



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 12:40 AM BST

PDB ID : 1FFT  
Title : The structure of ubiquinol oxidase from Escherichia coli  
Authors : Abramson, J.; Riistama, S.; Larsson, G.; Jasaitis, A.; Svensson-Ek, M.; Puustinen, A.; Iwata, S.; Wikstrom, M.  
Deposited on : 2000-07-26  
Resolution : 3.50 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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) : 2.13.1

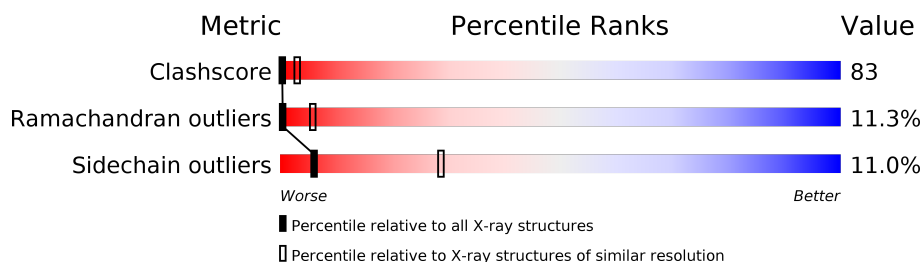
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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  $\geq 3$ , 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	663	16% 48% 11% • 24%
1	F	663	17% 47% 11% • 24%
2	B	315	16% 54% 10% • 18%
2	G	315	15% 54% 11% • 18%
3	C	204	22% 55% 12% • 9%
3	H	204	19% 58% 13% • 9%
4	D	109	70% 30%
4	I	109	70% 30%

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
7	HEO	A	1002	X	-	-	-
7	HEO	F	1002	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16136 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 OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	312	0	0
			3954	2654	630	639	31			
1	F	501	Total	C	N	O	S	312	0	0
			3954	2654	630	639	31			

- Molecule 2 is a protein called UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	155	0	0
			2015	1320	324	361	10			
2	G	257	Total	C	N	O	S	155	0	0
			2015	1320	324	361	10			

- Molecule 3 is a protein called UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	185	Total	C	N	O	S	157	0	0
			1451	970	229	240	12			
3	H	185	Total	C	N	O	S	157	0	0
			1451	970	229	240	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	cloning artifact	UNP P0ABJ3
C	2	ALA	-	cloning artifact	UNP P0ABJ3
C	3	THR	-	cloning artifact	UNP P0ABJ3
C	4	ASP	-	cloning artifact	UNP P0ABJ3
C	5	THR	-	cloning artifact	UNP P0ABJ3
C	6	LEU	-	cloning artifact	UNP P0ABJ3
C	7	THR	-	cloning artifact	UNP P0ABJ3
C	8	HIS	-	cloning artifact	UNP P0ABJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	ALA	-	cloning artifact	UNP P0ABJ3
C	10	THR	-	cloning artifact	UNP P0ABJ3
C	11	ALA	-	cloning artifact	UNP P0ABJ3
C	12	HIS	-	cloning artifact	UNP P0ABJ3
C	13	ALA	-	cloning artifact	UNP P0ABJ3
C	14	HIS	-	cloning artifact	UNP P0ABJ3
C	15	GLU	-	cloning artifact	UNP P0ABJ3
C	16	HIS	-	cloning artifact	UNP P0ABJ3
C	17	GLY	-	cloning artifact	UNP P0ABJ3
C	18	HIS	-	cloning artifact	UNP P0ABJ3
C	19	HIS	-	cloning artifact	UNP P0ABJ3
C	20	ASP	-	cloning artifact	UNP P0ABJ3
C	21	ALA	-	cloning artifact	UNP P0ABJ3
C	22	GLY	-	cloning artifact	UNP P0ABJ3
C	23	GLY	-	cloning artifact	UNP P0ABJ3
C	24	THR	-	cloning artifact	UNP P0ABJ3
H	1	MET	-	cloning artifact	UNP P0ABJ3
H	2	ALA	-	cloning artifact	UNP P0ABJ3
H	3	THR	-	cloning artifact	UNP P0ABJ3
H	4	ASP	-	cloning artifact	UNP P0ABJ3
H	5	THR	-	cloning artifact	UNP P0ABJ3
H	6	LEU	-	cloning artifact	UNP P0ABJ3
H	7	THR	-	cloning artifact	UNP P0ABJ3
H	8	HIS	-	cloning artifact	UNP P0ABJ3
H	9	ALA	-	cloning artifact	UNP P0ABJ3
H	10	THR	-	cloning artifact	UNP P0ABJ3
H	11	ALA	-	cloning artifact	UNP P0ABJ3
H	12	HIS	-	cloning artifact	UNP P0ABJ3
H	13	ALA	-	cloning artifact	UNP P0ABJ3
H	14	HIS	-	cloning artifact	UNP P0ABJ3
H	15	GLU	-	cloning artifact	UNP P0ABJ3
H	16	HIS	-	cloning artifact	UNP P0ABJ3
H	17	GLY	-	cloning artifact	UNP P0ABJ3
H	18	HIS	-	cloning artifact	UNP P0ABJ3
H	19	HIS	-	cloning artifact	UNP P0ABJ3
H	20	ASP	-	cloning artifact	UNP P0ABJ3
H	21	ALA	-	cloning artifact	UNP P0ABJ3
H	22	GLY	-	cloning artifact	UNP P0ABJ3
H	23	GLY	-	cloning artifact	UNP P0ABJ3
H	24	THR	-	cloning artifact	UNP P0ABJ3

