W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 10:02 pm BST

PDB ID	:	1L0N
Title	:	native structure of bovine mitochondrial cytochrome bc1 complex
Authors	:	Gao, X.; Wen, X.; Yu, C.A.; Esser, L.; Tsao, S.; Quinn, B.; Zhang, L.; Yu, L.; Xia, D.
Deposited on	:	2002-02-11
Resolution	:	2.60 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

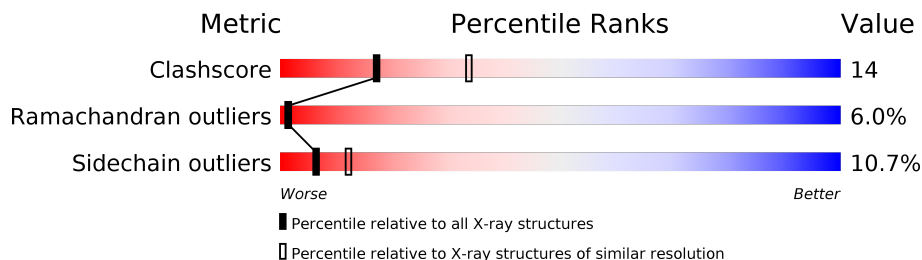|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		6.0%
Sidechain outliers		10.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	72% 23% •
2	B	439	69% 22% 5% • •
3	C	379	74% 20% 6% ••
4	D	241	52% 33% 13% •
5	E	196	49% 36% 12% •
6	F	110	59% 28% 8% 5%
7	G	81	63% 20% 7% • 7%
8	H	78	50% 31% 8% • 10%

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Mol	Chain	Length	Quality of chain
9	I	78	22% 21% 24% 6% 27%
10	J	62	55% 29% 8% · 6%
11	K	56	54% 21% 7% 5% 13%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 16577 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total 3458	C 2161	N 609	O 668	S 20	0	0	0

- Molecule 2 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total 3172	C 1993	N 562	O 610	S 7	0	0	0

- Molecule 3 is a protein called Cytochrome B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	377	Total 2996	C 2009	N 470	O 499	S 18	0	0	0

- Molecule 4 is a protein called Cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total 1919	C 1225	N 330	O 349	S 15	0	0	0

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

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

- 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 911	C 576	N 165	O 168	S 2	0	0	0

- 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	75	Total 628	C 410	N 118	O 99	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total 575	C 347	N 102	O 121	S 5	0	0	0

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE 8 KDA PROTEIN.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	58	Total 473	C 311	N 83	O 79	0	0	0

- Molecule 11 is a protein called cytochrome b-c1 complex 6.4K protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total 387	C 251	N 71	O 64	S 1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	THR	TYR	CONFLICT	UNP P07552

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

HEM
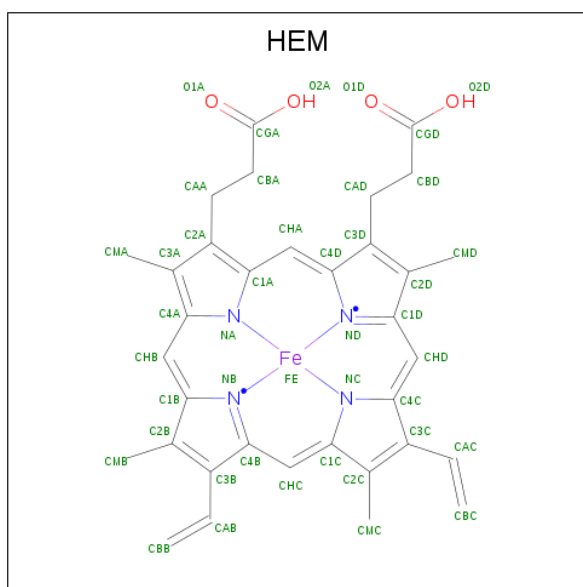
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

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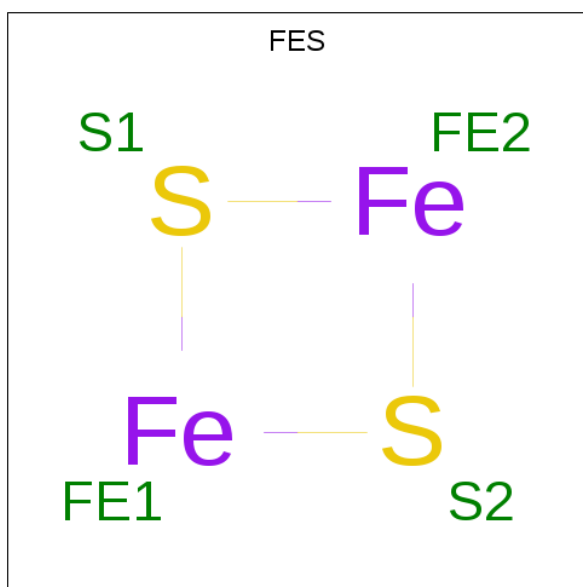
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots ⓘ

