEO:C4	2.14	0.59
2:J:212:CYS:HB2	2:J:222:PRO:HG2	1.83	0.59
1:E:345:GLU:HG2	1:E:346:PRO:CD	2.31	0.59
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.85	0.58
1:A:242:HIS:O	1:A:351:PRO:HA	2.03	0.58
1:I:350:ILE:HG13	1:I:351:PRO:HD2	1.86	0.58
1:E:350:ILE:HG13	1:E:351:PRO:HD2	1.84	0.58
4:H:44:THR:HG23	4:H:47:VAL:HG13	1.85	0.58
11:K:1129:HEM:HHA	11:K:1129:HEM:CBA	2.24	0.58
1:A:49:ALA:HA	5:A:601:FAD:C5X	2.34	0.58
1:E:49:ALA:HB3	1:E:142:GLY:HA3	1.86	0.56
1:I:242:HIS:O	1:I:351:PRO:HA	2.04	0.56
3:G:128:VAL:HG12	3:G:128:VAL:O	2.05	0.56
1:A:463:LEU:HD23	1:A:463:LEU:C	2.31	0.56
1:I:49:ALA:HA	5:I:601:FAD:N5	2.21	0.56
1:E:463:LEU:C	1:E:463:LEU:HD23	2.31	0.55
2:F:159:CYS:HB2	10:F:304:F3S:S2	2.46	0.55
4:L:44:THR:HG23	4:L:47:VAL:HG13	1.88	0.55
1:I:99:LEU:HD11	1:I:409:VAL:HG21	1.88	0.55
11:K:1129:HEM:HBA2	11:K:1129:HEM:CHA	2.19	0.55
1:A:173:GLN:CD	1:A:430:ARG:HH11	2.14	0.55
1:E:55:VAL:HG13	1:E:57:LEU:HG	1.88	0.55
1:A:49:ALA:HA	5:A:601:FAD:C6	2.38	0.54
4:D:112:VAL:C	4:D:114:GLY:H	2.15	0.53
1:I:345:GLU:HG2	1:I:346:PRO:CD	2.36	0.53
1:I:209:TYR:CD2	1:I:353:CYS:SG	2.97	0.53
2:J:58:GLY:CA	8:J:302:FES:S1	2.97	0.53
2:B:31:ARG:HG2	2:B:32:ASP:N	2.23	0.53
11:C:1129:HEM:HHH	11:C:1129:HEM:CBC	2.24	0.53
2:F:31:ARG:HG2	2:F:32:ASP:N	2.22	0.53
3:G:54:SER:HB2	3:G:55:PRO:CD	2.39	0.53
2:J:159:CYS:HB2	10:J:304:F3S:S2	2.48	0.53
1:A:208:ILE:HD12	1:A:467:MET:HE2	1.90	0.53
2:B:9:ARG:NH1	2:B:23:TYR:OH	2.42	0.53
3:K:127:LEU:O	3:K:127:LEU:HD23	2.09	0.53
1:I:51:GLY:CA	6:I:1589:TEO:O1A	2.55	0.53
3:K:128:VAL:O	3:K:128:VAL:CG1	2.56	0.53
3:C:128:VAL:HG12	3:C:128:VAL:O	2.09	0.52
1:A:43:ARG:HD3	2:B:60:CYS:O	2.10	0.52
3:G:83:TYR:CZ	3:G:87:VAL:HG21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:GLN:HA	1:I:134:THR:O	2.09	0.52
1:I:468:GLN:O	1:I:472:SER:HB2	2.10	0.52
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.92	0.52
4:D:44:THR:HG23	4:D:47:VAL:HG13	1.91	0.52
11:G:1129:HEM:HBB2	4:H:26:LEU:HD13	1.91	0.52
1:I:388:GLU:OE1	5:I:601:FAD:O3'	2.23	0.52
1:I:371:VAL:HA	1:I:376:GLU:O	2.09	0.52
1:E:286:ARG:HH22	6:E:1589:TEO:C3	2.23	0.51
1:A:78:TYR:CD1	1:A:583:PRO:HA	2.45	0.51
4:D:11:ASN:OD1	4:D:11:ASN:C	2.53	0.51
2:F:234:LEU:HD23	4:H:13:VAL:HG13	1.92	0.51
1:I:43:ARG:HD3	2:J:60:CYS:O	2.10	0.51
1:A:345:GLU:HG2	1:A:346:PRO:CD	2.37	0.51
3:C:54:SER:HB2	3:C:55:PRO:CD	2.40	0.51
1:E:20:MET:HE3	1:E:146:LEU:HD12	1.91	0.51
2:J:1:MET:O	2:J:1:MET:HG3	2.09	0.51
1:I:391:CYS:SG	1:I:393:SER:HB2	2.51	0.51
2:J:95:PRO:O	2:J:157:THR:HB	2.10	0.51
2:J:117:ILE:C	2:J:117:ILE:HD12	2.35	0.51
2:F:212:CYS:HB2	2:F:222:PRO:HG2	1.93	0.51
2:F:217:PRO:HD2	9:F:303:SF4:S2	2.51	0.51
1:I:578:ARG:NH1	1:I:581:PHE:CZ	2.79	0.51
2:F:1:MET:O	2:F:1:MET:HG3	2.10	0.51
2:J:9:ARG:NH1	2:J:23:TYR:OH	2.43	0.51
2:F:210:MET:HE3	2:F:223:THR:HG21	1.93	0.51
1:E:20:MET:CE	1:E:146:LEU:CD1	2.89	0.50
1:I:119:PHE:HZ	6:I:1589:TEO:O1A	1.94	0.50
1:I:257:CYS:HB3	1:I:315:LEU:HD21	1.93	0.50
2:B:160:PRO:HG2	2:B:209:ILE:HD13	1.93	0.50
2:F:117:ILE:HD12	2:F:117:ILE:C	2.36	0.50
1:I:237:GLU:OE1	1:I:529:SER:HB3	2.12	0.50
1:E:242:HIS:O	1:E:351:PRO:HA	2.10	0.50
4:H:112:VAL:C	4:H:114:GLY:H	2.20	0.50
2:F:55:CYS:O	2:F:56:ARG:HD2	2.12	0.50
3:K:52:LEU:HB3	4:L:115:VAL:HG21	1.93	0.50
1:A:408:LEU:HD11	5:A:601:FAD:H4'	1.94	0.49
3:K:83:TYR:CZ	3:K:87:VAL:HG21	2.47	0.49
11:K:1129:HEM:CBB	4:L:26:LEU:HD13	2.34	0.49
1:A:35:LEU:HD23	1:A:160:ILE:HG12	1.93	0.49
2:F:95:PRO:O	2:F:157:THR:HB	2.13	0.49
3:G:128:VAL:O	3:G:128:VAL:CG1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:112:VAL:C	4:L:114:GLY:H	2.18	0.49
4:H:11:ASN:C	4:H:11:ASN:OD1	2.55	0.49
2:B:210:MET:HE3	2:B:223:THR:HG21	1.95	0.49
1:E:1:MET:HE3	1:E:1:MET:HA	1.95	0.48
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.48	0.48
1:E:99:LEU:HD11	1:E:409:VAL:HG21	1.94	0.48
1:I:463:LEU:C	1:I:463:LEU:HD23	2.38	0.48
1:E:199:VAL:HG22	1:E:384:PHE:HB2	1.96	0.48
3:G:54:SER:HB2	3:G:55:PRO:HD2	1.95	0.48
1:I:166:ALA:N	5:I:601:FAD:N1A	2.50	0.48
3:C:54:SER:HB2	3:C:55:PRO:HD2	1.95	0.48
1:E:371:VAL:HA	1:E:376:GLU:O	2.14	0.48
2:J:5:PHE:HB2	2:J:23:TYR:HB2	1.96	0.48
1:E:20:MET:HE3	1:E:146:LEU:CD1	2.44	0.48
1:A:294:MET:O	1:A:298:ARG:HB2	2.13	0.48
2:B:8:TYR:CG	2:B:93:PRO:HD3	2.49	0.48
1:I:69:MET:O	1:I:73:VAL:HG23	2.14	0.47
2:J:52:ARG:O	2:J:63:ASP:HB3	2.13	0.47
2:J:217:PRO:HD2	9:J:303:SF4:S3	2.54	0.47
1:A:118:PRO:HA	1:A:132:ALA:HA	1.96	0.47
1:A:350:ILE:CG1	1:A:351:PRO:HD2	2.44	0.47
2:B:56:ARG:HD2	2:B:56:ARG:C	2.39	0.47
1:E:350:ILE:CG1	1:E:351:PRO:HD2	2.44	0.47
4:L:11:ASN:OD1	4:L:11:ASN:C	2.57	0.47
4:D:44:THR:HG23	4:D:47:VAL:HG22	1.96	0.47
1:I:208:ILE:HD12	1:I:467:MET:HE2	1.95	0.47
2:J:31:ARG:HG2	2:J:32:ASP:N	2.28	0.47
1:E:468:GLN:O	1:E:472:SER:HB2	2.13	0.47
1:I:266:ASN:HB2	1:I:301:ARG:O	2.14	0.47
2:J:8:TYR:CG	2:J:93:PRO:HD3	2.50	0.47
1:A:9:ASP:HB2	1:A:32:THR:O	2.15	0.47
1:I:405:LEU:HG	5:I:601:FAD:C2	2.44	0.47
4:L:40:SER:O	4:L:41:GLY:C	2.58	0.47
3:K:55:PRO:HA	4:L:45:TYR:CE1	2.50	0.47
1:E:271:ARG:O	1:E:271:ARG:HG2	2.15	0.46
11:K:1129:HEM:HHD	11:K:1129:HEM:CBC	2.40	0.46
11:K:1129:HEM:CBA	11:K:1129:HEM:CHA	2.89	0.46
1:A:99:LEU:HD11	1:A:409:VAL:HG21	1.97	0.46
1:E:20:MET:CE	1:E:146:LEU:HD11	2.45	0.46
3:K:54:SER:HB2	3:K:55:PRO:CD	2.45	0.46
1:E:78:TYR:CD1	1:E:583:PRO:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:VAL:HG13	1:I:57:LEU:HG	1.97	0.46
1:I:294:MET:O	1:I:298:ARG:HB2	2.16	0.46
1:A:401:GLY:HA2	6:A:1589:TEO:O4A	2.16	0.46
2:F:52:ARG:O	2:F:63:ASP:HB3	2.15	0.46
1:A:468:GLN:O	1:A:472:SER:HB2	2.16	0.46
2:B:117:ILE:C	2:B:117:ILE:HD12	2.41	0.46
3:G:127:LEU:HD23	3:G:127:LEU:O	2.16	0.46
1:E:116:GLN:HA	1:E:134:THR:O	2.16	0.46
4:D:80:LEU:HD11	4:D:97:ILE:HD12	1.97	0.45
1:I:1:MET:HE3	1:I:1:MET:HA	1.97	0.45
1:I:286:ARG:HH12	6:I:1589:TEO:C4	2.29	0.45
1:A:154:LEU:O	1:A:155:LYS:C	2.57	0.45
1:I:178:VAL:HG21	1:I:432:ALA:HB2	1.99	0.45
4:D:40:SER:O	4:D:41:GLY:C	2.59	0.45
4:H:40:SER:O	4:H:41:GLY:C	2.59	0.45
1:I:496:ASN:O	1:I:496:ASN:ND2	2.48	0.45
2:B:17:ALA:HB1	2:B:18:PRO:CD	2.46	0.45
1:E:40:PHE:CD1	1:E:41:PRO:HD2	2.51	0.45
1:E:208:ILE:HD12	1:E:467:MET:HE2	1.98	0.45
1:E:214:ASN:N	1:E:214:ASN:HD22	2.13	0.45
