



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 02:02 PM EDT

PDB ID : 2F9Q  
Title : Crystal Structure of Human Cytochrome P450 2D6  
Authors : Rowland, P.  
Deposited on : 2005-12-06  
Resolution : 3.00 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) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

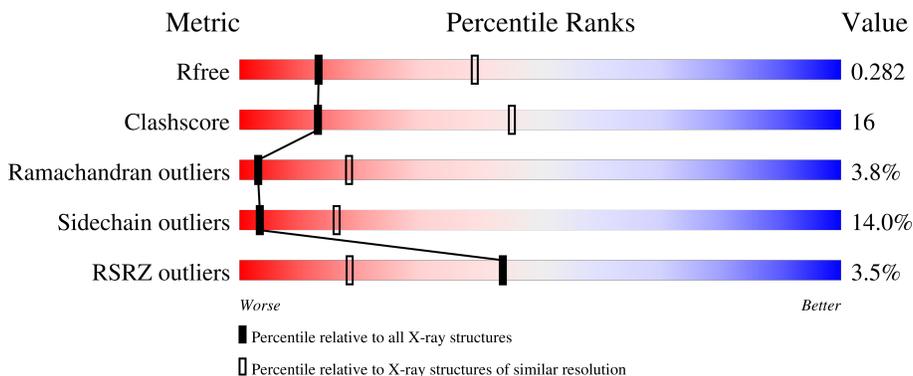
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	479	
1	B	479	
1	C	479	
1	D	479	

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
3	SO4	B	2000	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14421 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 Cytochrome P450 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3569	2281	634	639	15	0	0	0
1	B	451	3545	2265	630	635	15	0	0	0
1	C	454	3569	2281	634	639	15	0	0	0
1	D	451	3545	2265	630	635	15	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	HIS	cloning artifact	UNP P10635
A	25	LYS	ARG	cloning artifact	UNP P10635
A	26	LYS	ARG	cloning artifact	UNP P10635
A	27	THR	GLN	cloning artifact	UNP P10635
A	28	SER	ARG	cloning artifact	UNP P10635
A	29	SER	TRP	cloning artifact	UNP P10635
A	30	LYS	ALA	cloning artifact	UNP P10635
A	31	GLY	ALA	cloning artifact	UNP P10635
A	32	LYS	ARG	cloning artifact	UNP P10635
A	33	LEU	TYR	cloning artifact	UNP P10635
A	230	ASP	LEU	engineered mutation	UNP P10635
A	231	ARG	LEU	engineered mutation	UNP P10635
A	498	HIS	-	expression tag	UNP P10635
A	499	HIS	-	expression tag	UNP P10635
A	500	HIS	-	expression tag	UNP P10635
A	501	HIS	-	expression tag	UNP P10635
B	24	ALA	HIS	cloning artifact	UNP P10635
B	25	LYS	ARG	cloning artifact	UNP P10635
B	26	LYS	ARG	cloning artifact	UNP P10635
B	27	THR	GLN	cloning artifact	UNP P10635
B	28	SER	ARG	cloning artifact	UNP P10635

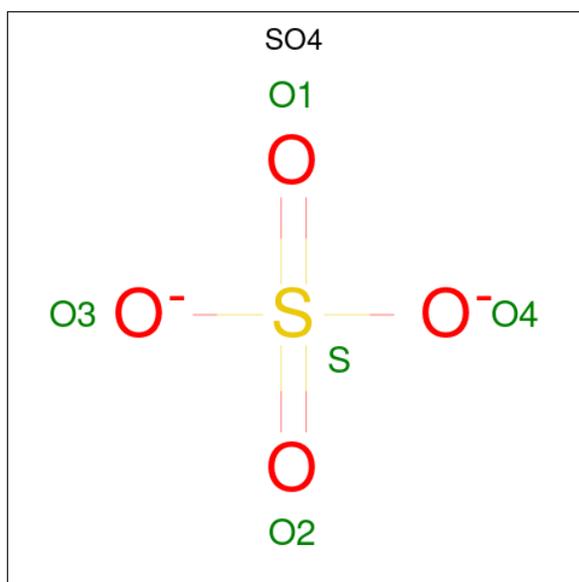
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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	TRP	cloning artifact	UNP P10635
B	30	LYS	ALA	cloning artifact	UNP P10635
B	31	GLY	ALA	cloning artifact	UNP P10635
B	32	LYS	ARG	cloning artifact	UNP P10635
B	33	LEU	TYR	cloning artifact	UNP P10635
B	230	ASP	LEU	engineered mutation	UNP P10635
B	231	ARG	LEU	engineered mutation	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP P10635
B	500	HIS	-	expression tag	UNP P10635
B	501	HIS	-	expression tag	UNP P10635
C	24	ALA	HIS	cloning artifact	UNP P10635
C	25	LYS	ARG	cloning artifact	UNP P10635
C	26	LYS	ARG	cloning artifact	UNP P10635
C	27	THR	GLN	cloning artifact	UNP P10635
C	28	SER	ARG	cloning artifact	UNP P10635
C	29	SER	TRP	cloning artifact	UNP P10635
C	30	LYS	ALA	cloning artifact	UNP P10635
C	31	GLY	ALA	cloning artifact	UNP P10635
C	32	LYS	ARG	cloning artifact	UNP P10635
C	33	LEU	TYR	cloning artifact	UNP P10635
C	230	ASP	LEU	engineered mutation	UNP P10635
C	231	ARG	LEU	engineered mutation	UNP P10635
C	498	HIS	-	expression tag	UNP P10635
C	499	HIS	-	expression tag	UNP P10635
C	500	HIS	-	expression tag	UNP P10635
C	501	HIS	-	expression tag	UNP P10635
D	24	ALA	HIS	cloning artifact	UNP P10635
D	25	LYS	ARG	cloning artifact	UNP P10635
D	26	LYS	ARG	cloning artifact	UNP P10635
D	27	THR	GLN	cloning artifact	UNP P10635
D	28	SER	ARG	cloning artifact	UNP P10635
D	29	SER	TRP	cloning artifact	UNP P10635
D	30	LYS	ALA	cloning artifact	UNP P10635
D	31	GLY	ALA	cloning artifact	UNP P10635
D	32	LYS	ARG	cloning artifact	UNP P10635
D	33	LEU	TYR	cloning artifact	UNP P10635
D	230	ASP	LEU	engineered mutation	UNP P10635
D	231	ARG	LEU	engineered mutation	UNP P10635
D	498	HIS	-	expression tag	UNP P10635
D	499	HIS	-	expression tag	UNP P10635
D	500	HIS	-	expression tag	UNP P10635

