Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 08:41 am BST

PDB ID	:	2WDR
Title	:	E. coli succinate:quinone oxidoreductase (SQR) with pentachlorophenol bound
Authors	:	Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on	:	2009-03-25
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 (i) symbol.

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

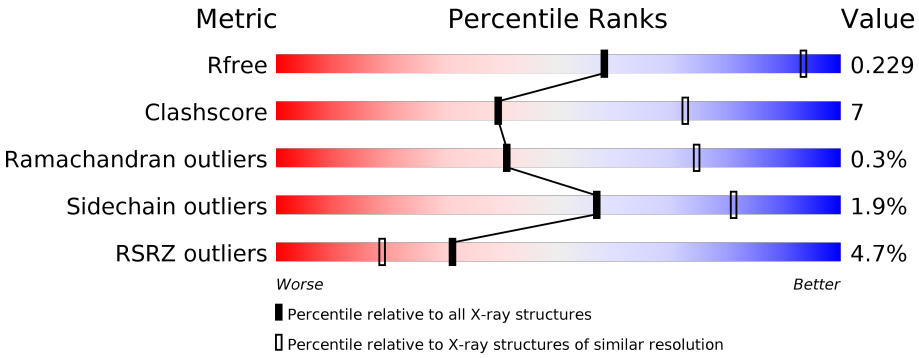
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	588	82% 18%
1	E	588	3% 80% 20%
1	I	588	10% 82% 18%
2	B	238	4% 82% 17%
2	F	238	3% 81% 18%
2	J	238	8% 85% 14%

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Mol	Chain	Length	Quality of chain
3	C	129	3% 79% 16% 5%
3	G	129	10% 76% 19% 5%
3	K	129	5% 78% 16% 5%
4	D	115	3% 71% 19% 9%
4	H	115	7% 67% 23% 9%
4	L	115	4% 72% 18% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	F3S	J	304	-	-	X	-
12	PCI	G	1131	-	X	-	-
6	TEO	A	1589	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 24936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 SUBUNIT.

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			

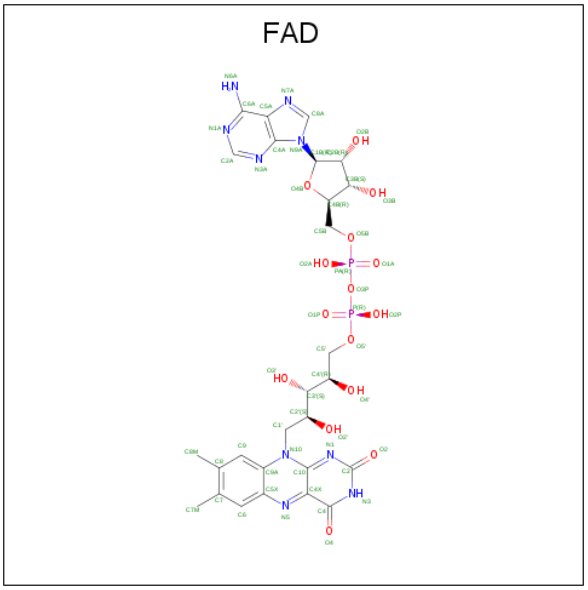
- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	122	Total	C	N	O	S	0	0	0
			948	630	153	160	5			
3	G	122	Total	C	N	O	S	0	0	0
			948	630	153	160	5			
3	K	122	Total	C	N	O	S	0	0	0
			948	630	153	160	5			

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

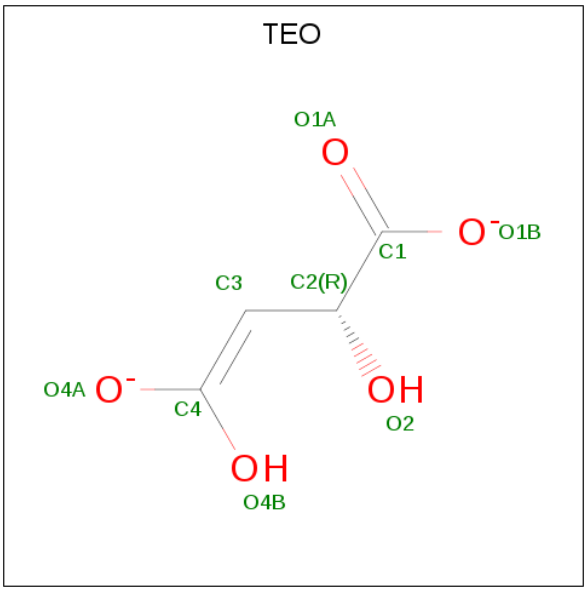
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total	C	N	O	S	0	0	0
			836	577	123	133	3			
4	H	105	Total	C	N	O	S	0	0	0
			836	577	123	133	3			
4	L	105	Total	C	N	O	S	0	0	0
			836	577	123	133	3			

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



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

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

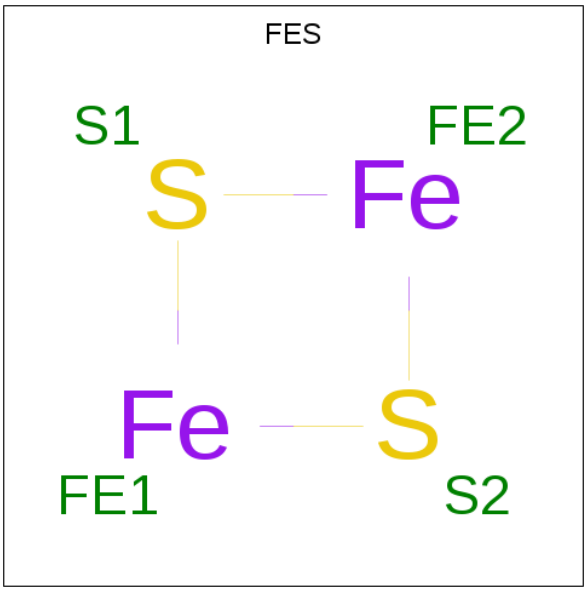


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 4 5	0	0
6	E	1	Total C O 9 4 5	0	0
6	I	1	Total C O 9 4 5	0	0

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

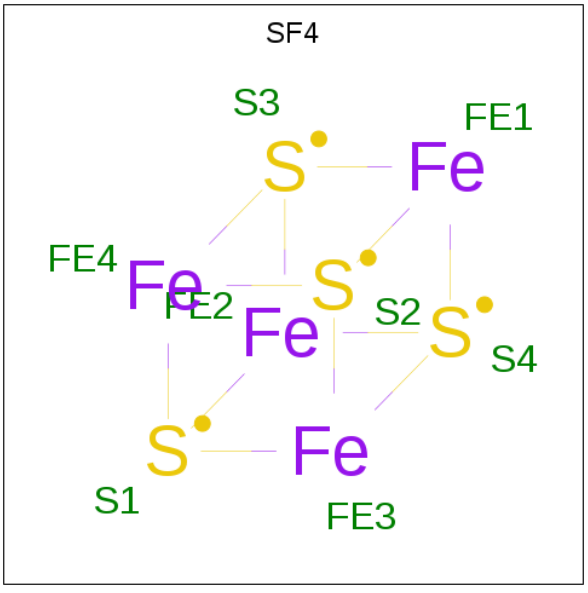
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total Na 1 1	0	0
7	A	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0

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



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

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



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

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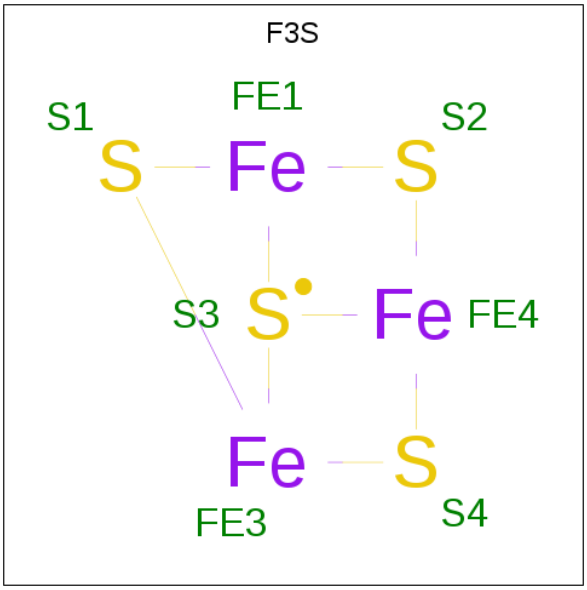
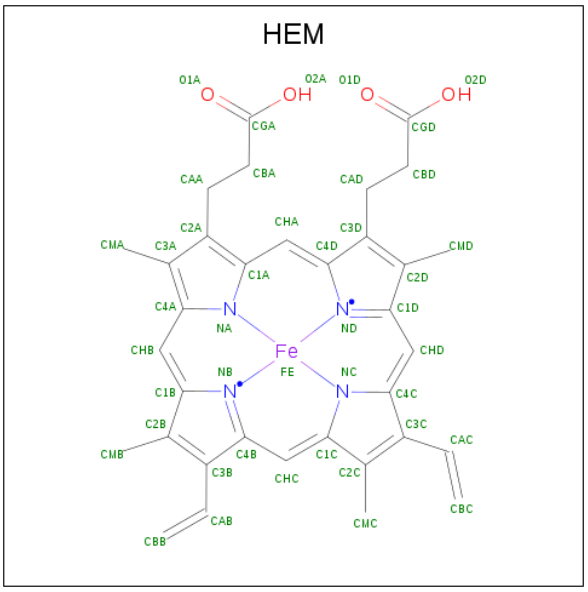
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Fe S 8 4 4	0	0
9	J	1	Total Fe S 8 4 4	0	0

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



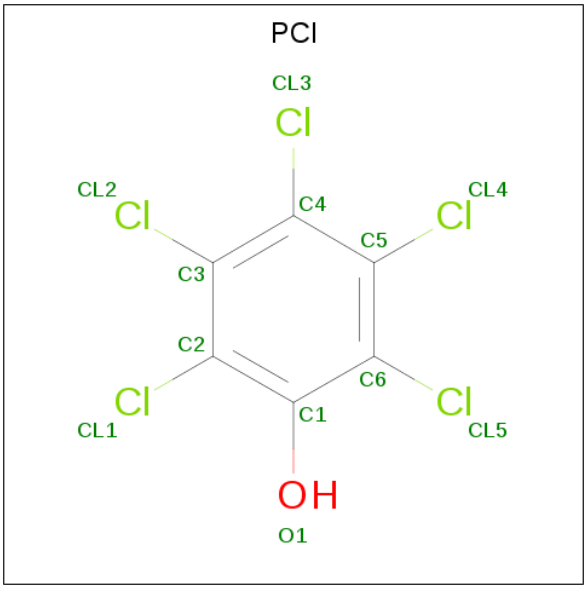
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe S 7 3 4	0	0
10	F	1	Total Fe S 7 3 4	0	0
10	J	1	Total Fe S 7 3 4	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 12 is PENTACHLOROPHENOL (three-letter code: PCI) (formula: C_6HCl_5O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Cl	O	0	0
			12	6	5	1		

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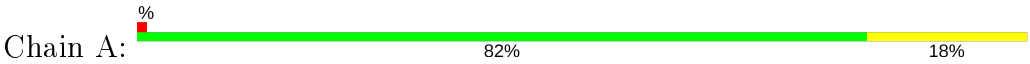
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	Cl	O	0	0
			12	6	5	1		
12	K	1	Total	C	Cl	O	0	0
			12	6	5	1		

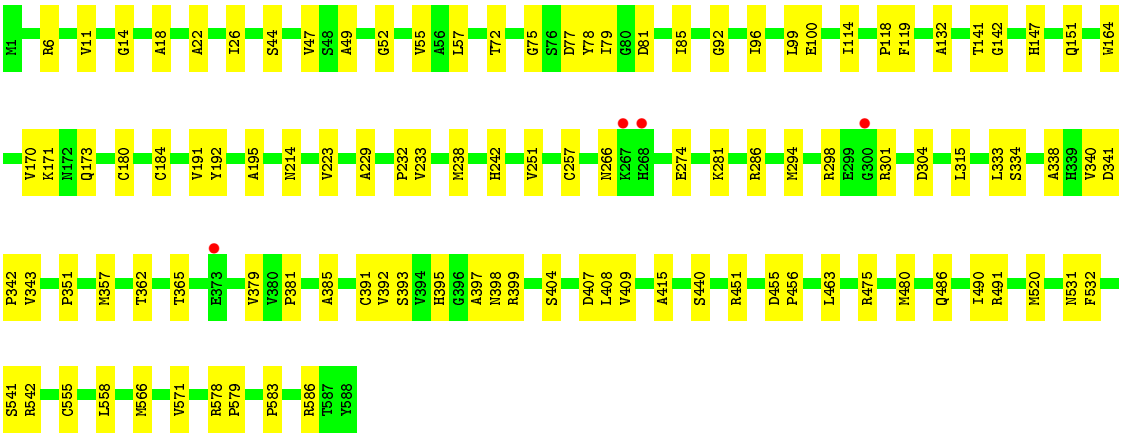
3 Residue-property plots (i)

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

• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

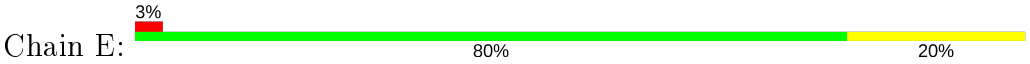
Chain A:

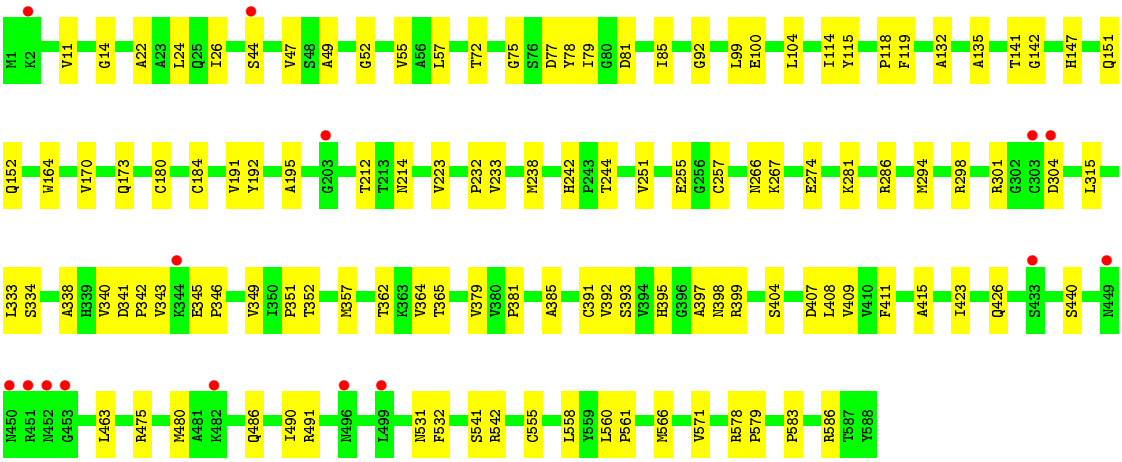




• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

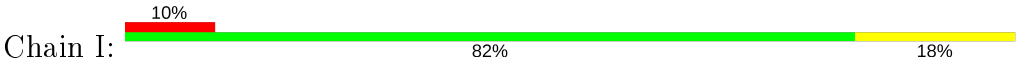
Chain E:

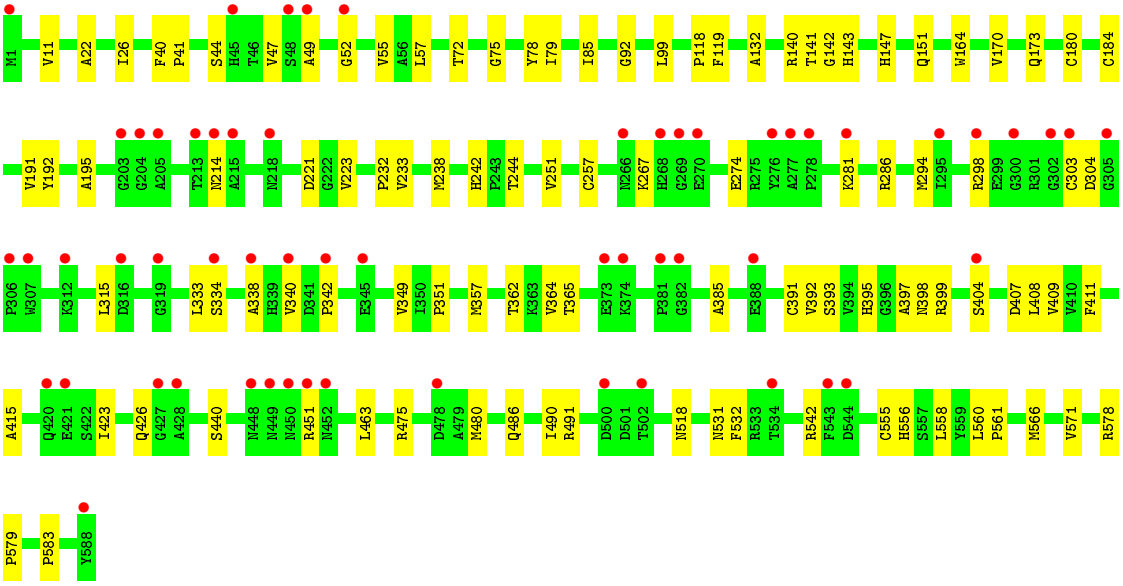




• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

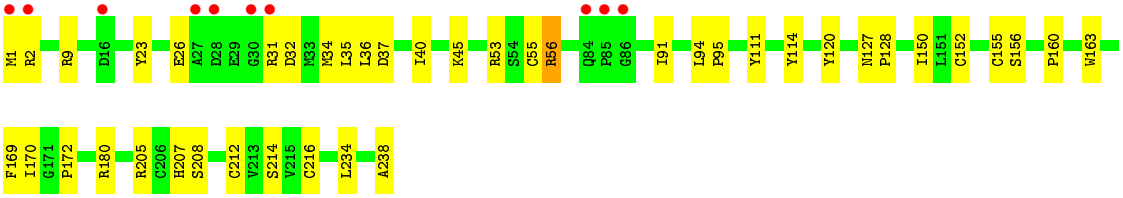
Chain I:





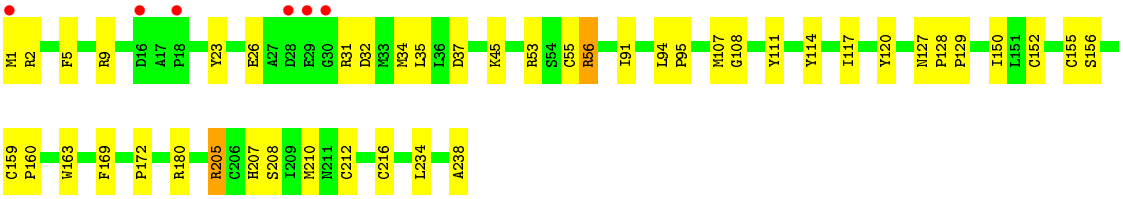
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain B:



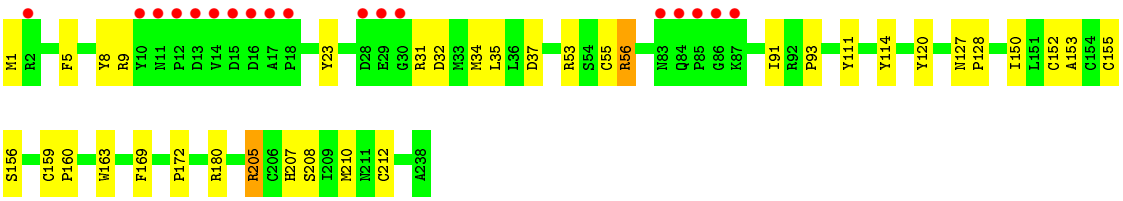
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain F:



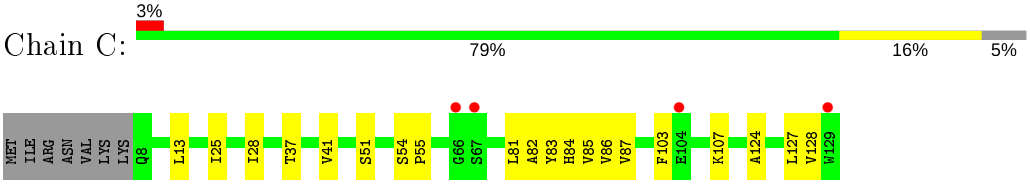
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain J:



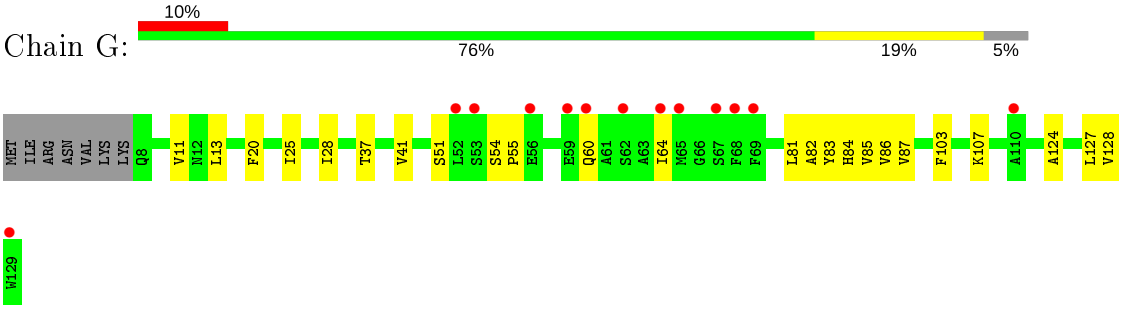
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain C:



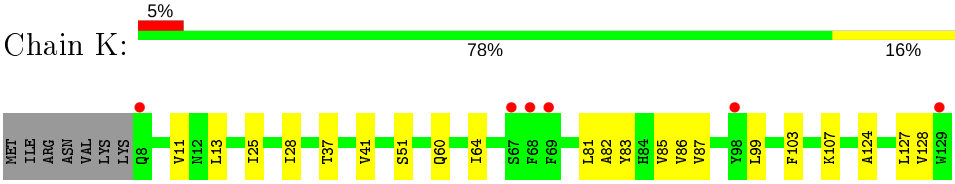
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain G:



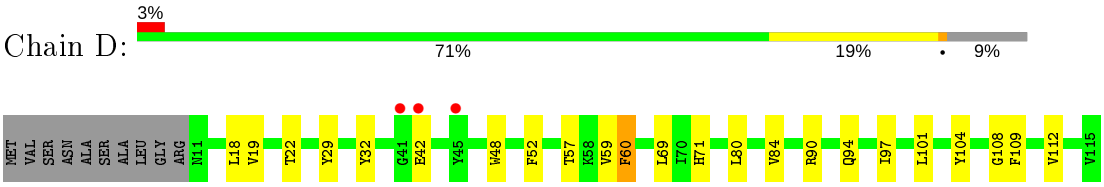
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain K:



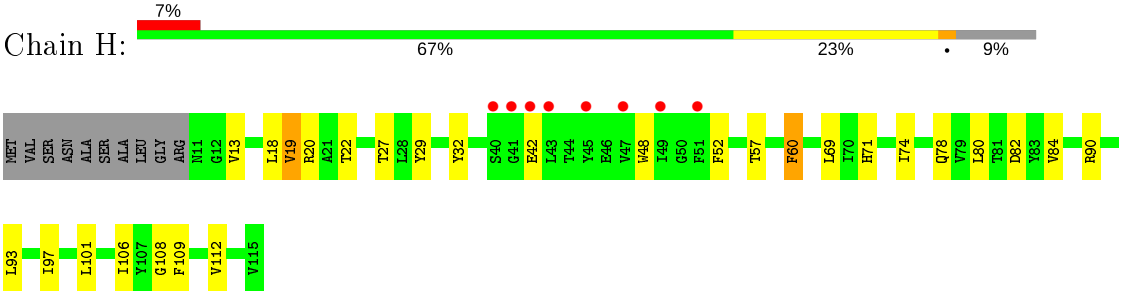
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain D:



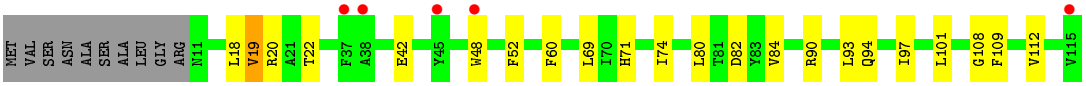
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain H:



• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain L:


MET
VAL
SER
ASN
ALA
SER
ALA
LEU
GLY
ARG
N11
L18
V19
R20
A21
T22
F37
A38
E42
Y45
W48
F52
F60
L69
I70
H71
I74
L80
T81
D82
Y83
V84
R90
L93
Q94
I97
L101
G108
F109
V112
V115

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.95Å 186.13Å 204.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.52 – 3.20 45.84 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.52-3.20) 99.3 (45.84-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.197 , 0.228 0.200 , 0.229	Depositor DCC
R_{free} test set	3828 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 89.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	24936	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/4611	0.56	0/6237
1	E	0.44	0/4611	0.53	0/6237
1	I	0.38	0/4611	0.50	0/6237
2	B	0.54	0/1908	0.60	0/2578
2	F	0.51	0/1908	0.58	0/2578
2	J	0.44	0/1908	0.55	0/2578
3	C	0.52	0/970	0.55	0/1316
3	G	0.47	0/970	0.54	0/1316
3	K	0.42	0/970	0.49	0/1316
4	D	0.46	0/859	0.50	0/1175
4	H	0.42	0/859	0.48	0/1175
4	L	0.42	0/859	0.47	0/1175
All	All	0.46	0/25044	0.54	0/33918