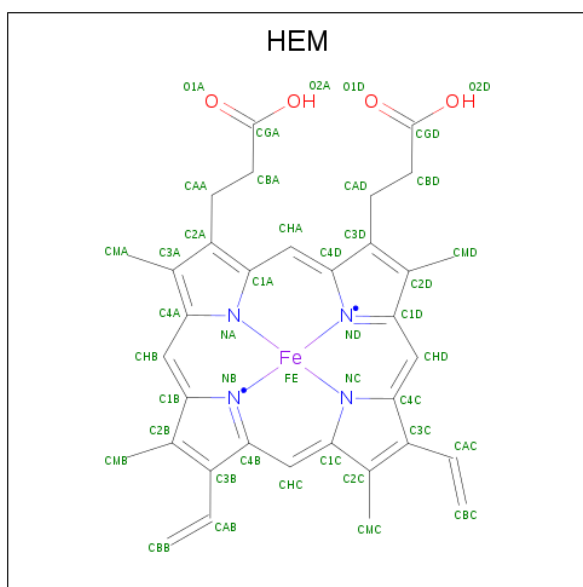
- Molecule 4 is a protein called UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	109	Total 545	C 327	N 109	O 109	0	0	0
4	I	109	Total 545	C 327	N 109	O 109	0	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

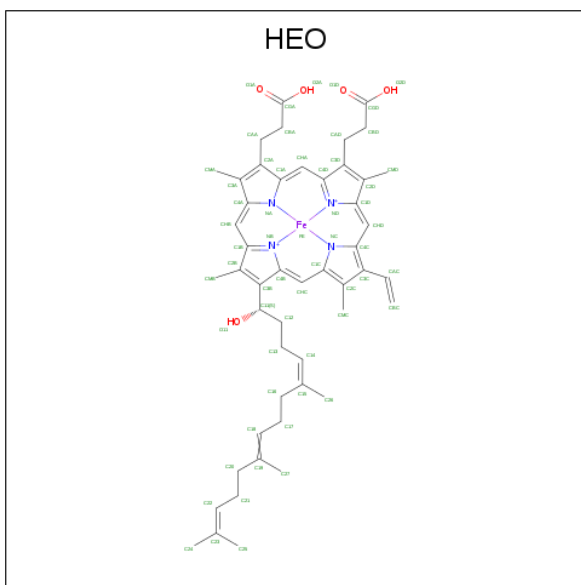
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cu 1 1	0	0
5	F	1	Total Cu 1 1	0	0

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is HEME O (three-letter code: HEO) (formula:  $\text{C}_{49}\text{H}_{58}\text{FeN}_4\text{O}_5$ ).



