



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:29 PM UTC

PDB ID : 2RGZ / pdb_00002rgz
Title : Ensemble refinement of the protein crystal structure of human heme oxygenase-2 C127A (HO-2) with bound heme
Authors : Bianchetti, C.M.; Bingman, C.A.; Bitto, E.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-10-05
Resolution : 2.61 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

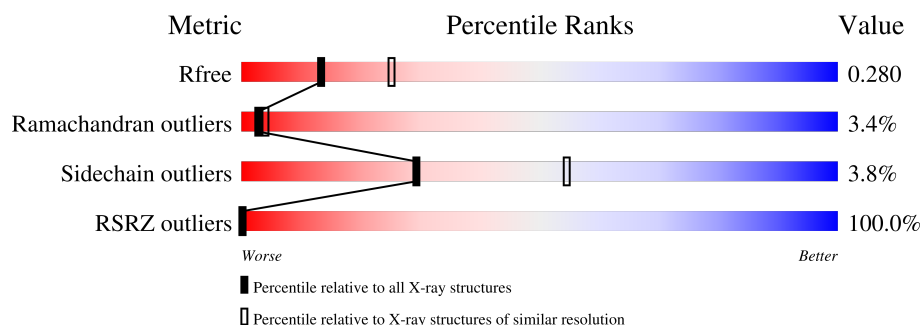
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	180053	4951 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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 $\leq 5\%$. 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	1-A	264	81% 77% 19%
1	1-B	264	83% 77% 6% 17%
1	10-A	264	78% 19%
1	10-B	264	77% 6% 17%
1	11-A	264	77% 19%
1	11-B	264	78% 5% 17%

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Mol	Chain	Length	Quality of chain
1	12-A	264	 78% 19%
1	12-B	264	 77% 17%
1	13-A	264	 77% 19%
1	13-B	264	 77% 17%
1	14-A	264	 76% 19%
1	14-B	264	 74% 17%
1	15-A	264	 75% 19%
1	15-B	264	 77% 17%
1	16-A	264	 77% 19%
1	16-B	264	 74% 17%
1	2-A	264	 77% 19%
1	2-B	264	 79% 17%
1	3-A	264	 77% 19%
1	3-B	264	 77% 17%
1	4-A	264	 76% 19%
1	4-B	264	 78% 17%
1	5-A	264	 77% 19%
1	5-B	264	 77% 17%
1	6-A	264	 76% 19%
1	6-B	264	 76% 17%
1	7-A	264	 77% 19%
1	7-B	264	 78% 17%
1	8-A	264	 77% 19%
1	8-B	264	 76% 17%
1	9-A	264	 75% 19%

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Mol	Chain	Length	Quality of chain
1	9-B	264	 77% 6% 17%

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
2	HEM	1-A	300	-	-	-	X
2	HEM	1-B	265	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 58291 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 Heme oxygenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	2-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	3-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	4-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	5-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	6-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	7-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	8-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	9-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	10-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	11-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	12-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	13-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	14-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	15-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	16-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			

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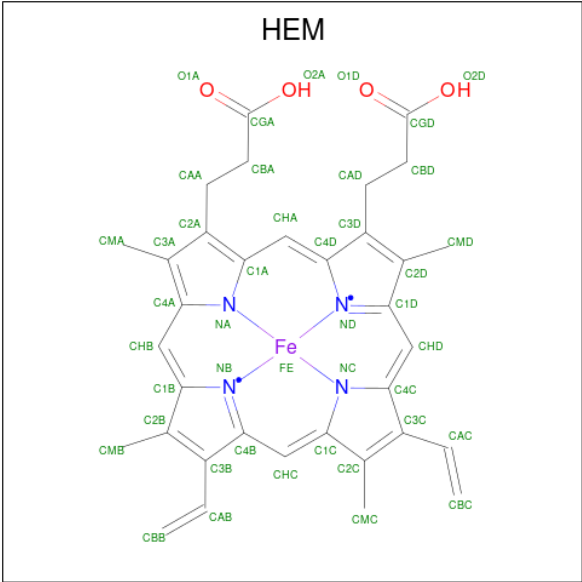
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	2-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	3-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	4-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	5-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	6-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	7-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	8-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	9-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	10-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	11-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	12-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	13-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	14-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	15-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	16-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	CYS	engineered mutation	UNP P30519
B	127	ALA	CYS	engineered mutation	UNP P30519

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	2-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	3-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	4-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	5-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	6-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	7-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	8-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	9-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	10-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	11-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	12-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	13-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	14-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	15-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	16-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	1-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	2-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	3-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	4-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	5-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	6-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	7-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	8-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	9-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	10-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	11-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	12-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	13-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	14-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	15-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	16-B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	49	Total 49	O 49	0	0

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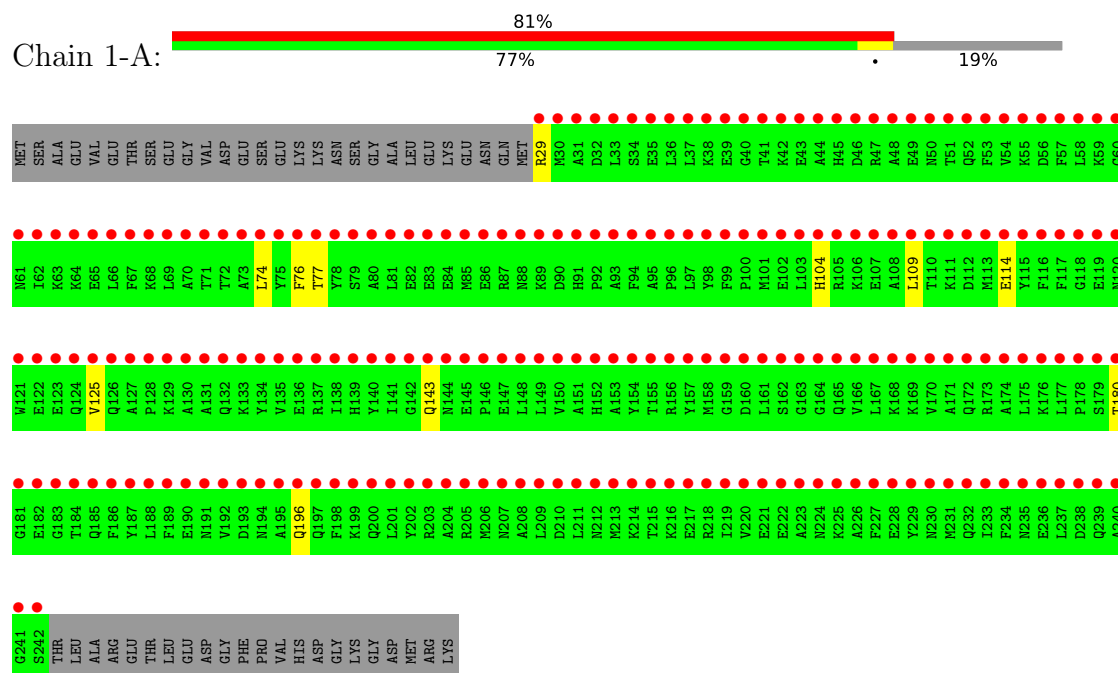
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-B	34	Total	O	0	0
			34	34		

