



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 11:50 PM EDT

PDB ID : 1NTK
Title : Crystal Structure of Mitochondrial Cytochrome bc1 in Complex with Antimycin A1
Authors : Gao, X.; Wen, X.; Esser, L.; Quinn, B.; Yu, L.; Yu, C.-A.; Xia, D.
Deposited on : 2003-01-30
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

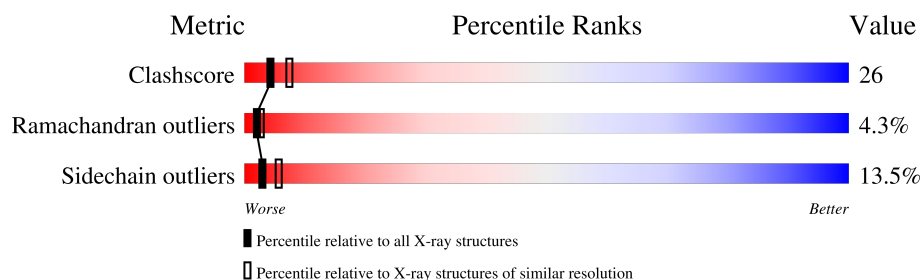
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	61% 33% 7%
2	B	439	57% 32% 6% .
3	C	379	55% 35% 7% .
4	D	241	42% 44% 11% .
5	E	196	74% 21% . .
6	F	110	50% 37% 8% 5%
7	G	81	58% 28% 11% .
8	H	78	47% 37% 12% . .

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Mol	Chain	Length	Quality of chain
9	I	57	<div><div></div><div>14%</div><div>42%</div><div>42%</div><div></div></div>
10	J	62	<div><div></div><div>53%</div><div>35%</div><div>8%</div><div></div></div>
11	K	56	<div><div></div><div>52%</div><div>29%</div><div>14%</div><div>5%</div></div>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 17118 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 Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3457	2161	609	667	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3171	1993	562	609	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			3003	2013	471	501	18			

- Molecule 4 is a protein called cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1918	1225	330	348	15			

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			910	576	165	167	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	79	Total	C	N	O	S	0	0	0
			659	430	122	106	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	76	Total	C	N	O	S	0	0	0
			626	378	109	134	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase 8 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	60	Total	C	N	O	0	0	0
			495	324	86	85			

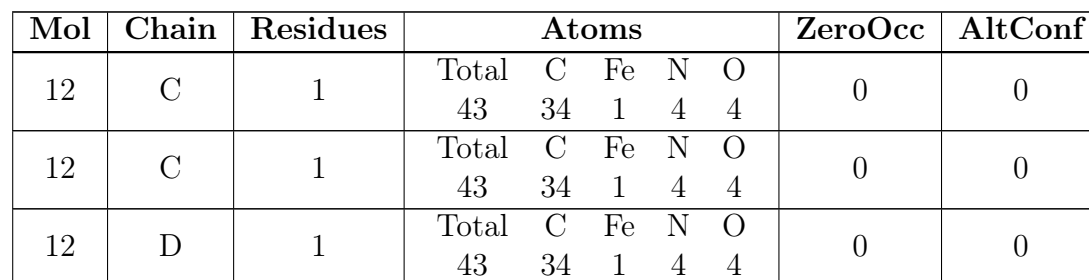
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			441	295	79	66	1			

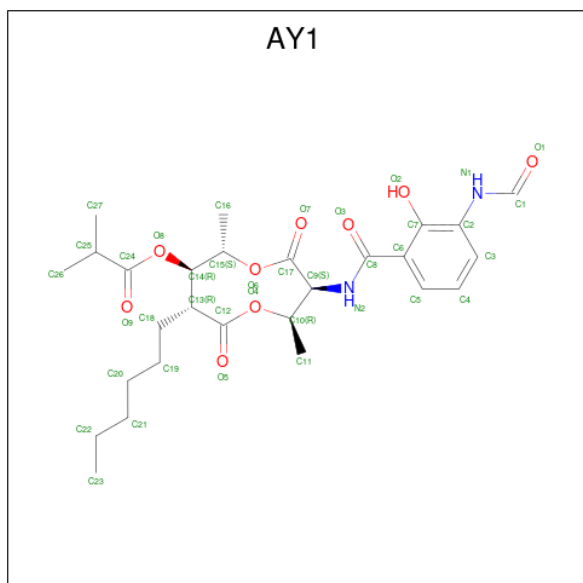
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	SEE REMARK 999	UNP P07552

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).