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

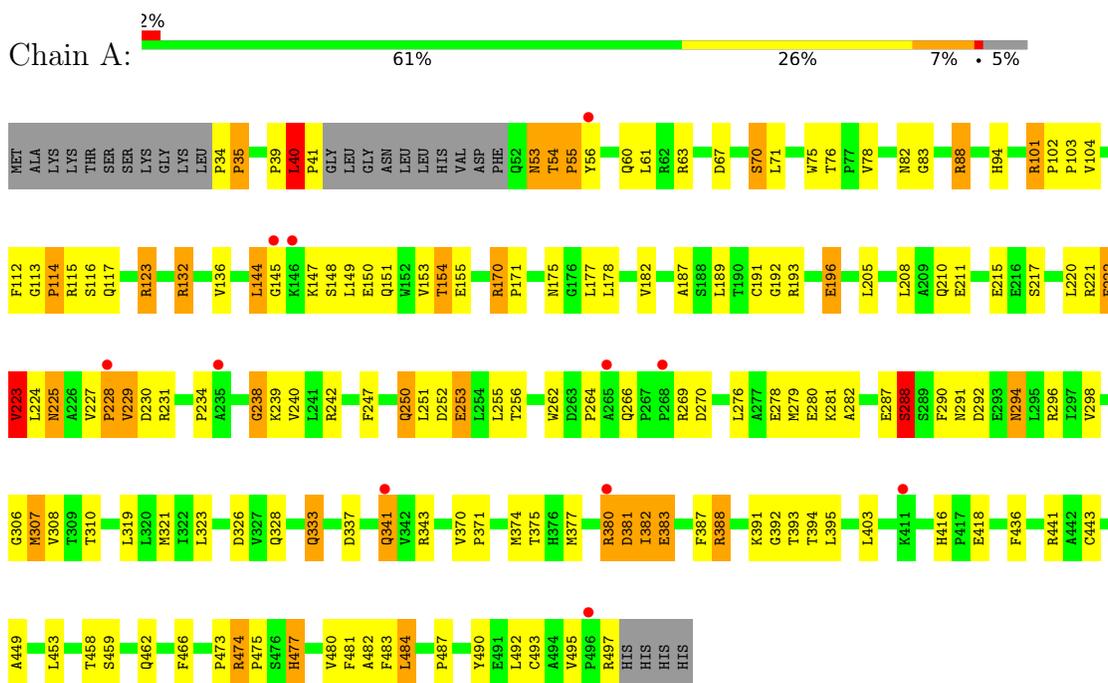
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	3	Total	O	0	0
			3	3		
4	C	2	Total	O	0	0
			2	2		
4	D	2	Total	O	0	0
			2	2		

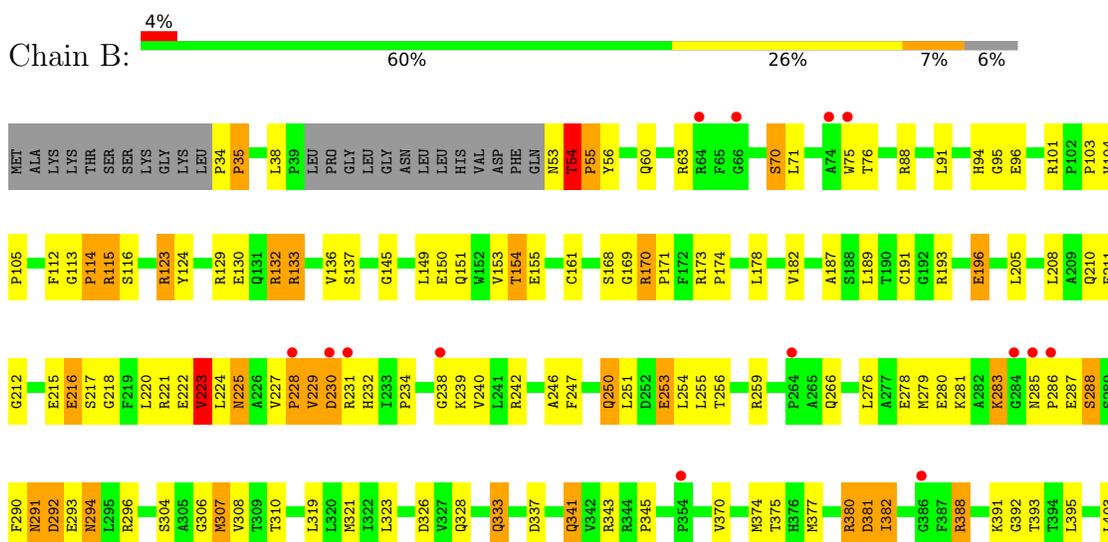
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Cytochrome P450 2D6