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4522	0	4426	67	0
1	I	4522	0	4426	63	0
2	B	1869	0	1850	24	0
2	F	1869	0	1850	30	0
2	J	1869	0	1850	24	0
3	C	948	0	989	13	0
3	G	948	0	989	14	0
3	K	948	0	989	12	0
4	D	836	0	875	12	0
4	H	836	0	875	19	0
4	L	836	0	875	14	0
5	A	53	0	29	7	0
5	E	53	0	30	5	0
5	I	53	0	29	6	0
6	A	9	0	3	4	0
6	E	9	0	3	2	0
6	I	9	0	3	2	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
8	B	4	0	0	0	0
8	F	4	0	0	0	0
8	J	4	0	0	0	0
9	B	8	0	0	1	0
9	F	8	0	0	1	0
9	J	8	0	0	1	0
10	B	7	0	0	1	0
10	F	7	0	0	1	0
10	J	7	0	0	2	0
11	C	43	0	30	7	0
11	G	43	0	30	7	0
11	K	43	0	30	4	0
12	C	12	0	1	0	0
12	G	12	0	0	1	0
12	K	12	0	0	0	0
All	All	24936	0	24608	368	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 (368) 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:1130:HEM:HBB2	11:C:1130:HEM:HHC	1.50	0.92
11:G:1130:HEM:HHC	11:G:1130:HEM:HBB2	1.55	0.87
2:F:55:CYS:O	2:F:56:ARG:HD3	1.75	0.86
1:E:555:CYS:HA	1:E:571:VAL:HG23	1.61	0.83
2:B:55:CYS:O	2:B:56:ARG:HD3	1.78	0.82
2:J:55:CYS:O	2:J:56:ARG:HD3	1.80	0.81
11:K:1130:HEM:HHC	11:K:1130:HEM:HBB2	1.62	0.80
1:I:555:CYS:HA	1:I:571:VAL:HG23	1.63	0.80
1:A:274:GLU:HG2	1:A:281:LYS:HE3	1.65	0.78
11:C:1130:HEM:HBD1	11:C:1130:HEM:HHA	1.66	0.77
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.65	0.77
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.68	0.76
1:A:555:CYS:HA	1:A:571:VAL:HG23	1.68	0.76
11:K:1130:HEM:HBD1	11:K:1130:HEM:HHA	1.69	0.75
1:E:274:GLU:HG2	1:E:281:LYS:HE3	1.67	0.74
1:I:274:GLU:HG2	1:I:281:LYS:HE3	1.70	0.74
1:I:49:ALA:HB3	1:I:142:GLY:HA3	1.69	0.73
1:E:49:ALA:HB3	1:E:142:GLY:HA3	1.68	0.73
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.72	0.72
1:E:392:VAL:N	1:E:393:SER:HA	2.05	0.71
4:D:69:LEU:HA	4:D:101:LEU:HD22	1.73	0.71
11:G:1130:HEM:HHD	11:G:1130:HEM:HBC2	1.73	0.69
1:A:147:HIS:O	1:A:151:GLN:HG3	1.91	0.69
1:E:147:HIS:O	1:E:151:GLN:HG3	1.91	0.69
2:J:56:ARG:HG2	2:J:56:ARG:O	1.93	0.69
1:I:392:VAL:N	1:I:393:SER:HA	2.06	0.69
2:F:56:ARG:HG2	2:F:56:ARG:O	1.94	0.67
1:I:286:ARG:HH22	6:I:1589:TEO:C3	2.07	0.67
2:B:55:CYS:O	2:B:56:ARG:CD	2.44	0.66
1:I:395:HIS:ND1	1:I:399:ARG:HG3	2.10	0.66
1:A:392:VAL:N	1:A:393:SER:HA	2.09	0.65
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.78	0.65
1:I:408:LEU:HD21	5:I:601:FAD:H5'2	1.79	0.64
1:E:395:HIS:ND1	1:E:399:ARG:HG3	2.12	0.64
5:A:601:FAD:N5	6:A:1589:TEO:H2	2.14	0.63
3:G:83:TYR:CZ	3:G:87:VAL:HG21	2.33	0.63
1:I:147:HIS:O	1:I:151:GLN:HG3	2.00	0.62
1:E:486:GLN:O	1:E:490:ILE:HG13	2.00	0.62
4:H:69:LEU:HA	4:H:101:LEU:HD22	1.80	0.62
11:G:1130:HEM:HBD1	11:G:1130:HEM:HHA	1.81	0.62
2:J:35:LEU:HD11	2:J:91:ILE:HD11	1.82	0.62
1:A:395:HIS:ND1	1:A:399:ARG:HG3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:1130:HEM:CBC	11:C:1130:HEM:HHD	2.31	0.61
3:K:83:TYR:CZ	3:K:87:VAL:HG21	2.35	0.61
1:A:391:CYS:SG	1:A:393:SER:HB2	2.40	0.61
1:I:99:LEU:HD11	1:I:409:VAL:HG21	1.83	0.61
4:L:69:LEU:HA	4:L:101:LEU:HD22	1.83	0.61
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.83	0.60
1:E:55:VAL:HG13	1:E:57:LEU:HG	1.83	0.60
11:C:1130:HEM:HBC2	11:C:1130:HEM:HHD	1.84	0.60
2:B:238:ALA:O	4:H:90:ARG:NH2	2.35	0.59
1:I:22:ALA:O	1:I:26:ILE:HG13	2.03	0.59
2:F:238:ALA:O	4:L:90:ARG:NH2	2.36	0.59
1:A:242:HIS:O	1:A:351:PRO:HA	2.02	0.58
1:E:22:ALA:O	1:E:26:ILE:HG13	2.03	0.58
1:A:79:ILE:HD11	1:A:397:ALA:HB2	1.86	0.58
1:I:49:ALA:HA	5:I:601:FAD:C6	2.33	0.58
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.38	0.58
1:I:191:VAL:HG12	1:I:192:TYR:N	2.18	0.58
1:I:232:PRO:HB2	1:I:558:LEU:HD11	1.85	0.58
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.39	0.58
2:F:35:LEU:HD11	2:F:91:ILE:HD11	1.86	0.58
1:E:286:ARG:HH22	6:E:1589:TEO:C3	2.17	0.57
1:E:404:SER:O	1:E:407:ASP:HB3	2.04	0.57
1:E:242:HIS:O	1:E:351:PRO:HA	2.05	0.57
1:E:79:ILE:HD11	1:E:397:ALA:HB2	1.87	0.57
1:A:480:MET:HB3	1:A:531:ASN:OD1	2.05	0.57
1:I:44:SER:O	1:I:47:VAL:HG12	2.05	0.57
4:L:80:LEU:HD11	4:L:97:ILE:HD12	1.87	0.56
1:E:408:LEU:HD11	5:E:601:FAD:H4'	1.86	0.56
1:I:49:ALA:HA	5:I:601:FAD:C5X	2.35	0.56
1:A:232:PRO:HB2	1:A:558:LEU:HD11	1.87	0.56
1:E:170:VAL:HG23	1:E:180:CYS:HA	1.86	0.56
11:G:1130:HEM:CBC	11:G:1130:HEM:HHD	2.36	0.56
1:I:75:GLY:O	1:I:398:ASN:HB3	2.06	0.56
1:I:55:VAL:HG13	1:I:57:LEU:HG	1.88	0.56
2:J:55:CYS:O	2:J:56:ARG:CD	2.54	0.56
11:K:1130:HEM:HBC2	11:K:1130:HEM:HHD	1.88	0.56
1:A:451:ARG:NH1	1:A:451:ARG:HG2	2.20	0.55
2:B:56:ARG:O	2:B:56:ARG:HG2	2.05	0.55
1:E:191:VAL:HG12	1:E:192:TYR:N	2.21	0.55
1:A:49:ALA:HA	5:A:601:FAD:C5X	2.37	0.55
2:F:234:LEU:HD23	4:H:13:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:170:VAL:HG23	1:I:180:CYS:HA	1.88	0.55
4:H:80:LEU:HD11	4:H:97:ILE:HD12	1.88	0.55
1:A:286:ARG:HH22	6:A:1589:TEO:C3	2.18	0.55
1:E:99:LEU:HD11	1:E:409:VAL:HG21	1.89	0.55
2:J:169:PHE:CD1	2:J:205:ARG:HB2	2.42	0.55
3:G:124:ALA:O	3:G:128:VAL:HG23	2.06	0.55
1:I:391:CYS:SG	1:I:393:SER:HB2	2.46	0.55
1:I:486:GLN:O	1:I:490:ILE:HG13	2.07	0.54
3:K:37:THR:O	3:K:41:VAL:HG23	2.07	0.54
1:A:191:VAL:HG12	1:A:192:TYR:N	2.23	0.54
4:D:108:GLY:O	4:D:112:VAL:HG22	2.07	0.54
1:I:242:HIS:O	1:I:351:PRO:HA	2.07	0.54
1:A:75:GLY:O	1:A:398:ASN:HB3	2.08	0.54
1:A:49:ALA:HA	5:A:601:FAD:C6	2.38	0.54
4:D:80:LEU:HD11	4:D:97:ILE:HD12	1.90	0.54
1:I:340:VAL:O	1:I:342:PRO:HD3	2.08	0.53
3:C:25:ILE:O	3:C:28:ILE:HG22	2.09	0.53
1:E:391:CYS:SG	1:E:393:SER:HB2	2.49	0.53
4:H:93:LEU:O	4:H:97:ILE:HG13	2.08	0.53
4:H:108:GLY:O	4:H:112:VAL:HG22	2.09	0.53
1:A:99:LEU:HD11	1:A:409:VAL:HG21	1.90	0.53
2:B:35:LEU:HD11	2:B:91:ILE:HD11	1.90	0.53
1:E:480:MET:HB3	1:E:531:ASN:OD1	2.09	0.52
1:I:79:ILE:HD11	1:I:397:ALA:HB2	1.91	0.52
4:D:101:LEU:O	4:D:104:TYR:HB2	2.09	0.52
4:D:22:THR:OG1	4:D:71:HIS:HB2	2.10	0.52
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.75	0.52
1:I:362:THR:HG21	1:I:385:ALA:HB3	1.92	0.52
3:K:25:ILE:O	3:K:28:ILE:HG22	2.10	0.52
4:L:108:GLY:O	4:L:112:VAL:HG22	2.09	0.52
1:A:294:MET:O	1:A:298:ARG:HG3	2.09	0.51
1:E:49:ALA:HA	5:E:601:FAD:C5X	2.41	0.51
1:A:340:VAL:O	1:A:342:PRO:HD3	2.11	0.51
2:J:159:CYS:HB2	10:J:304:F3S:S2	2.51	0.51
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.46	0.51
2:J:34:MET:O	2:J:37:ASP:HB2	2.10	0.51
3:K:124:ALA:O	3:K:128:VAL:HG23	2.11	0.51
1:A:14:GLY:HA2	5:A:601:FAD:H1B	1.93	0.51
1:I:480:MET:HB3	1:I:531:ASN:OD1	2.11	0.50
1:A:77:ASP:OD1	1:A:586:ARG:HD2	2.11	0.50
1:E:49:ALA:HA	5:E:601:FAD:C6	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:ALA:O	3:C:128:VAL:HG23	2.11	0.50
4:D:59:VAL:HG22	4:H:106:ILE:HG22	1.92	0.50
1:I:294:MET:O	1:I:298:ARG:HG3	2.11	0.50
1:E:232:PRO:HB2	1:E:558:LEU:HD11	1.93	0.50
3:G:37:THR:O	3:G:41:VAL:HG23	2.11	0.50
1:A:486:GLN:O	1:A:490:ILE:HG13	2.11	0.50
1:A:214:ASN:HD22	1:A:214:ASN:N	2.10	0.50
2:F:55:CYS:O	2:F:56:ARG:CD	2.54	0.50
1:I:392:VAL:H	1:I:393:SER:HA	1.77	0.50
2:F:155:CYS:SG	2:F:172:PRO:HB2	2.52	0.49
3:G:81:LEU:O	3:G:85:VAL:HG23	2.11	0.49
1:A:404:SER:O	1:A:407:ASP:HB3	2.12	0.49
1:A:78:TYR:CD1	1:A:583:PRO:HA	2.47	0.49
1:E:75:GLY:O	1:E:398:ASN:HB3	2.11	0.49
3:K:82:ALA:O	3:K:86:VAL:HG23	2.13	0.49
3:C:84:HIS:CE1	11:C:1130:HEM:NA	2.80	0.49
3:C:37:THR:O	3:C:41:VAL:HG23	2.12	0.49
3:G:25:ILE:O	3:G:28:ILE:HG22	2.12	0.49
2:J:208:SER:HA	10:J:304:F3S:S4	2.52	0.49
3:G:103:PHE:CE2	3:G:107:LYS:HE3	2.48	0.49
2:B:127:ASN:N	2:B:128:PRO:HD3	2.28	0.48
2:F:34:MET:O	2:F:37:ASP:HB2	2.13	0.48
1:I:364:VAL:HG22	1:I:411:PHE:HE1	1.79	0.48
2:B:207:HIS:O	2:B:208:SER:HB2	2.14	0.48
2:B:234:LEU:O	2:B:238:ALA:HB3	2.14	0.48
3:G:20:PHE:CE1	12:G:1131:PCI:CL2	3.04	0.48
2:J:31:ARG:HG2	2:J:32:ASP:N	2.29	0.48
4:L:48:TRP:CH2	4:L:52:PHE:HE2	2.32	0.48
1:A:463:LEU:C	1:A:463:LEU:HD23	2.34	0.48
4:L:22:THR:OG1	4:L:71:HIS:HB2	2.13	0.48
2:B:216:CYS:HA	9:B:303:SF4:S3	2.54	0.48
1:E:251:VAL:HG11	1:E:333:LEU:HD22	1.95	0.48
2:F:156:SER:HA	2:F:172:PRO:HD2	1.96	0.48
2:J:156:SER:OG	2:J:172:PRO:HD2	2.13	0.48
3:G:82:ALA:O	3:G:86:VAL:HG23	2.14	0.47
1:I:404:SER:O	1:I:407:ASP:HB3	2.13	0.47
1:A:578:ARG:NH1	1:A:579:PRO:O	2.47	0.47
4:H:22:THR:OG1	4:H:71:HIS:HB2	2.15	0.47
1:I:532:PHE:HB2	1:I:566:MET:HG3	1.97	0.47
2:J:127:ASN:N	2:J:128:PRO:HD3	2.29	0.47
3:K:127:LEU:HD23	3:K:127:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:ILE:HG13	2:B:152:CYS:HB3	1.96	0.47
1:E:334:SER:O	1:E:338:ALA:HB3	2.14	0.47
11:G:1130:HEM:HHA	11:G:1130:HEM:HBA2	1.96	0.47
1:I:251:VAL:HG11	1:I:333:LEU:HD22	1.95	0.47
1:I:49:ALA:HA	5:I:601:FAD:N5	2.29	0.47
1:E:340:VAL:O	1:E:342:PRO:HD3	2.14	0.47
3:C:81:LEU:O	3:C:85:VAL:HG23	2.15	0.47
1:E:44:SER:O	1:E:47:VAL:HG12	2.15	0.47
4:L:93:LEU:O	4:L:97:ILE:HG13	2.15	0.47
1:I:52:GLY:HA2	1:I:141:THR:HG21	1.96	0.47
3:C:103:PHE:CE2	3:C:107:LYS:HE3	2.50	0.47
3:G:60:GLN:O	3:G:64:ILE:HG13	2.15	0.47
11:K:1130:HEM:CBC	11:K:1130:HEM:HHD	2.45	0.47
1:I:399:ARG:CZ	1:I:404:SER:HB2	2.45	0.46
2:J:150:ILE:HG13	2:J:152:CYS:HB3	1.97	0.46
3:K:13:LEU:HD12	3:K:13:LEU:HA	1.78	0.46
1:E:81:ASP:O	1:E:85:ILE:HG13	2.15	0.46
2:J:160:PRO:HA	2:J:163:TRP:CE3	2.50	0.46
1:A:223:VAL:HG13	1:A:233:VAL:HG11	1.97	0.46
1:A:379:VAL:O	1:A:381:PRO:HD3	2.14	0.46
2:F:31:ARG:HG2	2:F:32:ASP:N	2.30	0.46
1:A:22:ALA:O	1:A:26:ILE:HG13	2.16	0.46
3:C:82:ALA:O	3:C:86:VAL:HG23	2.16	0.46
4:L:69:LEU:HD12	4:L:101:LEU:HB3	1.98	0.46
1:A:170:VAL:HG23	1:A:180:CYS:HA	1.96	0.46
1:A:362:THR:HG21	1:A:385:ALA:HB3	1.96	0.46
1:E:214:ASN:HD22	1:E:214:ASN:N	2.12	0.46
3:G:84:HIS:CE1	11:G:1130:HEM:NA	2.83	0.46
4:L:19:VAL:HG23	4:L:74:ILE:HG21	1.98	0.46
4:H:69:LEU:HD12	4:H:101:LEU:HB3	1.97	0.46
1:I:191:VAL:CG1	1:I:192:TYR:N	2.79	0.46
4:L:80:LEU:HD13	4:L:94:GLN:HG3	1.98	0.46
5:A:601:FAD:C4X	6:A:1589:TEO:H2	2.46	0.46
1:I:223:VAL:HG13	1:I:233:VAL:HG11	1.98	0.46
1:E:49:ALA:HA	5:E:601:FAD:N5	2.31	0.46
2:F:234:LEU:O	2:F:238:ALA:HB3	2.15	0.46
1:I:365:THR:O	1:I:415:ALA:HA	2.16	0.46
2:J:155:CYS:SG	2:J:172:PRO:HB2	2.56	0.46
2:F:216:CYS:HA	9:F:303:SF4:S3	2.55	0.45
1:A:49:ALA:HB3	1:A:142:GLY:CA	2.40	0.45
2:J:111:TYR:O	2:J:114:TYR:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:208:SER:O	2:F:210:MET:HG3	2.15	0.45
1:I:257:CYS:HB3	1:I:315:LEU:HD21	1.98	0.45
4:H:29:TYR:HD1	4:H:60:PHE:CD2	2.35	0.45
1:A:475:ARG:O	1:A:542:ARG:HA	2.17	0.45
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.52	0.45
1:I:334:SER:O	1:I:338:ALA:HB3	2.17	0.45
2:B:31:ARG:HG2	2:B:32:ASP:N	2.29	0.45
1:E:362:THR:HG21	1:E:385:ALA:HB3	1.98	0.45
1:E:392:VAL:H	1:E:393:SER:HA	1.78	0.45
1:E:294:MET:O	1:E:298:ARG:HG3	2.17	0.45
3:K:81:LEU:O	3:K:85:VAL:HG23	2.17	0.45
1:E:223:VAL:HG13	1:E:233:VAL:HG11	1.98	0.44
1:E:257:CYS:HB3	1:E:315:LEU:HD21	1.99	0.44
2:F:160:PRO:HA	2:F:163:TRP:CE3	2.51	0.44
1:I:78:TYR:CD1	1:I:583:PRO:HA	2.52	0.44
2:B:172:PRO:HG3	10:B:304:F3S:S3	2.57	0.44
1:E:341:ASP:OD1	1:E:343:VAL:HG23	2.18	0.44
2:J:9:ARG:NH1	2:J:23:TYR:OH	2.51	0.44
4:D:48:TRP:CH2	4:D:52:PHE:HE2	2.35	0.44
4:H:48:TRP:CH2	4:H:52:PHE:HE2	2.35	0.44
2:B:34:MET:O	2:B:37:ASP:HB2	2.18	0.44
4:H:18:LEU:HA	4:H:18:LEU:HD23	1.76	0.44
1:I:560:LEU:HA	1:I:561:PRO:HD3	1.84	0.44
1:A:118:PRO:HA	1:A:132:ALA:HA	2.00	0.44
2:B:111:TYR:O	2:B:114:TYR:HB3	2.17	0.44
1:E:49:ALA:HB3	1:E:142:GLY:CA	2.43	0.44
2:F:111:TYR:O	2:F:114:TYR:HB3	2.18	0.44
2:B:160:PRO:HA	2:B:163:TRP:CE3	2.53	0.44
1:E:72:THR:HG22	1:E:85:ILE:HD13	2.00	0.44
3:G:127:LEU:O	3:G:127:LEU:HD23	2.18	0.44
1:A:399:ARG:CZ	1:A:404:SER:HB2	2.47	0.44
2:B:156:SER:OG	2:B:172:PRO:HD2	2.18	0.44
2:F:127:ASN:N	2:F:128:PRO:HD3	2.32	0.44
2:F:150:ILE:HG13	2:F:152:CYS:HB3	1.99	0.44
4:D:80:LEU:HD13	4:D:94:GLN:HG3	2.00	0.43
1:E:578:ARG:NH1	1:E:579:PRO:O	2.51	0.43
2:F:128:PRO:HA	2:F:129:PRO:HD3	1.88	0.43
1:A:365:THR:O	1:A:415:ALA:HA	2.17	0.43
2:F:159:CYS:HB2	10:F:304:F3S:S2	2.59	0.43
2:F:2:ARG:HD3	2:F:26:GLU:OE2	2.18	0.43
1:I:118:PRO:HA	1:I:132:ALA:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:ARG:O	1:I:143:HIS:HB3	2.17	0.43
2:J:205:ARG:NH1	4:L:82:ASP:OD1	2.52	0.43
1:E:164:TRP:CZ2	1:E:184:CYS:HB2	2.53	0.43
1:I:286:ARG:HH22	6:I:1589:TEO:C4	2.30	0.43
3:K:128:VAL:O	3:K:128:VAL:HG12	2.19	0.43
1:A:455:ASP:HA	1:A:456:PRO:HD2	1.90	0.43
1:A:490:ILE:HG22	1:A:520:MET:HE1	2.01	0.43
1:E:78:TYR:CD1	1:E:583:PRO:HA	2.53	0.43
2:F:114:TYR:O	2:F:117:ILE:HG13	2.19	0.43
2:B:94:LEU:HA	2:B:95:PRO:HD3	1.84	0.43
4:D:18:LEU:HA	4:D:18:LEU:HD23	1.69	0.43
2:F:205:ARG:NH1	4:H:82:ASP:OD1	2.51	0.43
1:I:244:THR:HG22	1:I:349:VAL:HG21	2.01	0.43
1:I:475:ARG:O	1:I:542:ARG:HA	2.18	0.43
1:E:100:GLU:HG3	1:E:114:ILE:HD11	2.01	0.43
3:K:103:PHE:CE2	3:K:107:LYS:HE3	2.54	0.43
3:G:128:VAL:HG12	3:G:128:VAL:O	2.18	0.43
1:A:44:SER:O	1:A:47:VAL:HG12	2.19	0.43
1:E:255:GLU:N	6:E:1589:TEO:O1B	2.42	0.43
2:F:156:SER:OG	2:F:172:PRO:HD2	2.19	0.43
1:E:560:LEU:HA	1:E:561:PRO:HD3	1.84	0.43
2:F:9:ARG:NH1	2:F:23:TYR:OH	2.52	0.43
2:F:94:LEU:HA	2:F:95:PRO:HD3	1.90	0.43
11:G:1130:HEM:HAC	4:H:27:THR:OG1	2.18	0.43
4:L:19:VAL:HG12	4:L:20:ARG:N	2.33	0.43
5:A:601:FAD:C4	6:A:1589:TEO:C3	2.97	0.43
2:B:2:ARG:HD3	2:B:26:GLU:OE2	2.19	0.43
3:C:13:LEU:HD12	3:C:13:LEU:HA	1.78	0.43
4:H:32:TYR:HH	4:H:57:THR:HG1	1.66	0.43
1:I:214:ASN:N	1:I:214:ASN:HD22	2.17	0.43
2:J:152:CYS:O	2:J:153:ALA:HB3	2.19	0.43
1:A:164:TRP:CZ2	1:A:184:CYS:HB2	2.54	0.42
11:C:1130:HEM:CHD	11:C:1130:HEM:HBC2	2.47	0.42
1:E:365:THR:O	1:E:415:ALA:HA	2.19	0.42
1:E:77:ASP:OD1	1:E:586:ARG:HD2	2.19	0.42
4:H:19:VAL:HG12	4:H:20:ARG:N	2.34	0.42
1:I:164:TRP:CZ2	1:I:184:CYS:HB2	2.54	0.42
2:J:5:PHE:HB2	2:J:23:TYR:HB2	2.00	0.42
1:E:118:PRO:HA	1:E:132:ALA:HA	2.02	0.42
1:E:191:VAL:CG1	1:E:192:TYR:N	2.82	0.42
1:E:294:MET:HG2	1:E:351:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:VAL:O	1:E:381:PRO:HD3	2.19	0.42
1:E:14:GLY:HA2	5:E:601:FAD:H1B	2.02	0.42
1:I:578:ARG:NH1	1:I:579:PRO:O	2.52	0.42
1:A:100:GLU:HG3	1:A:114:ILE:HD11	2.02	0.42
1:A:52:GLY:HA2	1:A:141:THR:HG21	2.00	0.42
2:B:9:ARG:NH1	2:B:23:TYR:OH	2.53	0.42
1:E:345:GLU:HG2	1:E:346:PRO:N	2.34	0.42
4:H:19:VAL:HG23	4:H:74:ILE:HG21	2.00	0.42
1:I:267:LYS:HA	1:I:303:CYS:SG	2.59	0.42
1:A:72:THR:HG22	1:A:85:ILE:HD13	2.01	0.42
1:E:212:THR:HA	1:E:352:THR:HG22	2.00	0.42
1:E:244:THR:HG22	1:E:349:VAL:HG21	2.02	0.42
2:J:156:SER:HA	2:J:172:PRO:HD2	2.01	0.42
1:A:257:CYS:HB3	1:A:315:LEU:HD21	2.01	0.42
2:B:155:CYS:SG	2:B:172:PRO:HB2	2.59	0.42
3:C:128:VAL:HG12	3:C:128:VAL:O	2.20	0.42
3:G:13:LEU:HD12	3:G:13:LEU:HA	1.69	0.42
2:B:36:LEU:O	2:B:40:ILE:HG13	2.19	0.42
2:F:107:MET:HB2	2:F:111:TYR:CE2	2.54	0.42
1:A:266:ASN:HB2	1:A:301:ARG:O	2.20	0.42
3:C:127:LEU:O	3:C:127:LEU:HD23	2.20	0.42
1:E:266:ASN:HB2	1:E:301:ARG:O	2.19	0.42
1:E:463:LEU:C	1:E:463:LEU:HD23	2.41	0.42
1:E:475:ARG:O	1:E:542:ARG:HA	2.20	0.42
3:G:54:SER:HB2	3:G:55:PRO:CD	2.50	0.42
1:I:72:THR:HG22	1:I:85:ILE:HD13	2.02	0.42
1:A:334:SER:O	1:A:338:ALA:HB3	2.20	0.41
1:I:49:ALA:HB3	1:I:142:GLY:CA	2.44	0.41
5:I:601:FAD:H1'1	5:I:601:FAD:H9	1.64	0.41
2:F:207:HIS:O	2:F:208:SER:HB2	2.21	0.41
1:A:18:ALA:HB2	1:A:408:LEU:HD22	2.01	0.41
1:A:81:ASP:O	1:A:85:ILE:HG13	2.20	0.41
1:E:364:VAL:HG22	1:E:411:PHE:HE1	1.85	0.41
1:A:238:MET:O	1:A:357:MET:HB2	2.21	0.41
1:A:451:ARG:HH11	1:A:451:ARG:CG	2.33	0.41
1:A:49:ALA:HA	5:A:601:FAD:N5	2.36	0.41
4:D:32:TYR:HH	4:D:57:THR:HG1	1.58	0.41
1:E:24:LEU:HD21	1:E:152:GLN:HB3	2.02	0.41
4:H:84:VAL:O	4:H:90:ARG:HD3	2.19	0.41
3:K:60:GLN:O	3:K:64:ILE:HG13	2.20	0.41
3:C:54:SER:HB2	3:C:55:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:423:ILE:O	1:I:426:GLN:HG2	2.21	0.41
1:I:463:LEU:C	1:I:463:LEU:HD23	2.40	0.41
1:A:191:VAL:CG1	1:A:192:TYR:N	2.84	0.41
4:D:84:VAL:O	4:D:90:ARG:HD3	2.21	0.41
4:H:74:ILE:O	4:H:78:GLN:HG3	2.21	0.41
1:I:164:TRP:CH2	1:I:184:CYS:HB2	2.55	0.41
1:I:238:MET:O	1:I:357:MET:HB2	2.20	0.41
1:I:408:LEU:HD11	5:I:601:FAD:H4'	2.03	0.41
2:J:207:HIS:O	2:J:208:SER:HB2	2.21	0.41
4:L:84:VAL:O	4:L:90:ARG:HD3	2.21	0.41
1:A:171:LYS:HE3	1:A:229:ALA:O	2.21	0.41
1:A:532:PHE:HB2	1:A:566:MET:HG3	2.02	0.41
1:E:423:ILE:O	1:E:426:GLN:HG2	2.20	0.41
1:I:40:PHE:CD1	1:I:41:PRO:HD2	2.56	0.41
2:J:208:SER:O	2:J:210:MET:HG3	2.21	0.41
3:K:99:LEU:HA	3:K:99:LEU:HD23	1.81	0.41
2:B:214:SER:HB3	3:C:103:PHE:CZ	2.56	0.41
1:E:52:GLY:HA2	1:E:141:THR:HG21	2.03	0.41
1:I:221:ASP:OD1	1:I:518:ASN:ND2	2.41	0.41
11:C:1130:HEM:HBB2	11:C:1130:HEM:CHC	2.27	0.41
4:D:29:TYR:HD1	4:D:60:PHE:CD2	2.39	0.41
1:A:341:ASP:OD1	1:A:343:VAL:HG23	2.21	0.41
1:A:96:ILE:HD13	1:A:96:ILE:HA	1.88	0.41
2:F:5:PHE:HB2	2:F:23:TYR:HB2	2.03	0.41
1:I:451:ARG:HD3	1:I:451:ARG:HA	1.85	0.41
2:J:150:ILE:HG12	9:J:303:SF4:S1	2.60	0.41
1:E:115:TYR:O	1:E:135:ALA:HA	2.21	0.40
1:I:392:VAL:N	1:I:393:SER:CA	2.82	0.40
2:J:8:TYR:CG	2:J:93:PRO:HD3	2.57	0.40
2:B:170:ILE:HD13	2:B:170:ILE:HA	1.92	0.40
2:F:117:ILE:C	2:F:117:ILE:HD12	2.42	0.40
4:L:18:LEU:HA	4:L:18:LEU:HD23	1.73	0.40
1:E:104:LEU:C	1:E:104:LEU:HD23	2.42	0.40
1:I:79:ILE:O	1:I:556:HIS:CE1	2.75	0.40
1:A:6:ARG:HD2	1:A:191:VAL:HG11	2.03	0.40
1:A:251:VAL:HG11	1:A:333:LEU:HD22	2.02	0.40
1:E:267:LYS:HB2	1:E:267:LYS:HE3	1.84	0.40
1:E:238:MET:O	1:E:357:MET:HB2	2.22	0.40
1:E:532:PHE:HB2	1:E:566:MET:HG3	2.04	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%)	558 (95%)	27 (5%)	1 (0%)	47	79
1	E	586/588 (100%)	558 (95%)	27 (5%)	1 (0%)	47	79
1	I	586/588 (100%)	557 (95%)	28 (5%)	1 (0%)	47	79
2	B	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
2	F	236/238 (99%)	221 (94%)	14 (6%)	1 (0%)	34	69
2	J	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
3	C	120/129 (93%)	116 (97%)	3 (2%)	1 (1%)	19	58
3	G	120/129 (93%)	116 (97%)	3 (2%)	1 (1%)	19	58
3	K	120/129 (93%)	116 (97%)	3 (2%)	1 (1%)	19	58
4	D	103/115 (90%)	96 (93%)	6 (6%)	1 (1%)	15	54
4	H	103/115 (90%)	95 (92%)	7 (7%)	1 (1%)	15	54
4	L	103/115 (90%)	97 (94%)	5 (5%)	1 (1%)	15	54
All	All	3135/3210 (98%)	2972 (95%)	153 (5%)	10 (0%)	41	74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	GLY
1	E	92	GLY
1	I	92	GLY
4	D	42	GLU
4	H	42	GLU
4	L	42	GLU
3	C	51	SER
3	K	51	SER
3	G	51	SER
2	F	108	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	473/473 (100%)	467 (99%)	6 (1%)	69	87
1	E	473/473 (100%)	467 (99%)	6 (1%)	69	87
1	I	473/473 (100%)	468 (99%)	5 (1%)	73	88
2	B	208/208 (100%)	201 (97%)	7 (3%)	37	70
2	F	208/208 (100%)	200 (96%)	8 (4%)	33	67
2	J	208/208 (100%)	201 (97%)	7 (3%)	37	70
3	C	102/109 (94%)	102 (100%)	0	100	100
3	G	102/109 (94%)	101 (99%)	1 (1%)	76	90
3	K	102/109 (94%)	101 (99%)	1 (1%)	76	90
4	D	88/96 (92%)	85 (97%)	3 (3%)	37	70
4	H	88/96 (92%)	85 (97%)	3 (3%)	37	70
4	L	88/96 (92%)	85 (97%)	3 (3%)	37	70
All	All	2613/2658 (98%)	2563 (98%)	50 (2%)	57	81