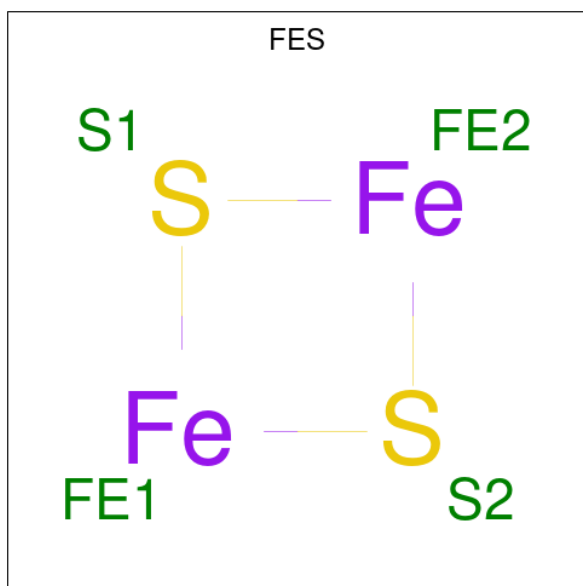


- Molecule 13 is [(2R,3S,6S,7R,8R)-3-[(3-formamido-2-oxidanyl-phenyl)carbonylamino]-8-hexyl-2,6-dimethyl-4,9-bis(oxidanylidene)-1,5-dioxonan-7-yl] 2-methylpropanoate (three-letter code: AY1) (formula: C₂₇H₃₈N₂O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			38	27	2	9		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	95	Total	O	0	0
			95	95		
15	B	83	Total	O	0	0
			83	83		
15	C	61	Total	O	0	0
			61	61		
15	D	27	Total	O	0	0
			27	27		
15	E	3	Total	O	0	0
			3	3		
15	F	30	Total	O	0	0
			30	30		
15	G	22	Total	O	0	0
			22	22		
15	I	6	Total	O	0	0
			6	6		

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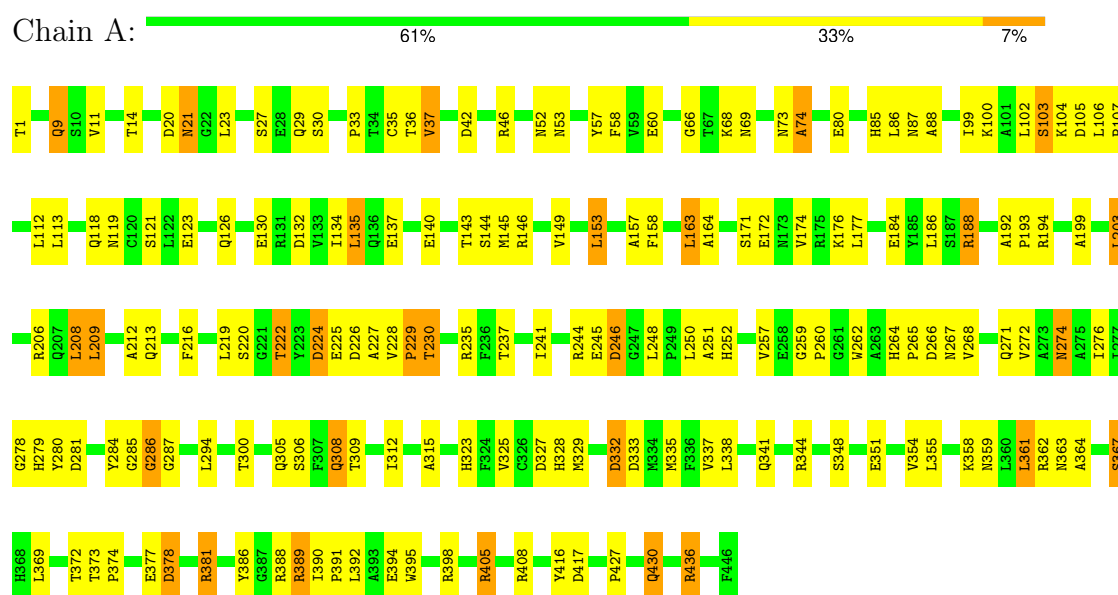
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	5	Total	O	0	0
			5	5		
15	K	10	Total	O	0	0
			10	10		

3 Residue-property plots

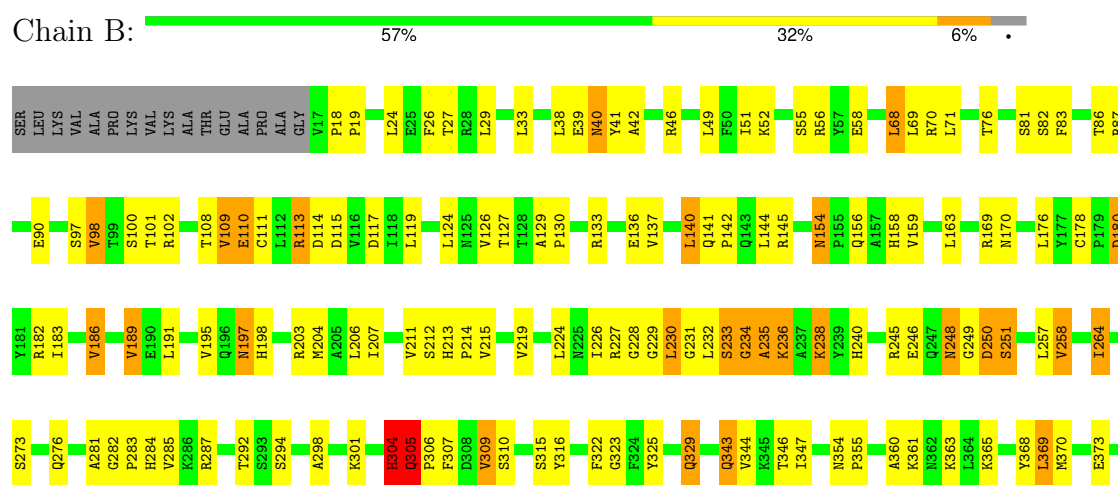
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

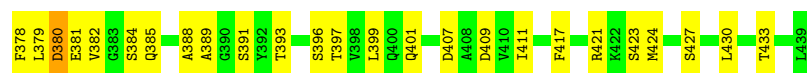
Note EDS was not executed.

- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial



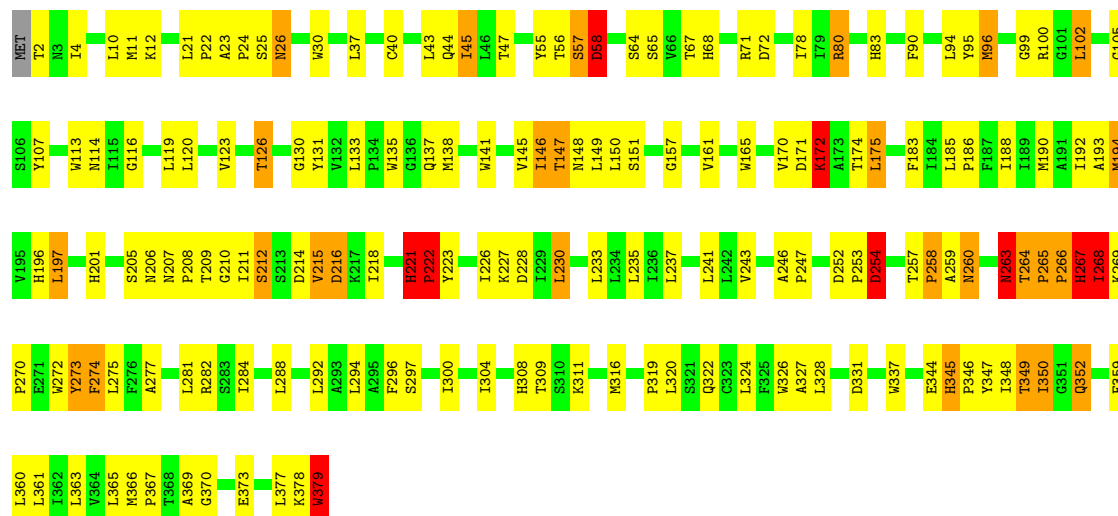
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial