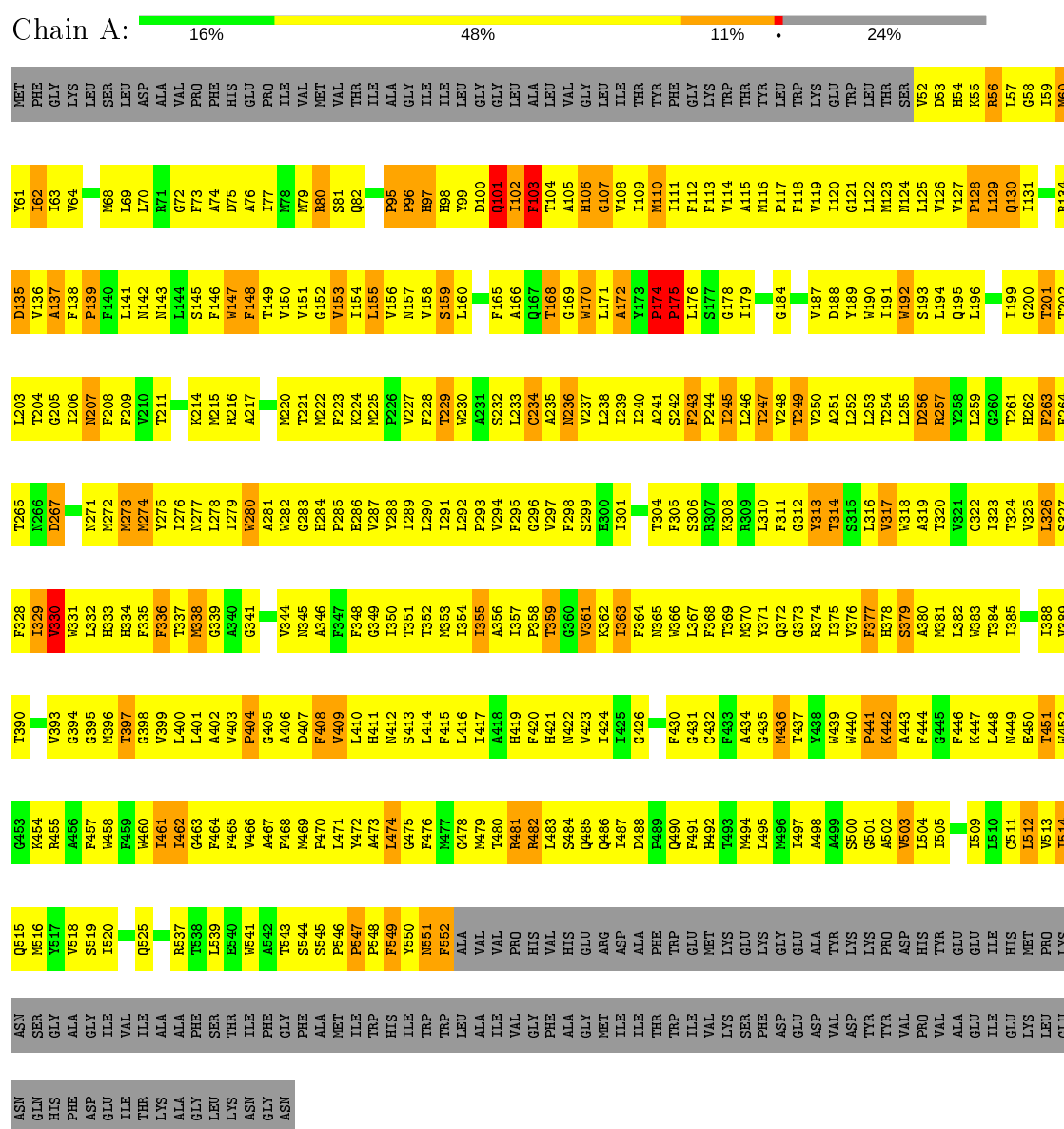
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 59	C 49	Fe 1	N 4	O 5	0	0
7	F	1	Total 59	C 49	Fe 1	N 4	O 5	0	0