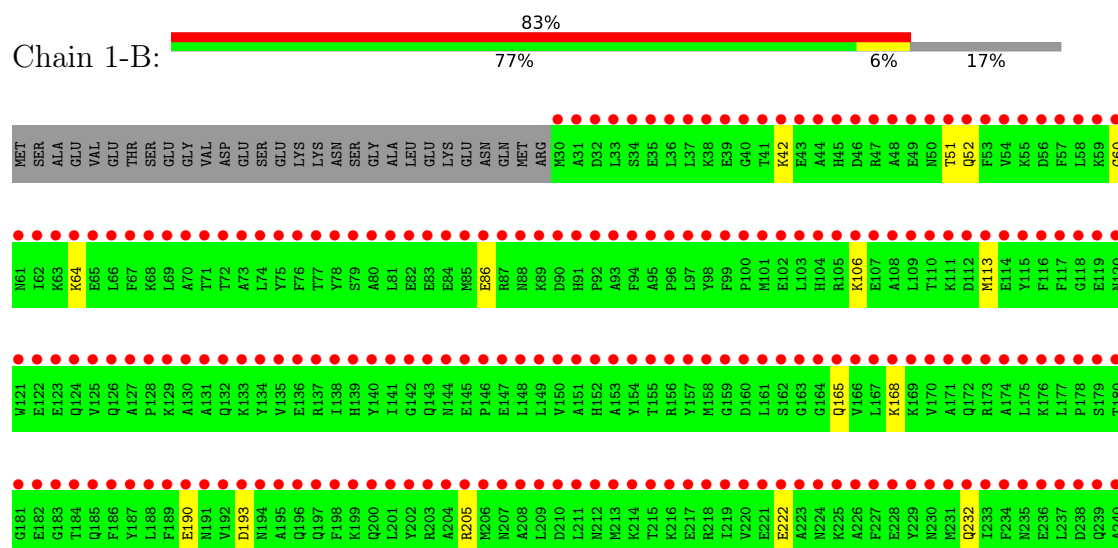
3 Residue-property plots [i](#)

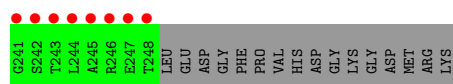
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Heme oxygenase 2

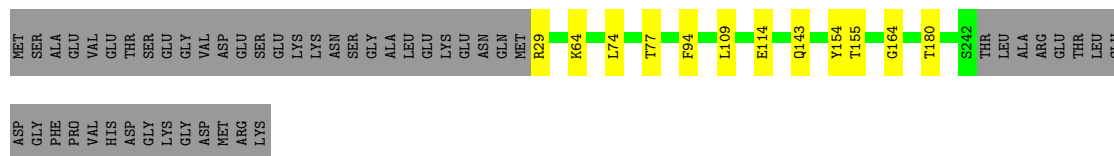
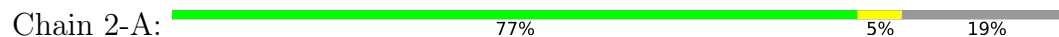


• Molecule 1: Heme oxygenase 2

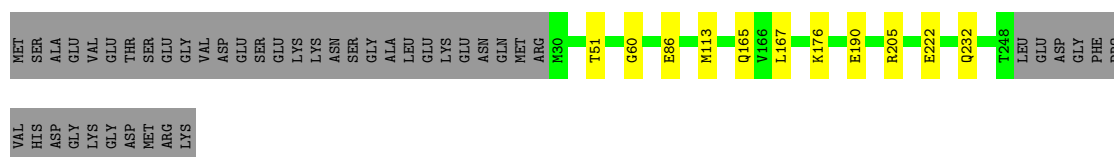
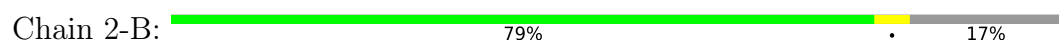




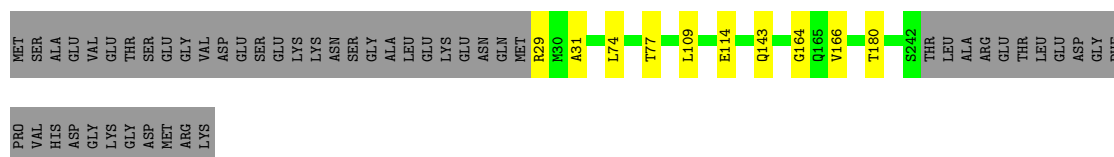
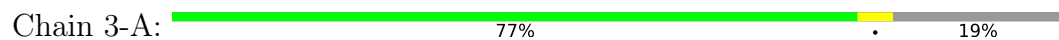
- Molecule 1: Heme oxygenase 2