2:F:216:CYS:HA	9:F:303:SF4:S2	2.57	0.45
1:E:404:SER:O	1:E:407:ASP:HB3	2.16	0.45
1:I:9:ASP:HB2	1:I:32:THR:O	2.16	0.45
11:C:1129:HEM:HHC	11:C:1129:HEM:HBB2	1.97	0.45
1:A:103:GLY:O	1:A:104:LEU:C	2.59	0.45
2:F:9:ARG:NH1	2:F:23:TYR:OH	2.50	0.45
4:H:38:ALA:O	4:H:39:THR:HG23	2.16	0.45
1:I:399:ARG:CZ	1:I:404:SER:HB2	2.47	0.45
3:C:128:VAL:O	3:C:128:VAL:CG1	2.65	0.45
1:E:257:CYS:HB3	1:E:315:LEU:HD21	1.99	0.45
1:E:49:ALA:HA	5:E:601:FAD:N5	2.32	0.44
1:E:69:MET:O	1:E:73:VAL:HG23	2.17	0.44
1:E:242:HIS:CD2	6:E:1589:TEO:O2	2.71	0.44
2:B:56:ARG:C	2:B:56:ARG:CD	2.90	0.44
1:E:266:ASN:HB2	1:E:301:ARG:O	2.17	0.44
1:A:116:GLN:HA	1:A:134:THR:O	2.17	0.44
2:B:212:CYS:HB2	2:B:222:PRO:HG2	1.99	0.44
3:K:54:SER:HB2	3:K:55:PRO:HD2	1.99	0.44
1:E:533:ARG:NH1	1:E:535:GLU:OE2	2.47	0.44
4:H:41:GLY:O	4:H:42:GLU:C	2.60	0.44
3:C:12:ASN:OD1	3:C:12:ASN:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:ASP:HB2	1:E:32:THR:O	2.17	0.44
2:F:1:MET:HE3	2:F:1:MET:HB2	1.66	0.44
1:I:168:ASP:HA	1:I:225:MET:HG2	1.99	0.44
1:E:49:ALA:HA	5:E:601:FAD:C5X	2.48	0.44
1:E:103:GLY:O	1:E:104:LEU:C	2.61	0.44
1:I:20:MET:HE3	1:I:146:LEU:HD12	2.00	0.44
1:I:404:SER:HB3	5:I:601:FAD:N1	2.33	0.44
2:J:35:LEU:HD11	2:J:91:ILE:HD11	2.00	0.44
4:L:44:THR:HG23	4:L:47:VAL:HG22	1.99	0.44
1:A:1:MET:HE3	1:A:1:MET:HA	1.99	0.44
4:H:44:THR:HG23	4:H:47:VAL:HG22	1.99	0.44
4:L:80:LEU:HD11	4:L:97:ILE:HD12	1.99	0.44
3:G:12:ASN:OD1	3:G:12:ASN:C	2.60	0.43
2:B:160:PRO:HA	2:B:163:TRP:CE3	2.54	0.43
1:I:262:GLY:HA3	1:I:315:LEU:HD23	2.00	0.43
3:K:12:ASN:OD1	3:K:12:ASN:C	2.61	0.43
1:A:399:ARG:CZ	1:A:404:SER:HB2	2.48	0.43
1:I:407:ASP:O	1:I:408:LEU:C	2.61	0.43
4:L:38:ALA:O	4:L:39:THR:HG23	2.19	0.43
1:I:49:ALA:HA	5:I:601:FAD:C5X	2.49	0.43
4:H:44:THR:CG2	4:H:47:VAL:HG13	2.48	0.43
2:J:17:ALA:HB1	2:J:18:PRO:CD	2.49	0.43
2:J:210:MET:HE3	2:J:223:THR:HG21	1.99	0.43
2:B:63:ASP:OD2	2:B:74:ALA:HB3	2.19	0.43
1:I:22:ALA:O	1:I:26:ILE:HG13	2.19	0.43
1:A:48:SER:HB3	5:A:601:FAD:HM72	2.01	0.43
2:B:127:ASN:N	2:B:128:PRO:CD	2.82	0.43
1:A:549:ASP:OD1	1:A:549:ASP:C	2.61	0.43
1:I:40:PHE:CD1	1:I:41:PRO:HD2	2.54	0.43
1:I:404:SER:O	1:I:407:ASP:HB3	2.19	0.43
1:A:507:ASN:OD1	1:A:507:ASN:C	2.62	0.42
1:E:237:GLU:OE1	1:E:529:SER:HB3	2.19	0.42
5:I:601:FAD:H9	5:I:601:FAD:H1'1	1.80	0.42
1:E:522:THR:O	1:E:523:ALA:C	2.62	0.42
2:B:111:TYR:O	2:B:114:TYR:HB3	2.20	0.42
1:E:578:ARG:NH1	1:E:581:PHE:CZ	2.87	0.42
2:F:8:TYR:CG	2:F:93:PRO:HD3	2.54	0.42
1:I:75:GLY:O	1:I:398:ASN:HB3	2.19	0.42
2:F:5:PHE:HB2	2:F:23:TYR:HB2	2.01	0.42
2:F:56:ARG:CD	2:F:56:ARG:C	2.93	0.42
2:B:52:ARG:O	2:B:63:ASP:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:LEU:HB3	4:D:105:VAL:HG22	2.00	0.42
1:I:78:TYR:CD1	1:I:583:PRO:HA	2.54	0.42
1:A:404:SER:O	1:A:407:ASP:HB3	2.19	0.42
3:G:13:LEU:HD12	3:G:13:LEU:HA	1.86	0.42
1:I:59:ASN:HB2	1:I:116:GLN:OE1	2.20	0.42
2:J:71:ASN:OD1	2:J:94:LEU:HD23	2.20	0.42
2:J:160:PRO:HA	2:J:163:TRP:CE3	2.55	0.42
2:F:94:LEU:HA	2:F:95:PRO:HD3	1.91	0.42
2:J:35:LEU:HD11	2:J:91:ILE:CD1	2.50	0.42
1:E:191:VAL:HG12	1:E:192:TYR:N	2.35	0.42
3:G:37:THR:HG22	11:G:1129:HEM:HMB3	2.01	0.42
1:A:266:ASN:HB2	1:A:301:ARG:O	2.20	0.41
2:B:101:ARG:O	2:B:102:ASP:C	2.63	0.41
1:E:399:ARG:CZ	1:E:404:SER:HB2	2.49	0.41
1:E:549:ASP:OD1	1:E:549:ASP:C	2.62	0.41
5:E:601:FAD:C4	6:E:1589:TEO:C3	2.98	0.41
2:J:56:ARG:C	2:J:56:ARG:HD2	2.45	0.41
2:J:127:ASN:N	2:J:128:PRO:CD	2.84	0.41
1:A:251:VAL:HG11	1:A:333:LEU:HD22	2.02	0.41
4:D:26:LEU:HD23	4:D:26:LEU:HA	1.91	0.41
1:A:257:CYS:HB3	1:A:315:LEU:HD21	2.03	0.41
1:I:494:LEU:HD21	1:I:517:ASP:HA	2.02	0.41
1:A:92:GLY:O	1:A:93:PRO:C	2.61	0.41
2:B:98:PRO:HB2	2:B:106:ASP:HB3	2.02	0.41
2:B:103:LEU:HA	2:B:103:LEU:HD23	1.87	0.41
2:B:136:MET:O	2:B:137:PRO:C	2.61	0.41
3:C:52:LEU:HB3	4:D:115:VAL:HG21	2.02	0.41
1:E:61:HIS:O	1:E:62:GLU:C	2.61	0.41
1:I:451:ARG:HA	1:I:451:ARG:HD3	1.89	0.41
2:J:216:CYS:SG	2:J:220:LEU:N	2.80	0.41
3:C:25:ILE:O	3:C:26:ALA:C	2.63	0.41
1:E:43:ARG:HD3	2:F:60:CYS:O	2.20	0.41
2:F:56:ARG:HD2	2:F:56:ARG:C	2.46	0.41
1:I:20:MET:CE	1:I:146:LEU:CD1	2.99	0.41
1:E:262:GLY:HA3	1:E:315:LEU:HD23	2.03	0.41
4:H:65:LEU:HB3	4:H:105:VAL:HG22	2.03	0.41
1:I:118:PRO:HA	1:I:132:ALA:HA	2.02	0.41
1:I:191:VAL:CG1	1:I:192:TYR:N	2.84	0.41
1:I:350:ILE:CG1	1:I:351:PRO:HD2	2.48	0.41
1:A:303:CYS:O	1:A:309:PRO:HA	2.21	0.41
2:F:189:GLU:O	2:F:190:THR:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ARG:CG	2:B:32:ASP:N	2.84	0.41
1:E:46:THR:OG1	5:E:601:FAD:O2A	2.38	0.41
1:E:118:PRO:HA	1:E:132:ALA:HA	2.03	0.41
1:E:395:HIS:O	1:E:396:GLY:C	2.64	0.41
1:I:49:ALA:HB3	1:I:142:GLY:CA	2.50	0.41
2:J:1:MET:HB2	2:J:1:MET:HE3	1.67	0.41
2:B:207:HIS:O	2:B:208:SER:HB2	2.20	0.41
2:J:56:ARG:C	2:J:56:ARG:CD	2.94	0.41
2:F:136:MET:O	2:F:137:PRO:C	2.62	0.40
1:I:423:ILE:O	1:I:426:GLN:HG2	2.20	0.40
2:B:95:PRO:O	2:B:157:THR:HB	2.20	0.40
3:G:126:VAL:C	3:G:128:VAL:H	2.29	0.40
1:A:72:THR:HG22	1:A:85:ILE:HD13	2.04	0.40
4:D:112:VAL:C	4:D:114:GLY:N	2.78	0.40
2:J:67:MET:HE1	2:J:77:THR:OG1	2.21	0.40
3:K:58:PHE:CD2	3:K:58:PHE:C	2.99	0.40
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.57	0.40
2:F:183:ILE:HD12	2:F:183:ILE:C	2.47	0.40
1:I:48:SER:HB3	5:I:601:FAD:HM72	2.02	0.40
1:I:365:THR:O	1:I:415:ALA:HA	2.22	0.40
1:I:463:LEU:HD12	1:I:520:MET:HE2	2.03	0.40
2:B:1:MET:HE3	2:B:1:MET:HB2	1.67	0.40
2:B:94:LEU:HA	2:B:95:PRO:HD3	1.92	0.40
1:E:191:VAL:CG1	1:E:192:TYR:N	2.84	0.40
1:I:38:LYS:HE3	1:I:217:ILE:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/588 (100%)	567 (97%)	18 (3%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	586/588 (100%)	563 (96%)	21 (4%)	2 (0%)	36	68
1	I	586/588 (100%)	562 (96%)	23 (4%)	1 (0%)	43	73
2	B	236/238 (99%)	221 (94%)	14 (6%)	1 (0%)	30	62
2	F	236/238 (99%)	220 (93%)	16 (7%)	0	100	100
2	J	236/238 (99%)	220 (93%)	14 (6%)	2 (1%)	16	50
3	C	119/129 (92%)	115 (97%)	4 (3%)	0	100	100
3	G	119/129 (92%)	115 (97%)	3 (2%)	1 (1%)	16	50
3	K	119/129 (92%)	115 (97%)	4 (3%)	0	100	100
4	D	103/115 (90%)	94 (91%)	8 (8%)	1 (1%)	12	45
4	H	103/115 (90%)	95 (92%)	7 (7%)	1 (1%)	12	45
4	L	103/115 (90%)	95 (92%)	6 (6%)	2 (2%)	6	33
All	All	3132/3210 (98%)	2982 (95%)	138 (4%)	12 (0%)	30	62