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. 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
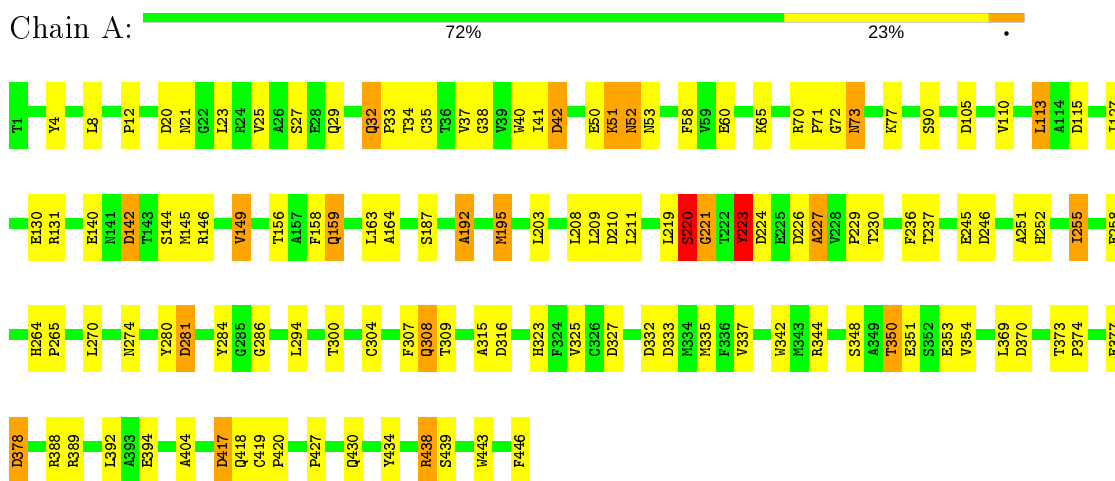
Chain A:

• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:

• Molecule 3: Cytochrome B

Chain C:

MET THR N3 I4 P24 S25 N26 W30 W31 N32 F33 L36 C40 L41 I42 L43 Q44 I45 L46 L51 D72 I78 I79 R80 F90 M96 R100 G101 L102 Y103 Y104 N114 L119 V123 V132 L133 G136 Q137 M138 S139 V145 I146 T447