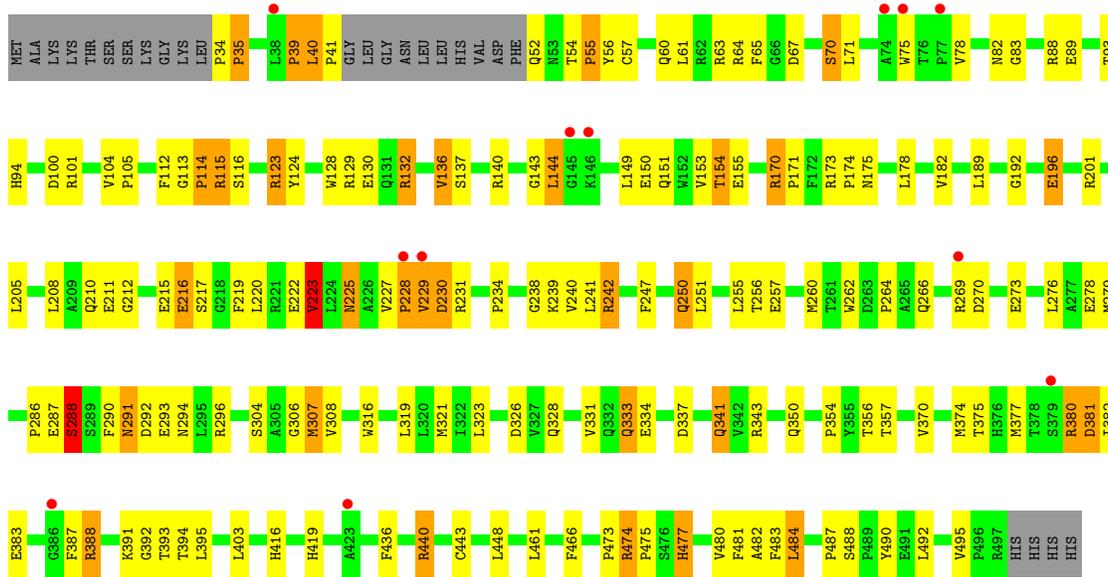


#### • Molecule 1: Cytochrome P450 2D6

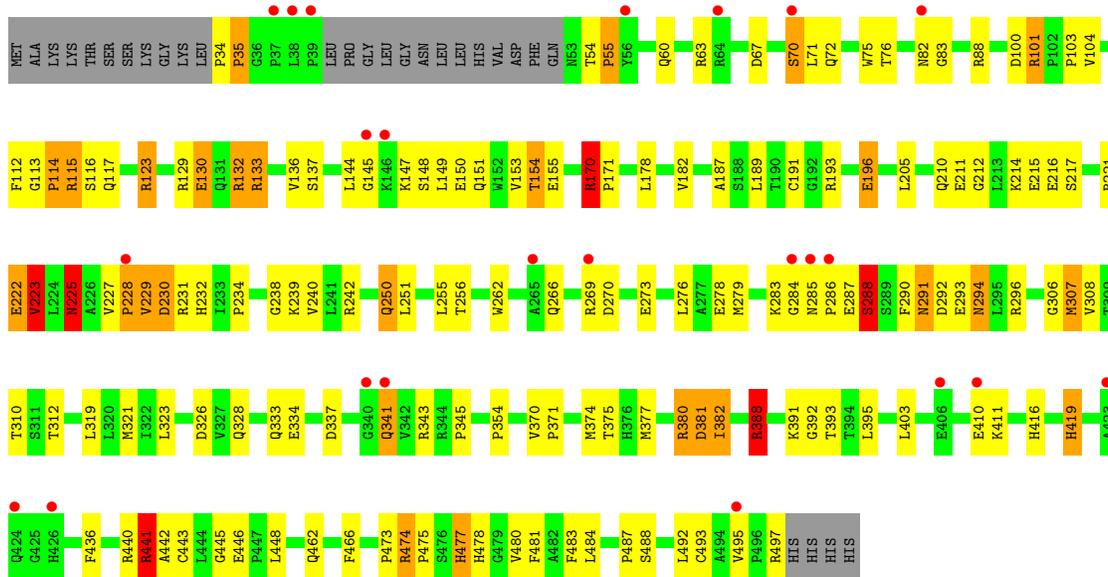




• Molecule 1: Cytochrome P450 2D6



• Molecule 1: Cytochrome P450 2D6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.07Å 155.50Å 95.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.00 – 3.00 39.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (106.00-3.00) 89.6 (39.97-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.230 , 0.286 0.230 , 0.282	Depositor DCC
$R_{free}$ test set	1601 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtrriage
Anisotropy	0.268	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 80.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14421	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.79	0/3664	0.82	1/4982 (0.0%)
1	B	0.72	1/3639 (0.0%)	0.80	3/4947 (0.1%)
1	C	0.79	1/3664 (0.0%)	0.84	1/4982 (0.0%)
1	D	0.77	2/3639 (0.1%)	0.82	6/4947 (0.1%)
All	All	0.77	4/14606 (0.0%)	0.82	11/19858 (0.1%)

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	4
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	269	ARG	CZ-NH1	15.49	1.53	1.33
1	C	57	CYS	CB-SG	-5.78	1.72	1.81
1	D	269	ARG	CZ-NH2	5.50	1.40	1.33
1	B	161	CYS	CB-SG	-5.42	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	269	ARG	NE-CZ-NH2	-13.90	113.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	D	441	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	D	388	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	234	PRO	N-CA-CB	6.54	111.15	103.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	GLY	Peptide
1	A	40	LEU	Peptide
1	A	53	ASN	Peptide
1	A	83	GLY	Peptide
1	B	113	GLY	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	3569	0	3513	126	0
1	B	3545	0	3487	116	0
1	C	3569	0	3513	139	0
1	D	3545	0	3487	125	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
2	C	43	0	30	5	0
2	D	43	0	30	8	0
3	B	10	0	0	2	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	14421	0	14120	468	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 16.

The worst 5 of 468 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:B:227:VAL:HB	1:C:227:VAL:CB	1.75	1.16
1:B:227:VAL:CB	1:C:227:VAL:HB	1.75	1.15
1:A:60:GLN:NE2	1:B:60:GLN:HE21	1.49	1.11
1:C:60:GLN:HE21	1:D:60:GLN:NE2	1.53	1.05
1:A:60:GLN:NE2	1:B:60:GLN:NE2	2.06	1.03

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	450/479 (94%)	396 (88%)	34 (8%)	20 (4%)	2	15
1	B	447/479 (93%)	397 (89%)	33 (7%)	17 (4%)	3	18
1	C	450/479 (94%)	397 (88%)	38 (8%)	15 (3%)	4	21
1	D	447/479 (93%)	395 (88%)	36 (8%)	16 (4%)	3	19
All	All	1794/1916 (94%)	1585 (88%)	141 (8%)	68 (4%)	3	18

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PRO
1	A	40	LEU
1	A	114	PRO
1	A	145	GLY
1	A	229	VAL

### 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	380/409 (93%)	330 (87%)	50 (13%)	4	18
1	B	377/409 (92%)	322 (85%)	55 (15%)	3	15
1	C	380/409 (93%)	328 (86%)	52 (14%)	3	17
1	D	377/409 (92%)	322 (85%)	55 (15%)	3	15
All	All	1514/1636 (92%)	1302 (86%)	212 (14%)	3	16

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	130	GLU
1	C	370	VAL
1	D	382	ILE
1	C	154	THR
1	C	266	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	294	ASN
1	D	60	GLN
1	C	333	GLN
1	C	424	GLN
1	D	166	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](#)