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	PHE
1	A	173	GLN
1	A	304	ASP
1	A	440	SER
1	A	491	ARG
1	A	541	SER
2	B	1	MET
2	B	45	LYS
2	B	53	ARG
2	B	56	ARG
2	B	120	TYR
2	B	180	ARG
2	B	212	CYS
4	D	19	VAL

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Mol	Chain	Res	Type
4	D	60	PHE
4	D	109	PHE
1	E	119	PHE
1	E	173	GLN
1	E	304	ASP
1	E	440	SER
1	E	491	ARG
1	E	541	SER
2	F	1	MET
2	F	45	LYS
2	F	53	ARG
2	F	56	ARG
2	F	120	TYR
2	F	180	ARG
2	F	205	ARG
2	F	212	CYS
3	G	11	VAL
4	H	19	VAL
4	H	60	PHE
4	H	109	PHE
1	I	119	PHE
1	I	173	GLN
1	I	304	ASP
1	I	440	SER
1	I	491	ARG
2	J	1	MET
2	J	53	ARG
2	J	56	ARG
2	J	120	TYR
2	J	180	ARG
2	J	205	ARG
2	J	212	CYS
3	K	11	VAL
4	L	19	VAL
4	L	60	PHE
4	L	109	PHE

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

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	HEM	K	1130	3,4	27,50,50	2.26	6 (22%)	17,82,82	1.53	3 (17%)
12	PCI	C	1131	-	12,12,12	2.00	4 (33%)	18,18,18	1.22	1 (5%)
10	F3S	F	304	2	0,9,9	0.00	-	-		
8	FES	J	302	2	0,4,4	0.00	-	-		
6	TEO	I	1589	-	1,8,8	0.61	0	0,10,10	0.00	-
8	FES	B	302	2	0,4,4	0.00	-	-		
9	SF4	J	303	2	0,12,12	0.00	-	-		
6	TEO	A	1589	-	1,8,8	0.24	0	0,10,10	0.00	-
6	TEO	E	1589	-	1,8,8	0.35	0	0,10,10	0.00	-
5	FAD	I	601	1	51,58,58	1.53	8 (15%)	60,89,89	1.81	11 (18%)
11	HEM	C	1130	3,4	27,50,50	2.18	6 (22%)	17,82,82	1.81	3 (17%)
11	HEM	G	1130	3,4	27,50,50	2.33	6 (22%)	17,82,82	1.80	5 (29%)
5	FAD	E	601	1	51,58,58	1.49	5 (9%)	60,89,89	1.77	12 (20%)
9	SF4	F	303	2	0,12,12	0.00	-	-		
8	FES	F	302	2	0,4,4	0.00	-	-		
5	FAD	A	601	1	51,58,58	1.45	6 (11%)	60,89,89	1.78	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SF4	B	303	2	0,12,12	0.00	-	-		
10	F3S	J	304	2	0,9,9	0.00	-	-		
12	PCI	K	1131	-	12,12,12	2.14	5 (41%)	18,18,18	1.14	2 (11%)
12	PCI	G	1131	-	12,12,12	2.21	6 (50%)	18,18,18	2.03	7 (38%)
10	F3S	B	304	2	0,9,9	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEM	K	1130	3,4	-	2/6/54/54	-
12	PCI	C	1131	-	-	-	0/1/1/1
6	TEO	E	1589	-	-	2/2/8/8	-
8	FES	J	302	2	-	-	0/1/1/1
6	TEO	I	1589	-	-	1/2/8/8	-
10	F3S	B	304	2	-	-	0/3/3/3
5	FAD	E	601	1	-	5/30/50/50	0/6/6/6
8	FES	B	302	2	-	-	0/1/1/1
9	SF4	J	303	2	-	-	0/6/5/5
5	FAD	I	601	1	-	9/30/50/50	0/6/6/6
12	PCI	K	1131	-	-	-	0/1/1/1
11	HEM	G	1130	3,4	-	4/6/54/54	-
11	HEM	C	1130	3,4	-	2/6/54/54	-
9	SF4	F	303	2	-	-	0/6/5/5
8	FES	F	302	2	-	-	0/1/1/1
9	SF4	B	303	2	-	-	0/6/5/5
5	FAD	A	601	1	-	4/30/50/50	0/6/6/6
10	F3S	J	304	2	-	-	0/3/3/3
10	F3S	F	304	2	-	-	0/3/3/3
12	PCI	G	1131	-	-	-	0/1/1/1
6	TEO	A	1589	-	-	2/2/8/8	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1130	HEM	C3B-C2B	-5.63	1.32	1.40
11	G	1130	HEM	C3C-C2C	-5.49	1.32	1.40
11	K	1130	HEM	C3D-C2D	5.34	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	1130	HEM	C3B-C2B	-5.30	1.33	1.40
11	K	1130	HEM	C3B-C2B	-5.29	1.33	1.40
11	G	1130	HEM	C3D-C2D	5.11	1.52	1.37
5	E	601	FAD	C4X-N5	5.04	1.40	1.33
5	A	601	FAD	C4X-N5	5.03	1.40	1.33
11	C	1130	HEM	C3C-C2C	-5.02	1.33	1.40
11	C	1130	HEM	C3D-C2D	4.91	1.52	1.37
5	E	601	FAD	C10-N1	4.87	1.39	1.33
5	I	601	FAD	C10-N1	4.72	1.39	1.33
5	I	601	FAD	C4X-N5	4.58	1.39	1.33
11	K	1130	HEM	C3C-C2C	-4.26	1.34	1.40
5	I	601	FAD	C2A-N3A	4.21	1.38	1.32
12	C	1131	PCI	C4-CL3	3.74	1.80	1.72
5	A	601	FAD	C10-N1	3.73	1.38	1.33
11	G	1130	HEM	C3B-CAB	3.71	1.55	1.47
5	A	601	FAD	C2A-N3A	3.58	1.37	1.32
11	K	1130	HEM	C3B-CAB	3.55	1.55	1.47
5	E	601	FAD	C2A-N3A	3.53	1.37	1.32
5	I	601	FAD	C4-N3	3.43	1.39	1.33
12	G	1131	PCI	C6-CL5	3.42	1.80	1.72
11	K	1130	HEM	C3C-CAC	3.41	1.54	1.47
12	K	1131	PCI	C4-CL3	3.38	1.80	1.72
5	E	601	FAD	C4-N3	3.38	1.38	1.33
12	G	1131	PCI	C5-CL4	3.31	1.80	1.72
12	K	1131	PCI	C2-CL1	3.30	1.80	1.72
12	K	1131	PCI	C6-CL5	3.25	1.79	1.72
12	K	1131	PCI	C5-CL4	3.17	1.79	1.72
12	G	1131	PCI	C2-CL1	3.15	1.79	1.72
12	G	1131	PCI	C3-CL2	3.15	1.79	1.72
5	A	601	FAD	C5X-N5	3.03	1.40	1.35
12	C	1131	PCI	C5-CL4	3.00	1.79	1.72
11	G	1130	HEM	C3C-CAC	3.00	1.54	1.47
5	A	601	FAD	C4-N3	2.94	1.38	1.33
11	C	1130	HEM	C3B-CAB	2.75	1.53	1.47
12	K	1131	PCI	C3-CL2	2.72	1.78	1.72
5	I	601	FAD	C5X-N5	2.65	1.39	1.35
5	A	601	FAD	C2A-N1A	2.64	1.38	1.33
5	I	601	FAD	C2A-N1A	2.59	1.38	1.33
12	C	1131	PCI	C6-CL5	2.49	1.78	1.72
5	I	601	FAD	C1'-N10	2.48	1.50	1.48
12	C	1131	PCI	C2-CL1	2.40	1.78	1.72
12	G	1131	PCI	C4-CL3	2.34	1.77	1.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1130	HEM	C3C-CAC	2.33	1.52	1.47
5	I	601	FAD	C4X-C10	2.28	1.41	1.38
5	E	601	FAD	C5X-N5	2.26	1.39	1.35
11	C	1130	HEM	CAA-C2A	2.20	1.55	1.52
11	K	1130	HEM	CAD-C3D	2.05	1.55	1.52
11	G	1130	HEM	C1C-C2C	2.04	1.47	1.42
12	G	1131	PCI	C5-C4	-2.01	1.35	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	601	FAD	C4-N3-C2	7.81	121.74	115.14
5	A	601	FAD	C4-N3-C2	7.20	121.22	115.14
5	E	601	FAD	C4-N3-C2	5.71	119.96	115.14
5	A	601	FAD	N3A-C2A-N1A	-5.32	120.36	128.68
12	G	1131	PCI	C1-C6-CL5	5.29	124.02	118.08
5	E	601	FAD	N3A-C2A-N1A	-5.20	120.56	128.68
5	I	601	FAD	N3A-C2A-N1A	-4.90	121.03	128.68
11	C	1130	HEM	CAD-CBD-CGD	-4.63	104.91	112.67
5	E	601	FAD	C4X-N5-C5X	3.82	120.58	116.77
11	G	1130	HEM	CBA-CAA-C2A	-3.77	105.54	112.49
5	E	601	FAD	C4-C4X-N5	3.69	122.81	118.60
11	K	1130	HEM	CBA-CAA-C2A	-3.67	105.72	112.49
5	I	601	FAD	C5X-C9A-N10	3.55	120.29	117.72
11	G	1130	HEM	CAD-CBD-CGD	-3.48	106.84	112.67
5	A	601	FAD	C4X-N5-C5X	3.47	120.24	116.77
5	A	601	FAD	C4-C4X-N5	3.44	122.53	118.60
11	C	1130	HEM	C4C-C3C-C2C	3.40	109.28	106.90
5	E	601	FAD	C10-C4X-N5	-3.39	118.91	121.26
5	I	601	FAD	C10-C4X-N5	-3.33	118.96	121.26
5	A	601	FAD	C5X-C9A-N10	3.32	120.12	117.72
5	I	601	FAD	C4-C4X-N5	3.31	122.39	118.60
5	E	601	FAD	C5X-C9A-N10	3.29	120.10	117.72
5	I	601	FAD	C4X-C4-N3	-3.17	119.10	123.43
5	A	601	FAD	C4'-C3'-C2'	-3.16	106.79	113.36
5	E	601	FAD	C5'-C4'-C3'	-3.14	106.13	112.20
5	A	601	FAD	C6-C5X-N5	3.11	122.48	119.05
12	G	1131	PCI	C4-C3-CL2	-3.08	114.07	119.98
5	I	601	FAD	C4X-N5-C5X	3.05	119.82	116.77
5	E	601	FAD	P-O3P-PA	-3.04	122.39	132.83
5	I	601	FAD	C1'-N10-C10	3.03	121.12	118.41
5	E	601	FAD	C4'-C3'-C2'	-2.94	107.25	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	1131	PCI	C1-C2-CL1	2.90	121.33	118.08
12	G	1131	PCI	C2-C3-CL2	2.87	125.49	119.98
12	C	1131	PCI	C1-C2-CL1	2.86	121.29	118.08
5	E	601	FAD	C4A-C5A-N7A	-2.85	106.43	109.40
5	A	601	FAD	C4-C4X-C10	-2.82	118.08	119.95
12	K	1131	PCI	C1-C6-CL5	2.81	121.23	118.08
11	G	1130	HEM	C1D-C2D-C3D	-2.77	105.07	107.00
5	A	601	FAD	C4X-C4-N3	-2.76	119.66	123.43
5	A	601	FAD	C10-C4X-N5	-2.71	119.38	121.26
11	K	1130	HEM	C4C-C3C-C2C	2.70	108.78	106.90
5	E	601	FAD	C4-C4X-C10	-2.54	118.27	119.95
5	A	601	FAD	C1'-N10-C9A	2.50	120.26	118.29
11	C	1130	HEM	CBA-CAA-C2A	-2.49	107.90	112.49
11	K	1130	HEM	CBD-CAD-C3D	2.34	116.80	112.48
5	I	601	FAD	C4'-C3'-C2'	-2.34	108.49	113.36
12	G	1131	PCI	C1-C2-CL1	2.31	120.67	118.08
5	I	601	FAD	C6-C5X-N5	2.29	121.57	119.05
11	G	1130	HEM	C4C-C3C-C2C	2.26	108.48	106.90
5	I	601	FAD	C4A-C5A-N7A	-2.19	107.11	109.40
12	G	1131	PCI	C6-C5-CL4	2.14	124.10	119.98
12	G	1131	PCI	C1-C2-C3	-2.09	119.43	121.15
5	E	601	FAD	C6-C5X-N5	2.06	121.32	119.05
5	A	601	FAD	C9A-C5X-N5	-2.05	119.15	122.36
12	G	1131	PCI	C5-C6-CL5	-2.05	116.04	119.98
11	G	1130	HEM	CAA-CBA-CGA	-2.02	109.29	112.67