### 3 Residue-property plots

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

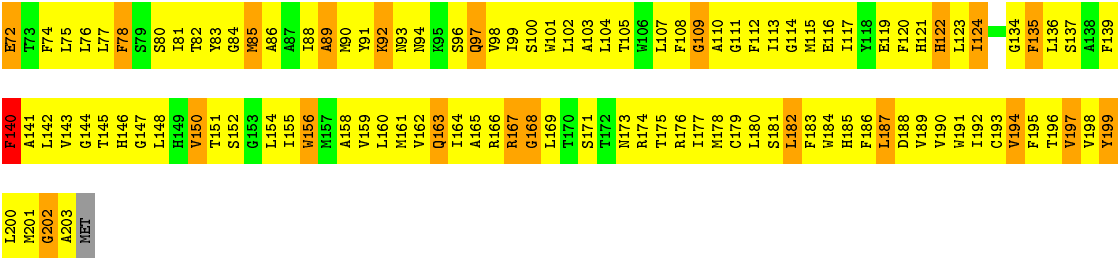


#### • Molecule 1: UBIQUINOL OXIDASE

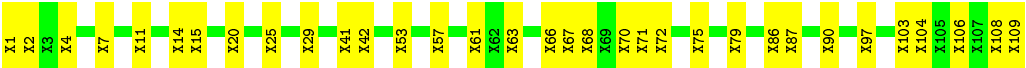








● Molecule 4: UBIQUINOL OXIDASE



● Molecule 4: UBIQUINOL OXIDASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.10 Å   372.50 Å   232.70 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.50)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program		Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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, HEO, CU

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	0.46	1/4086 (0.0%)	0.71	4/5573 (0.1%)
1	F	0.44	0/4086	0.68	2/5573 (0.0%)
2	B	0.43	0/2074	0.65	0/2825
2	G	0.43	0/2074	0.67	0/2825
3	C	0.47	0/1494	0.66	0/2030
3	H	0.43	0/1494	0.65	0/2030
All	All	0.45	1/15308 (0.0%)	0.68	6/20856 (0.0%)

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
1	A	0	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	PRO	C-N	-9.24	1.16	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	PRO	C-N-CD	-12.28	93.59	120.60
1	A	175	PRO	CB-CA-C	7.79	131.48	112.00
1	F	175	PRO	CB-CA-C	7.42	130.56	112.00
1	F	174	PRO	C-N-CD	-6.30	106.74	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	PRO	CA-N-CD	-6.28	102.72	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	PRO	Mainchain
1	F	174	PRO	Mainchain

## 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	3954	0	3975	658	0
1	F	3954	0	3975	661	0
2	B	2015	0	2016	317	0
2	G	2015	0	2016	348	0
3	C	1451	0	1458	254	0
3	H	1451	0	1458	265	0
4	D	545	0	114	57	0
4	I	545	0	115	55	0
5	A	1	0	0	0	0
5	F	1	0	0	0	0
6	A	43	0	30	18	0
6	F	43	0	30	17	0
7	A	59	0	56	16	0
7	F	59	0	56	14	0
All	All	16136	0	15299	2417	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 83.