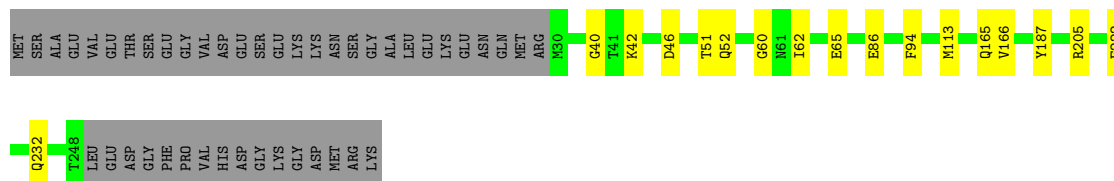
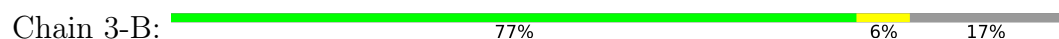
- Molecule 1: Heme oxygenase 2



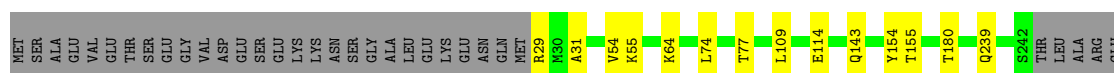
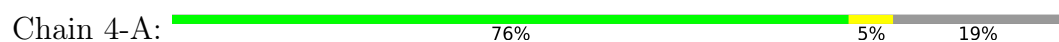
- Molecule 1: Heme oxygenase 2



- Molecule 1: Heme oxygenase 2



- Molecule 1: Heme oxygenase 2



THR
LEU
GLU
ASP
GLY
PHE
PRO
VAL
HIS
GLY
ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

Chain 4-B:  78% 5% 17%

MET SER ALA VAL THR SER GLY VAL ASP GLU LYS ASN SER GLY ALA LEU LYS GLU LYS ASN GLN MET MET ARG M30 A44 T51 V54 K63 K64 E86 M113 Q165 V170 P178 R205 E222 Q232 E247 T248 LEU

ASP
GLY
PHE
PRO
VAL
HIS
ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

Chain 5-A:  77% 5% 19%

MET SER ALA VAL THR SER GLY VAL ASP GLU LYS ASN SER GLY ALA LEU LYS GLU LYS ASN GLN MET MET ARG R29 L74 T77 F94 L109 E114 I138 Q143 T180 E190 N191 G241 S242 THR LEU ALA ARG GLU THR LEU ASP

GLY
PHE
PRO
VAL
HIS
ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

Chain 5-B:  77% 6% 17%

MET SER ALA VAL THR SER GLY VAL ASP GLU LYS ASN SER GLY ALA LEU LYS GLU LYS ASN GLN MET MET ARG M30 G40 T51 I62 K63 K64 E86 M113 E119 G164 Q165 P178 S179 E182 R205 E222 Q232 T243

T248
LEU
GLU
PHE
PRO
VAL
HIS
ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

Chain 6-A:  76% 5% 19%

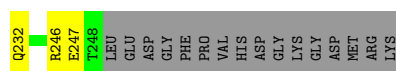
MET SER ALA VAL THR SER GLY VAL ASP GLU LYS ASN SER GLY ALA LEU LYS GLU LYS ASN GLN MET MET ARG R29 M30 A31 L74 T77 P100 M101 L109 E114 Q143 S162 G163 K176 T180 S242 THR LEU ALA ARG GLU THR LEU

GLU
ASP
GLY
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ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

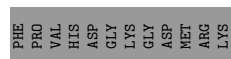
Chain 6-B:  76% 7% 17%

MET SER ALA VAL THR SER GLY VAL ASP GLU LYS ASN SER GLY ALA LEU LYS GLU LYS ASN GLN MET MET ARG M30 T51 Q52 K64 E86 F99 H104 R105 M113 Q165 L175 P178 S179 V192 R205 N212 E222



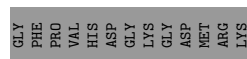
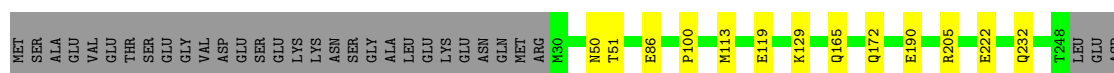
- Molecule 1: Heme oxygenase 2

Chain 7-A: 77% 19%



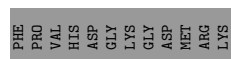
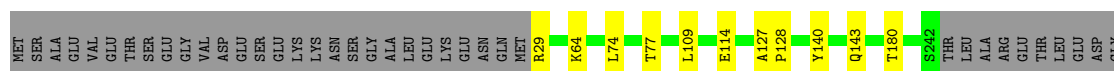
- Molecule 1: Heme oxygenase 2

Chain 7-B: 78% 5% 17%



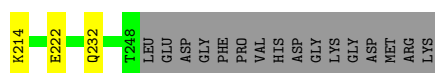
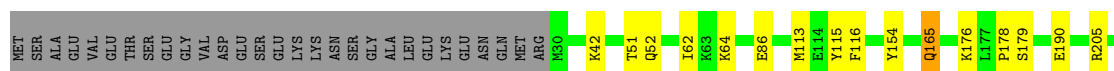
- Molecule 1: Heme oxygenase 2