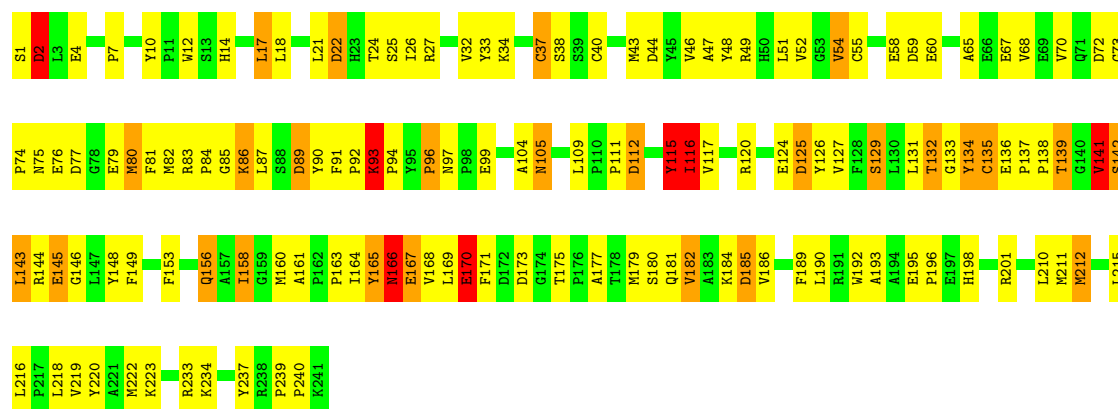
• Molecule 3: Cytochrome b

Chain C: 55% 35% 7% •



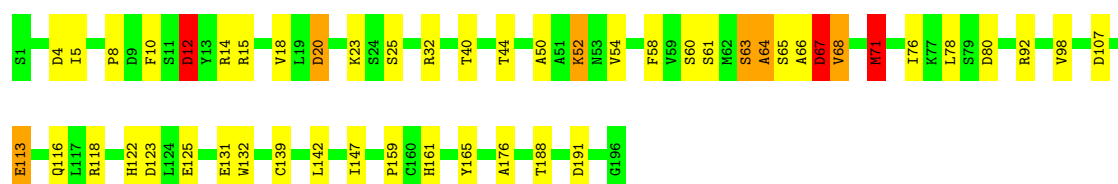
• Molecule 4: cytochrome c1

Chain D: 42% 44% 11% •

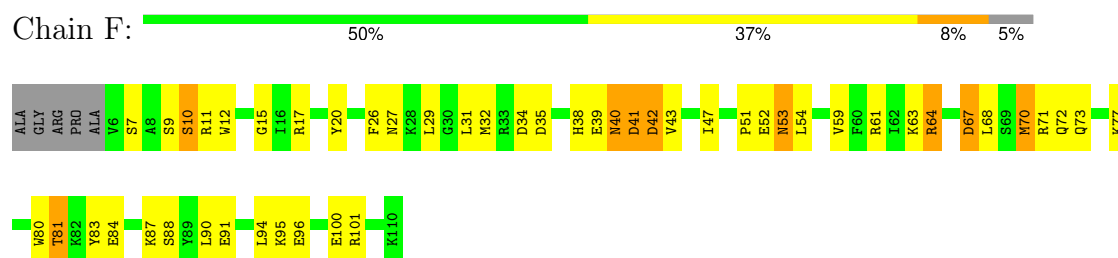


• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, MITOCHONDRIAL

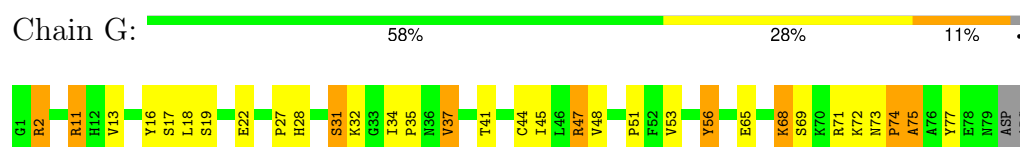
Chain E: 74% 21% • •



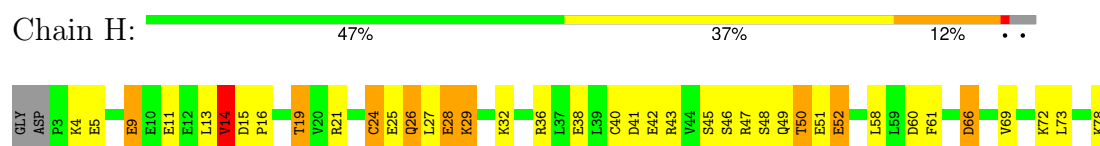
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



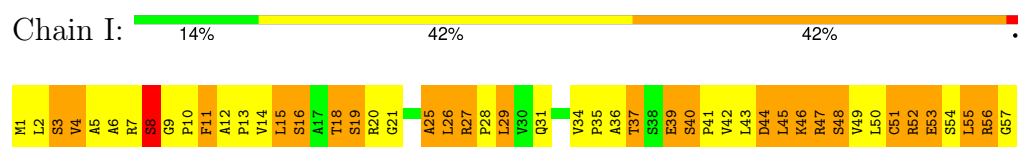
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



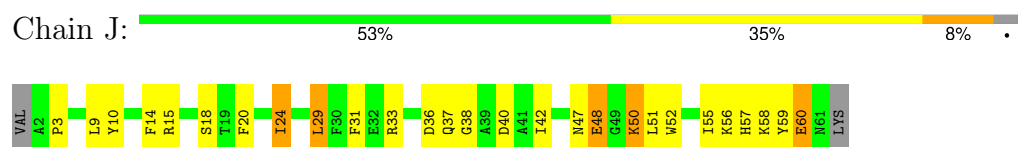
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein



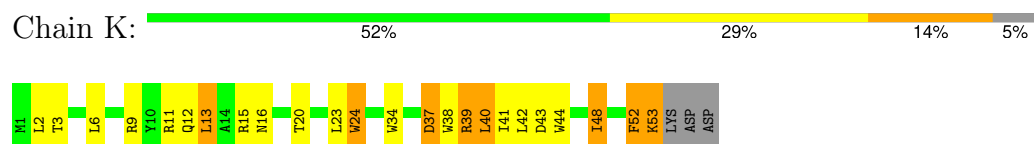
- Molecule 9: Ubiquinol-cytochrome C reductase 8 kDa protein



- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein



- Molecule 11: Ubiquinol-cytochrome C reductase complex 6.4 kDa protein



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.78Å 153.78Å 592.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.5 (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.233 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17118	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AY1, FES, HEM

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	0.84	2/3530 (0.1%)	0.85	11/4792 (0.2%)
2	B	1.11	1/3231 (0.0%)	0.94	11/4386 (0.3%)
3	C	0.78	3/3100 (0.1%)	0.82	9/4242 (0.2%)
4	D	0.60	0/1977	0.87	11/2684 (0.4%)
5	E	0.53	0/1553	0.78	8/2100 (0.4%)
6	F	0.96	0/929	0.91	5/1246 (0.4%)
7	G	0.77	0/681	0.79	0/922
8	H	0.56	0/632	0.83	3/847 (0.4%)
9	I	1.07	1/411 (0.2%)	1.18	1/558 (0.2%)
10	J	0.56	0/508	0.76	2/686 (0.3%)
11	K	0.66	0/457	0.77	2/625 (0.3%)
All	All	0.83	7/17009 (0.0%)	0.86	63/23088 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	1	0
3	C	2	2
7	G	2	0
9	I	1	0
All	All	6	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	25	ALA	CA-CB	-6.95	1.37	1.52
3	C	26	ASN	CB-CG	-6.36	1.36	1.51
3	C	194	MET	SD-CE	5.82	2.10	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	159	VAL	CB-CG2	-5.71	1.40	1.52
3	C	379	TRP	CB-CG	-5.44	1.40	1.50

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	42	ASP	CB-CG-OD2	7.55	125.10	118.30
3	C	345	HIS	N-CA-C	6.71	129.12	111.00
1	A	333	ASP	CB-CG-OD2	6.66	124.30	118.30
3	C	252	ASP	CB-CG-OD2	6.55	124.19	118.30
5	E	67	ASP	CB-CG-OD2	6.40	124.06	118.30

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	304	HIS	CA
3	C	58	ASP	CA
3	C	221	HIS	CA
7	G	11	ARG	CA
7	G	73	ASN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	221	HIS	Mainchain,Peptide

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	3457	0	3356	229	0
2	B	3171	0	3152	199	0
3	C	3003	0	3065	153	0
4	D	1918	0	1870	113	0
5	E	1519	0	1504	34	0
6	F	910	0	904	43	0
7	G	659	0	658	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	626	0	595	25	0
9	I	406	0	435	260	0
10	J	495	0	493	27	0
11	K	441	0	450	18	0
12	C	86	0	60	16	0
12	D	43	0	30	6	0
13	C	38	0	37	12	0
14	E	4	0	0	1	0
15	A	95	0	0	10	0
15	B	83	0	0	21	0
15	C	61	0	0	7	0
15	D	27	0	0	2	0
15	E	3	0	0	2	0
15	F	30	0	0	4	0
15	G	22	0	0	3	0
15	I	6	0	0	3	0
15	J	5	0	0	0	0
15	K	10	0	0	2	0
All	All	17118	0	16609	883	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 26.