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	56	ARG
2	B	56	ARG
4	H	41	GLY
4	L	41	GLY
4	D	41	GLY
1	E	92	GLY
1	E	472	SER
3	G	127	LEU
1	I	92	GLY
4	L	40	SER
1	A	92	GLY
2	J	108	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%)	466 (98%)	7 (2%)	57	76
1	E	473/473 (100%)	462 (98%)	11 (2%)	44	70
1	I	473/473 (100%)	460 (97%)	13 (3%)	39	68
2	B	208/208 (100%)	198 (95%)	10 (5%)	23	56
2	F	208/208 (100%)	198 (95%)	10 (5%)	23	56
2	J	208/208 (100%)	198 (95%)	10 (5%)	23	56
3	C	101/109 (93%)	97 (96%)	4 (4%)	28	61
3	G	101/109 (93%)	99 (98%)	2 (2%)	48	72
3	K	101/109 (93%)	99 (98%)	2 (2%)	48	72
4	D	88/96 (92%)	85 (97%)	3 (3%)	32	64
4	H	88/96 (92%)	85 (97%)	3 (3%)	32	64
4	L	88/96 (92%)	85 (97%)	3 (3%)	32	64
All	All	2610/2658 (98%)	2532 (97%)	78 (3%)	36	66

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ASP
1	A	325	SER
1	A	363	LYS
1	A	378	VAL
1	A	423	ILE
1	A	541	SER
1	A	573	MET
2	B	1	MET
2	B	2	ARG
2	B	53	ARG
2	B	56	ARG
2	B	87	LYS
2	B	138	GLU
2	B	161	SER
2	B	180	ARG
2	B	205	ARG
2	B	212	CYS
3	C	11	VAL
3	C	13	LEU
3	C	19	ARG
3	C	28	ILE
4	D	34	VAL

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Mol	Chain	Res	Type
4	D	44	THR
4	D	110	VAL
1	E	119	PHE
1	E	252	LEU
1	E	304	ASP
1	E	325	SER
1	E	363	LYS
1	E	364	VAL
1	E	440	SER
1	E	491	ARG
1	E	541	SER
1	E	563	SER
1	E	573	MET
2	F	1	MET
2	F	2	ARG
2	F	53	ARG
2	F	56	ARG
2	F	87	LYS
2	F	120	TYR
2	F	138	GLU
2	F	161	SER
2	F	180	ARG
2	F	212	CYS
3	G	11	VAL
3	G	19	ARG
4	H	34	VAL
4	H	44	THR
4	H	110	VAL
1	I	2	LYS
1	I	304	ASP
1	I	325	SER
1	I	363	LYS
1	I	364	VAL
1	I	378	VAL
1	I	423	ILE
1	I	440	SER
1	I	491	ARG
1	I	496	ASN
1	I	535	GLU
1	I	541	SER
1	I	573	MET
2	J	1	MET

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Mol	Chain	Res	Type
2	J	2	ARG
2	J	53	ARG
2	J	56	ARG
2	J	87	LYS
2	J	138	GLU
2	J	161	SER
2	J	180	ARG
2	J	205	ARG
2	J	212	CYS
3	K	11	VAL
3	K	19	ARG
4	L	34	VAL
4	L	44	THR
4	L	110	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	156	ASN
1	A	216	HIS
1	A	339	HIS
1	A	531	ASN
2	B	41	GLN
2	B	135	GLN
2	B	237	ASN
3	C	91	HIS
1	E	216	HIS
1	E	531	ASN
2	F	41	GLN
2	F	135	GLN
2	F	228	HIS
2	F	237	ASN
1	I	216	HIS
1	I	531	ASN
2	J	41	GLN
2	J	113	GLN
2	J	135	GLN
2	J	237	ASN
3	K	91	HIS
4	L	78	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	TEO	I	1589	-	6,8,8	1.13	0	4,10,10	1.55	1 (25%)
9	SF4	B	303	2	0,12,12	-	-	-		
9	SF4	J	303	2	0,12,12	-	-	-		
6	TEO	E	1589	-	6,8,8	1.15	1 (16%)	4,10,10	1.17	0
5	FAD	A	601	1	56,58,58	1.20	4 (7%)	81,89,89	1.84	20 (24%)
5	FAD	I	601	1	56,58,58	1.13	5 (8%)	81,89,89	1.86	19 (23%)
10	F3S	B	304	2	0,9,9	-	-	-		
10	F3S	J	304	2	0,9,9	-	-	-		
8	FES	F	302	2	0,4,4	-	-	-		
8	FES	J	302	2	0,4,4	-	-	-		
8	FES	B	302	2	0,4,4	-	-	-		
11	HEM	C	1129	4,3	50,50,50	1.75	8 (16%)	66,82,82	1.25	6 (9%)
11	HEM	G	1129	4,3	50,50,50	1.74	9 (18%)	66,82,82	1.46	8 (12%)
11	HEM	K	1129	4,3	50,50,50	1.89	10 (20%)	66,82,82	1.46	7 (10%)
10	F3S	F	304	2	0,9,9	-	-	-		
5	FAD	E	601	1	56,58,58	1.23	5 (8%)	81,89,89	1.93	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TEO	A	1589	-	6,8,8	1.33	1 (16%)	4,10,10	2.07	1 (25%)
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
6	TEO	I	1589	-	-	1/6/8/8	-
9	SF4	B	303	2	-	-	0/6/5/5
9	SF4	J	303	2	-	-	0/6/5/5
6	TEO	E	1589	-	-	5/6/8/8	-
5	FAD	A	601	1	-	10/34/50/50	0/6/6/6
5	FAD	I	601	1	-	3/34/50/50	0/6/6/6
10	F3S	B	304	2	-	-	0/3/3/3
10	F3S	J	304	2	-	-	0/3/3/3
8	FES	F	302	2	-	-	0/1/1/1
8	FES	J	302	2	-	-	0/1/1/1
11	HEM	C	1129	4,3	-	7/14/54/54	-
11	HEM	G	1129	4,3	-	5/14/54/54	-
11	HEM	K	1129	4,3	-	4/14/54/54	-
8	FES	B	302	2	-	-	0/1/1/1
10	F3S	F	304	2	-	-	0/3/3/3
5	FAD	E	601	1	-	7/34/50/50	0/6/6/6
6	TEO	A	1589	-	-	4/6/8/8	-
9	SF4	F	303	2	-	-	0/6/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	1129	HEM	C3D-C2D	7.77	1.53	1.36
11	C	1129	HEM	C3D-C2D	7.53	1.52	1.36
11	G	1129	HEM	C3D-C2D	7.43	1.52	1.36
5	A	601	FAD	C4X-N5	5.16	1.40	1.30
5	E	601	FAD	C4X-N5	4.90	1.40	1.30
11	K	1129	HEM	FE-ND	4.84	2.09	1.94
5	I	601	FAD	C4X-N5	4.35	1.39	1.30
11	C	1129	HEM	FE-NB	4.12	2.07	1.94
11	K	1129	HEM	FE-NC	3.92	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	1129	HEM	FE-NB	3.72	2.06	1.94
11	C	1129	HEM	FE-NA	3.62	2.07	1.95
11	G	1129	HEM	FE-NA	3.56	2.07	1.95
11	G	1129	HEM	FE-ND	3.47	2.05	1.94
5	E	601	FAD	C10-N1	3.14	1.39	1.33
5	I	601	FAD	C2A-N3A	3.08	1.39	1.33
11	G	1129	HEM	CAC-C3C	2.99	1.55	1.47
11	G	1129	HEM	CAB-C3B	2.95	1.55	1.47
5	A	601	FAD	C2A-N1A	2.90	1.39	1.33
11	K	1129	HEM	CAC-C3C	2.78	1.55	1.47
5	A	601	FAD	C2A-N3A	2.75	1.39	1.33
5	E	601	FAD	C2A-N1A	2.62	1.38	1.33
11	C	1129	HEM	CAB-C3B	2.61	1.54	1.47
11	K	1129	HEM	CAB-C3B	2.58	1.54	1.47
5	E	601	FAD	C2A-N3A	2.56	1.38	1.33
5	I	601	FAD	C10-N1	2.55	1.38	1.33
11	C	1129	HEM	C3B-C2B	-2.50	1.32	1.37
11	C	1129	HEM	CAC-C3C	2.47	1.54	1.47
11	G	1129	HEM	C3B-C2B	-2.46	1.32	1.37
11	K	1129	HEM	C3B-C2B	-2.40	1.32	1.37
6	A	1589	TEO	C2-C1	-2.36	1.49	1.54
5	A	601	FAD	O4B-C4B	-2.33	1.39	1.45
5	I	601	FAD	C2A-N1A	2.29	1.38	1.33
11	G	1129	HEM	C2A-C3A	-2.24	1.32	1.38
11	K	1129	HEM	CMD-C2D	2.24	1.55	1.50
11	G	1129	HEM	CMC-C2C	2.22	1.55	1.50
11	C	1129	HEM	CMA-C3A	2.17	1.55	1.50
11	K	1129	HEM	CMC-C2C	2.15	1.55	1.50
5	I	601	FAD	C8A-N7A	2.12	1.35	1.31
6	E	1589	TEO	O1B-C1	-2.10	1.23	1.30
11	K	1129	HEM	CMA-C3A	2.06	1.55	1.50
5	E	601	FAD	C8A-N7A	2.04	1.35	1.31
11	C	1129	HEM	CMC-C2C	2.03	1.55	1.50
11	G	1129	HEM	CMB-C2B	2.02	1.55	1.50