The worst 5 of 2417 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)
3:H:86:ALA:HB1	3:H:91:TYR:CD1	1.43	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:83:TYR:HE1	4:I:14:UNK:CB	1.44	1.30
3:C:78:PHE:HZ	4:D:57:UNK:CB	1.44	1.30
1:A:55:LYS:NZ	1:A:551:ASN:HA	1.44	1.29
3:C:78:PHE:CZ	4:D:57:UNK:CB	2.20	1.24

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/663 (75%)	331 (66%)	110 (22%)	58 (12%)	0	5
1	F	499/663 (75%)	333 (67%)	108 (22%)	58 (12%)	0	5
2	B	255/315 (81%)	162 (64%)	66 (26%)	27 (11%)	0	7
2	G	255/315 (81%)	167 (66%)	58 (23%)	30 (12%)	0	5
3	C	183/204 (90%)	112 (61%)	52 (28%)	19 (10%)	0	7
3	H	183/204 (90%)	107 (58%)	56 (31%)	20 (11%)	0	6
All	All	1874/2364 (79%)	1212 (65%)	450 (24%)	212 (11%)	0	6

5 of 212 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	102	ILE
1	A	106	HIS
1	A	135	ASP
1	A	175	PRO

### 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	413/547 (76%)	373 (90%)	40 (10%)	8	33
1	F	413/547 (76%)	373 (90%)	40 (10%)	8	33
2	B	215/262 (82%)	188 (87%)	27 (13%)	4	22
2	G	215/262 (82%)	187 (87%)	28 (13%)	4	21
3	C	152/166 (92%)	133 (88%)	19 (12%)	4	23
3	H	152/166 (92%)	134 (88%)	18 (12%)	5	25
All	All	1560/1950 (80%)	1388 (89%)	172 (11%)	6	29

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	122	HIS
1	F	159	SER
3	H	46	THR
3	C	156	TRP
1	F	56	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	268	ASN
1	F	142	ASN
3	H	94	ASN
3	C	97	GLN
1	F	143	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
7	HEO	F	1002	1	51,66,66	1.13	3 (5%)	54,102,102	1.24	6 (11%)
7	HEO	A	1002	1	51,66,66	1.12	2 (3%)	54,102,102	1.25	6 (11%)
6	HEM	A	1001	1	27,50,50	1.74	4 (14%)	17,82,82	0.91	0
6	HEM	F	1001	1	27,50,50	1.75	4 (14%)	17,82,82	0.99	0

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
7	HEO	F	1002	1	2/2/17/25	2/28/114/114	-
7	HEO	A	1002	1	2/2/17/25	1/28/114/114	-
6	HEM	A	1001	1	-	0/6/54/54	-
6	HEM	F	1001	1	-	0/6/54/54	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1002	HEO	C3C-CAC	-4.12	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	1002	HEO	C3C-CAC	-4.07	1.39	1.47
6	F	1001	HEM	C3B-C2B	-3.91	1.35	1.40
6	F	1001	HEM	C3C-CAC	-3.90	1.39	1.47
6	A	1001	HEM	C3C-CAC	-3.85	1.39	1.47

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1002	HEO	C1D-ND-C4D	-2.94	102.03	105.07
7	F	1002	HEO	C1D-ND-C4D	-2.86	102.12	105.07
7	A	1002	HEO	C3C-C4C-NC	2.52	112.47	109.21
7	F	1002	HEO	C3C-C4C-NC	2.45	112.37	109.21
7	A	1002	HEO	C3D-C4D-ND	2.34	112.62	110.36

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	F	1002	HEO	ND
7	F	1002	HEO	NB
7	A	1002	HEO	ND
7	A	1002	HEO	NB

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	1002	HEO	C15-C16-C17-C18
7	A	1002	HEO	C15-C16-C17-C18
7	F	1002	HEO	C26-C15-C16-C17