Chain 8-A: 77% 19%



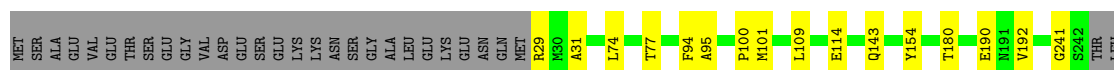
- Molecule 1: Heme oxygenase 2

Chain 8-B: 76% 7% 17%



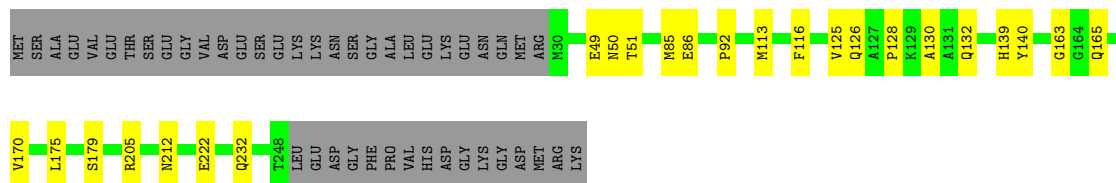
- Molecule 1: Heme oxygenase 2

Chain 9-A: 75% 6% 19%



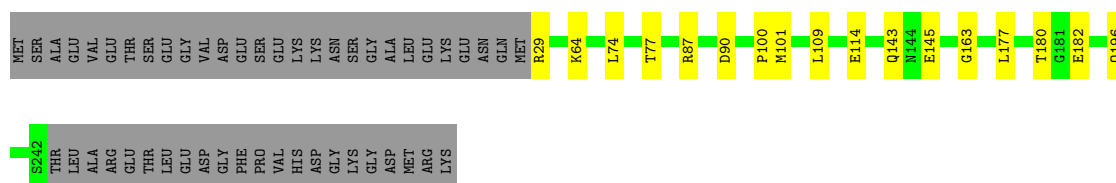
- Molecule 1: Heme oxygenase 2

Chain 14-B:  74% 9% 17%



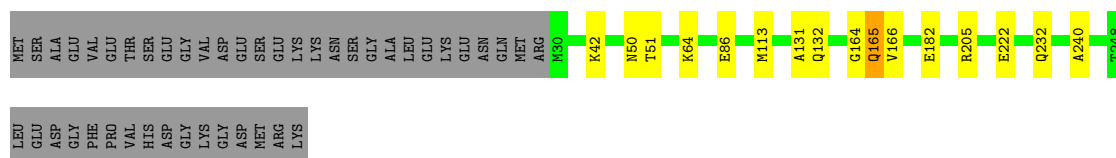
- Molecule 1: Heme oxygenase 2

Chain 15-A:  75% 6% 19%



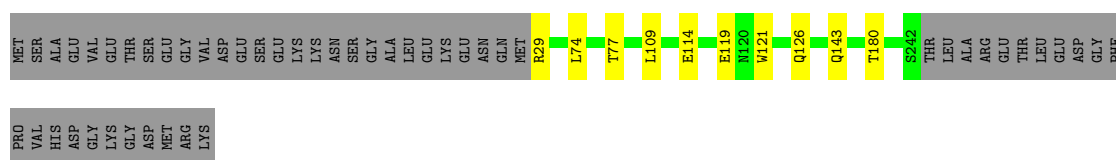
- Molecule 1: Heme oxygenase 2

Chain 15-B:  77% 6% 17%



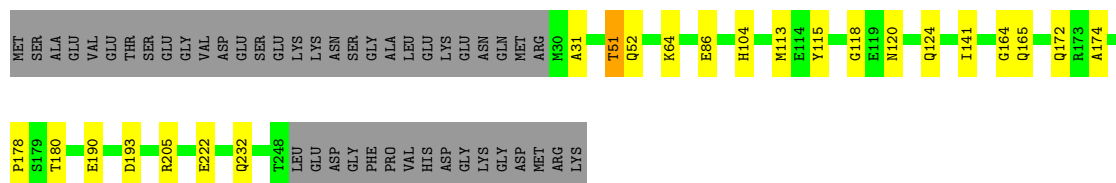
- Molecule 1: Heme oxygenase 2

Chain 16-A:  77% 6% 19%



- Molecule 1: Heme oxygenase 2

Chain 16-B:  74% 8% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.98Å 85.09Å 97.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.02 – 2.61 39.02 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.02-2.61) 99.3 (39.02-2.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.161 , 0.249 0.209 , 0.280	Depositor DCC
R_{free} test set	1005 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.52	EDS
Total number of atoms	58291	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1-A	0.19	0/1794	0.32	0/2410
1	1-B	0.18	0/1830	0.29	0/2460
1	2-A	0.19	0/1794	0.32	0/2410
1	2-B	0.18	0/1830	0.29	0/2460
1	3-A	0.19	0/1794	0.32	0/2410
1	3-B	0.18	0/1830	0.29	0/2460
1	4-A	0.19	0/1794	0.32	0/2410
1	4-B	0.18	0/1830	0.29	0/2460
1	5-A	0.19	0/1794	0.32	0/2410
1	5-B	0.18	0/1830	0.29	0/2460
1	6-A	0.19	0/1794	0.32	0/2410
1	6-B	0.18	0/1830	0.29	0/2460
1	7-A	0.19	0/1794	0.32	0/2410
1	7-B	0.18	0/1830	0.29	0/2460
1	8-A	0.19	0/1794	0.32	0/2410
1	8-B	0.18	0/1830	0.29	0/2460
1	9-A	0.19	0/1794	0.32	0/2410
1	9-B	0.18	0/1830	0.29	0/2460
1	10-A	0.19	0/1794	0.32	0/2410
1	10-B	0.18	0/1830	0.29	0/2460
1	11-A	0.19	0/1794	0.32	0/2410
1	11-B	0.18	0/1830	0.29	0/2460
1	12-A	0.19	0/1794	0.32	0/2410
1	12-B	0.18	0/1830	0.29	0/2460
1	13-A	0.19	0/1794	0.32	0/2410
1	13-B	0.18	0/1830	0.29	0/2460
1	14-A	0.19	0/1794	0.32	0/2410
1	14-B	0.18	0/1830	0.29	0/2460
1	15-A	0.19	0/1794	0.32	0/2410
1	15-B	0.18	0/1830	0.29	0/2460
1	16-A	0.19	0/1794	0.32	0/2410
1	16-B	0.18	0/1830	0.29	0/2460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.19	0/57984	0.31	0/77920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1-A	1758	0	1717	0	0
1	1-B	1794	0	1753	0	0
1	2-A	1758	0	1717	0	0
1	2-B	1794	0	1753	0	0
1	3-A	1758	0	1717	0	0
1	3-B	1794	0	1753	0	0
1	4-A	1758	0	1717	0	0
1	4-B	1794	0	1753	0	0
1	5-A	1758	0	1717	0	0
1	5-B	1794	0	1753	0	0
1	6-A	1758	0	1717	0	0
1	6-B	1794	0	1753	0	0
1	7-A	1758	0	1717	0	0
1	7-B	1794	0	1753	0	0
1	8-A	1758	0	1717	0	0
1	8-B	1794	0	1753	0	0
1	9-A	1758	0	1717	0	0
1	9-B	1794	0	1753	0	0
1	10-A	1758	0	1717	0	0
1	10-B	1794	0	1753	0	0
1	11-A	1758	0	1717	0	0
1	11-B	1794	0	1753	0	0
1	12-A	1758	0	1717	0	0
1	12-B	1794	0	1753	0	0
1	13-A	1758	0	1717	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13-B	1794	0	1753	0	0
1	14-A	1758	0	1717	0	0
1	14-B	1794	0	1753	0	0
1	15-A	1758	0	1717	0	0
1	15-B	1794	0	1753	0	0
1	16-A	1758	0	1717	0	0
1	16-B	1794	0	1753	0	0
2	1-A	43	0	30	0	0
2	1-B	43	0	30	0	0
2	2-A	43	0	30	0	0
2	2-B	43	0	30	0	0
2	3-A	43	0	30	0	0
2	3-B	43	0	30	0	0
2	4-A	43	0	30	0	0
2	4-B	43	0	30	0	0
2	5-A	43	0	30	0	0
2	5-B	43	0	30	0	0
2	6-A	43	0	30	0	0
2	6-B	43	0	30	0	0
2	7-A	43	0	30	0	0
2	7-B	43	0	30	0	0
2	8-A	43	0	30	0	0
2	8-B	43	0	30	0	0
2	9-A	43	0	30	0	0
2	9-B	43	0	30	0	0
2	10-A	43	0	30	0	0
2	10-B	43	0	30	0	0
2	11-A	43	0	30	0	0
2	11-B	43	0	30	0	0
2	12-A	43	0	30	0	0
2	12-B	43	0	30	0	0
2	13-A	43	0	30	0	0
2	13-B	43	0	30	0	0
2	14-A	43	0	30	0	0
2	14-B	43	0	30	0	0
2	15-A	43	0	30	0	0
2	15-B	43	0	30	0	0
2	16-A	43	0	30	0	0
2	16-B	43	0	30	0	0
3	1-A	49	0	0	0	0
3	1-B	34	0	0	0	0
All	All	58291	0	56480	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	212/264 (80%)	185 (87%)	23 (11%)	4 (2%)	6	12