6 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
2	HEM	B	600	1	27,50,50	2.40	8 (29%)	17,82,82	1.52	3 (17%)
2	HEM	A	600	1	27,50,50	2.21	9 (33%)	17,82,82	1.77	5 (29%)
2	HEM	C	600	1	27,50,50	2.35	8 (29%)	17,82,82	1.83	6 (35%)
3	SO4	B	2001	-	4,4,4	0.31	0	6,6,6	0.82	0
3	SO4	B	2000	-	4,4,4	0.31	0	6,6,6	1.11	1 (16%)
2	HEM	D	600	1	27,50,50	2.37	9 (33%)	17,82,82	1.51	6 (35%)

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
2	HEM	D	600	1	-	0/6/54/54	-
2	HEM	B	600	1	-	0/6/54/54	-
2	HEM	A	600	1	-	0/6/54/54	-
2	HEM	C	600	1	-	0/6/54/54	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	C3D-C2D	5.40	1.53	1.37
2	A	600	HEM	C3D-C2D	5.24	1.53	1.37
2	D	600	HEM	C3D-C2D	4.88	1.52	1.37
2	C	600	HEM	C3B-CAB	4.55	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	C3C-C2C	-4.53	1.34	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	C4C-C3C-C2C	3.48	109.33	106.90
2	C	600	HEM	C4A-C3A-C2A	3.05	109.12	107.00
2	A	600	HEM	CBD-CAD-C3D	-2.94	107.06	112.48
2	C	600	HEM	C1D-C2D-C3D	-2.93	104.96	107.00
2	C	600	HEM	CMC-C2C-C3C	2.86	130.04	124.68

There are no chirality outliers.

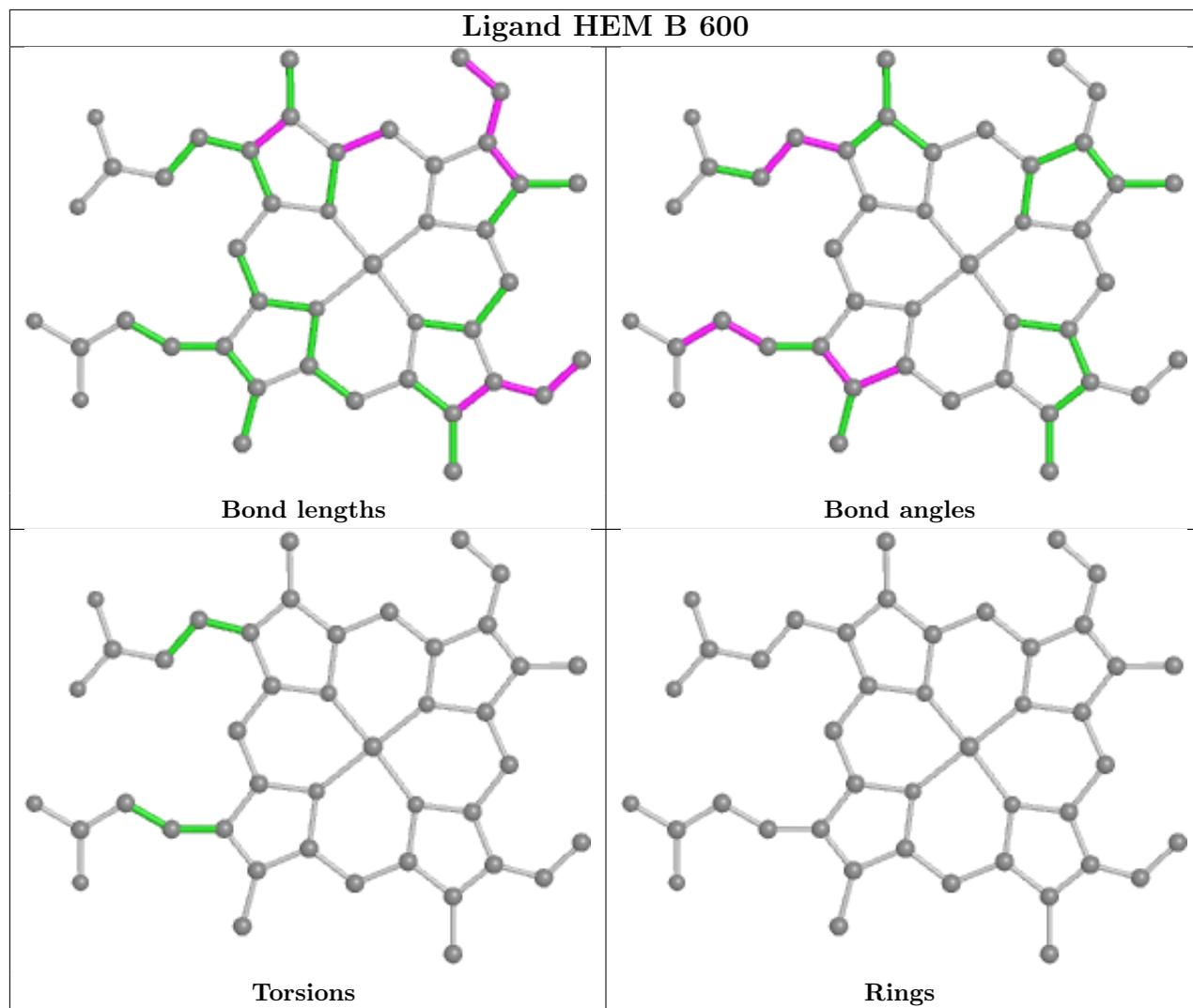
There are no torsion outliers.