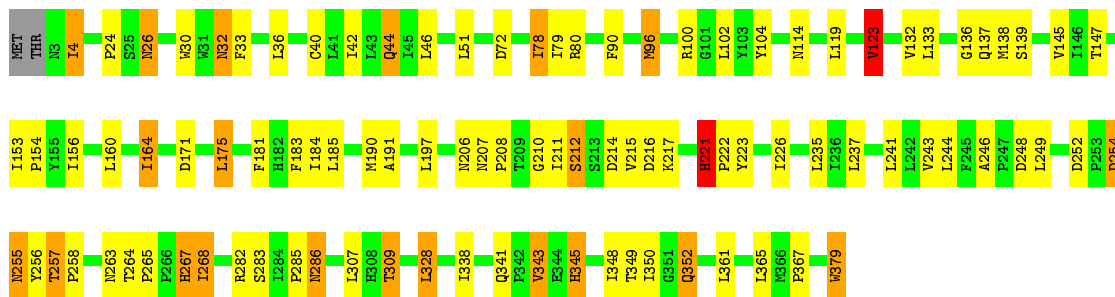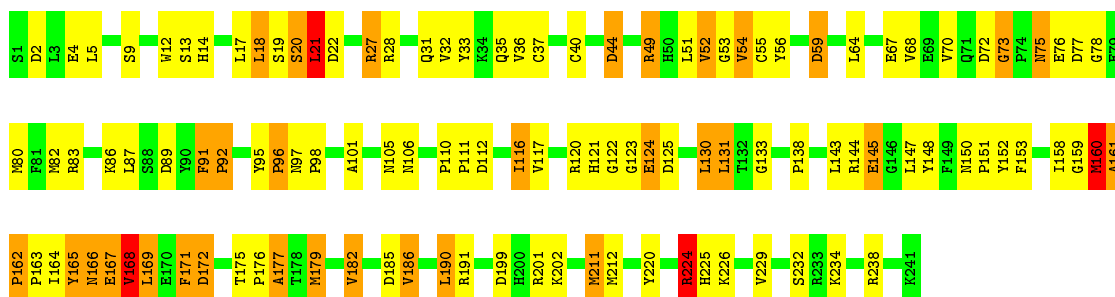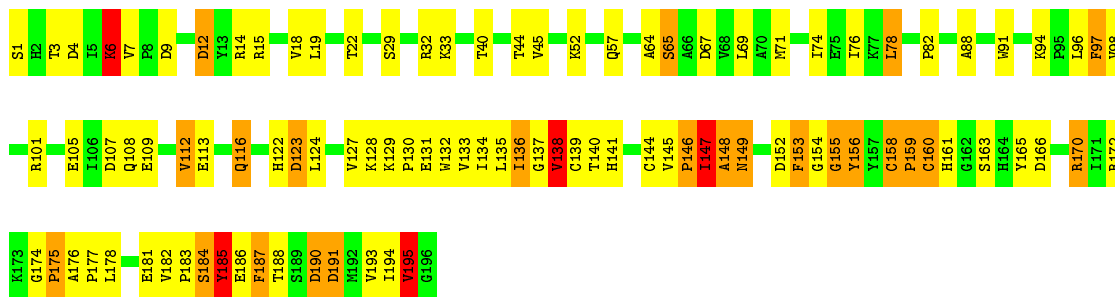I153 P154 Y155 I156 L160 I164 D171 L175 F181 H182 F183 I184 L185 M190 A191 L197 N206 P207 P208 T209 G210 Q211 S212 S213 D214 V215 D216 K217 H221 P222 Y223 I226 L235 I236 L237 L241 L242 V243 L244 F245 A246 P247 D248 L249 D252 P253 D254

N255 Y256 T257 P258 N263 T264 P265 H267 I268 R282 S283 I284 P285 N286 L307 H308 T309 L328 I338 Q341 P342 V343 E344 H345 I348 T349 I350 G351 Q352 L361 L365 M366 P367 W379

• Molecule 4: Cytochrome c1, heme protein

Chain D: 52% 33% 13% •

S1 D2 L3 E4 L5 S9 W12 S13 H14 L17 L18 S19 S20 L21 D22 R27 R28 Q31 V32 Y33 K34 Q35 V36 C37 C40 D44 R49 H50 L51 V52 G53 V54 C55 Y56 D59 L64 E67 V68 E69 V70 Q71 D72 G73 P74 N75 E76 D77 G78 E79

M80 F81 M82 R83 K86 L87 S88 D89 Y90 F91 P92 Y95 P96 N97 P98 A101 N105 N106 P110 P111 D112 I116 V117 R120 H121 G122 G123 E124 D125 L130 L131 T132 G133 P138 L143 R144 E145 G146 L147 Y148 F149 N150 Y152 F153 I158 G159 M160 A161

P162 P163 I164 Y165 N166 E167 V168 L169 E170 F171 D172 T175 P176 A177 T178 M179 V182 D185 V186 L190 R191 D199 H200 R201 K202 M211 M212 Y220 R224 H225 K226 V229 S232 R233 K234 R238 K241

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

Chain E: 49% 36% 12% •

S1 H2 T3 D4 I5 A6 V7 P8 D9 D12 Y13 R14 R15 V18 L19 T22 S29 R32 K33 T40 T44 V45 K52 Q57 A64 S65 D67 V68 L69 A70 M71 I74 E75 I76 K77 L78 P82 A88 W91 K94 P95 L96 F97 V98

R101 E105 I106 D107 Q108 E109 V112 E113 Q116 H122 D123 L124 V127 K128 K129 P130 E131 W132 V133 I134 L135 I136 G137 V138 C139 T140 H141 C144 V145 P146 I147 A148 N149 D152 F153 G154 G155 Y156 Y157 C158 P159 C160 H161 G162 S163 H164 Y165 D166 R170 I171 R172