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	601	FAD	C5A-C4A-N3A	-6.72	117.98	126.75
5	E	601	FAD	C4'-C3'-C2'	-5.37	102.19	113.36
5	E	601	FAD	N3A-C2A-N1A	-5.30	120.31	128.60
11	K	1129	HEM	C4D-ND-C1D	5.28	110.52	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	1129	HEM	C4D-ND-C1D	5.27	110.52	105.07
5	I	601	FAD	N3A-C4A-N9A	4.90	135.15	127.08
5	A	601	FAD	N3A-C2A-N1A	-4.85	121.01	128.60
5	I	601	FAD	N3A-C2A-N1A	-4.84	121.03	128.60
5	A	601	FAD	C4-C4X-N5	4.63	124.82	118.23
5	I	601	FAD	N9A-C8A-N7A	-4.56	107.68	113.91
5	A	601	FAD	N9A-C8A-N7A	-4.39	107.90	113.91
5	I	601	FAD	C5A-N7A-C8A	4.37	109.72	103.51
11	C	1129	HEM	C4D-ND-C1D	4.35	109.56	105.07
5	A	601	FAD	C5A-C4A-N3A	-4.34	121.09	126.75
5	E	601	FAD	C5A-C4A-N3A	-4.33	121.11	126.75
5	E	601	FAD	N9A-C8A-N7A	-4.32	108.00	113.91
5	I	601	FAD	C2A-N3A-C4A	4.21	121.71	111.75
5	A	601	FAD	C4X-C10-N10	4.05	122.41	116.48
5	E	601	FAD	C4-C4X-N5	4.04	123.98	118.23
11	G	1129	HEM	CAD-CBD-CGD	-3.93	105.14	113.60
11	K	1129	HEM	CAD-CBD-CGD	-3.63	105.78	113.60
5	E	601	FAD	C4-N3-C2	-3.51	119.15	125.64
5	E	601	FAD	C4X-C4-N3	3.37	121.74	113.19
5	E	601	FAD	C5A-N7A-C8A	3.35	108.28	103.51
5	A	601	FAD	C4'-C3'-C2'	-3.35	106.39	113.36
5	A	601	FAD	N3A-C4A-N9A	3.35	132.60	127.08
5	E	601	FAD	N3A-C4A-N9A	3.34	132.58	127.08
5	E	601	FAD	C10-C4X-N5	-3.33	117.79	124.86
5	E	601	FAD	C2A-N3A-C4A	3.32	119.60	111.75
5	A	601	FAD	C4-N3-C2	-3.28	119.59	125.64
5	A	601	FAD	C10-C4X-N5	-3.27	117.92	124.86
5	A	601	FAD	C5A-N7A-C8A	3.22	108.08	103.51
5	I	601	FAD	C4'-C3'-C2'	-3.21	106.68	113.36
5	A	601	FAD	C5A-C6A-N6A	-3.16	116.56	123.43
5	A	601	FAD	C2A-N3A-C4A	3.10	119.08	111.75
5	A	601	FAD	C4A-N9A-C8A	3.08	109.07	105.73
11	G	1129	HEM	C3B-C2B-C1B	3.07	108.77	106.49
5	I	601	FAD	C4-N3-C2	-3.07	119.98	125.64
5	A	601	FAD	C4X-C4-N3	3.06	120.97	113.19
6	A	1589	TEO	O1A-C1-C2	-3.05	115.06	122.42
5	E	601	FAD	C4A-N9A-C8A	3.05	109.03	105.73
5	E	601	FAD	C5A-C6A-N6A	-2.97	116.97	123.43
5	I	601	FAD	C4X-C4-N3	2.95	120.69	113.19
5	A	601	FAD	O3B-C3B-C4B	-2.88	102.71	111.05
11	C	1129	HEM	CMB-C2B-C1B	2.87	129.41	125.04
5	E	601	FAD	P-O3P-PA	-2.85	123.06	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	1129	HEM	C3B-C2B-C1B	2.77	108.54	106.49
11	K	1129	HEM	CAD-C3D-C4D	2.75	129.46	124.66
5	E	601	FAD	C9A-C5X-N5	-2.75	119.45	122.43
5	I	601	FAD	C9A-C5X-N5	-2.67	119.53	122.43
5	A	601	FAD	O4-C4-N3	-2.66	115.02	120.12
11	C	1129	HEM	CAD-CBD-CGD	-2.63	107.94	113.60
5	I	601	FAD	C5A-C6A-N6A	-2.54	117.91	123.43
5	A	601	FAD	O2'-C2'-C3'	-2.52	102.97	109.10
5	I	601	FAD	C10-C4X-N5	-2.51	119.53	124.86
5	I	601	FAD	C4A-C5A-N7A	-2.50	107.58	110.62
5	I	601	FAD	C4-C4X-N5	2.47	121.75	118.23
5	E	601	FAD	O3B-C3B-C4B	-2.45	103.96	111.05
5	E	601	FAD	O4-C4-N3	-2.45	115.43	120.12
5	A	601	FAD	P-O3P-PA	-2.43	124.48	132.83
5	E	601	FAD	C6-C5X-N5	2.43	122.75	118.51
5	A	601	FAD	C2B-C3B-C4B	2.43	107.36	102.64
11	G	1129	HEM	CAD-C3D-C4D	2.41	128.87	124.66
5	I	601	FAD	C4X-C10-N10	2.41	120.00	116.48
6	I	1589	TEO	O1A-C1-C2	-2.41	116.62	122.42
5	E	601	FAD	C9-C9A-N10	-2.37	118.63	121.84
11	K	1129	HEM	C1B-NB-C4B	2.37	107.52	105.07
5	E	601	FAD	C4X-C10-N1	-2.33	119.32	124.73
5	I	601	FAD	C6A-C5A-C4A	2.33	120.32	117.18
5	E	601	FAD	C4X-C10-N10	2.31	119.85	116.48
5	E	601	FAD	C1'-N10-C9A	-2.29	116.70	120.51
5	E	601	FAD	C5X-N5-C4X	2.28	121.86	118.07
11	K	1129	HEM	O1A-CGA-CBA	-2.27	115.79	123.08
11	K	1129	HEM	CBA-CAA-C2A	-2.25	106.37	112.63
5	I	601	FAD	C4A-N9A-C8A	2.22	108.14	105.73
5	A	601	FAD	C6A-C5A-C4A	2.18	120.11	117.18
11	G	1129	HEM	O2A-CGA-CBA	2.13	120.86	114.03
5	I	601	FAD	O4-C4-C4X	-2.12	120.99	126.60
11	C	1129	HEM	C4C-C3C-C2C	2.11	108.48	106.75
11	C	1129	HEM	CMB-C2B-C3B	-2.09	123.18	128.30
5	E	601	FAD	C10-N1-C2	2.08	121.06	116.90
5	I	601	FAD	O3'-C3'-C4'	2.07	113.81	108.81
11	G	1129	HEM	CMD-C2D-C1D	2.06	128.18	125.04
11	C	1129	HEM	C4D-C3D-C2D	-2.05	103.90	106.90
11	G	1129	HEM	O1A-CGA-CBA	-2.04	116.53	123.08
11	G	1129	HEM	CAA-CBA-CGA	-2.00	109.29	113.60

There are no chirality outliers.