1	1-B	217/264 (82%)	190 (88%)	19 (9%)	8 (4%)	2	3
1	2-A	212/264 (80%)	184 (87%)	23 (11%)	5 (2%)	4	8
1	2-B	217/264 (82%)	183 (84%)	30 (14%)	4 (2%)	6	13
1	3-A	212/264 (80%)	192 (91%)	17 (8%)	3 (1%)	9	17
1	3-B	217/264 (82%)	174 (80%)	33 (15%)	10 (5%)	2	2
1	4-A	212/264 (80%)	188 (89%)	17 (8%)	7 (3%)	3	4
1	4-B	217/264 (82%)	175 (81%)	35 (16%)	7 (3%)	3	4
1	5-A	212/264 (80%)	189 (89%)	18 (8%)	5 (2%)	4	8
1	5-B	217/264 (82%)	186 (86%)	22 (10%)	9 (4%)	2	2
1	6-A	212/264 (80%)	181 (85%)	25 (12%)	6 (3%)	4	6
1	6-B	217/264 (82%)	167 (77%)	38 (18%)	12 (6%)	1	1
1	7-A	212/264 (80%)	182 (86%)	26 (12%)	4 (2%)	6	12
1	7-B	217/264 (82%)	183 (84%)	28 (13%)	6 (3%)	4	6
1	8-A	212/264 (80%)	187 (88%)	21 (10%)	4 (2%)	6	12
1	8-B	217/264 (82%)	183 (84%)	21 (10%)	13 (6%)	1	1
1	9-A	212/264 (80%)	179 (84%)	24 (11%)	9 (4%)	2	2
1	9-B	217/264 (82%)	184 (85%)	23 (11%)	10 (5%)	2	2
1	10-A	212/264 (80%)	189 (89%)	20 (9%)	3 (1%)	9	17
1	10-B	217/264 (82%)	185 (85%)	23 (11%)	9 (4%)	2	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11-A	212/264 (80%)	185 (87%)	24 (11%)	3 (1%)	9	17
1	11-B	217/264 (82%)	184 (85%)	28 (13%)	5 (2%)	5	8
1	12-A	212/264 (80%)	198 (93%)	12 (6%)	2 (1%)	14	28
1	12-B	217/264 (82%)	174 (80%)	33 (15%)	10 (5%)	2	2
1	13-A	212/264 (80%)	186 (88%)	21 (10%)	5 (2%)	4	8
1	13-B	217/264 (82%)	182 (84%)	26 (12%)	9 (4%)	2	2
1	14-A	212/264 (80%)	176 (83%)	30 (14%)	6 (3%)	4	6
1	14-B	217/264 (82%)	165 (76%)	35 (16%)	17 (8%)	1	0
1	15-A	212/264 (80%)	176 (83%)	26 (12%)	10 (5%)	2	2
1	15-B	217/264 (82%)	171 (79%)	36 (17%)	10 (5%)	2	2
1	16-A	212/264 (80%)	177 (84%)	32 (15%)	3 (1%)	9	17
1	16-B	217/264 (82%)	172 (79%)	28 (13%)	17 (8%)	1	0
All	All	6864/8448 (81%)	5812 (85%)	817 (12%)	235 (3%)	3	4

5 of 235 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-B	64	LYS
1	2-A	64	LYS
1	3-B	46	ASP
1	3-B	52	GLN
1	3-B	65	GLU

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	1-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	1-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	2-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	2-B	186/224 (83%)	179 (96%)	7 (4%)	29	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	3-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	4-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	4-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	5-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	5-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	6-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	6-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	7-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	7-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	8-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	8-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	9-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	9-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	10-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	10-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	11-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	11-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	12-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	12-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	13-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	13-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	14-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	14-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	15-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	15-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	16-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	16-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
All	All	5888/7168 (82%)	5664 (96%)	224 (4%)	29	54