The worst 5 of 883 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:TYR:HE1	9:I:20:ARG:CG	1.09	1.65
1:A:284:TYR:CE1	9:I:20:ARG:HG3	1.24	1.61
1:A:279:HIS:CE1	9:I:52:ARG:HB2	1.56	1.40
2:B:283:PRO:HG3	9:I:31:GLN:CG	1.52	1.39
3:C:194:MET:SD	3:C:194:MET:CE	2.10	1.38

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	444/446 (100%)	396 (89%)	42 (10%)	6 (1%)	9	19
2	B	421/439 (96%)	389 (92%)	24 (6%)	8 (2%)	6	13
3	C	376/379 (99%)	317 (84%)	37 (10%)	22 (6%)	1	1
4	D	239/241 (99%)	172 (72%)	47 (20%)	20 (8%)	0	0
5	E	194/196 (99%)	181 (93%)	9 (5%)	4 (2%)	5	11
6	F	103/110 (94%)	95 (92%)	8 (8%)	0	100	100
7	G	77/81 (95%)	65 (84%)	8 (10%)	4 (5%)	1	2
8	H	74/78 (95%)	58 (78%)	11 (15%)	5 (7%)	1	1
9	I	55/57 (96%)	25 (46%)	17 (31%)	13 (24%)	0	0
10	J	58/62 (94%)	46 (79%)	8 (14%)	4 (7%)	1	1
11	K	51/56 (91%)	41 (80%)	7 (14%)	3 (6%)	1	1
All	All	2092/2145 (98%)	1785 (85%)	218 (10%)	89 (4%)	2	3

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ALA
1	A	225	GLU
2	B	234	GLY
2	B	304	HIS
2	B	305	GLN

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	370/370 (100%)	324 (88%)	46 (12%)	4	7
2	B	332/343 (97%)	291 (88%)	41 (12%)	4	8
3	C	326/327 (100%)	286 (88%)	40 (12%)	4	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	206/206 (100%)	172 (84%)	34 (16%)	2	3
5	E	168/168 (100%)	158 (94%)	10 (6%)	16	35
6	F	96/98 (98%)	81 (84%)	15 (16%)	2	3
7	G	68/71 (96%)	53 (78%)	15 (22%)	1	1
8	H	73/74 (99%)	62 (85%)	11 (15%)	2	4
9	I	44/44 (100%)	33 (75%)	11 (25%)	0	1
10	J	50/52 (96%)	45 (90%)	5 (10%)	6	13
11	K	43/46 (94%)	31 (72%)	12 (28%)	0	0
All	All	1776/1799 (99%)	1536 (86%)	240 (14%)	3	6

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	281	LEU
9	I	47	ARG
4	D	135	CYS
9	I	27	ARG
11	K	41	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	248	ASN
11	K	12	GLN
3	C	44	GLN
9	I	31	GLN
6	F	53	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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
12	HEM	D	242	4	42,50,50	3.19	21 (50%)	46,82,82	2.60	17 (36%)
13	AY1	C	383	-	39,39,39	2.24	10 (25%)	33,53,53	2.45	11 (33%)
12	HEM	C	381	3	42,50,50	3.17	22 (52%)	46,82,82	2.79	20 (43%)
14	FES	E	197	5	0,4,4	-	-	-	-	-
12	HEM	C	382	3	42,50,50	3.13	19 (45%)	46,82,82	2.44	11 (23%)

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
12	HEM	D	242	4	-	4/12/54/54	-
13	AY1	C	383	-	-	5/38/53/53	0/1/2/2
12	HEM	C	381	3	-	8/12/54/54	-
14	FES	E	197	5	-	-	0/1/1/1
12	HEM	C	382	3	-	4/12/54/54	-

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	C4D-C3D	-7.87	1.31	1.45
12	D	242	HEM	C4D-C3D	-7.51	1.32	1.45
12	C	382	HEM	C3C-C4C	-6.66	1.31	1.41
12	C	382	HEM	C4D-C3D	-6.63	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	383	AY1	C1-N1	6.58	1.43	1.34

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	382	HEM	C4C-CHD-C1D	-9.85	109.56	122.56
12	C	381	HEM	C4B-CHC-C1C	-8.27	111.64	122.56
12	C	381	HEM	C4C-CHD-C1D	-7.67	112.43	122.56
12	D	242	HEM	C4C-CHD-C1D	-7.50	112.66	122.56
12	D	242	HEM	C4B-CHC-C1C	-7.30	112.92	122.56

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	381	HEM	C2B-C3B-CAB-CBB
12	C	381	HEM	C4B-C3B-CAB-CBB
13	C	383	AY1	C9-C10-O4-C12
12	C	381	HEM	C3D-CAD-CBD-CGD
12	C	381	HEM	C2A-CAA-CBA-CGA