All (46) 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	O3'-C3'-C4'-C5'
5	A	601	FAD	O4'-C4'-C5'-O5'
5	E	601	FAD	N10-C1'-C2'-O2'
5	E	601	FAD	N10-C1'-C2'-C3'
5	E	601	FAD	O4'-C4'-C5'-O5'
5	I	601	FAD	N10-C1'-C2'-O2'
6	A	1589	TEO	C1-C2-C3-C4
6	E	1589	TEO	C1-C2-C3-C4
6	I	1589	TEO	O2-C2-C3-C4
11	K	1129	HEM	C1A-C2A-CAA-CBA
5	A	601	FAD	O3'-C3'-C4'-O4'
11	K	1129	HEM	C3A-C2A-CAA-CBA
5	A	601	FAD	C2'-C3'-C4'-C5'
5	A	601	FAD	C2'-C3'-C4'-O4'
6	A	1589	TEO	O1A-C1-C2-O2
6	A	1589	TEO	O1B-C1-C2-O2
11	C	1129	HEM	C4C-C3C-CAC-CBC
11	G	1129	HEM	C4C-C3C-CAC-CBC
11	C	1129	HEM	C1A-C2A-CAA-CBA
5	A	601	FAD	O4B-C4B-C5B-O5B
5	E	601	FAD	P-O3P-PA-O2A
6	E	1589	TEO	O1A-C1-C2-O2
11	C	1129	HEM	C3D-CAD-CBD-CGD
11	G	1129	HEM	CAA-CBA-CGA-O1A
6	A	1589	TEO	O2-C2-C3-C4
6	E	1589	TEO	O2-C2-C3-C4
11	G	1129	HEM	CAA-CBA-CGA-O2A
11	K	1129	HEM	CAD-CBD-CGD-O2D
5	E	601	FAD	P-O3P-PA-O1A
11	G	1129	HEM	C1A-C2A-CAA-CBA
11	K	1129	HEM	CAD-CBD-CGD-O1D
6	E	1589	TEO	O1B-C1-C2-O2
5	A	601	FAD	C3B-C4B-C5B-O5B
11	C	1129	HEM	CAA-CBA-CGA-O1A
11	C	1129	HEM	CAA-CBA-CGA-O2A
5	E	601	FAD	O4B-C4B-C5B-O5B
5	A	601	FAD	C3'-C4'-C5'-O5'
5	E	601	FAD	C5B-O5B-PA-O1A
5	I	601	FAD	O4B-C4B-C5B-O5B
11	C	1129	HEM	CAD-CBD-CGD-O2D

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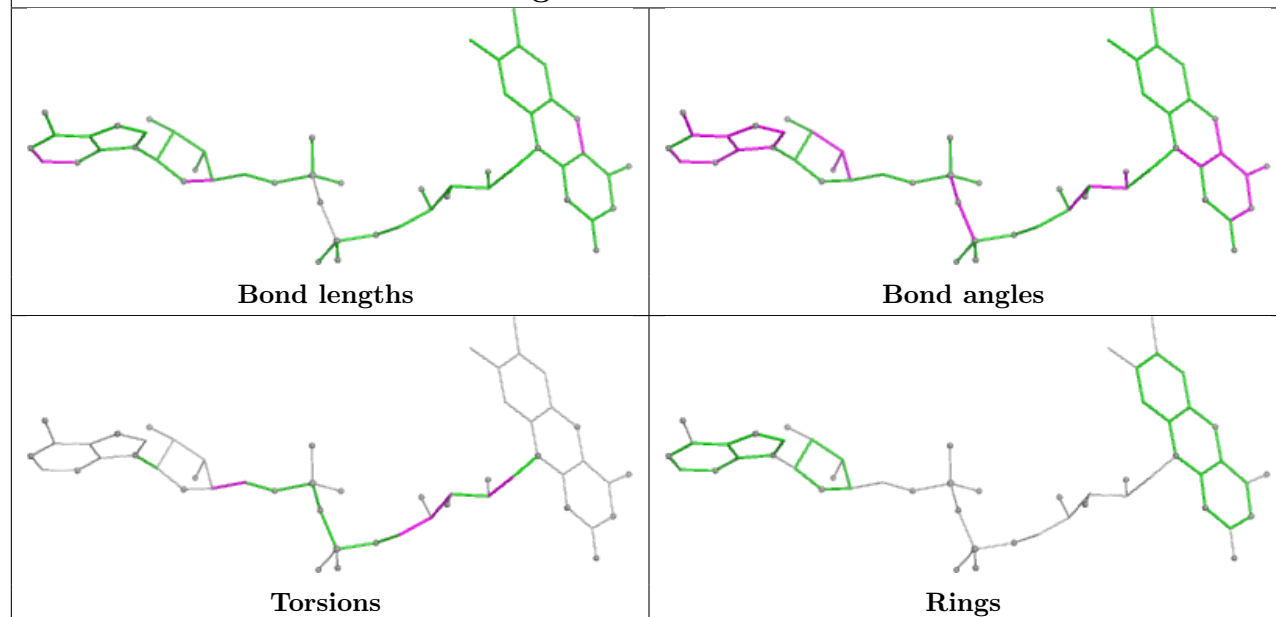
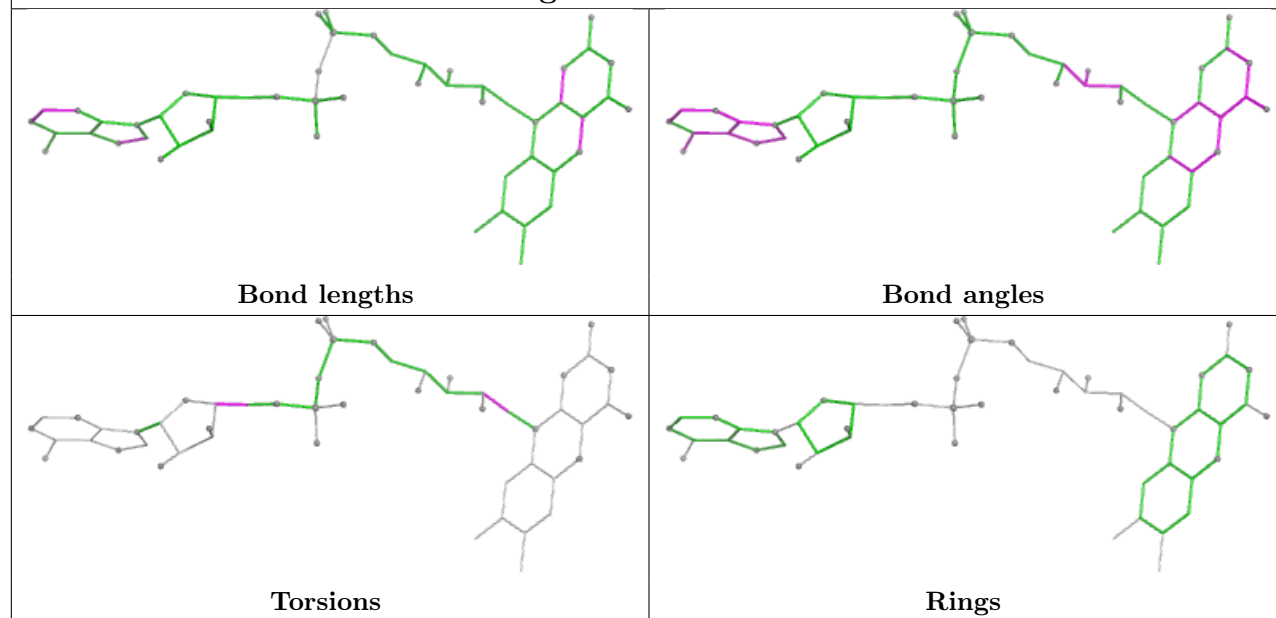
Mol	Chain	Res	Type	Atoms
6	E	1589	TEO	O1B-C1-C2-C3
5	I	601	FAD	N10-C1'-C2'-C3'
11	C	1129	HEM	C3A-C2A-CAA-CBA
11	G	1129	HEM	C3A-C2A-CAA-CBA

There are no ring outliers.

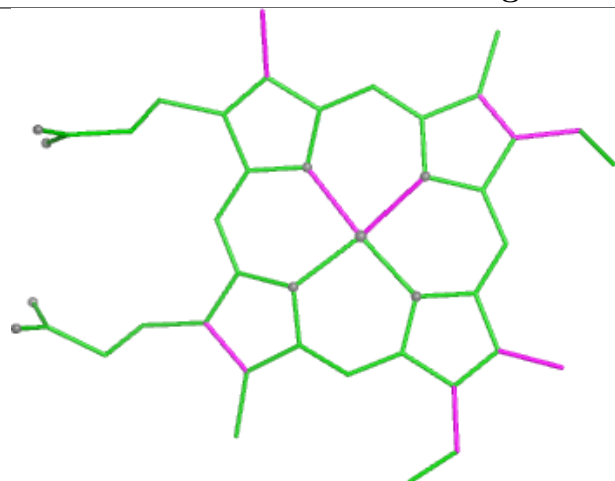
14 monomers are involved in 52 short contacts:

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

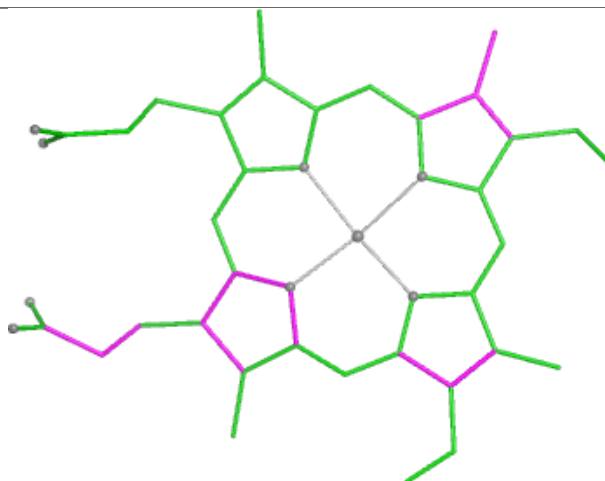
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A 601**Ligand FAD I 601**