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1589	TEO	C1-C2-C3-C4
11	K	1130	HEM	C2D-C3D-CAD-CBD
11	K	1130	HEM	C4D-C3D-CAD-CBD
11	G	1130	HEM	C1A-C2A-CAA-CBA
11	G	1130	HEM	C3A-C2A-CAA-CBA
11	G	1130	HEM	C2D-C3D-CAD-CBD
11	G	1130	HEM	C4D-C3D-CAD-CBD
5	E	601	FAD	PA-O3P-P-O5'
5	A	601	FAD	O4B-C4B-C5B-O5B
6	A	1589	TEO	C1-C2-C3-C4
5	I	601	FAD	N10-C1'-C2'-O2'
5	I	601	FAD	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
5	I	601	FAD	C2'-C3'-C4'-O4'
5	I	601	FAD	C2'-C3'-C4'-C5'
5	I	601	FAD	O3'-C3'-C4'-C5'
5	I	601	FAD	O4'-C4'-C5'-O5'
11	C	1130	HEM	C2D-C3D-CAD-CBD
11	C	1130	HEM	C4D-C3D-CAD-CBD
5	I	601	FAD	O3'-C3'-C4'-O4'
5	I	601	FAD	O4B-C4B-C5B-O5B
5	A	601	FAD	C3B-C4B-C5B-O5B
5	E	601	FAD	P-O3P-PA-O2A
5	E	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	N10-C1'-C2'-O2'
5	I	601	FAD	C3B-C4B-C5B-O5B
6	I	1589	TEO	O2-C2-C3-C4
6	E	1589	TEO	O2-C2-C3-C4
6	A	1589	TEO	O2-C2-C3-C4
5	A	601	FAD	P-O3P-PA-O1A
5	E	601	FAD	P-O3P-PA-O1A
5	E	601	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

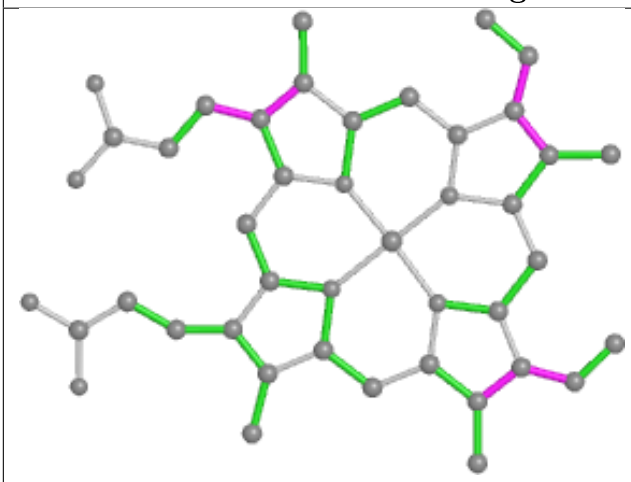
16 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1130	HEM	4	0
10	F	304	F3S	1	0
6	I	1589	TEO	2	0
9	J	303	SF4	1	0
6	A	1589	TEO	4	0
6	E	1589	TEO	2	0
5	I	601	FAD	6	0
11	C	1130	HEM	7	0
11	G	1130	HEM	7	0
5	E	601	FAD	5	0
9	F	303	SF4	1	0
5	A	601	FAD	7	0
9	B	303	SF4	1	0
10	J	304	F3S	2	0
12	G	1131	PCI	1	0
10	B	304	F3S	1	0

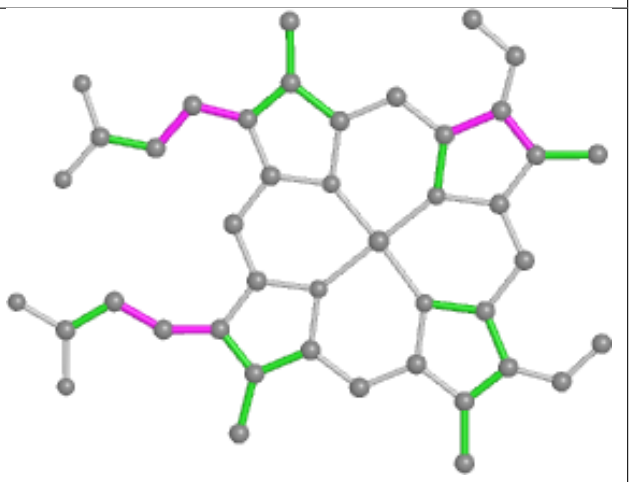
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

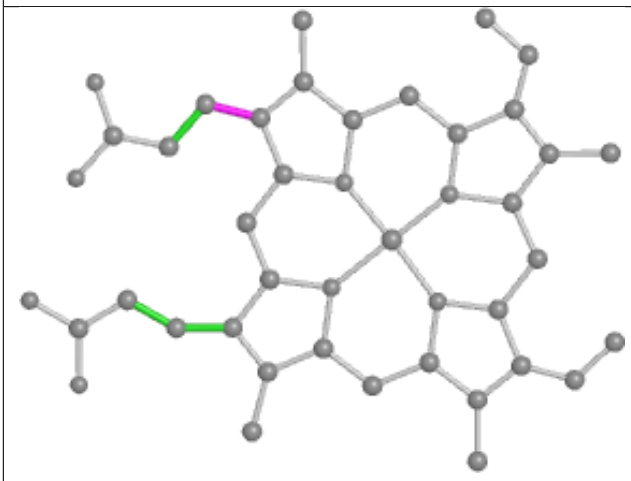
Ligand HEM K 1130



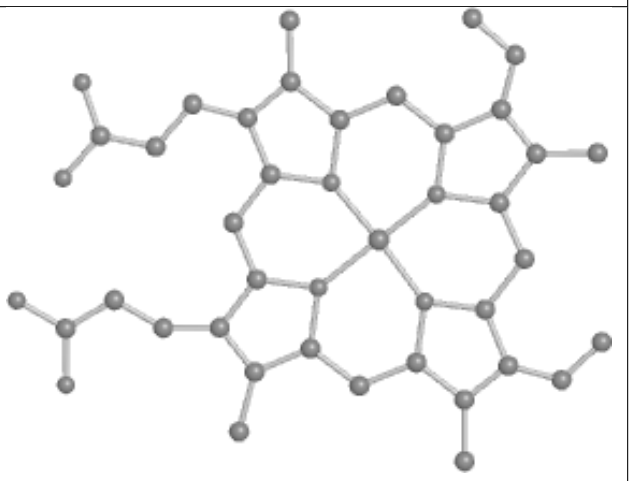
Bond lengths



Bond angles

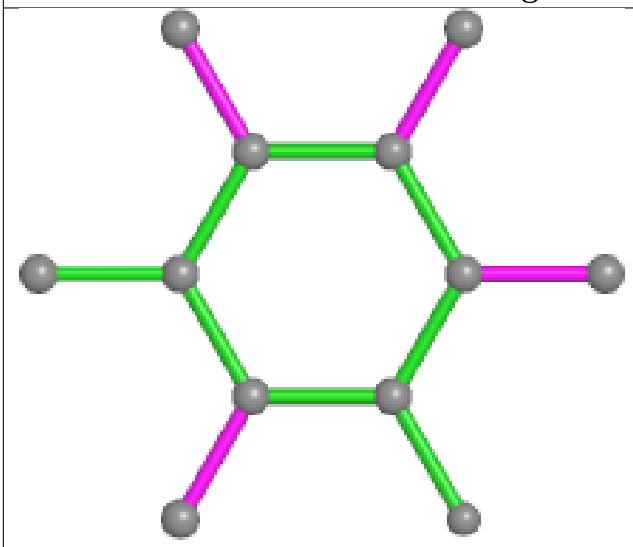


Torsions

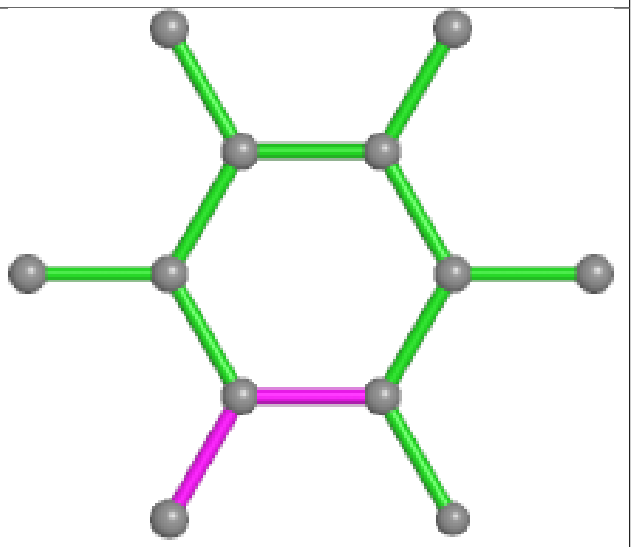


Rings

Ligand PCI C 1131



Bond lengths



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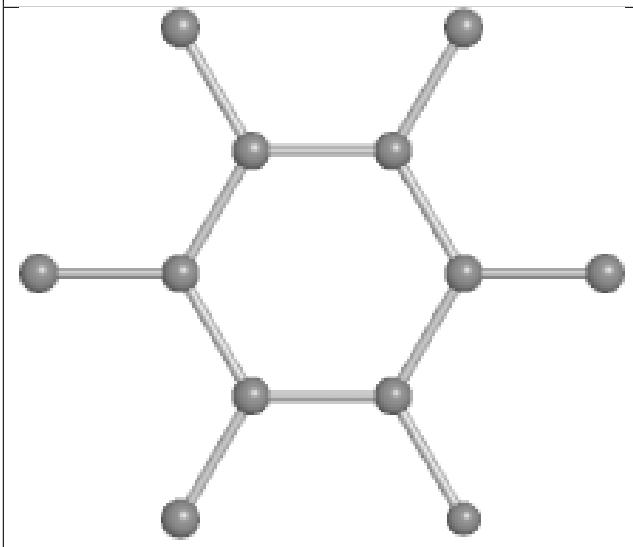

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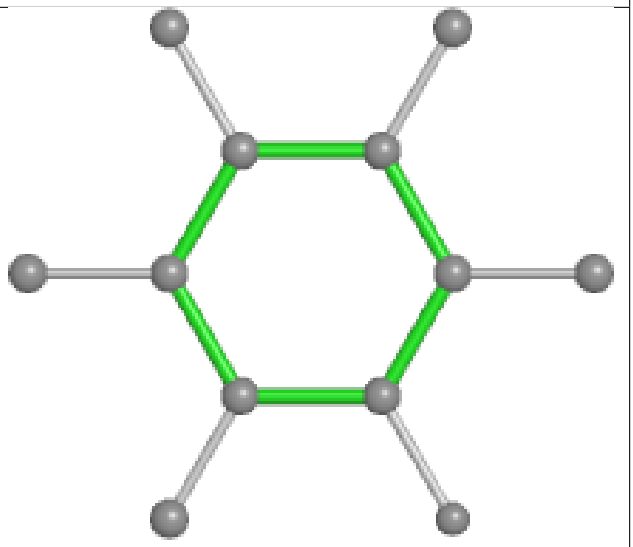
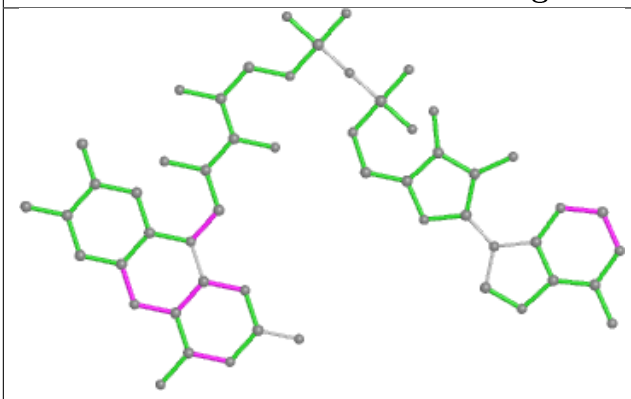


Rings

Ligand FAD I 601



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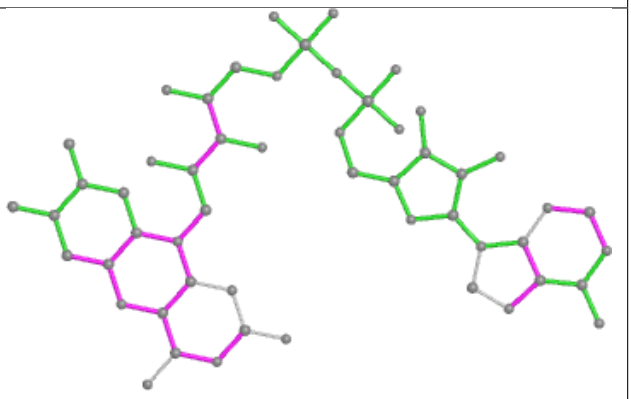
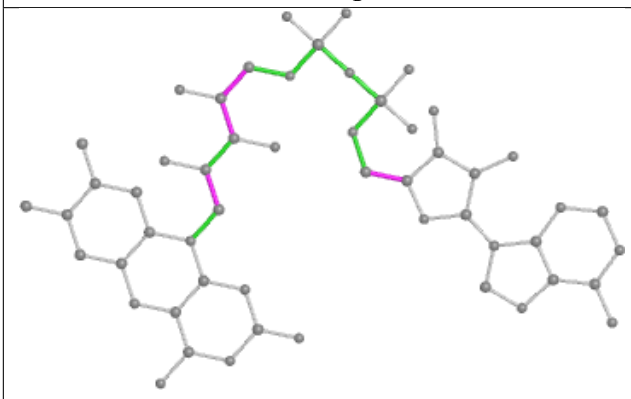


Bond angles



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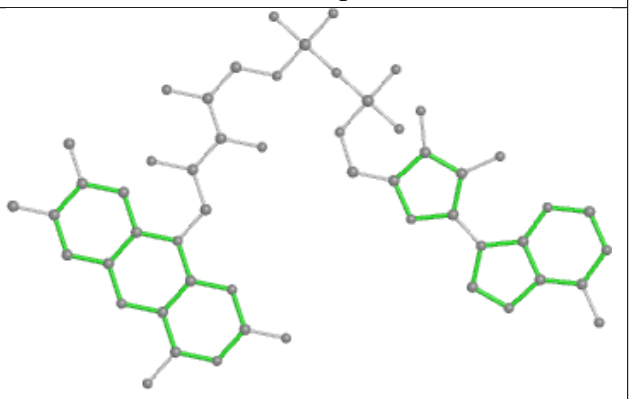
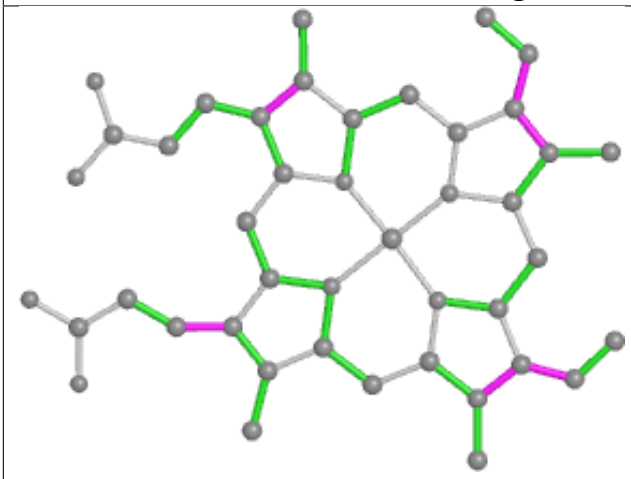