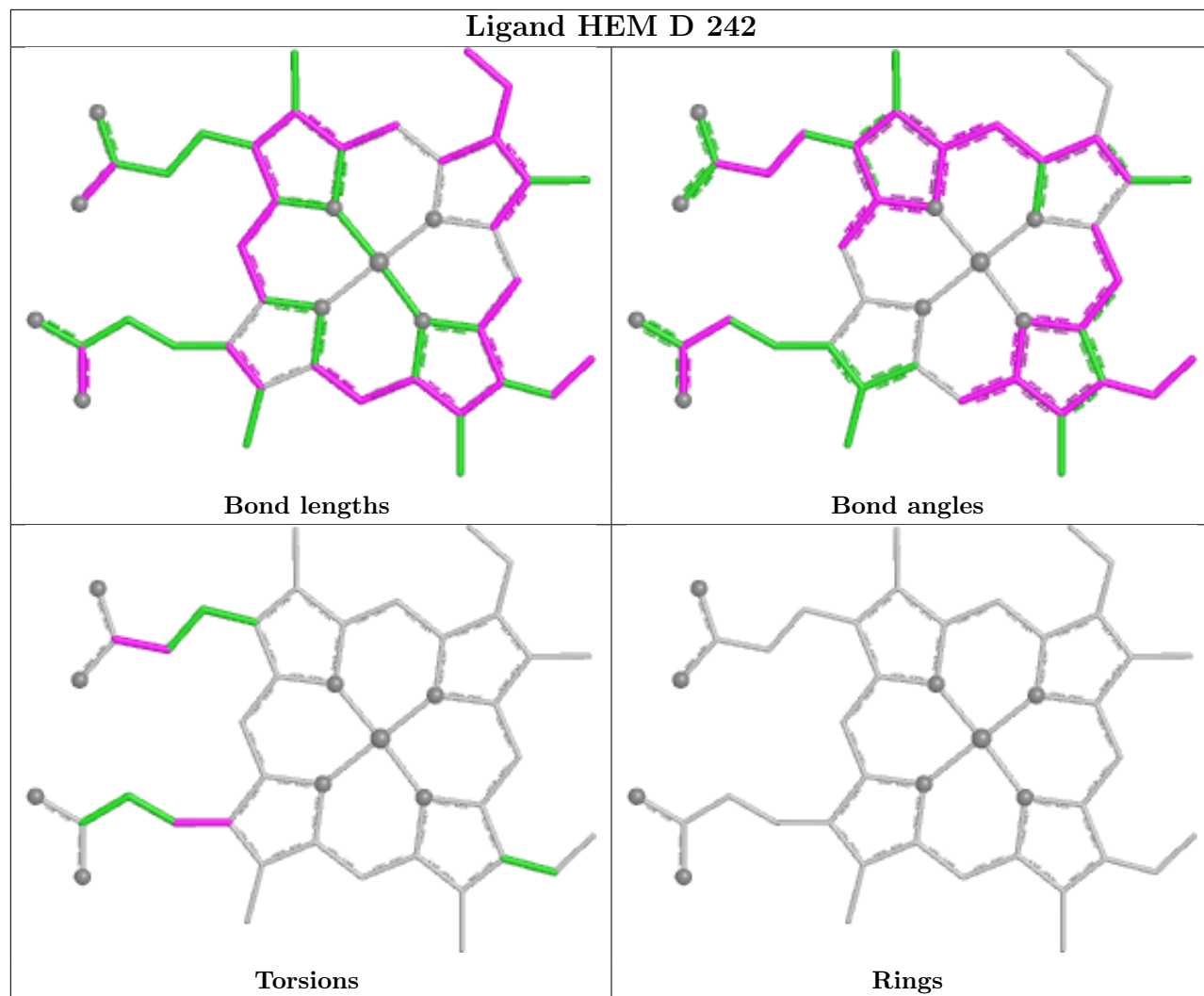
There are no ring outliers.

5 monomers are involved in 35 short contacts:

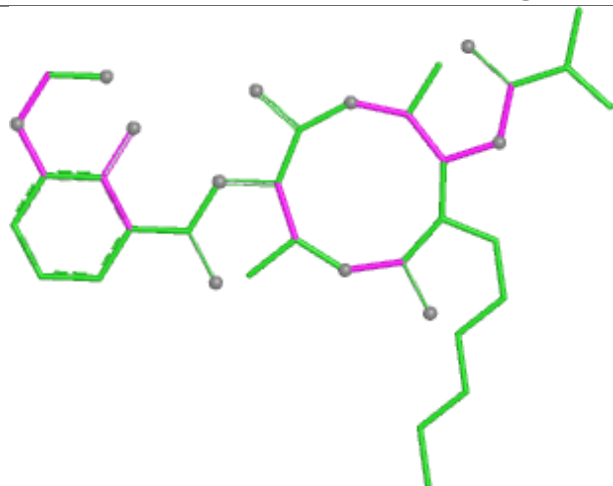
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	242	HEM	6	0
13	C	383	AY1	12	0
12	C	381	HEM	9	0
14	E	197	FES	1	0
12	C	382	HEM	7	0