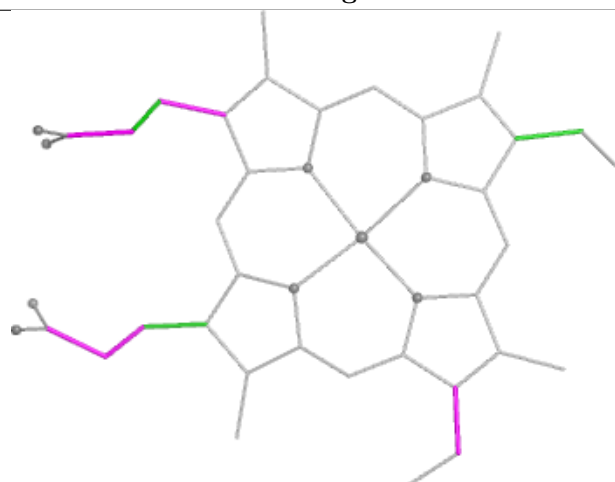
Ligand HEM C 1129



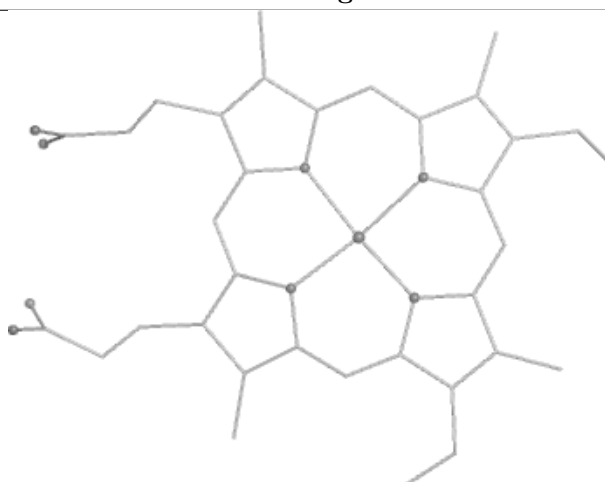
Bond lengths



Bond angles

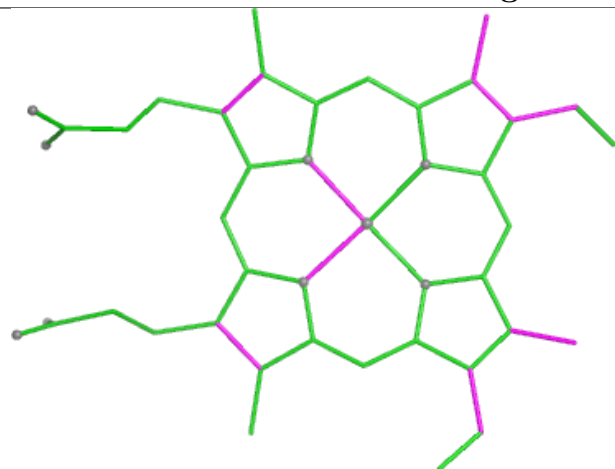


Torsions

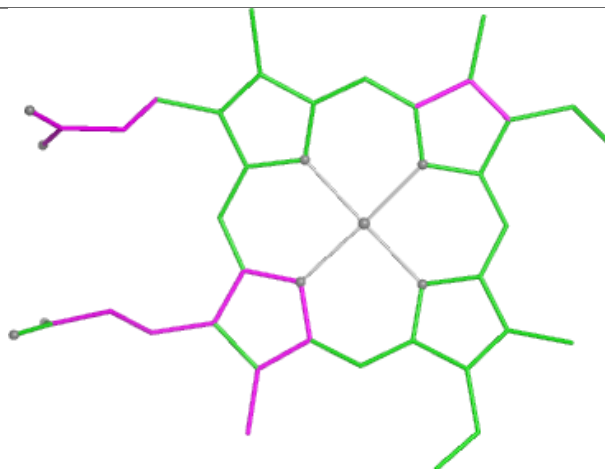


Rings

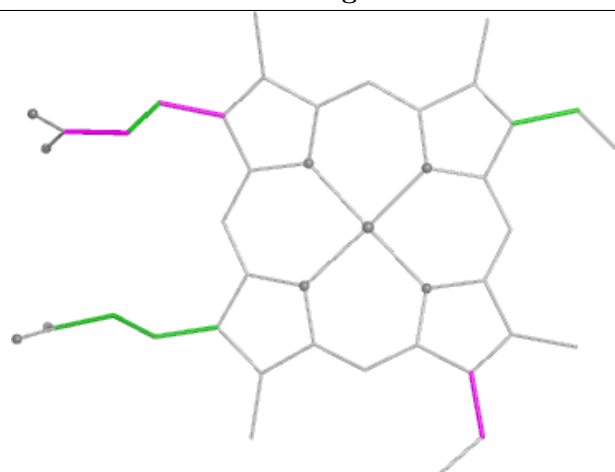
Ligand HEM G 1129



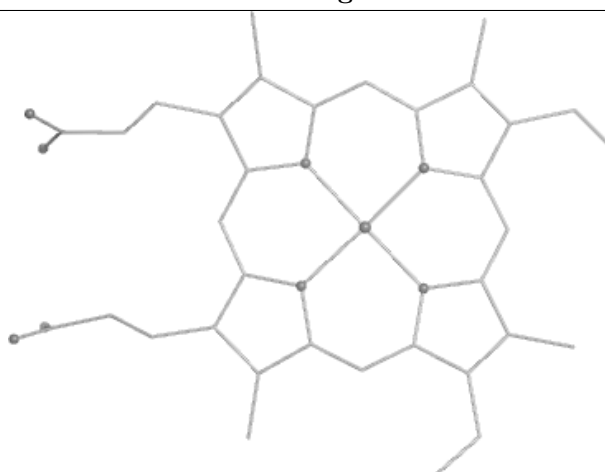
Bond lengths



Bond angles

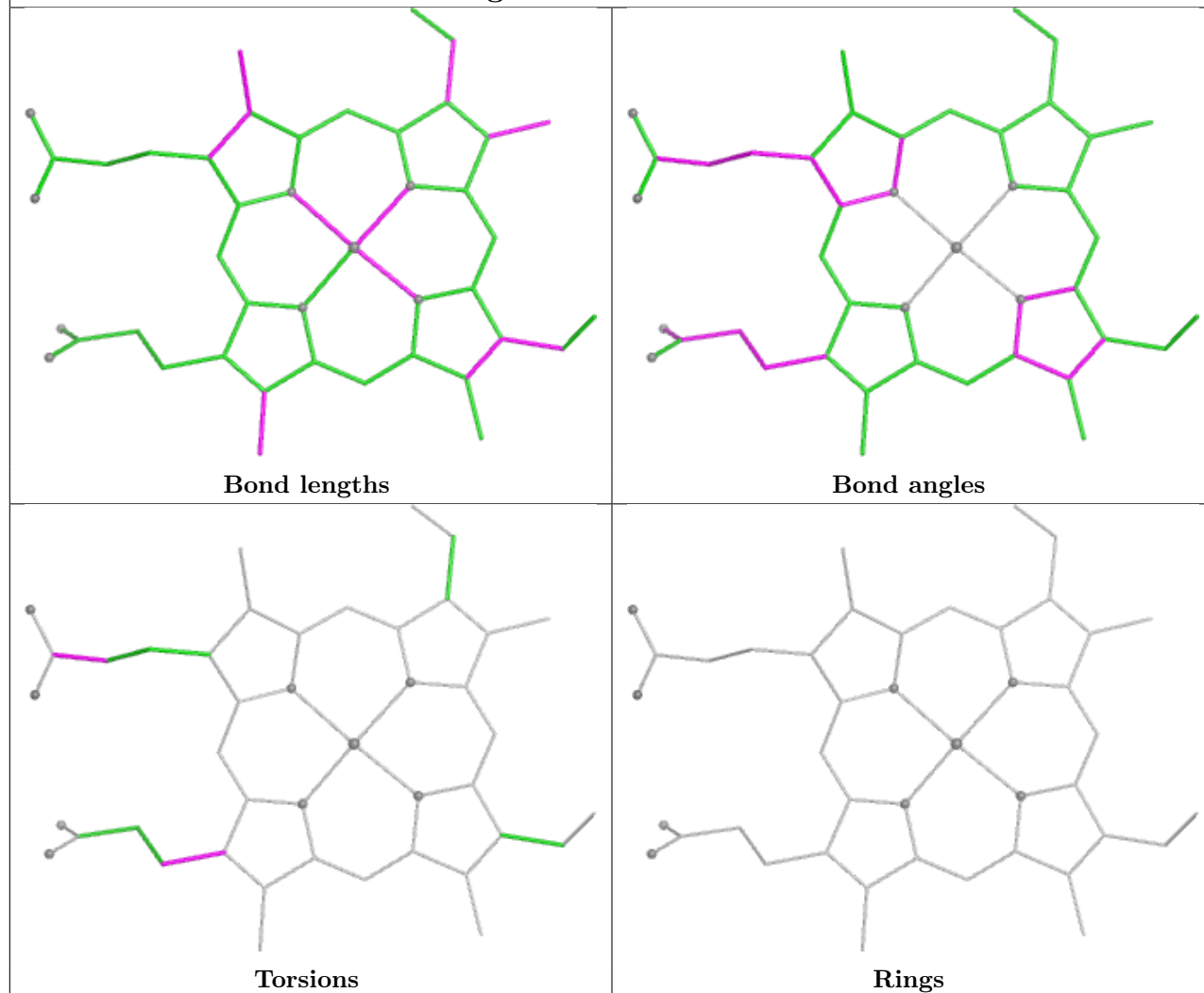


Torsions

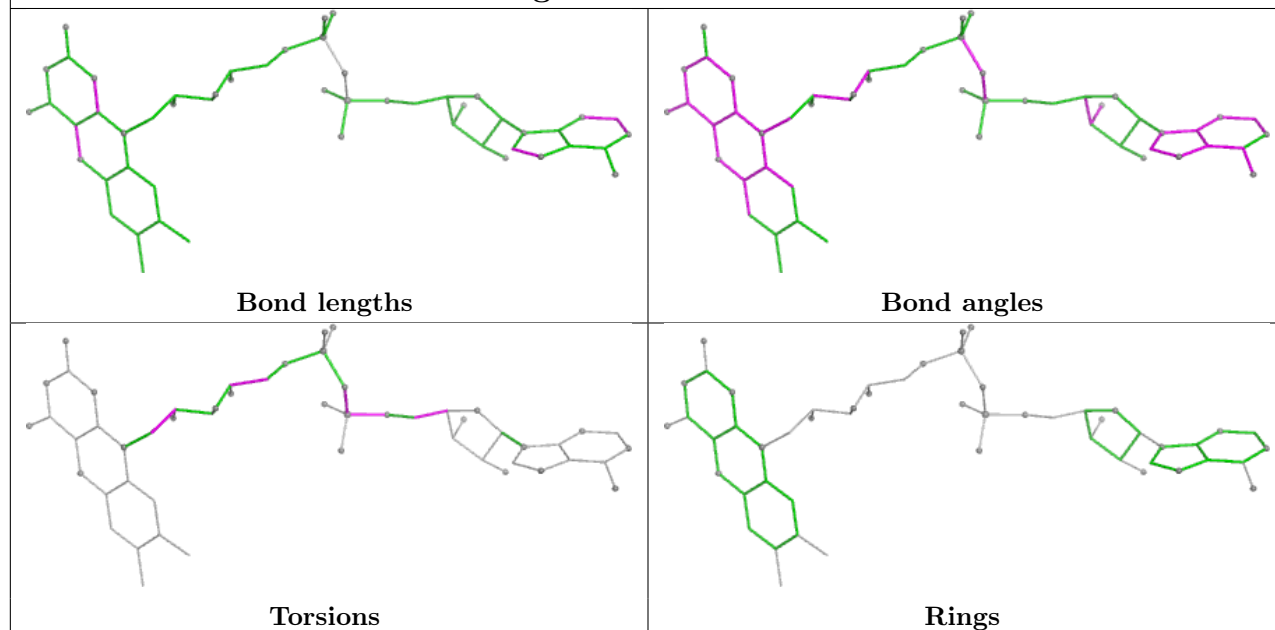


Rings

Ligand HEM K 1129



Ligand FAD E 601



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.03	5 (0%) 81 64	54, 55, 56, 58	0
1	E	588/588 (100%)	0.28	2 (0%) 90 81	54, 55, 56, 58	0
1	I	588/588 (100%)	1.27	106 (18%) 3 3	54, 55, 56, 58	0
2	B	238/238 (100%)	0.21	4 (1%) 69 49	53, 55, 56, 57	0
2	F	238/238 (100%)	0.37	1 (0%) 88 79	54, 55, 56, 57	0
2	J	238/238 (100%)	1.18	41 (17%) 4 3	54, 55, 56, 57	0
3	C	121/129 (93%)	0.82	14 (11%) 9 7	54, 55, 56, 56	0
3	G	121/129 (93%)	0.64	4 (3%) 49 30	54, 55, 56, 56	0
3	K	121/129 (93%)	0.78	7 (5%) 29 18	54, 55, 56, 56	0
4	D	105/115 (91%)	0.52	3 (2%) 53 35	54, 55, 56, 57	0
4	H	105/115 (91%)	0.79	6 (5%) 29 19	54, 55, 56, 57	0
4	L	105/115 (91%)	0.46	4 (3%) 44 27	54, 55, 56, 57	0
All	All	3156/3210 (98%)	0.56	197 (6%) 26 17	53, 55, 56, 58	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	MET	6.9
1	I	334	SER	5.1
1	I	246	ILE	4.7
3	G	68	PHE	4.7
3	C	10	PRO	4.6
1	I	338	ALA	4.4
2	J	134	LEU	4.3
1	I	245	GLY	3.9
1	I	337	PHE	3.9
1	I	585	ILE	3.9
1	I	208	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	588	TYR	3.6
1	I	511	VAL	3.6
3	C	66	GLY	3.6
1	I	209	TYR	3.6
1	I	460	ARG	3.6
1	I	470	ASN	3.5
1	I	448	ASN	3.5
1	I	403	ASN	3.5
4	H	11	ASN	3.5
1	I	347	ILE	3.5
1	I	176	ALA	3.4
2	J	69	GLY	3.4
1	I	583	PRO	3.4
1	I	353	CYS	3.3
1	I	284	ALA	3.3
2	B	238	ALA	3.3
1	I	456	PRO	3.2
2	J	154	CYS	3.2
4	L	38	ALA	3.2
1	I	565	SER	3.2
1	I	478	ASP	3.1
1	I	513	CYS	3.1
3	C	52	LEU	3.1
4	H	42	GLU	3.1
1	I	336	THR	3.0
1	I	395	HIS	3.0
1	I	502	THR	3.0
1	I	322	VAL	3.0
3	C	8	GLN	3.0
1	I	462	ALA	2.9
1	I	56	ALA	2.9
1	A	300	GLY	2.9
3	C	16	GLN	2.9
2	J	130	ALA	2.9
1	I	288	VAL	2.9
1	I	24	LEU	2.9
3	G	53	SER	2.8
1	I	463	LEU	2.8
2	J	25	LEU	2.8
4	D	42	GLU	2.8
2	J	212	CYS	2.8
1	I	400	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	223	THR	2.8
2	J	211	ASN	2.7
1	E	466	CYS	2.7
3	K	22	ILE	2.7
1	I	587	THR	2.7
1	I	527	ALA	2.7
1	I	444	LEU	2.7
1	I	464	GLN	2.7
1	I	251	VAL	2.7
1	I	496	ASN	2.7
1	I	471	PHE	2.7
1	I	109	LEU	2.7
2	J	184	ASP	2.7
3	C	68	PHE	2.6
1	I	62	GLU	2.6
1	I	481	ALA	2.6