Rings

Ligand HEM C 1130



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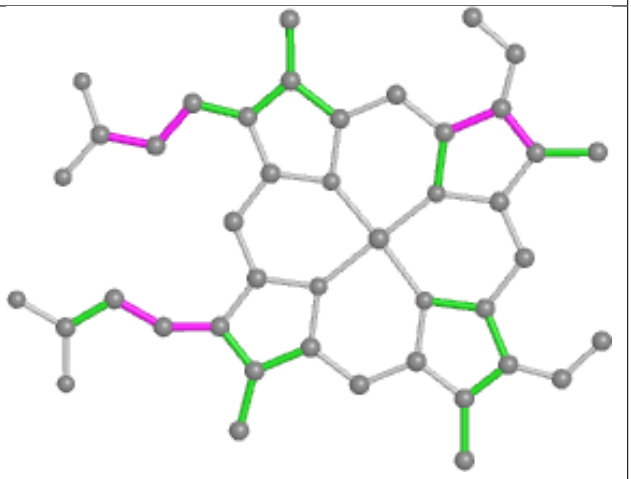
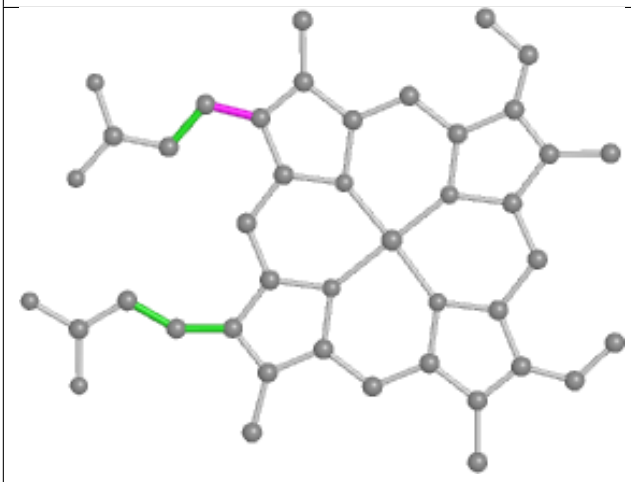


Bond angles



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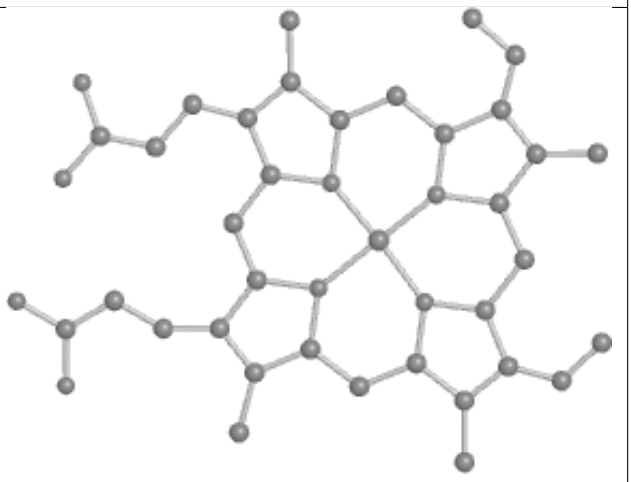
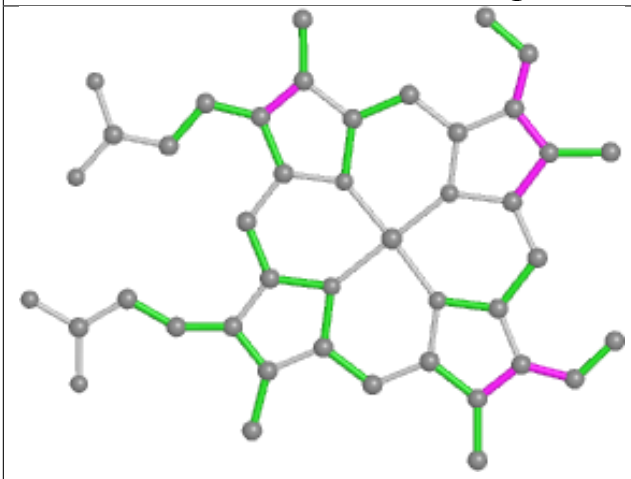


Rings

Ligand HEM G 1130



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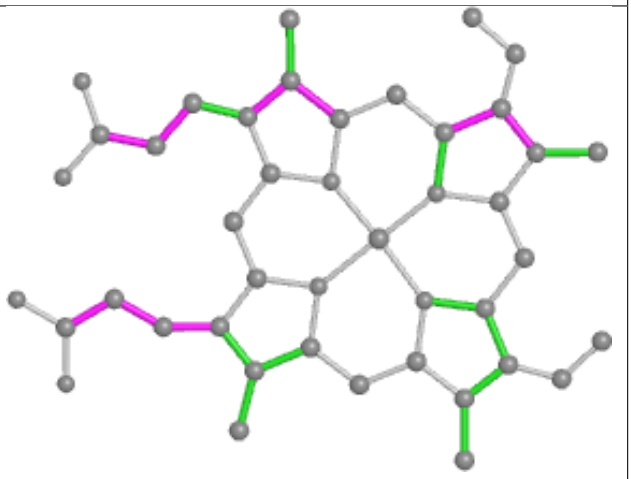

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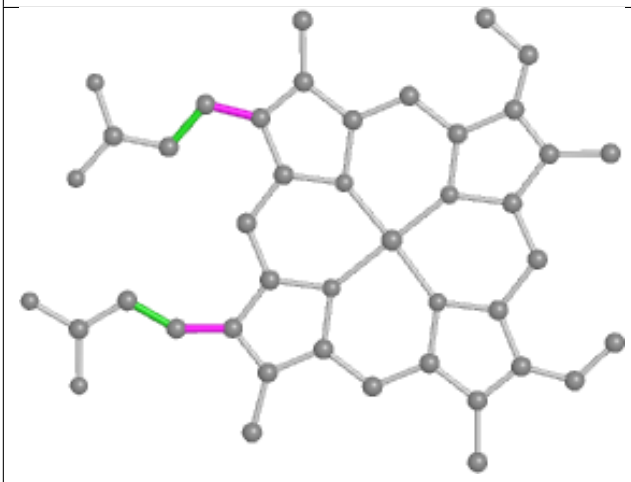

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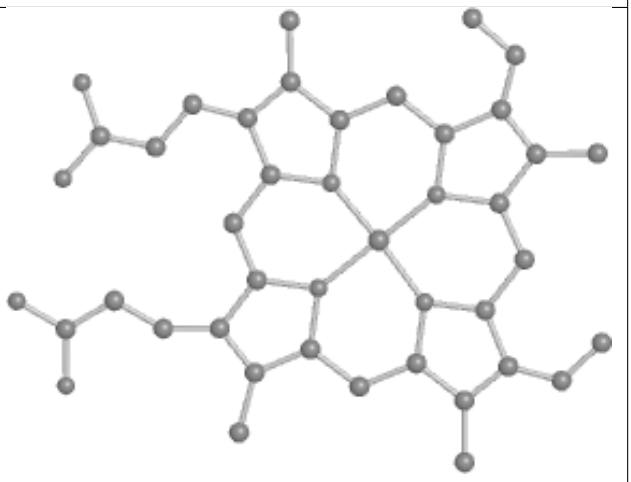
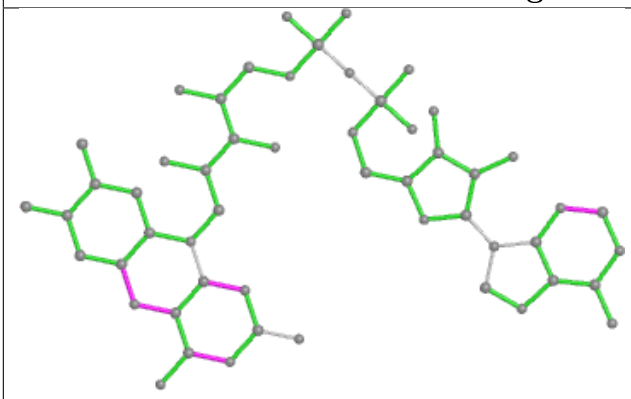


Rings

Ligand FAD E 601



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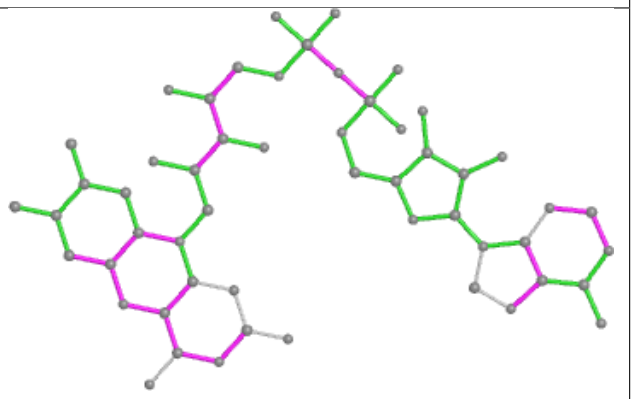
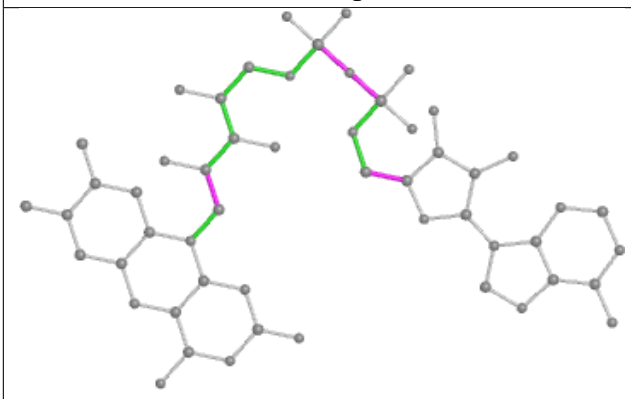


Bond angles



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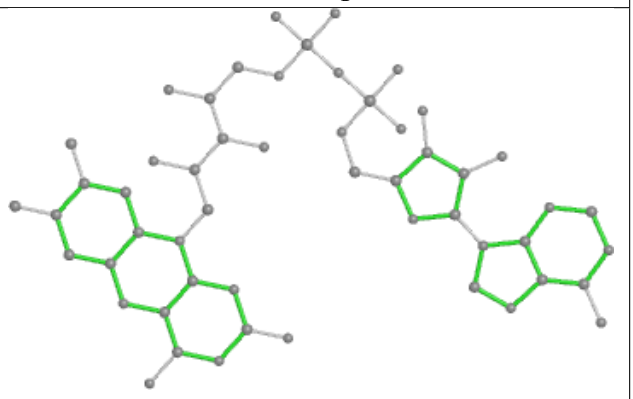
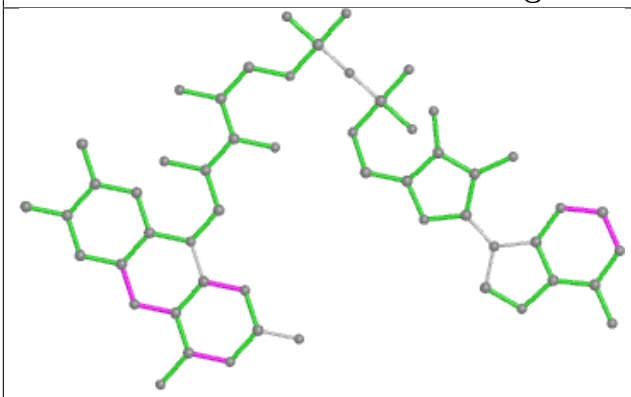


Rings

Ligand FAD A 601



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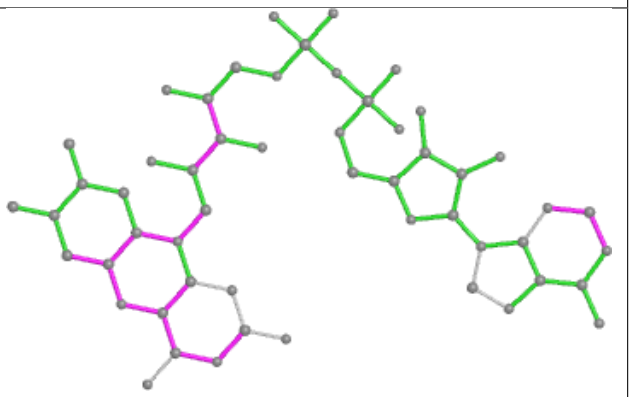
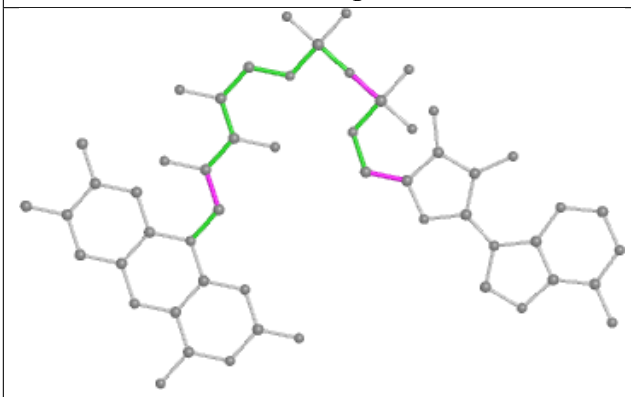
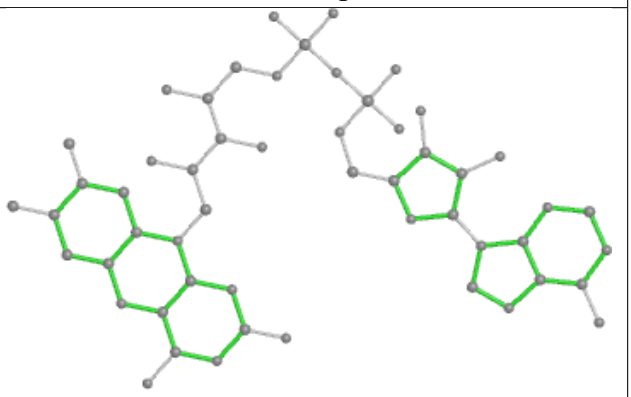