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9-A	109	LEU
1	16-B	205	ARG
1	11-A	109	LEU
1	16-B	113	MET
1	15-A	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 203 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-B	104	HIS
1	11-B	152	HIS
1	16-B	172	GLN
1	9-B	194	ASN
1	10-B	172	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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	5-A	300	1	50,50,50	1.11	4 (8%)	67,82,82	0.94	2 (2%)
2	HEM	13-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.92	1 (1%)
2	HEM	4-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.94	2 (2%)
2	HEM	3-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.93	1 (1%)
2	HEM	12-B	265	1	50,50,50	1.21	4 (8%)	67,82,82	0.89	1 (1%)
2	HEM	5-B	265	1	50,50,50	1.17	4 (8%)	67,82,82	0.89	1 (1%)
2	HEM	11-B	265	1	50,50,50	1.16	4 (8%)	67,82,82	0.93	1 (1%)
2	HEM	7-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.90	1 (1%)
2	HEM	15-B	265	1	50,50,50	1.20	4 (8%)	67,82,82	0.94	1 (1%)
2	HEM	9-B	265	1	50,50,50	1.20	4 (8%)	67,82,82	0.92	1 (1%)
2	HEM	6-A	300	1	50,50,50	1.13	4 (8%)	67,82,82	0.97	1 (1%)
2	HEM	14-A	300	1	50,50,50	1.18	5 (10%)	67,82,82	0.98	1 (1%)
2	HEM	13-A	300	1	50,50,50	1.20	4 (8%)	67,82,82	0.94	1 (1%)
2	HEM	16-A	300	1	50,50,50	1.10	4 (8%)	67,82,82	0.98	1 (1%)
2	HEM	6-B	265	1	50,50,50	1.16	4 (8%)	67,82,82	0.89	2 (2%)
2	HEM	1-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.91	1 (1%)
2	HEM	10-B	265	1	50,50,50	1.20	4 (8%)	67,82,82	0.92	1 (1%)
2	HEM	8-A	300	1	50,50,50	1.13	4 (8%)	67,82,82	0.98	1 (1%)
2	HEM	11-A	300	1	50,50,50	1.13	4 (8%)	67,82,82	0.97	1 (1%)
2	HEM	3-A	300	1	50,50,50	1.14	4 (8%)	67,82,82	0.96	1 (1%)
2	HEM	9-A	300	1	50,50,50	1.21	4 (8%)	67,82,82	0.95	1 (1%)
2	HEM	8-B	265	1	50,50,50	1.17	4 (8%)	67,82,82	0.89	1 (1%)
2	HEM	10-A	300	1	50,50,50	1.10	4 (8%)	67,82,82	0.95	1 (1%)
2	HEM	12-A	300	1	50,50,50	1.14	4 (8%)	67,82,82	0.97	1 (1%)
2	HEM	16-B	265	1	50,50,50	1.23	4 (8%)	67,82,82	0.96	1 (1%)
2	HEM	14-B	265	1	50,50,50	1.25	5 (10%)	67,82,82	1.06	3 (4%)
2	HEM	15-A	300	1	50,50,50	1.13	4 (8%)	67,82,82	0.97	3 (4%)
2	HEM	2-A	300	1	50,50,50	1.11	4 (8%)	67,82,82	0.96	1 (1%)
2	HEM	1-A	300	1	50,50,50	1.10	4 (8%)	67,82,82	0.95	1 (1%)
2	HEM	2-B	265	1	50,50,50	1.20	4 (8%)	67,82,82	0.92	1 (1%)
2	HEM	7-A	300	1	50,50,50	1.12	4 (8%)	67,82,82	0.97	1 (1%)
2	HEM	4-A	300	1	50,50,50	1.21	4 (8%)	67,82,82	0.94	1 (1%)

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	5-A	300	1	-	2/14/54/54	-
2	HEM	13-B	265	1	-	6/14/54/54	-
2	HEM	4-B	265	1	-	10/14/54/54	-
2	HEM	3-B	265	1	-	11/14/54/54	-
2	HEM	12-B	265	1	-	11/14/54/54	-
2	HEM	5-B	265	1	-	8/14/54/54	-
2	HEM	11-B	265	1	-	6/14/54/54	-
2	HEM	7-B	265	1	-	8/14/54/54	-
2	HEM	15-B	265	1	-	8/14/54/54	-
2	HEM	9-B	265	1	-	7/14/54/54	-
2	HEM	6-A	300	1	-	6/14/54/54	-
2	HEM	14-A	300	1	-	4/14/54/54	-
2	HEM	13-A	300	1	-	5/14/54/54	-
2	HEM	16-A	300	1	-	5/14/54/54	-
2	HEM	6-B	265	1	-	6/14/54/54	-
2	HEM	1-B	265	1	-	9/14/54/54	-
2	HEM	10-B	265	1	-	9/14/54/54	-
2	HEM	8-A	300	1	-	2/14/54/54	-
2	HEM	11-A	300	1	-	6/14/54/54	-
2	HEM	3-A	300	1	-	7/14/54/54	-
2	HEM	9-A	300	1	-	7/14/54/54	-
2	HEM	8-B	265	1	-	8/14/54/54	-
2	HEM	10-A	300	1	-	2/14/54/54	-
2	HEM	12-A	300	1	-	7/14/54/54	-
2	HEM	16-B	265	1	-	11/14/54/54	-
2	HEM	14-B	265	1	-	5/14/54/54	-
2	HEM	15-A	300	1	-	2/14/54/54	-
2	HEM	2-A	300	1	-	5/14/54/54	-
2	HEM	1-A	300	1	-	2/14/54/54	-
2	HEM	2-B	265	1	-	7/14/54/54	-
2	HEM	7-A	300	1	-	4/14/54/54	-
2	HEM	4-A	300	1	-	8/14/54/54	-

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	12-B	265	HEM	CAB-C3B	-3.50	1.38	1.47
2	14-B	265	HEM	CBB-CAB	3.44	1.46	1.30
2	12-B	265	HEM	CBC-CAC	3.44	1.46	1.30
2	1-B	265	HEM	CAB-C3B	-3.36	1.38	1.47
2	9-B	265	HEM	CAB-C3B	-3.36	1.38	1.47

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-A	300	HEM	C3B-C4B-NB	4.17	112.46	109.47
2	16-A	300	HEM	C3B-C4B-NB	3.80	112.20	109.47
2	2-A	300	HEM	C3B-C4B-NB	3.63	112.07	109.47
2	13-A	300	HEM	C3B-C4B-NB	3.61	112.06	109.47
2	12-A	300	HEM	C3B-C4B-NB	3.46	111.95	109.47

There are no chirality outliers.