1	I	477	GLY	2.6
1	A	62	GLU	2.6
2	J	85	PRO	2.6
1	A	332	GLU	2.6
1	I	497	ALA	2.6
1	I	355	TYR	2.6
2	J	86	GLY	2.6
4	L	115	VAL	2.6
3	C	55	PRO	2.6
1	I	501	ASP	2.6
3	C	11	VAL	2.6
1	I	350	ILE	2.5
1	I	529	SER	2.5
4	L	43	LEU	2.5
2	J	238	ALA	2.5
1	I	57	LEU	2.5
1	I	242	HIS	2.5
1	E	345	GLU	2.5
4	L	46	GLU	2.5
1	I	118	PRO	2.5
2	J	45	LYS	2.5
3	K	98	TYR	2.5
2	F	238	ALA	2.5
1	I	522	THR	2.5
4	H	73	TRP	2.5
1	I	354	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	125	GLY	2.5
1	I	201	ALA	2.4
1	I	325	SER	2.4
1	A	345	GLU	2.4
1	I	417	LEU	2.4
3	K	65	MET	2.4
2	J	122	LEU	2.4
1	I	130	GLN	2.4
2	B	29	GLU	2.4
1	I	339	HIS	2.4
2	J	88	LYS	2.4
2	J	235	GLN	2.4
1	I	265	LEU	2.4
1	I	333	LEU	2.4
2	J	65	LEU	2.4
1	I	67	TRP	2.4
1	I	247	ALA	2.4
3	K	112	ILE	2.4
2	J	180	ARG	2.4
1	I	351	PRO	2.4
2	J	197	LEU	2.3
2	J	209	ILE	2.3
1	I	577	LEU	2.3
2	J	220	LEU	2.3
1	I	528	VAL	2.3
1	I	112	GLY	2.3
2	J	47	PRO	2.3
1	I	467	MET	2.3
3	C	13	LEU	2.3
1	I	2	LYS	2.3
3	C	59	GLU	2.3
1	I	541	SER	2.3
1	I	394	VAL	2.3
2	J	44	GLU	2.2
1	I	88	MET	2.2
1	I	452	ASN	2.2
2	J	61	GLY	2.2
3	K	10	PRO	2.2
1	I	283	LEU	2.2
2	J	121	LEU	2.2
3	C	15	LEU	2.2
2	J	131	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	208	SER	2.2
1	I	293	ILE	2.2
1	I	154	LEU	2.2
2	B	86	GLY	2.2
4	H	87	LEU	2.2
1	I	239	TRP	2.2
1	I	313	LEU	2.2
1	I	205	ALA	2.2
1	I	428	ALA	2.2
2	B	30	GLY	2.2
1	I	136	ALA	2.2
2	J	183	ILE	2.1
1	I	102	MET	2.1
1	I	382	GLY	2.1
2	J	237	ASN	2.1
3	K	70	VAL	2.1
1	I	114	ILE	2.1
1	I	297	ILE	2.1
2	J	142	LYS	2.1
2	J	136	MET	2.1
1	I	433	SER	2.1
2	J	72	GLY	2.1
4	H	40	SER	2.1
1	I	241	PHE	2.1
4	H	84	VAL	2.1
1	A	502	THR	2.1
1	I	96	ILE	2.1
1	I	558	LEU	2.1
2	J	89	ILE	2.1
1	I	566	MET	2.1
1	I	121	GLY	2.1
3	C	49	GLY	2.1
4	D	37	PHE	2.1
1	I	63	ASP	2.1
1	I	331	LEU	2.1
1	I	544	ASP	2.1
3	K	99	LEU	2.1
2	J	153	ALA	2.1
1	I	562	GLU	2.1
1	I	579	PRO	2.1
1	I	582	PRO	2.1
2	J	93	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	231	VAL	2.1
1	I	487	LEU	2.1
4	D	87	LEU	2.1
1	I	60	THR	2.1
3	G	98	TYR	2.1
1	I	379	VAL	2.0
1	I	586	ARG	2.0
1	I	14	GLY	2.0
1	I	152	GLN	2.0
2	J	203	VAL	2.0
2	J	39	LEU	2.0
2	J	221	ASN	2.0
3	C	65	MET	2.0
2	J	60	CYS	2.0
1	I	73	VAL	2.0
3	G	56	GLU	2.0
2	J	193	ARG	2.0
3	C	9	ARG	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 [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($\text{\AA}^2$)	Q<0.9
6	TEO	I	1589	9/9	0.76	0.12	122,123,124,124	0
5	FAD	I	601	53/53	0.82	0.16	70,80,90,93	0
6	TEO	E	1589	9/9	0.88	0.26	43,45,47,48	0
6	TEO	A	1589	9/9	0.92	0.18	33,35,35,38	0
5	FAD	E	601	53/53	0.94	0.13	26,40,50,53	0