Bond angles

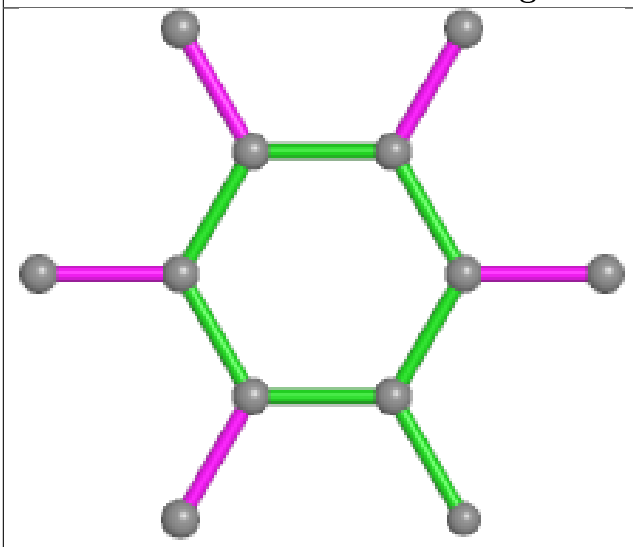


Torsions

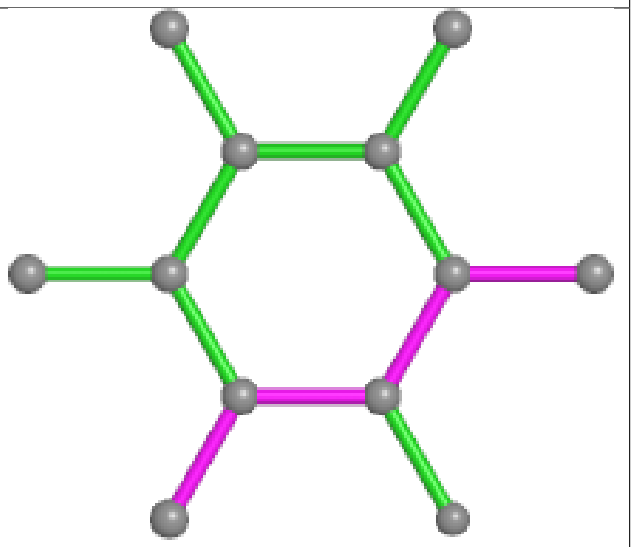


Rings

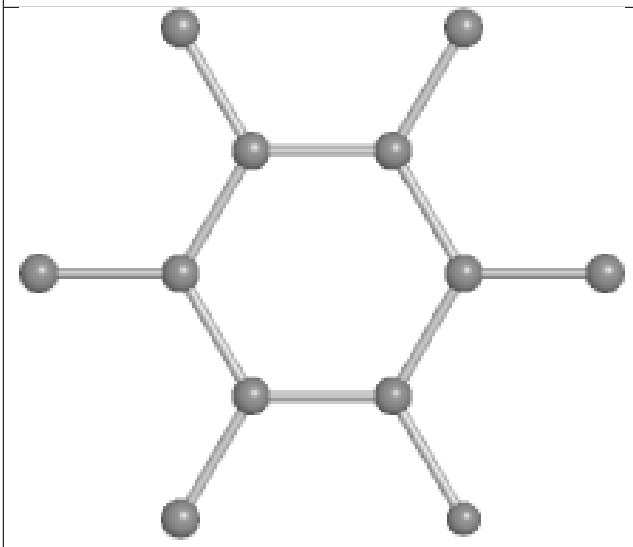
Ligand PCI K 1131



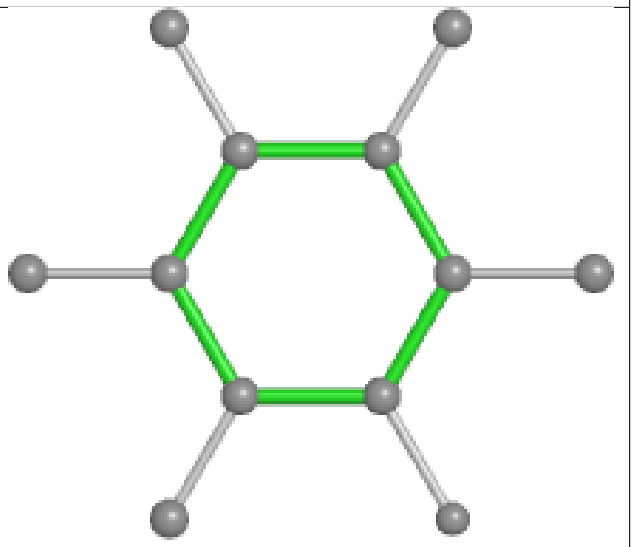
Bond lengths



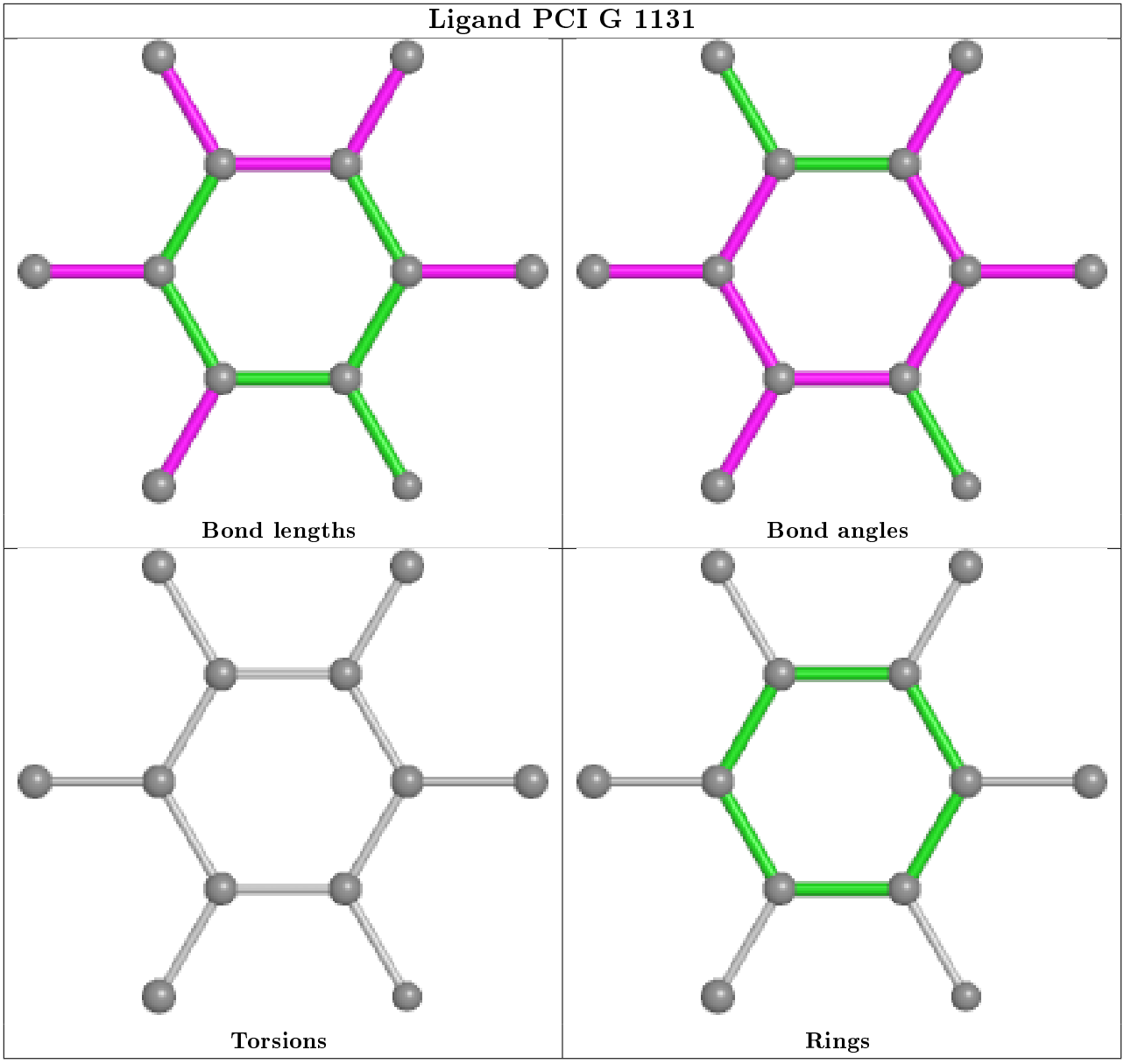
Bond angles



Torsions



Rings



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, 95^{th} 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%)	-0.01	4 (0%) 87 81	47, 48, 49, 51	0
1	E	588/588 (100%)	0.14	15 (2%) 56 40	47, 48, 49, 51	0
1	I	588/588 (100%)	0.51	58 (9%) 7 4	47, 48, 49, 51	0
2	B	238/238 (100%)	-0.02	10 (4%) 36 23	47, 48, 49, 50	0
2	F	238/238 (100%)	0.03	6 (2%) 57 43	47, 48, 49, 50	0
2	J	238/238 (100%)	0.32	18 (7%) 13 7	47, 48, 49, 50	0
3	C	122/129 (94%)	0.09	4 (3%) 46 30	47, 48, 49, 49	0
3	G	122/129 (94%)	0.47	13 (10%) 6 3	47, 48, 49, 49	0
3	K	122/129 (94%)	0.36	6 (4%) 29 17	47, 48, 49, 49	0
4	D	105/115 (91%)	-0.02	3 (2%) 51 36	47, 48, 49, 50	0
4	H	105/115 (91%)	0.10	8 (7%) 13 7	47, 48, 49, 50	0
4	L	105/115 (91%)	0.05	5 (4%) 30 18	47, 48, 49, 49	0
All	All	3159/3210 (98%)	0.18	150 (4%) 31 19	47, 48, 49, 51	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	68	PHE	5.5
3	K	129	TRP	5.3
1	I	204	GLY	5.1
1	I	268	HIS	4.9
3	C	129	TRP	4.6
1	I	334	SER	4.6
3	G	129	TRP	4.5
1	I	266	ASN	4.3
1	I	1	MET	4.0
4	H	42	GLU	4.0
3	K	68	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	450	ASN	3.6
1	E	451	ARG	3.5
1	E	304	ASP	3.4
4	H	41	GLY	3.4
1	I	306	PRO	3.4
1	I	420	GLN	3.4
4	L	48	TRP	3.4
2	J	18	PRO	3.4
3	K	8	GLN	3.3
2	B	1	MET	3.3
2	J	85	PRO	3.3
2	J	84	GLN	3.2
2	J	30	GLY	3.2
1	I	340	VAL	3.2
4	L	37	PHE	3.2
2	J	86	GLY	3.1
1	I	452	ASN	3.1
1	A	268	HIS	3.0
2	J	16	ASP	3.0
1	I	303	CYS	3.0
1	E	449	ASN	3.0
1	E	452	ASN	3.0
1	I	281	LYS	3.0
2	B	30	GLY	3.0
1	I	421	GLU	3.0
2	B	16	ASP	3.0
1	I	48	SER	3.0
1	I	345	GLU	3.0
1	I	205	ALA	2.9
1	I	298	ARG	2.9
1	I	316	ASP	2.9
2	J	28	ASP	2.9
2	J	83	ASN	2.9
4	D	42	GLU	2.9
2	F	1	MET	2.9
1	I	544	ASP	2.9
1	E	453	GLY	2.9
1	I	338	ALA	2.9
2	B	28	ASP	2.9
3	G	56	GLU	2.8
1	I	307	TRP	2.8
4	D	45	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	214	ASN	2.8
2	B	85	PRO	2.8
4	L	115	VAL	2.8
2	F	30	GLY	2.8
1	A	300	GLY	2.7
1	I	270	GLU	2.7
1	I	276	TYR	2.7
3	G	67	SER	2.7
3	G	69	PHE	2.7
2	J	13	ASP	2.6
1	I	388	GLU	2.6
4	H	49	ILE	2.6
1	I	534	THR	2.6
1	I	269	GLY	2.6
4	L	38	ALA	2.6
1	E	303	CYS	2.6
2	J	29	GLU	2.6
1	E	2	LYS	2.6
3	K	69	PHE	2.6
1	I	302	GLY	2.6
4	H	45	TYR	2.6
1	E	203	GLY	2.5
4	D	41	GLY	2.5
3	G	64	ILE	2.5
2	B	86	GLY	2.5
1	I	502	THR	2.5
2	F	16	ASP	2.5
2	F	29	GLU	2.5
1	I	218	ASN	2.5
1	E	344	LYS	2.4
1	I	543	PHE	2.4
3	G	62	SER	2.4
3	G	65	MET	2.4
1	I	478	ASP	2.4
1	E	496	ASN	2.4
2	J	11	ASN	2.4
2	J	87	LYS	2.4
3	G	59	GLU	2.4
1	I	427	GLY	2.4
1	I	49	ALA	2.4
1	I	295	ILE	2.4
1	I	300	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	203	GLY	2.3
4	H	40	SER	2.3
1	I	381	PRO	2.3
4	H	47	VAL	2.3
1	I	213	THR	2.3
1	I	428	ALA	2.3
1	I	448	ASN	2.3
1	I	451	ARG	2.3
1	I	500	ASP	2.3
2	B	2	ARG	2.3
1	I	588	TYR	2.3
2	B	84	GLN	2.3
1	A	373	GLU	2.2
1	I	319	GLY	2.2
1	I	382	GLY	2.2
2	J	12	PRO	2.2
4	H	51	PHE	2.2
1	I	312	LYS	2.2
3	G	53	SER	2.2
1	I	277	ALA	2.2
3	K	67	SER	2.2
1	I	215	ALA	2.2
4	L	45	TYR	2.2
1	I	342	PRO	2.2
2	J	15	ASP	2.2
2	J	17	ALA	2.2
4	H	43	LEU	2.2
1	I	52	GLY	2.2
1	E	433	SER	2.2
1	I	45	HIS	2.2
1	I	374	LYS	2.1
1	A	267	LYS	2.1
3	C	67	SER	2.1
3	G	60	GLN	2.1
2	J	2	ARG	2.1
2	J	10	TYR	2.1
1	I	404	SER	2.1
3	G	110	ALA	2.1
3	K	98	TYR	2.0
1	I	450	ASN	2.0
3	G	52	LEU	2.0
1	E	44	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	28	ASP	2.0
2	B	27	ALA	2.0
1	E	482	LYS	2.0
2	F	18	PRO	2.0
3	C	66	GLY	2.0
2	B	31	ARG	2.0
1	I	373	GLU	2.0
1	I	305	GLY	2.0
1	I	278	PRO	2.0
1	I	449	ASN	2.0
3	C	104	GLU	2.0
1	E	499	LEU	2.0
2	J	14	VAL	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 carbohydrates 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, 95^{th} 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	0.24	67,70,71,71	0
7	NA	I	1590	1/1	0.94	0.21	21,21,21,21	0
6	TEO	E	1589	9/9	0.94	0.18	38,39,39,41	0
12	PCI	G	1131	12/12	0.94	0.21	46,48,50,51	0
12	PCI	K	1131	12/12	0.94	0.25	56,58,60,61	0
5	FAD	I	601	53/53	0.95	0.19	42,50,57,58	0
6	TEO	A	1589	9/9	0.95	0.18	26,27,30,32	0
12	PCI	C	1131	12/12	0.96	0.20	40,42,44,48	0
11	HEM	K	1130	43/43	0.96	0.21	46,48,59,61	0
7	NA	A	1590	1/1	0.97	0.08	2,2,2,2	0

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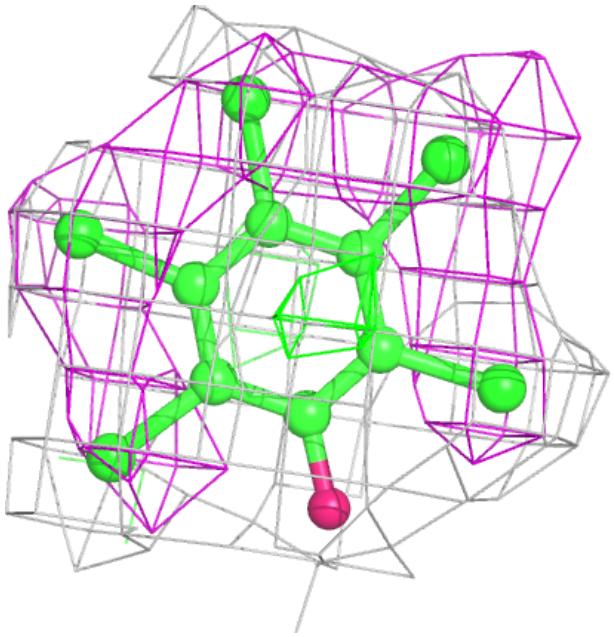
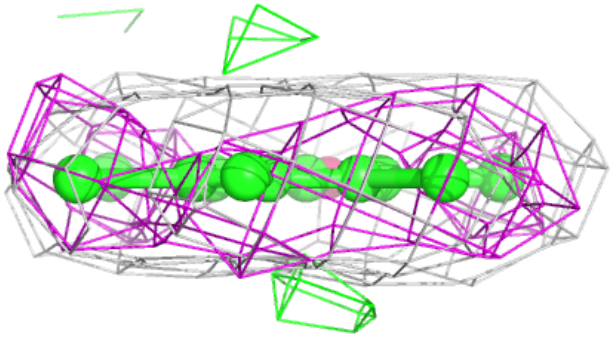
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FAD	E	601	53/53	0.97	0.15	26,38,42,44	0
5	FAD	A	601	53/53	0.97	0.15	20,24,34,39	0
11	HEM	C	1130	43/43	0.97	0.24	37,41,46,48	0
11	HEM	G	1130	43/43	0.97	0.20	43,47,53,56	0
10	F3S	J	304	7/7	0.98	0.09	47,50,53,56	0
10	F3S	F	304	7/7	0.98	0.07	43,46,48,51	0
10	F3S	B	304	7/7	0.98	0.07	39,39,41,41	0
7	NA	E	1590	1/1	0.98	0.07	12,12,12,12	0
8	FES	J	302	4/4	0.99	0.05	55,56,58,58	0
9	SF4	B	303	8/8	0.99	0.10	27,29,31,31	0
9	SF4	F	303	8/8	0.99	0.07	35,36,38,38	0
8	FES	F	302	4/4	0.99	0.10	38,39,42,44	0
9	SF4	J	303	8/8	0.99	0.07	46,48,50,50	0
8	FES	B	302	4/4	0.99	0.11	31,32,33,36	0

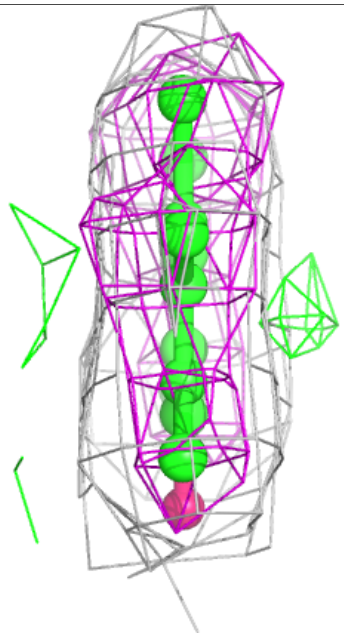
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PCI G 1131:

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

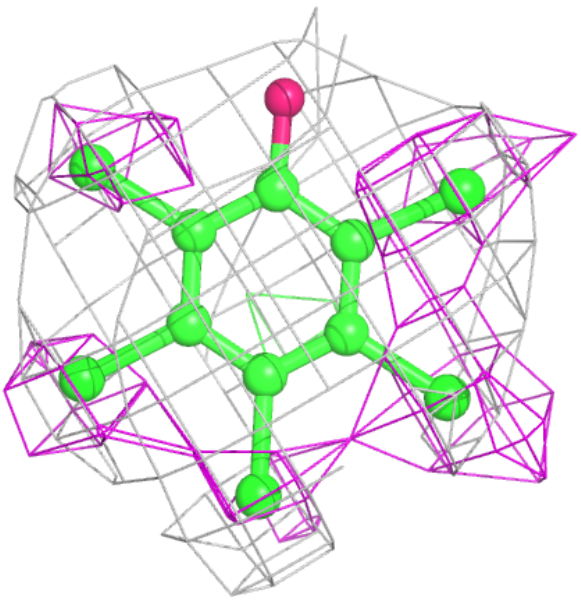


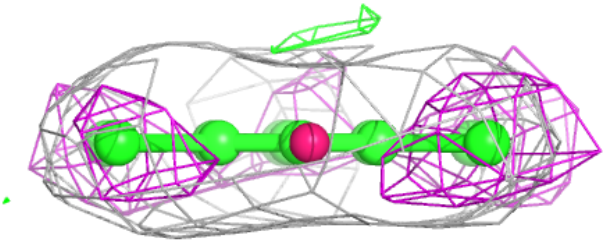


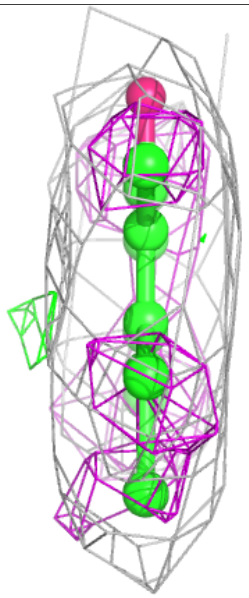


Electron density around PCI K 1131:

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

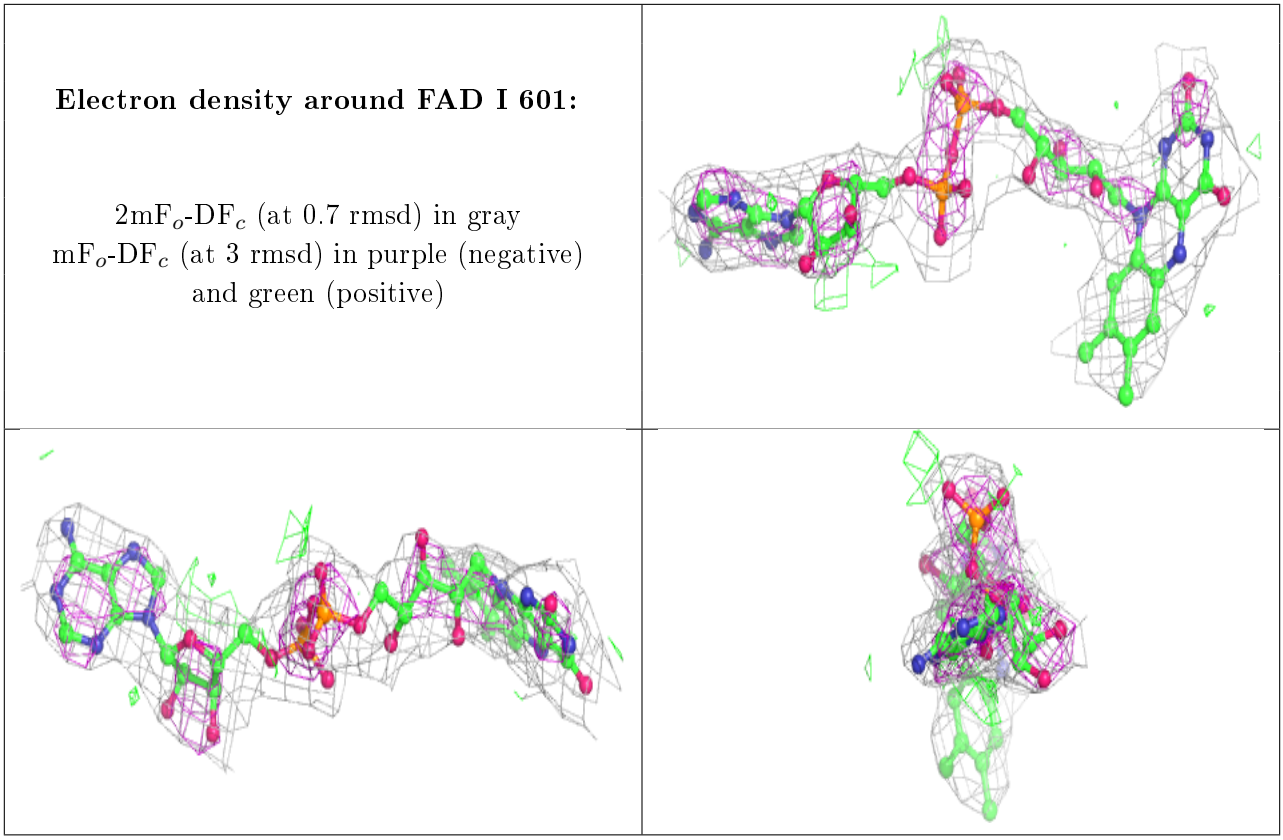






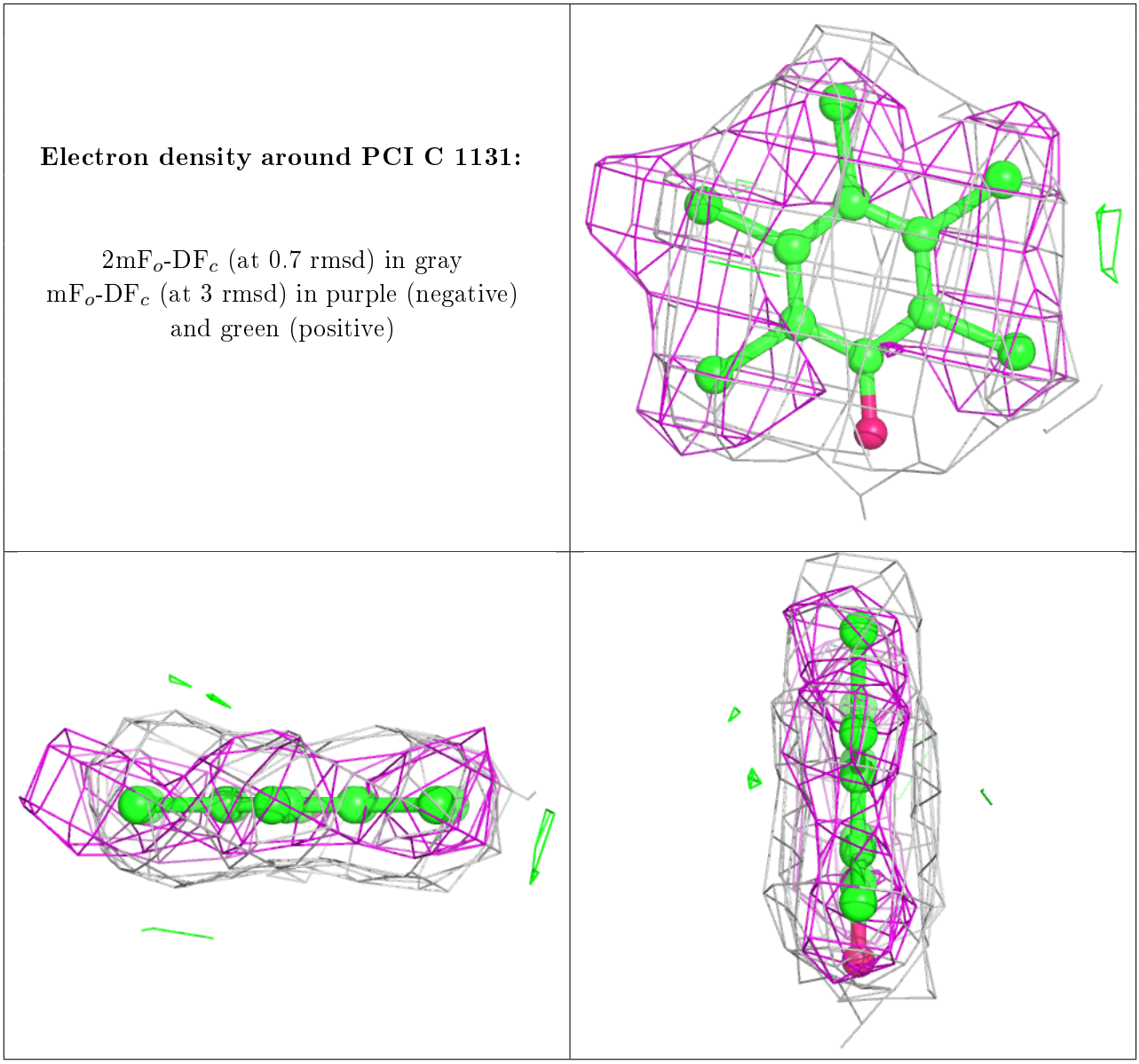
Electron density around FAD I 601:

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



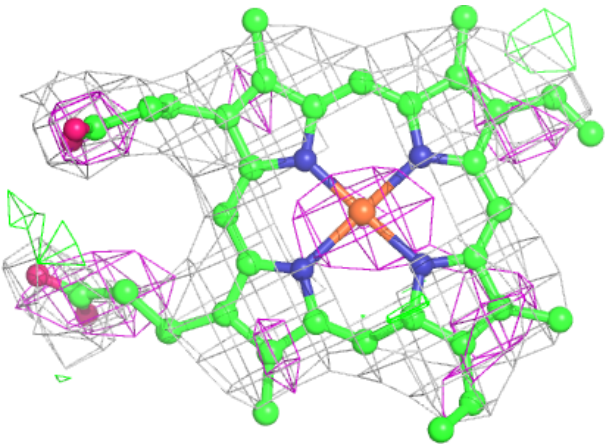
Electron density around PCI C 1131:

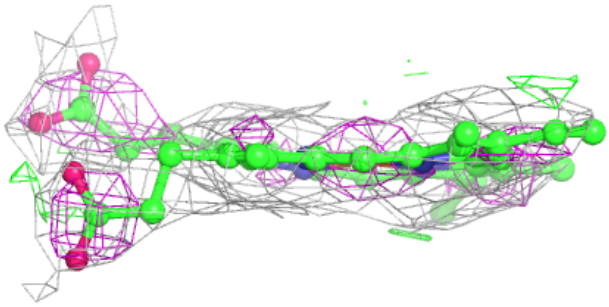
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

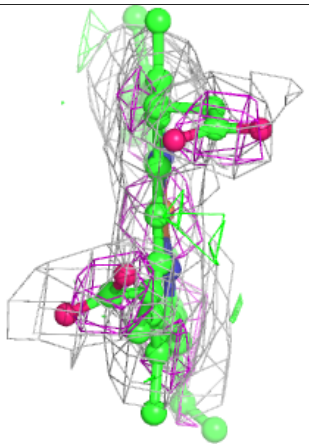


Electron density around HEM K 1130:

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

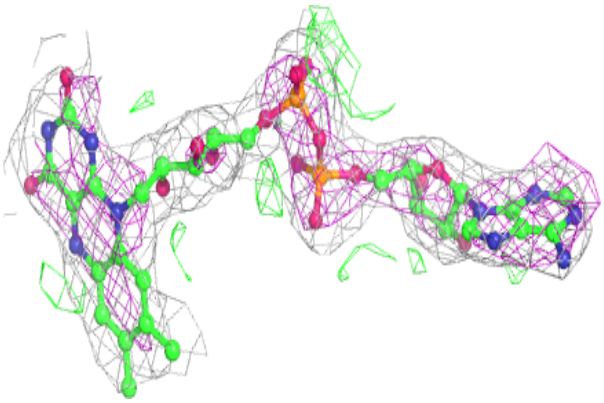


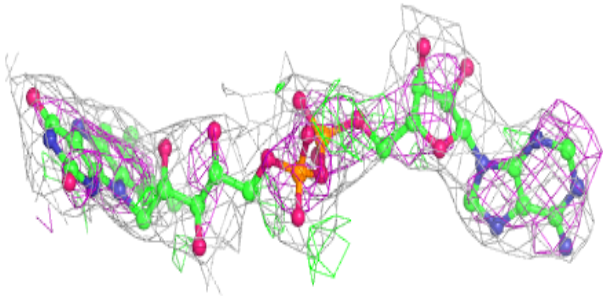


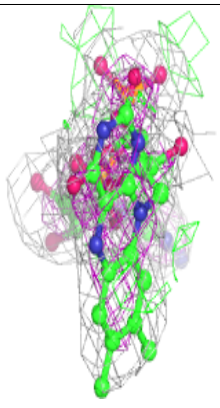


Electron density around FAD E 601:

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

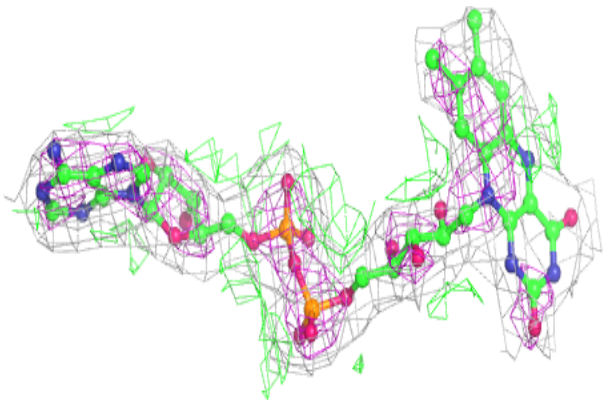


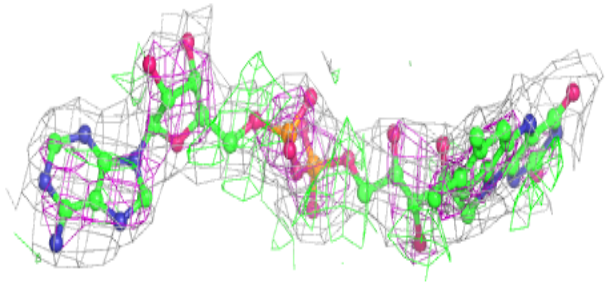


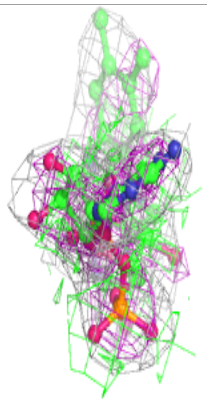


Electron density around FAD A 601:

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

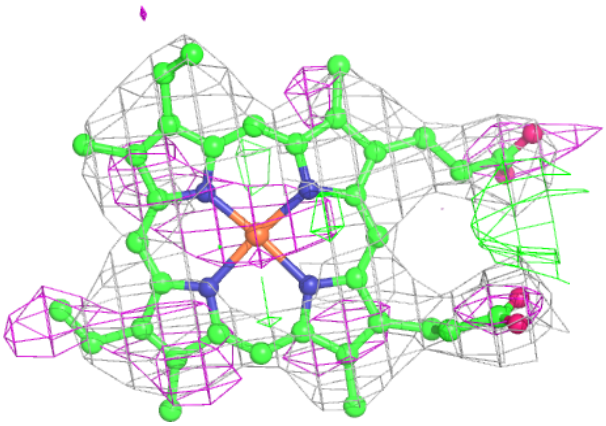


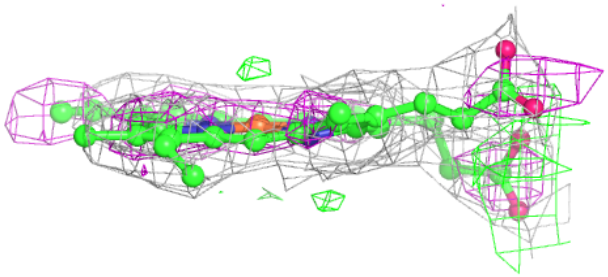


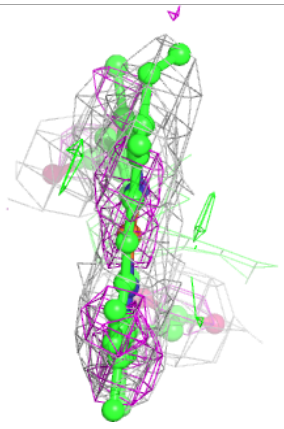


Electron density around HEM C 1130:

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

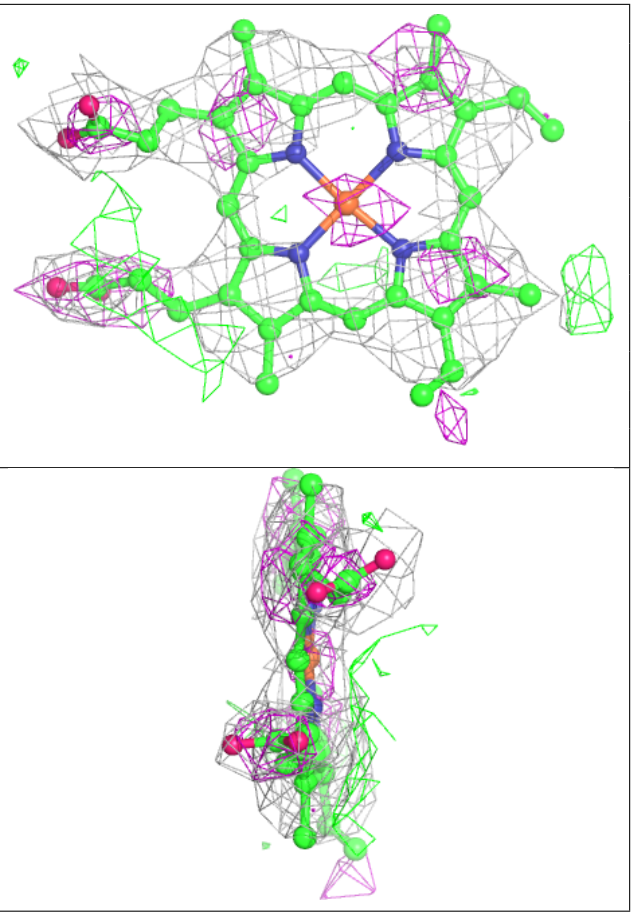






Electron density around HEM G 1130:

$2mF_o$-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

There are no such residues in this entry.