K173 G174 P175 A176 P177 L178 E181 V182 P183 S184 Y185 E186 F187 T188 S189 D190 D191 M192 V193 I194 V195 G196

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

Chain F: 59% 28% 8% 5%

ALA GLY ARG PRO ALA V6 S7 A8 S9 S10 R11 W12 I16 N22 M27 K28 L31 D34 D35 T36 I37 N40 D41 D42 V43 A46 R49 N53 L54 Y55 D56 D57 R58 V59 F60 R61 I62 K63 R64 A65 L66 D67 R71 Q72 Q73 I74 E78 T81

K82 Y83 E84 E85 L90 L94 E100 K110
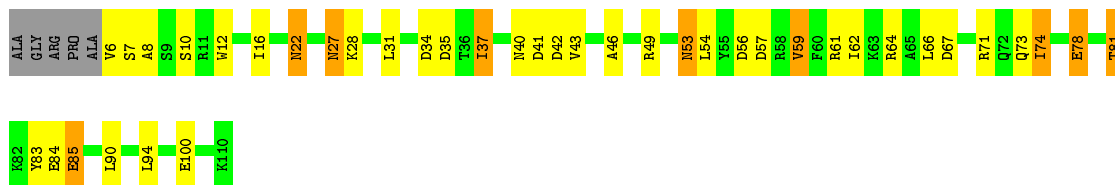
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G: 63% 20% 7% • 7%

G1 R2 Q3 F4 L7 V10 L18 S19 P20 Q23 R24 A25 F26 P27 H28 Y29 F30 S31 K32 G33 I34 V37 L38 R39 R40 T41 I45 P50 P51 F52 V53 N73 P74 A75 ALA TYR GLU ASN ASP ARG

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

Chain H: 50%   31%   8% • 10%

GLY ASP PRO LYS GLU GLU GLU E9 E10 E11 E12 L13 V14 L17 R21 E25 Q26 L27 E28 K29 C30 R34 L37 C40 D41 V44 S45 S46 Q49 D53 C54 L58 L59 D60 F61 R65 D66 H67 C68 H71 K72 L73 F74 N75 K78

• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE 8 KDA PROTEIN

Chain I: 22%   21%   24%   6%   27%

M1 L2 S3 V4 A5 A6 R7 S8 G9 P10 F11 A12 P13 V14 L15 S16 A17 T18 S19 R20 G21 G24 A25 L26 R27 P28 L29 V30 Q31 A32 A33 V34 P35 A36 T37 S38 E39 S40 P41 V42 L43 D44 L45 K46 R47 S48 C51 R52 E53 S54 L55 R56 G57 GLN ALA ALA GLY ARG

PRO LEU VAL ALA SER VAL SER LEU ASN VAL PRO ALA SER VAL ARG TYR

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

Chain J: 55%   29%   8% • 6%

V1 A2 P3 T4 L5 T6 Y10 L13 F14 T17 S18 T19 T23 A28 R33 Q37 A41 I42 Y43 E44 H45 I46 N47 E48 G49 K50 H54 K58 TYR GLU ASN LYS

• Molecule 11: cytochrome b-c1 complex 6.4K protein

Chain K: 54%   21%   7% 5%   13%

M1 Q12 L13 W17 L23 W24 V27 A35 T36 D37 S38 R39 L40 I41 L42 D43 W44 V45 P46 T47 I48 N49 GLY LYS PHE LYS LYS ASP ASP

4 Data and refinement statistics (i)

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	153.83Å 153.83Å 596.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 − 2.60	Depositor
% Data completeness (in resolution range)	100.0 (28.99-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.261 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16577	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

5   Model quality (i)

5.1   Standard geometry (i)

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

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	0.98	4/3531 (0.1%)	0.89	17/4792 (0.4%)
2	B	1.22	9/3232 (0.3%)	0.98	18/4386 (0.4%)
3	C	0.89	3/3093 (0.1%)	0.85	7/4232 (0.2%)
4	D	0.80	3/1978 (0.2%)	1.17	19/2684 (0.7%)
5	E	0.82	3/1553 (0.2%)	0.98	11/2100 (0.5%)
6	F	1.01	1/930 (0.1%)	0.97	6/1246 (0.5%)
7	G	0.93	0/649	0.87	1/878 (0.1%)
8	H	0.70	0/580	0.97	5/777 (0.6%)
9	I	1.24	3/411 (0.7%)	1.50	8/558 (1.4%)
10	J	0.79	0/485	0.80	1/655 (0.2%)
11	K	0.77	0/397	0.97	3/544 (0.6%)
All	All	0.97	26/16839 (0.2%)	0.97	96/22852 (0.4%)