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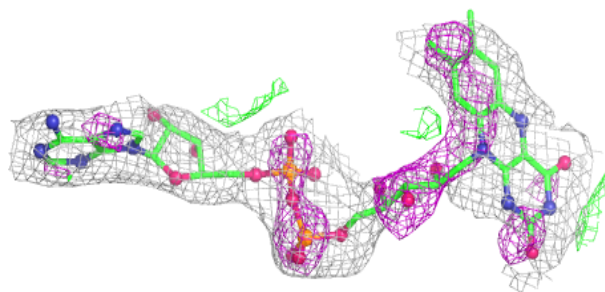
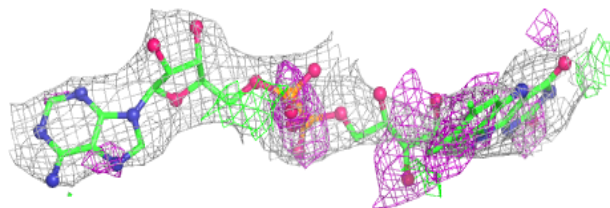
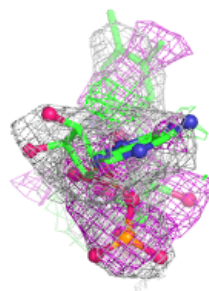
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NA	I	1590	1/1	0.94	0.13	41,41,41,41	0
11	HEM	G	1129	43/43	0.94	0.13	55,59,63,65	0
11	HEM	K	1129	43/43	0.94	0.13	54,55,65,65	0
8	FES	J	302	4/4	0.95	0.14	70,71,72,73	0
5	FAD	A	601	53/53	0.96	0.10	17,21,30,40	0
11	HEM	C	1129	43/43	0.96	0.12	43,46,55,58	0
10	F3S	J	304	7/7	0.97	0.11	61,64,66,69	0
9	SF4	J	303	8/8	0.98	0.10	60,61,64,64	0
10	F3S	F	304	7/7	0.98	0.09	47,48,50,53	0
10	F3S	B	304	7/7	0.99	0.08	43,45,49,49	0
8	FES	F	302	4/4	0.99	0.08	32,33,40,41	0
7	NA	E	1590	1/1	0.99	0.21	9,9,9,9	0
9	SF4	B	303	8/8	0.99	0.04	28,28,30,33	0
9	SF4	F	303	8/8	0.99	0.06	37,38,41,42	0
8	FES	B	302	4/4	0.99	0.06	30,31,34,35	0
7	NA	A	1590	1/1	1.00	0.20	2,2,2,2	0

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

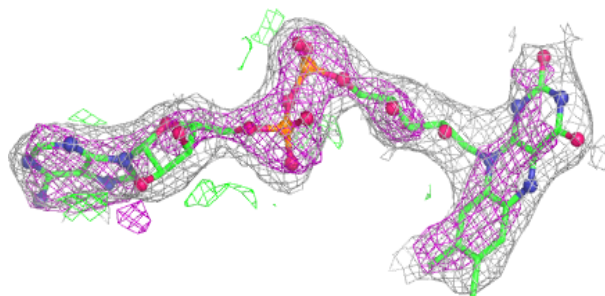
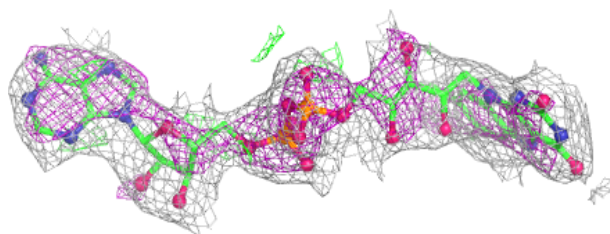
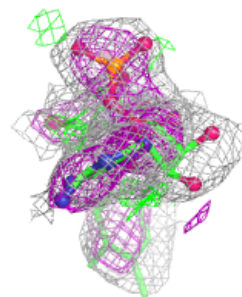
Electron density around FAD I 601:

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

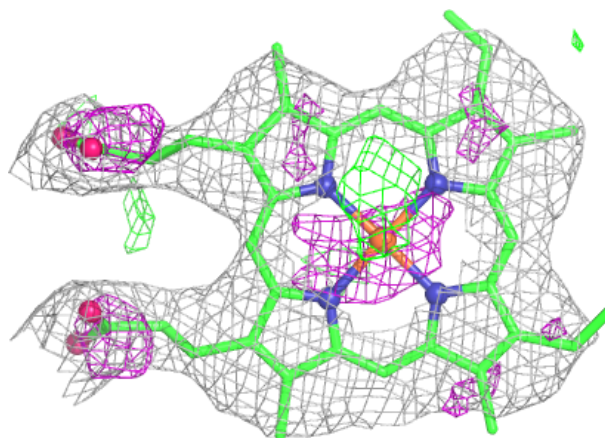
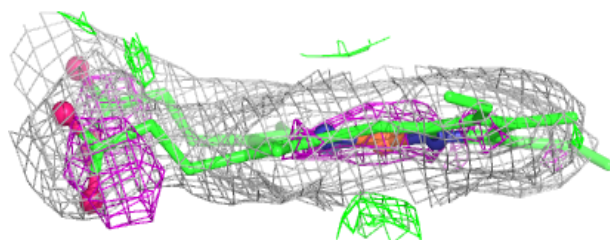


Electron density around FAD E 601:

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

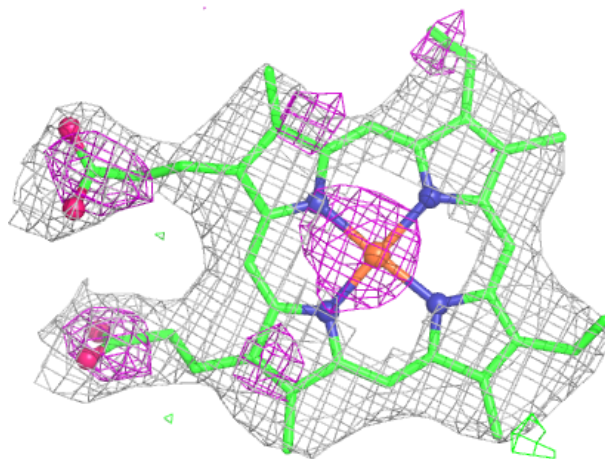
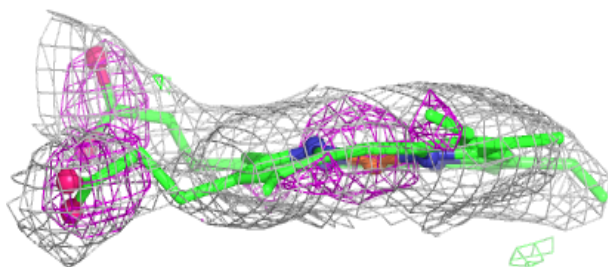
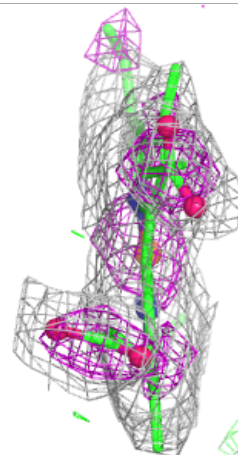
**Electron density around HEM G 1129:**

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



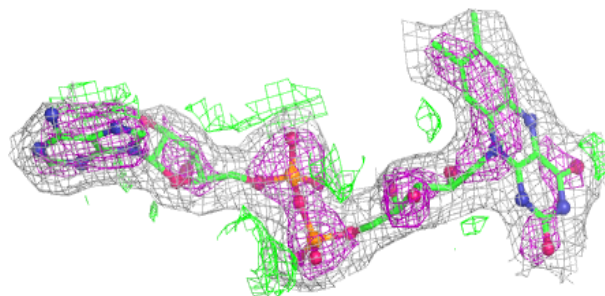
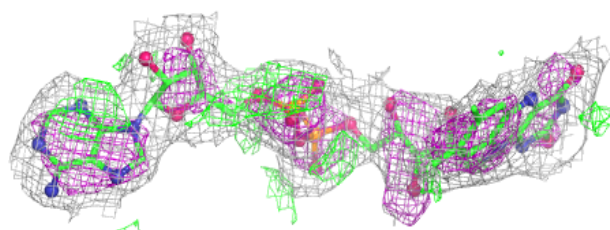
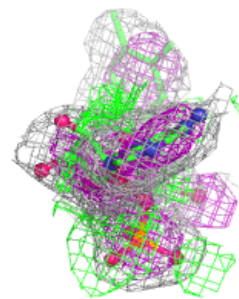
Electron density around HEM K 1129:

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



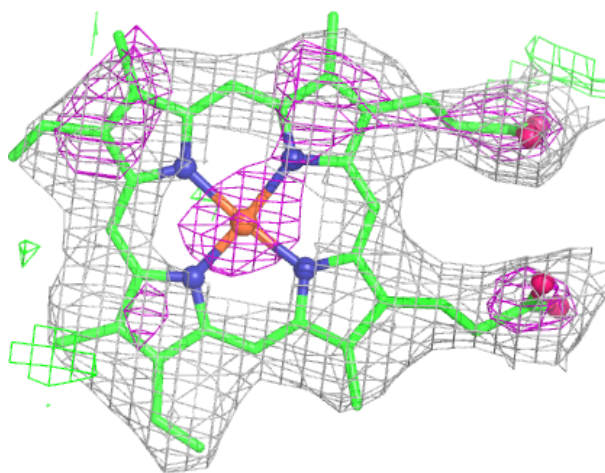
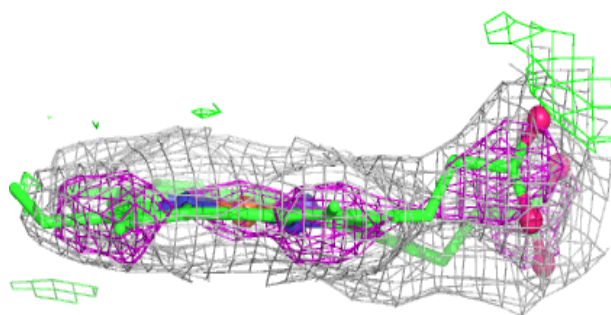
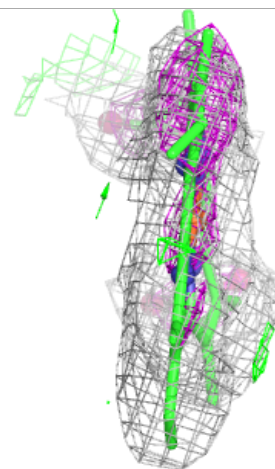
Electron density around FAD A 601:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.