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

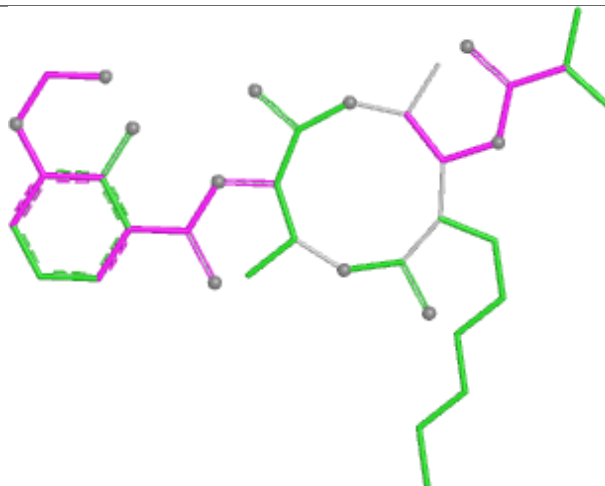
equivalents in the CSD to analyse the geometry.



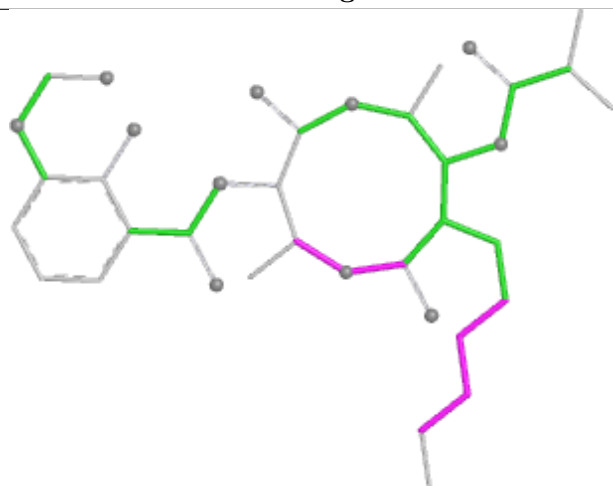
Ligand AY1 C 383