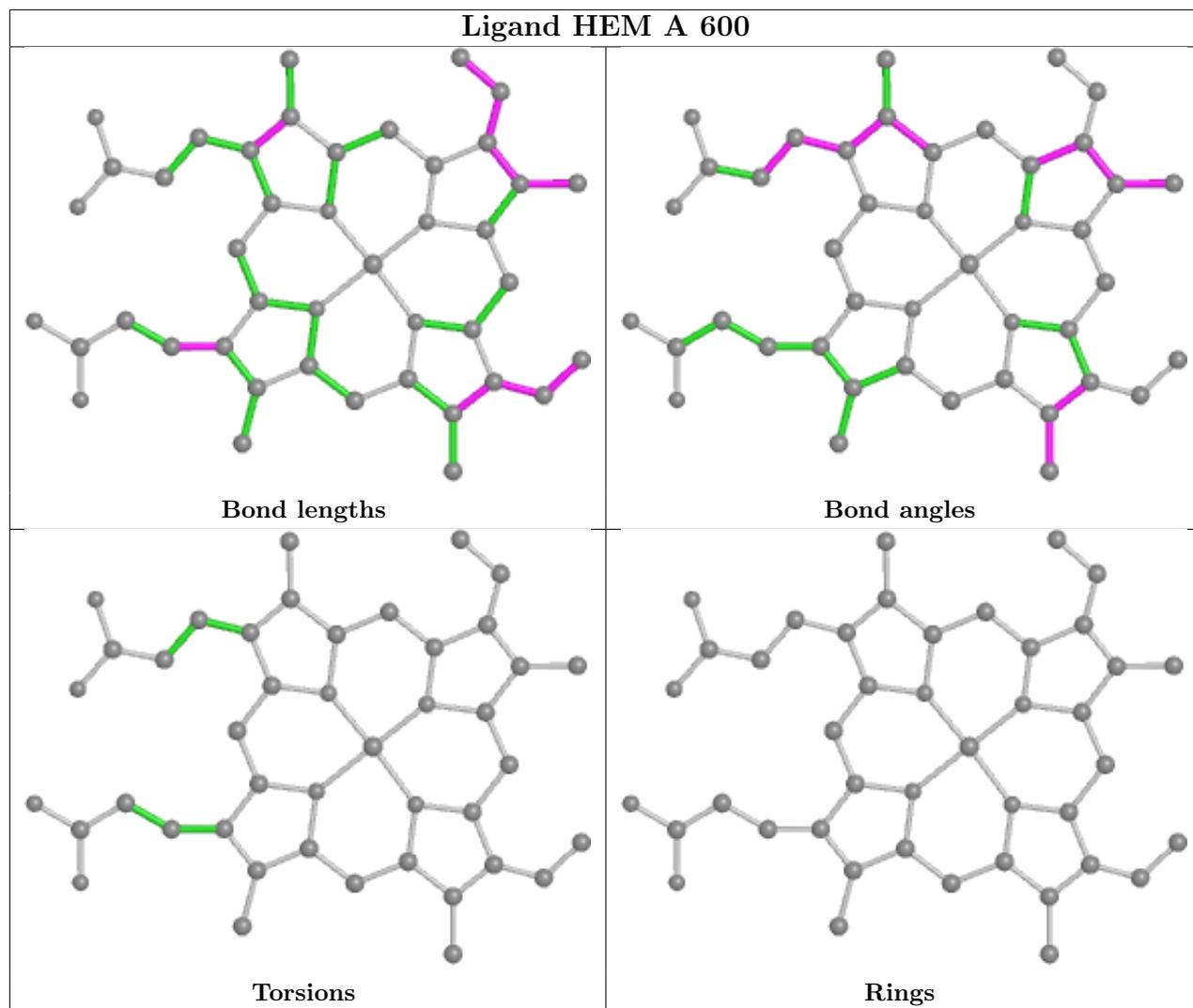
There are no ring outliers.

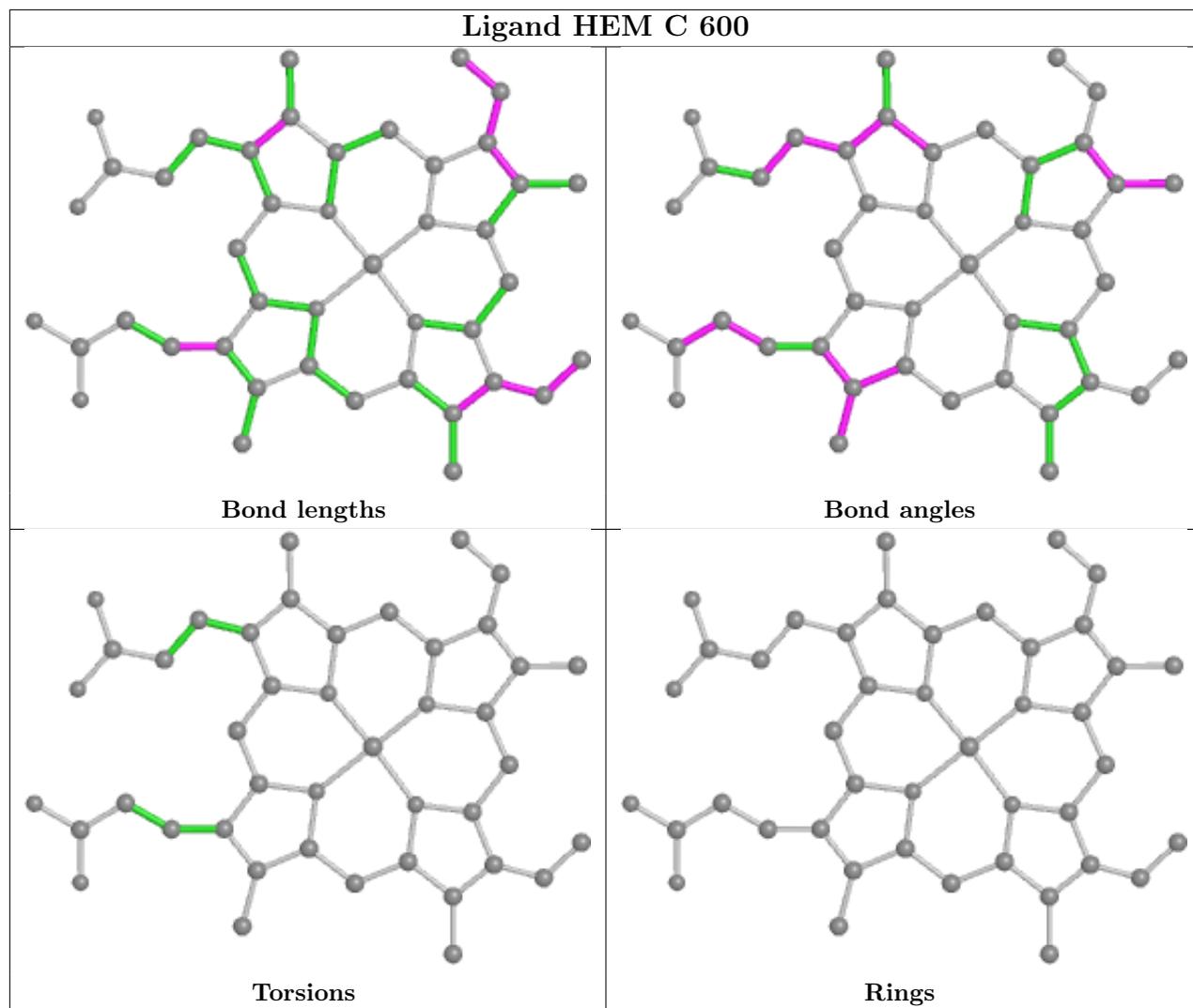
5 monomers are involved in 26 short contacts:

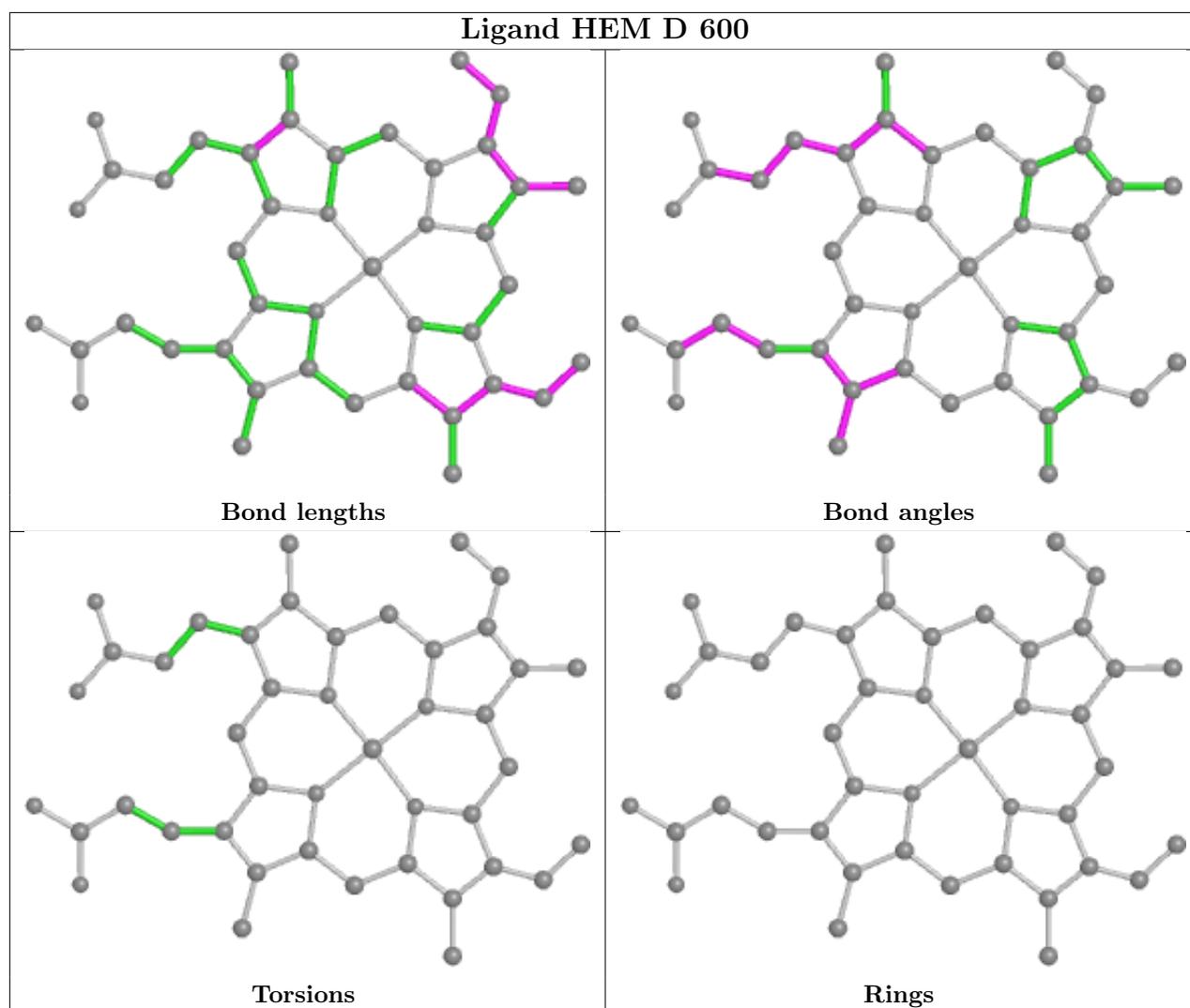
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	HEM	6	0
2	A	600	HEM	5	0
2	C	600	HEM	5	0
3	B	2000	SO4	2	0
2	D	600	HEM	8	0

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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	454/479 (94%)	0.10	11 (2%) 59 30	50, 57, 63, 77	0
1	B	451/479 (94%)	0.24	17 (3%) 40 16	46, 57, 63, 71	0
1	C	454/479 (94%)	0.06	12 (2%) 56 27	49, 57, 63, 75	0
1	D	451/479 (94%)	0.19	23 (5%) 28 10	48, 57, 63, 72	0
All	All	1810/1916 (94%)	0.15	63 (3%) 44 18	46, 57, 63, 77	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	228	PRO	4.9
1	B	424	GLN	4.4
1	B	286	PRO	4.2
1	C	228	PRO	4.0
1	C	145	GLY	3.7