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
3	C	0	1
4	D	1	0
All	All	1	1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	26	ASN	CB-CG	-7.32	1.34	1.51
9	I	25	ALA	CA-CB	-7.28	1.37	1.52
4	D	92	PRO	CB-CG	-7.26	1.13	1.50
2	B	325	TYR	CE2-CZ	-6.84	1.29	1.38
3	C	379	TRP	CB-CG	-6.41	1.38	1.50

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	91	PHE	C-N-CD	-23.89	68.03	120.60
9	I	42	VAL	O-C-N	12.05	141.98	122.70
4	D	168	VAL	O-C-N	10.28	139.15	122.70
4	D	92	PRO	CA-N-CD	-10.23	97.18	111.50
9	I	42	VAL	CA-C-N	-10.16	94.85	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	171	PHE	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	221	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	71	0
2	B	3172	0	3152	85	0
3	C	2996	0	3058	57	0
4	D	1919	0	1867	82	0
5	E	1519	0	1505	72	0
6	F	911	0	904	24	0
7	G	628	0	636	18	0
8	H	575	0	550	15	0
9	I	406	0	437	62	0
10	J	473	0	484	22	0
11	K	387	0	400	19	0
12	C	86	0	60	2	0
12	D	43	0	30	5	0
13	E	4	0	0	1	0
All	All	16577	0	16439	460	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 14.

The worst 5 of 460 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)
2:B:305:GLN:NE2	2:B:305:GLN:HA	1.52	1.10
5:E:52:LYS:HE2	11:K:35:ALA:HA	1.22	1.10
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.28	1.08
4:D:167:GLU:HG2	4:D:169:LEU:HD23	1.08	1.05
4:D:167:GLU:HG2	4:D:169:LEU:CD2	1.86	1.05

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%)	407 (92%)	23 (5%)	14 (3%)	4	6
2	B	421/439 (96%)	391 (93%)	22 (5%)	8 (2%)	8	15
3	C	375/379 (99%)	335 (89%)	28 (8%)	12 (3%)	4	6
4	D	239/241 (99%)	177 (74%)	36 (15%)	26 (11%)	0	0
5	E	194/196 (99%)	127 (66%)	43 (22%)	24 (12%)	0	0
6	F	103/110 (94%)	96 (93%)	6 (6%)	1 (1%)	15	32
7	G	73/81 (90%)	62 (85%)	6 (8%)	5 (7%)	1	1
8	H	68/78 (87%)	50 (74%)	9 (13%)	9 (13%)	0	0
9	I	55/78 (70%)	26 (47%)	15 (27%)	14 (26%)	0	0
10	J	56/62 (90%)	43 (77%)	7 (12%)	6 (11%)	0	0
11	K	47/56 (84%)	32 (68%)	9 (19%)	6 (13%)	0	0
All	All	2075/2166 (96%)	1746 (84%)	204 (10%)	125 (6%)	1	1

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	220	SER
1	A	227	ALA
2	B	305	GLN
3	C	212	SER

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	370/370 (100%)	342 (92%)	28 (8%)	13	26
2	B	332/343 (97%)	299 (90%)	33 (10%)	8	15
3	C	325/327 (99%)	298 (92%)	27 (8%)	11	22
4	D	206/206 (100%)	175 (85%)	31 (15%)	3	5
5	E	168/168 (100%)	148 (88%)	20 (12%)	5	9
6	F	96/98 (98%)	87 (91%)	9 (9%)	8	17
7	G	66/71 (93%)	58 (88%)	8 (12%)	5	9
8	H	67/74 (90%)	58 (87%)	9 (13%)	4	6
9	I	44/60 (73%)	35 (80%)	9 (20%)	1	2
10	J	48/52 (92%)	41 (85%)	7 (15%)	3	5
11	K	40/46 (87%)	32 (80%)	8 (20%)	1	2
All	All	1762/1815 (97%)	1573 (89%)	189 (11%)	6	12

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	350	ILE
4	D	124	GLU
10	J	4	THR
4	D	4	GLU
4	D	36	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	284	HIS
2	B	385	GLN
9	I	31	GLN
2	B	342	ASN
2	B	401	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	27,50,50	2.12	7 (25%)	17,82,82	1.83	3 (17%)
13	FES	E	197	5	0,4,4	0.00	-	-		
12	HEM	C	381	3	27,50,50	2.05	8 (29%)	17,82,82	1.84	5 (29%)
12	HEM	C	382	3	27,50,50	2.16	5 (18%)	17,82,82	1.49	3 (17%)