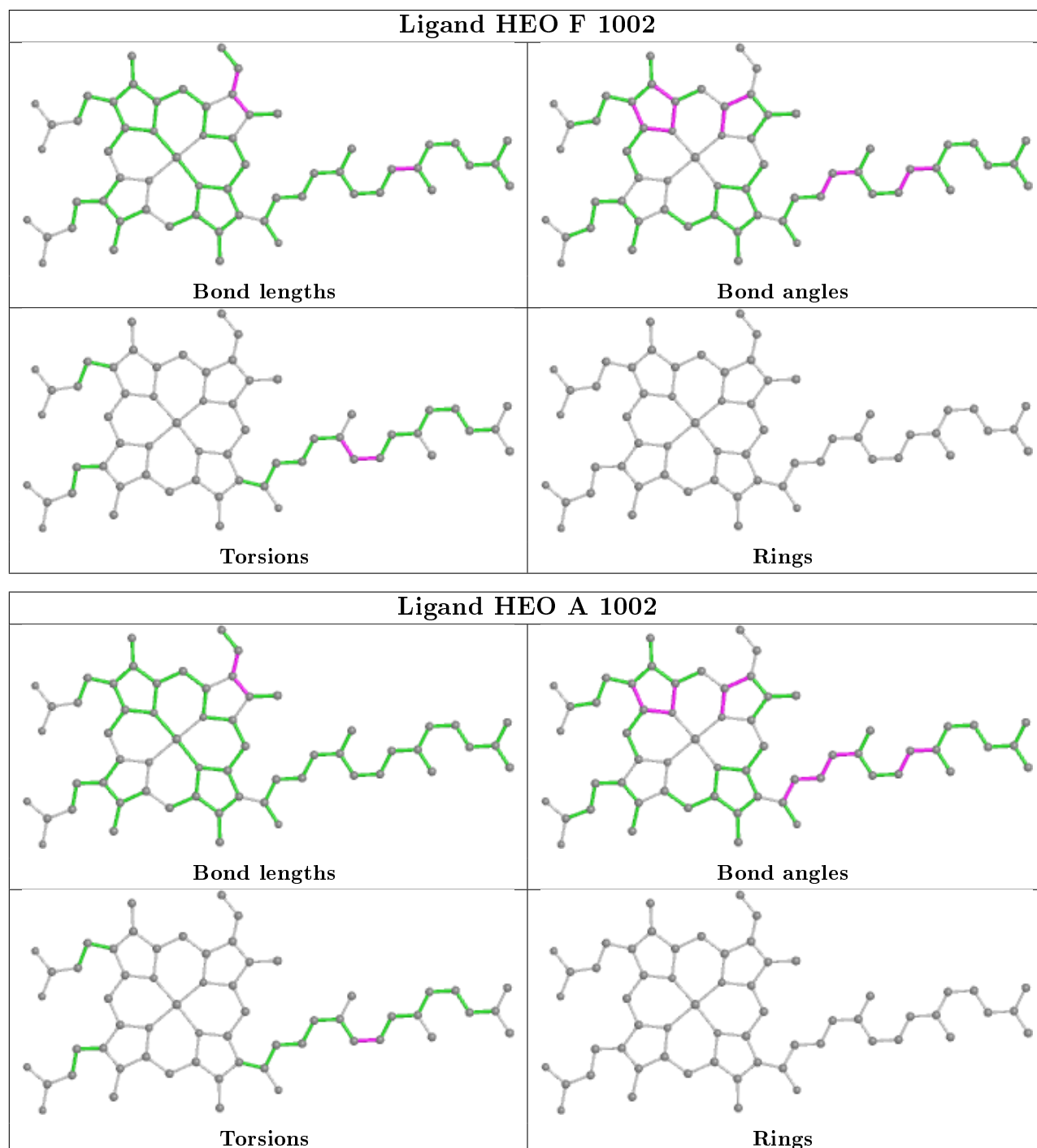
There are no ring outliers.