### 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](#)

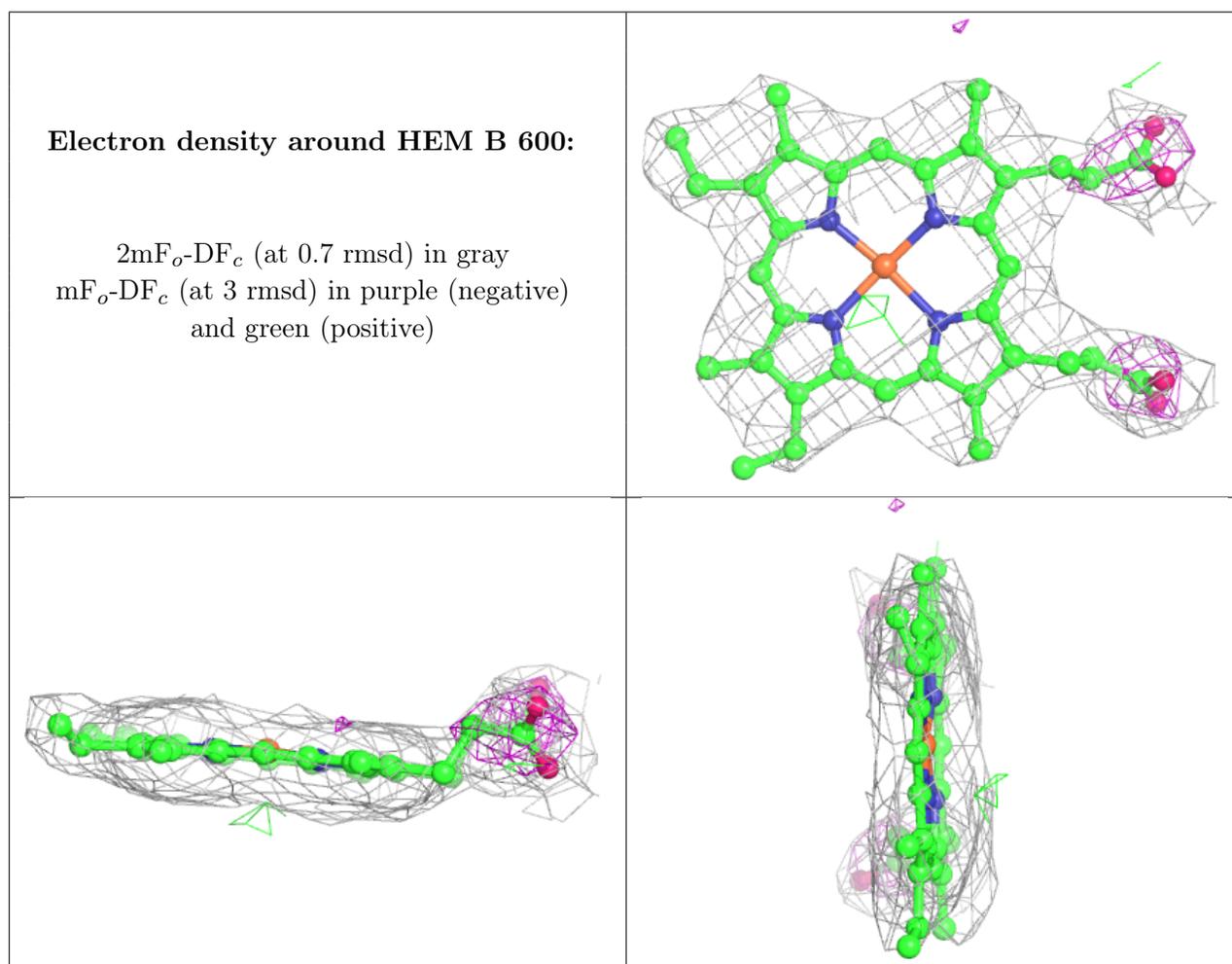
There are no monosaccharides in this entry.

### 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

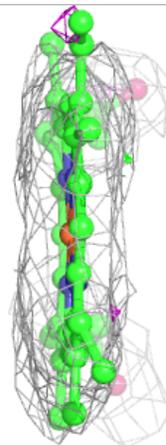
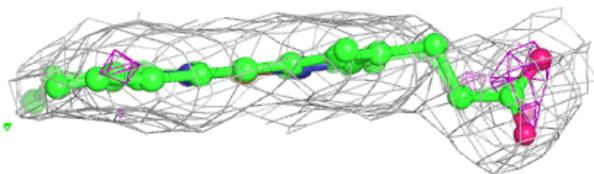
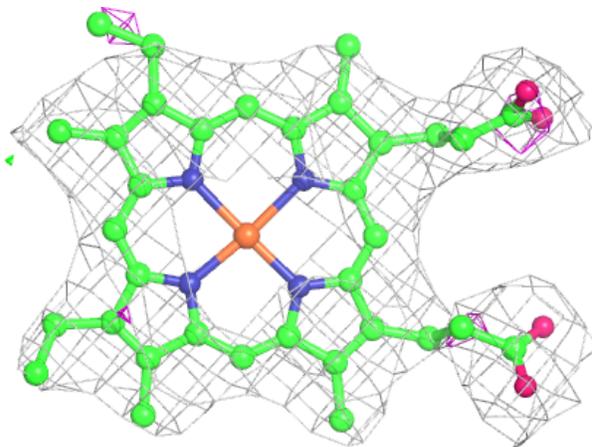
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	2001	5/5	0.92	0.18	52,54,57,58	0
2	HEM	B	600	43/43	0.95	0.22	48,52,55,56	0
2	HEM	A	600	43/43	0.95	0.23	48,52,55,56	0
2	HEM	D	600	43/43	0.96	0.19	48,52,55,56	0
3	SO4	B	2000	5/5	0.97	0.13	46,51,54,54	0
2	HEM	C	600	43/43	0.97	0.18	48,52,55,56	0