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	-	2/6/54/54	-
13	FES	E	197	5	-	-	0/1/1/1
12	HEM	C	381	3	-	2/6/54/54	-
12	HEM	C	382	3	-	1/6/54/54	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	382	HEM	C3C-C2C	-5.49	1.32	1.40
12	C	382	HEM	C3D-C2D	5.32	1.53	1.37
12	D	242	HEM	C3B-C2B	-5.14	1.33	1.40
12	D	242	HEM	C3D-C2D	4.76	1.51	1.37
12	C	381	HEM	C3C-C2C	-4.68	1.33	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	242	HEM	CAD-CBD-CGD	-4.25	105.54	112.67
12	D	242	HEM	CAA-CBA-CGA	-4.06	105.86	112.67
12	C	381	HEM	CBD-CAD-C3D	-3.87	105.36	112.48
12	C	381	HEM	CAA-CBA-CGA	-3.43	106.92	112.67
12	C	382	HEM	C4C-C3C-C2C	3.39	109.26	106.90

There are no chirality outliers.
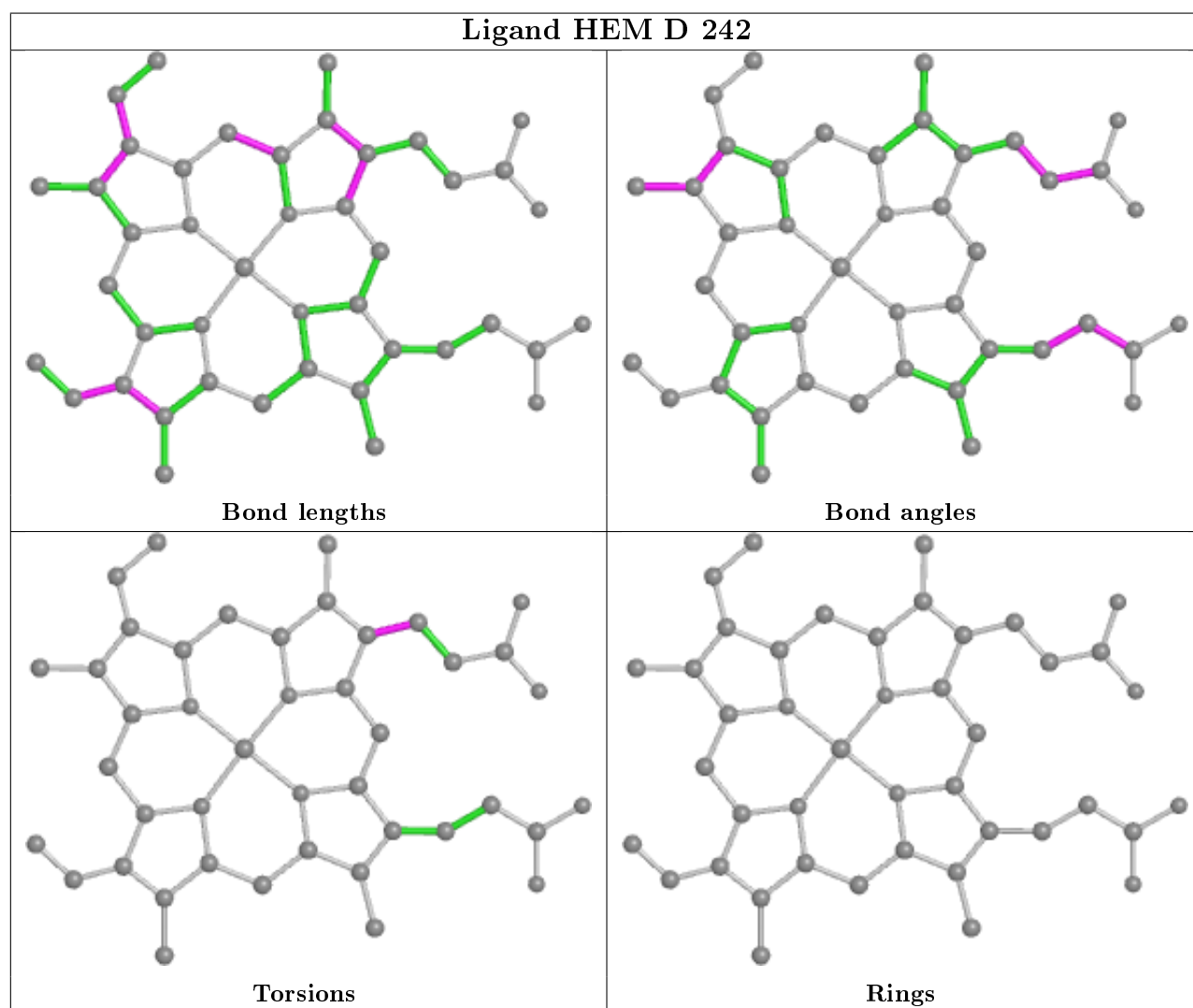
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	242	HEM	C2D-C3D-CAD-CBD
12	D	242	HEM	C4D-C3D-CAD-CBD
12	C	381	HEM	C1A-C2A-CAA-CBA
12	C	381	HEM	C3A-C2A-CAA-CBA
12	C	382	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	242	HEM	5	0
13	E	197	FES	1	0
12	C	381	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 D 242