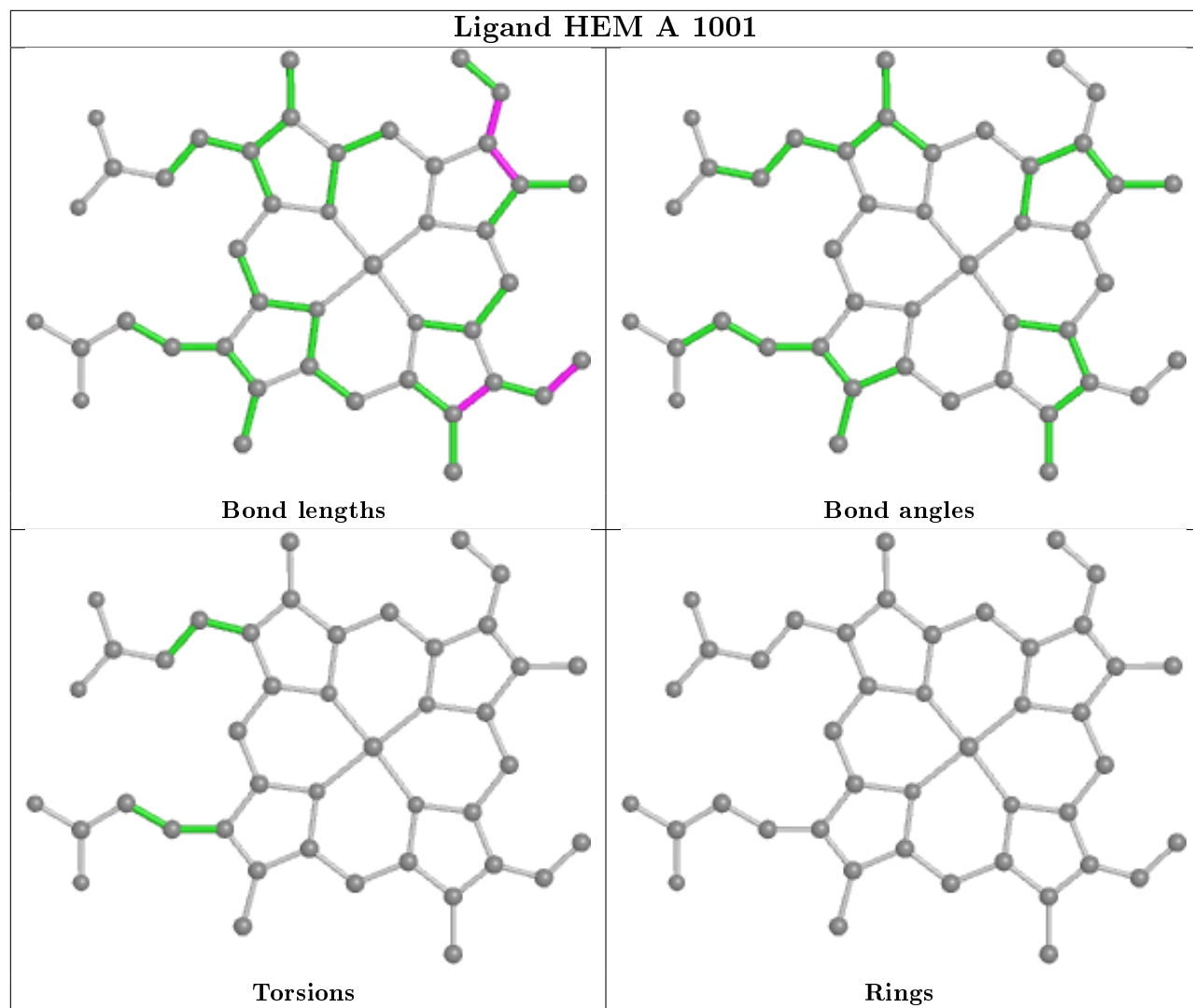
4 monomers are involved in 65 short contacts:

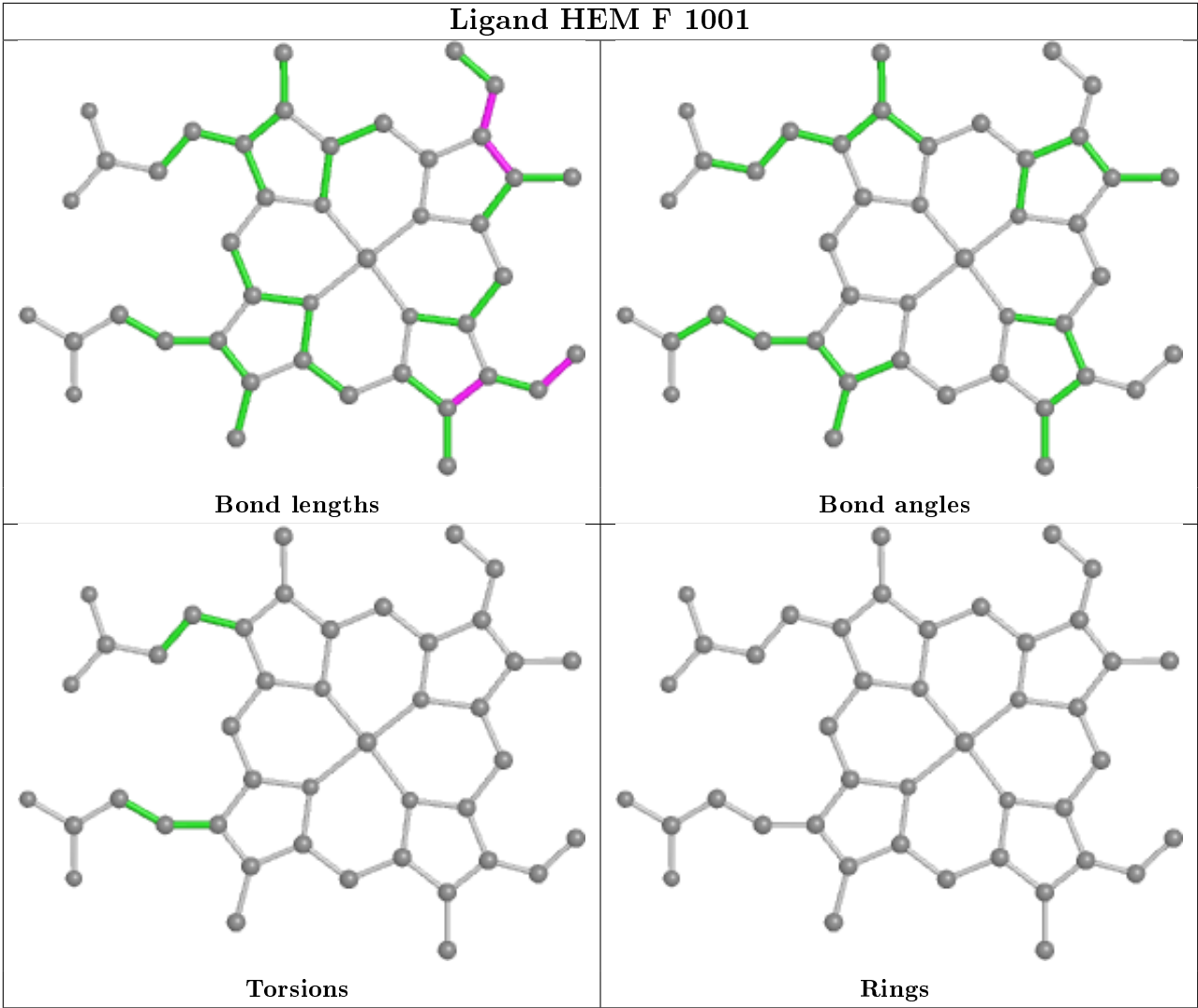
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1002	HEO	14	0
7	A	1002	HEO	16	0
6	A	1001	HEM	18	0
6	F	1001	HEM	17	0

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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	174:PRO	C	175:PRO	N	1.16

## 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.