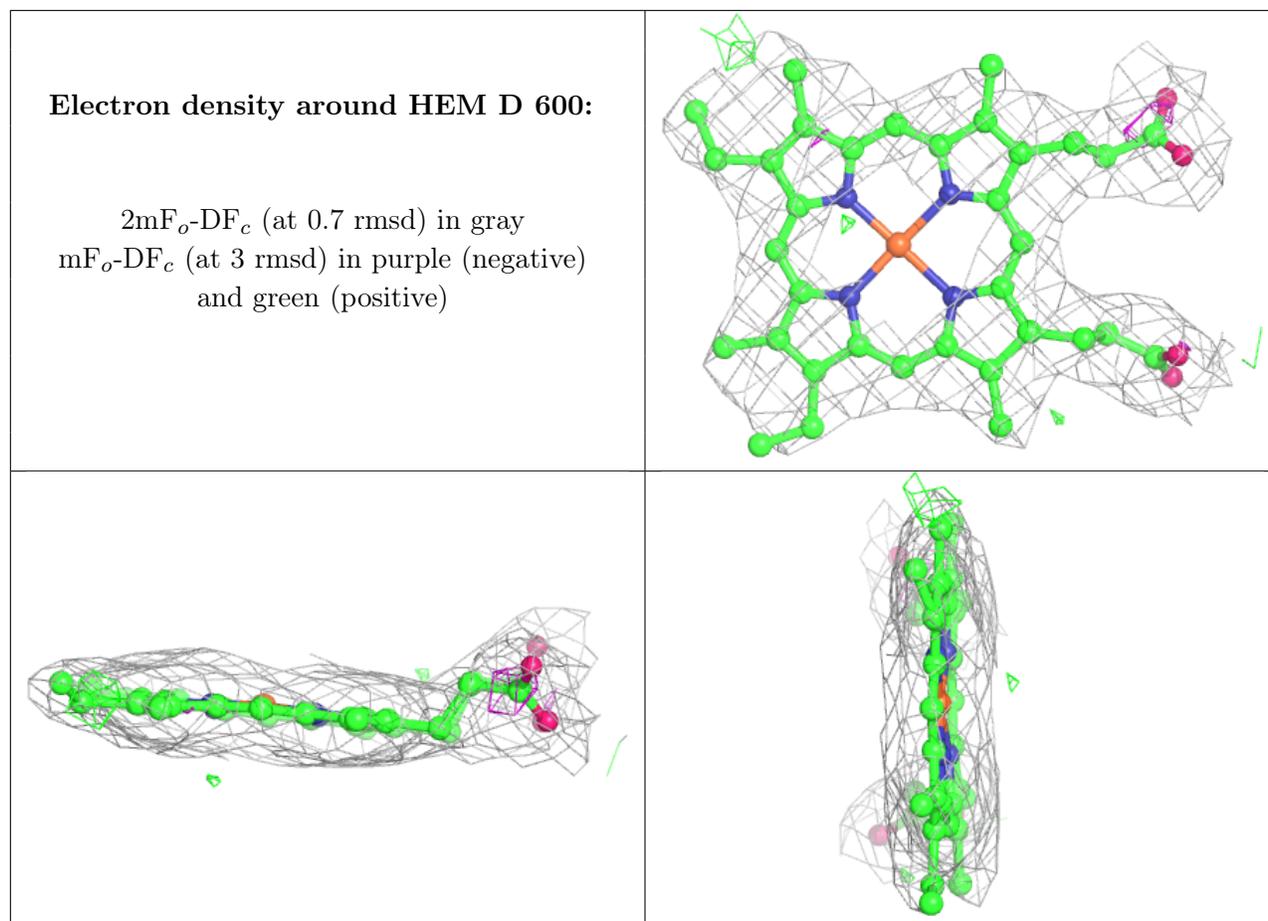
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

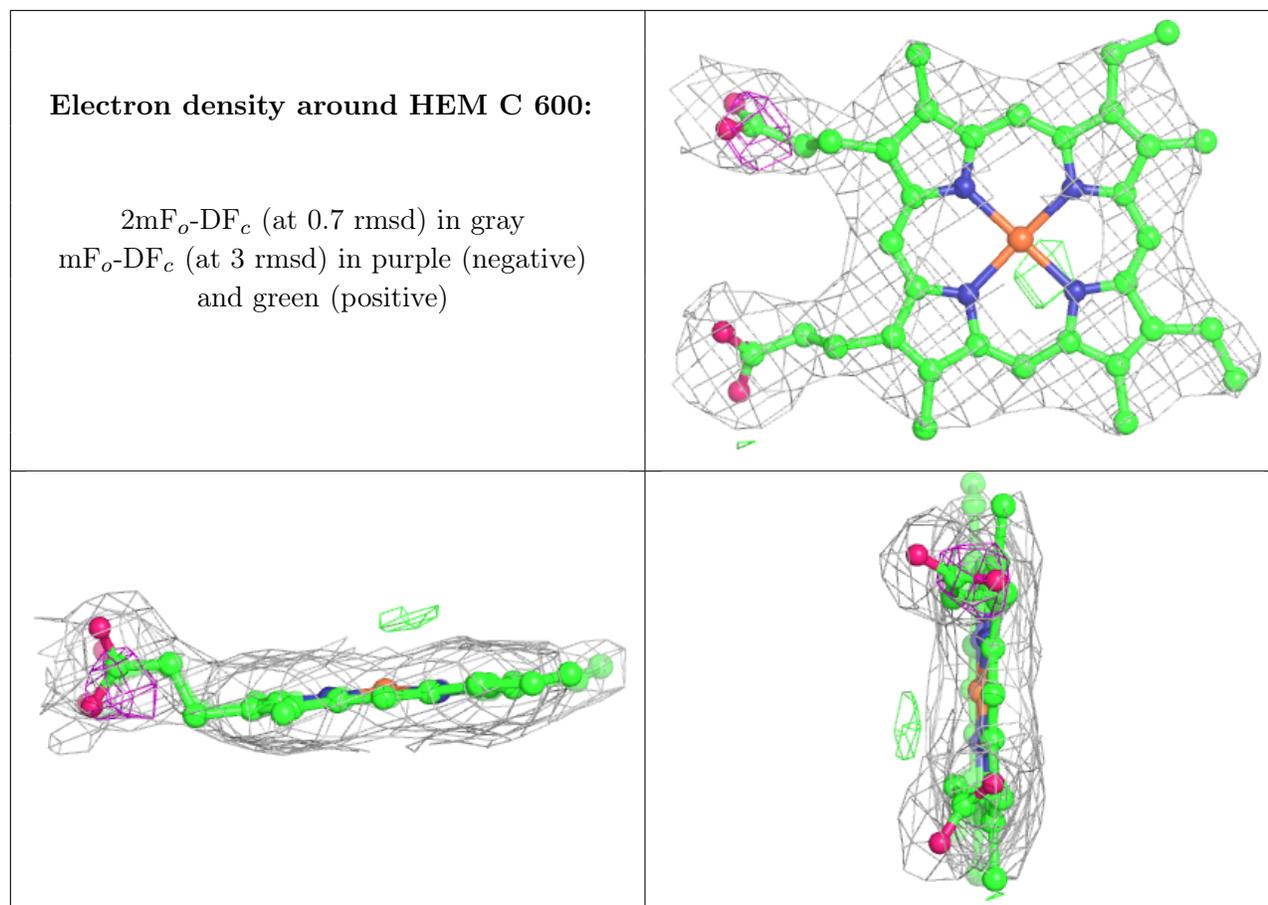


**Electron density around HEM A 600:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.