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 381

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 382

Bond lengths

Bond angles

Torsions

Rings
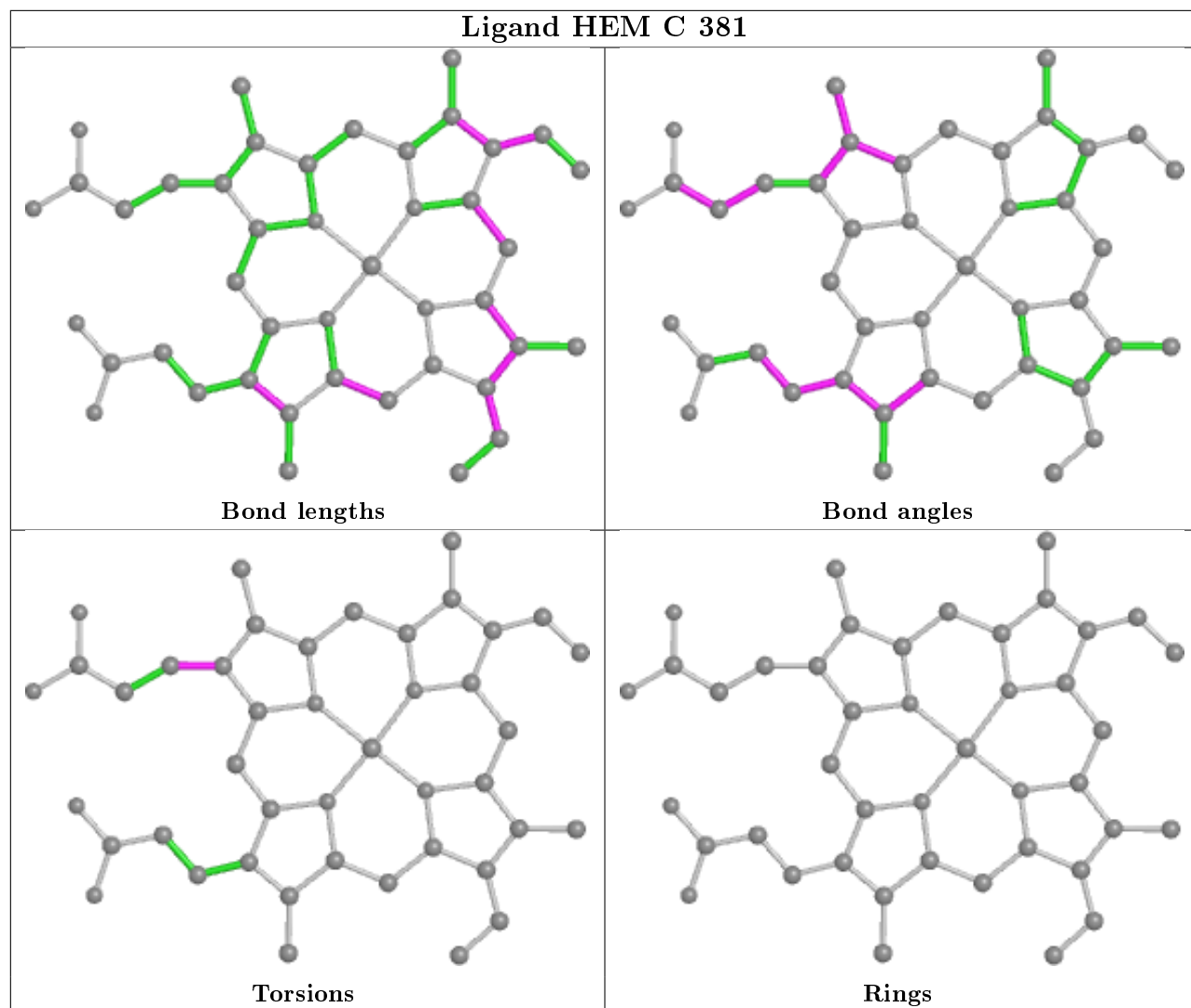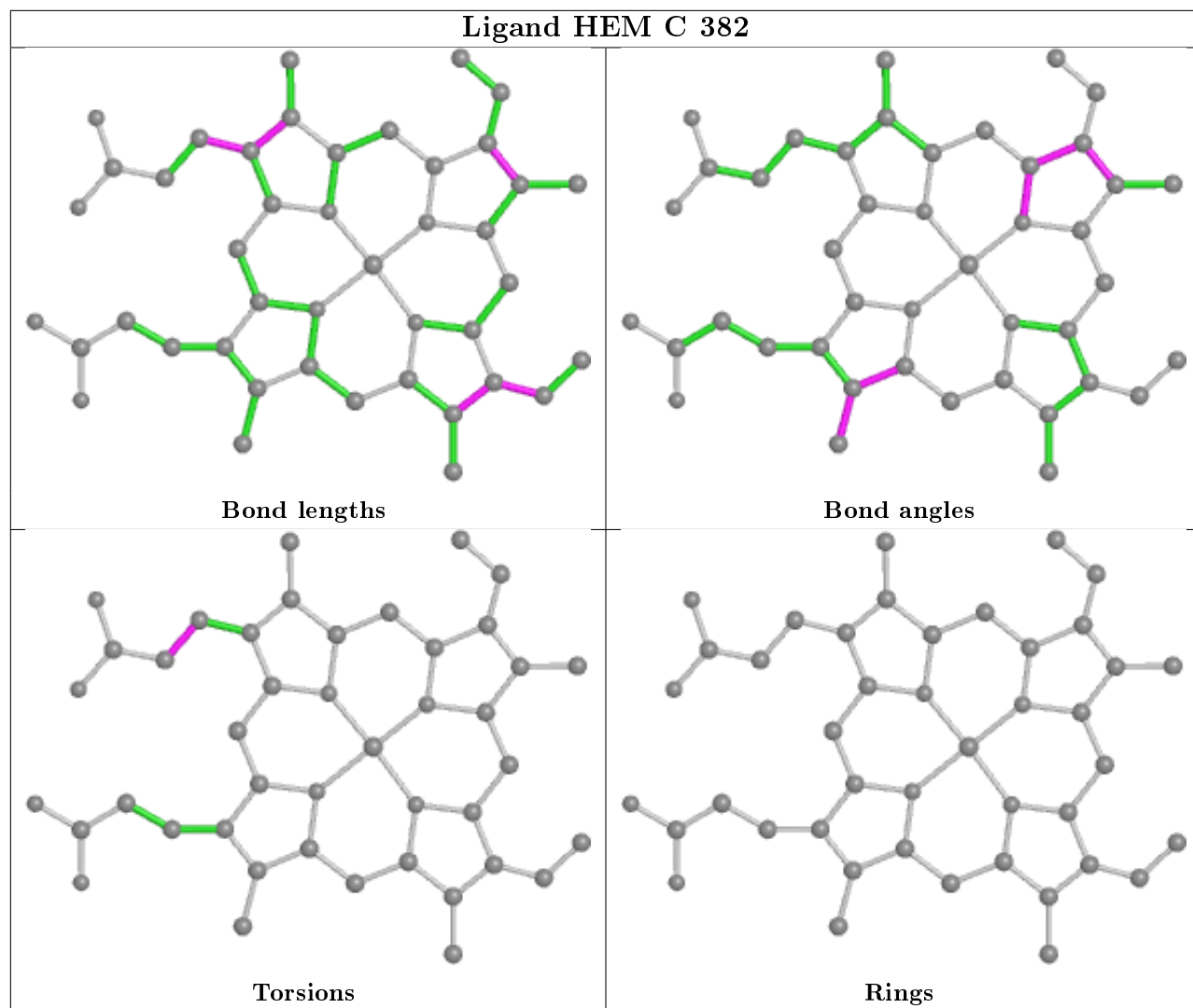
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.