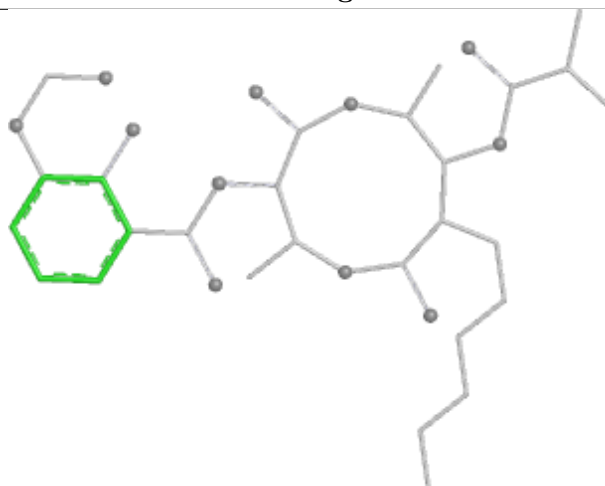
Bond lengths



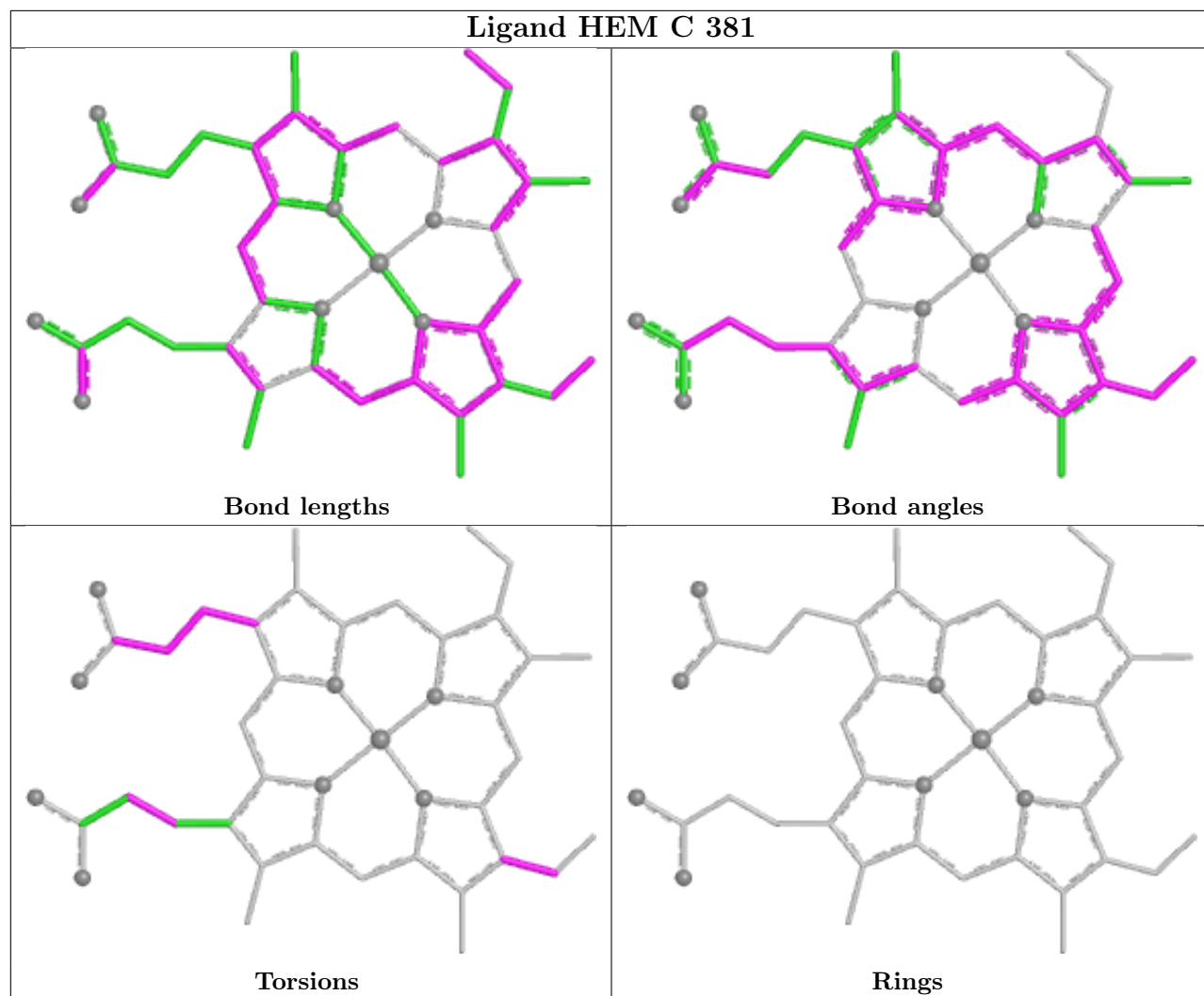
Bond angles

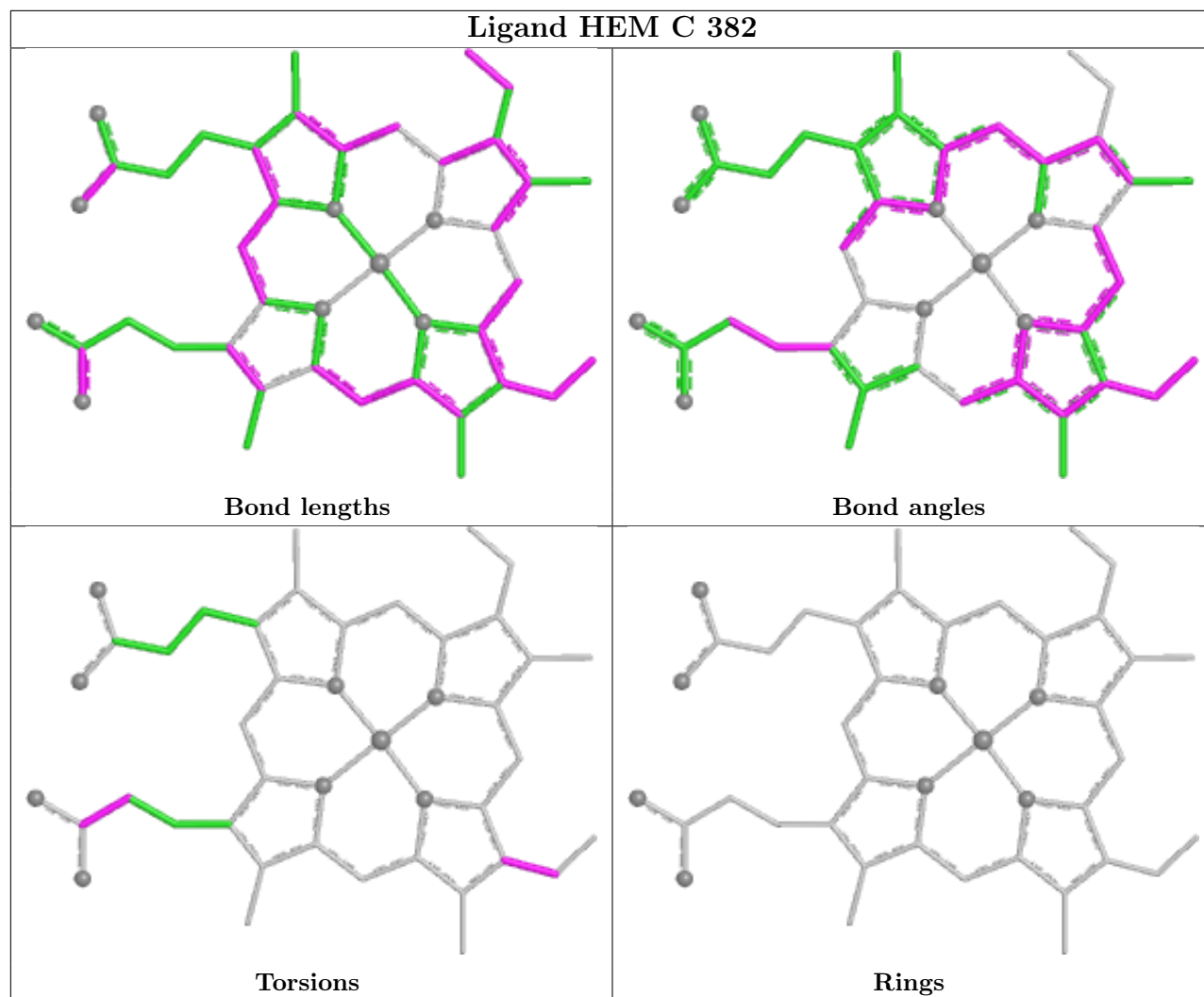


Torsions



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.