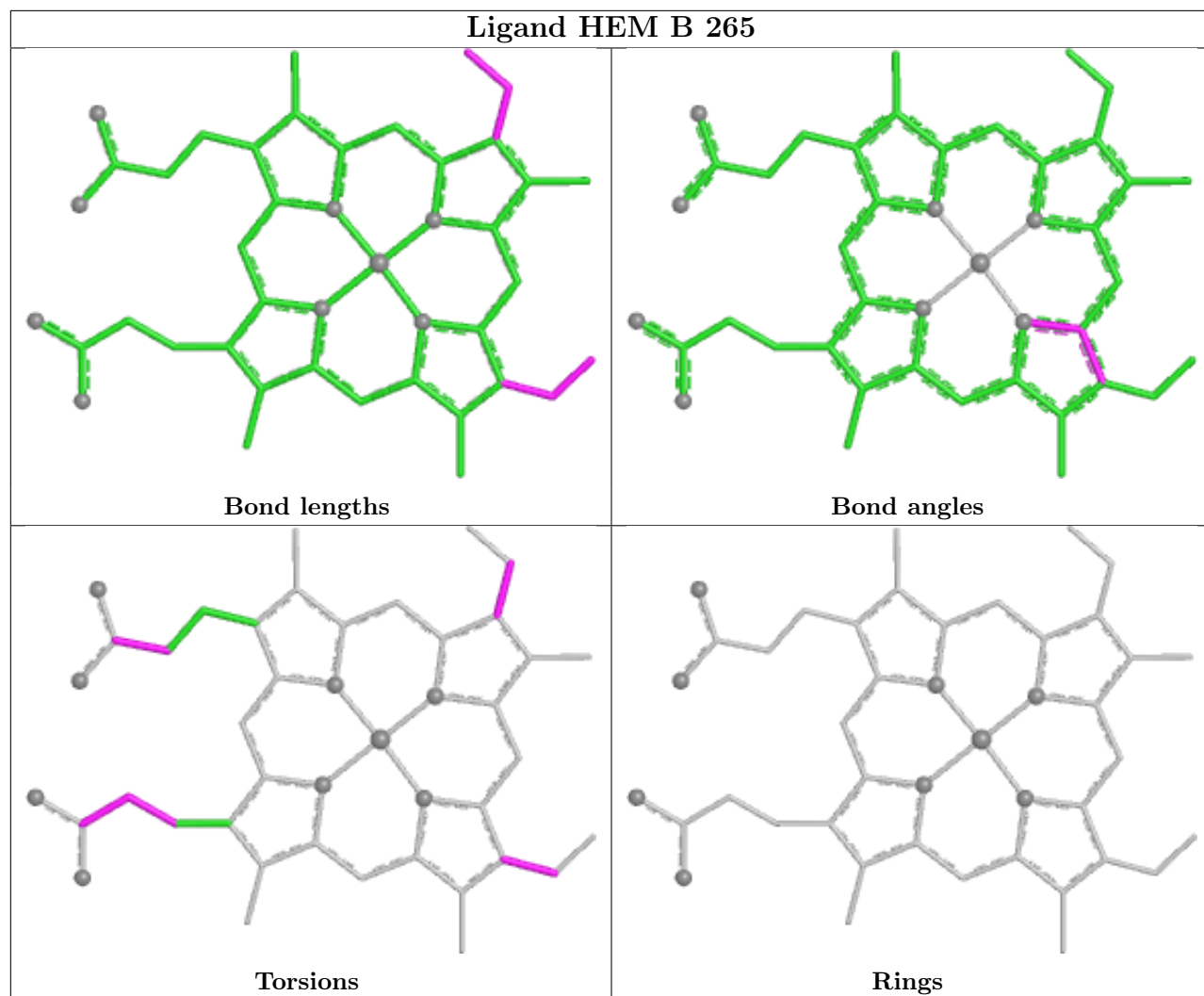
5 of 204 torsion outliers are listed below:

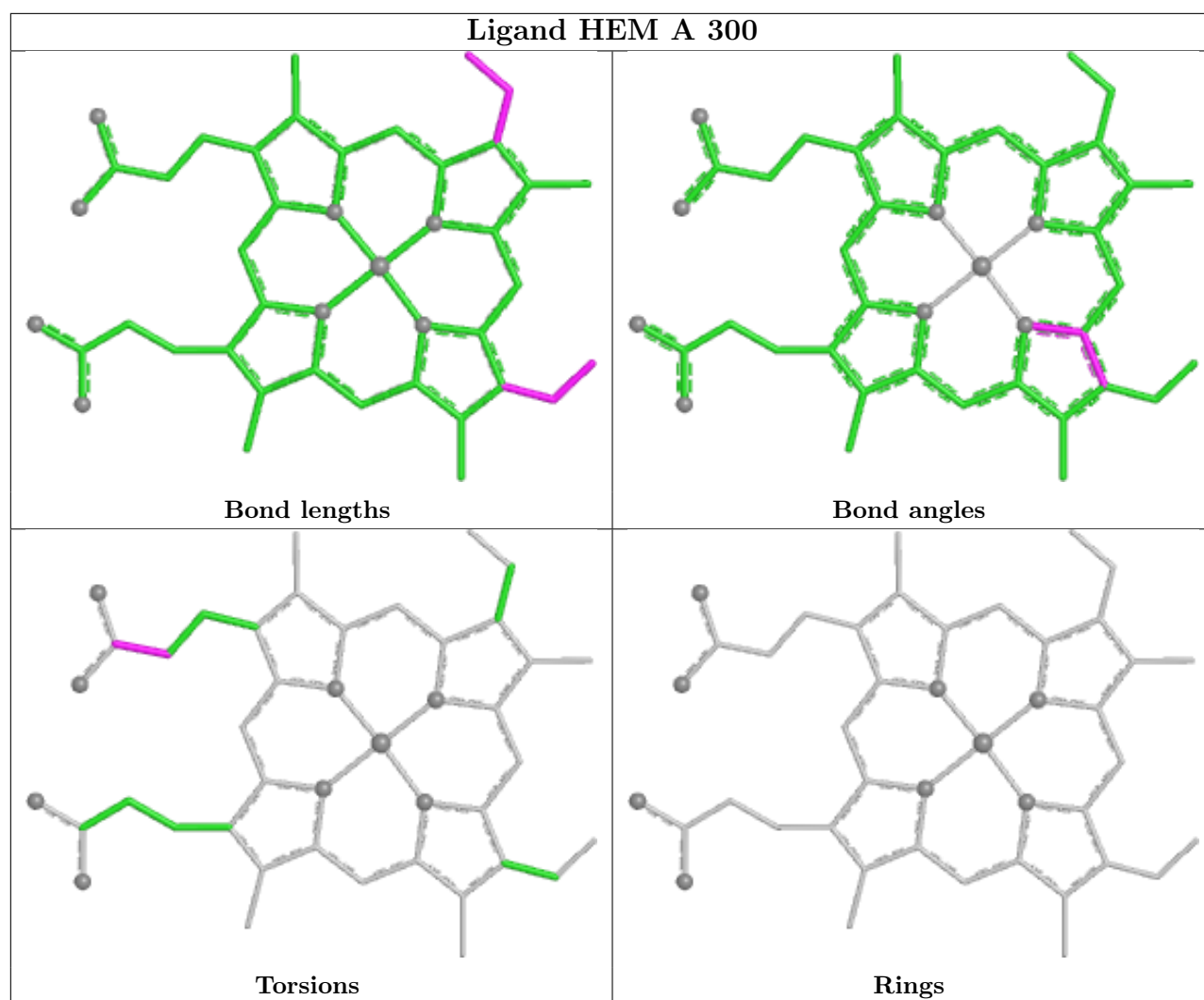
Mol	Chain	Res	Type	Atoms
2	6-A	300	HEM	C2C-C3C-CAC-CBC
2	6-A	300	HEM	C4C-C3C-CAC-CBC
2	7-A	300	HEM	C2C-C3C-CAC-CBC
2	7-A	300	HEM	C4C-C3C-CAC-CBC
2	11-A	300	HEM	C2C-C3C-CAC-CBC

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	214/264 (81%)	13.20	214 (100%) 0 0	2, 3, 4, 4	214 (100%)
1	1-B	219/264 (82%)	13.05	219 (100%) 0 0	3, 4, 5, 5	219 (100%)
1	2-A	0/264	-	-	-	-
1	2-B	0/264	-	-	-	-
1	3-A	0/264	-	-	-	-
1	3-B	0/264	-	-	-	-
1	4-A	0/264	-	-	-	-
1	4-B	0/264	-	-	-	-
1	5-A	0/264	-	-	-	-
1	5-B	0/264	-	-	-	-
1	6-A	0/264	-	-	-	-
1	6-B	0/264	-	-	-	-
1	7-A	0/264	-	-	-	-
1	7-B	0/264	-	-	-	-
1	8-A	0/264	-	-	-	-
1	8-B	0/264	-	-	-	-
1	9-A	0/264	-	-	-	-
1	9-B	0/264	-	-	-	-
1	10-A	0/264	-	-	-	-
1	10-B	0/264	-	-	-	-
1	11-A	0/264	-	-	-	-
1	11-B	0/264	-	-	-	-
1	12-A	0/264	-	-	-	-
1	12-B	0/264	-	-	-	-
1	13-A	0/264	-	-	-	-
1	13-B	0/264	-	-	-	-
1	14-A	0/264	-	-	-	-
1	14-B	0/264	-	-	-	-
1	15-A	0/264	-	-	-	-
1	15-B	0/264	-	-	-	-
1	16-A	0/264	-	-	-	-
1	16-B	0/264	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	433/8448 (5%)	13.13	433 (100%) 0 0	2, 3, 5, 5	433 (100%)

The worst 5 of 433 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	229	TYR	35.3
1	1-A	172	GLN	30.2
1	1-B	48	ALA	29.8
1	1-B	219	ILE	29.6
1	1-B	227	PHE	29.3

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	1-B	265	43/43	0.60	0.61	57,64,65,65	43
2	HEM	2-A	300	43/43	-	-	47,52,56,56	43
2	HEM	3-A	300	43/43	-	-	42,51,53,54	43
2	HEM	4-A	300	43/43	-	-	43,49,53,57	43
2	HEM	5-A	300	43/43	-	-	47,53,60,61	43
2	HEM	6-A	300	43/43	-	-	47,53,59,60	43
2	HEM	7-A	300	43/43	-	-	48,53,59,60	43
2	HEM	8-A	300	43/43	-	-	47,52,55,56	43
2	HEM	9-A	300	43/43	-	-	45,50,52,53	43
2	HEM	10-A	300	43/43	-	-	47,53,59,60	43
2	HEM	11-A	300	43/43	-	-	47,53,58,60	43
2	HEM	12-A	300	43/43	-	-	47,53,59,60	43
2	HEM	13-A	300	43/43	-	-	44,49,53,55	43

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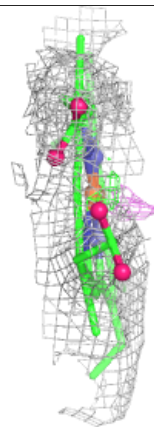
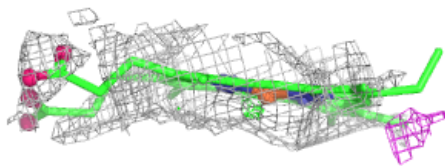
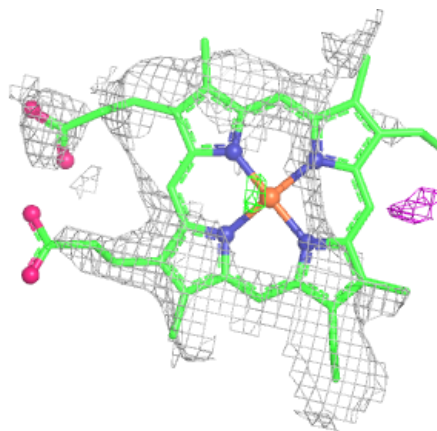
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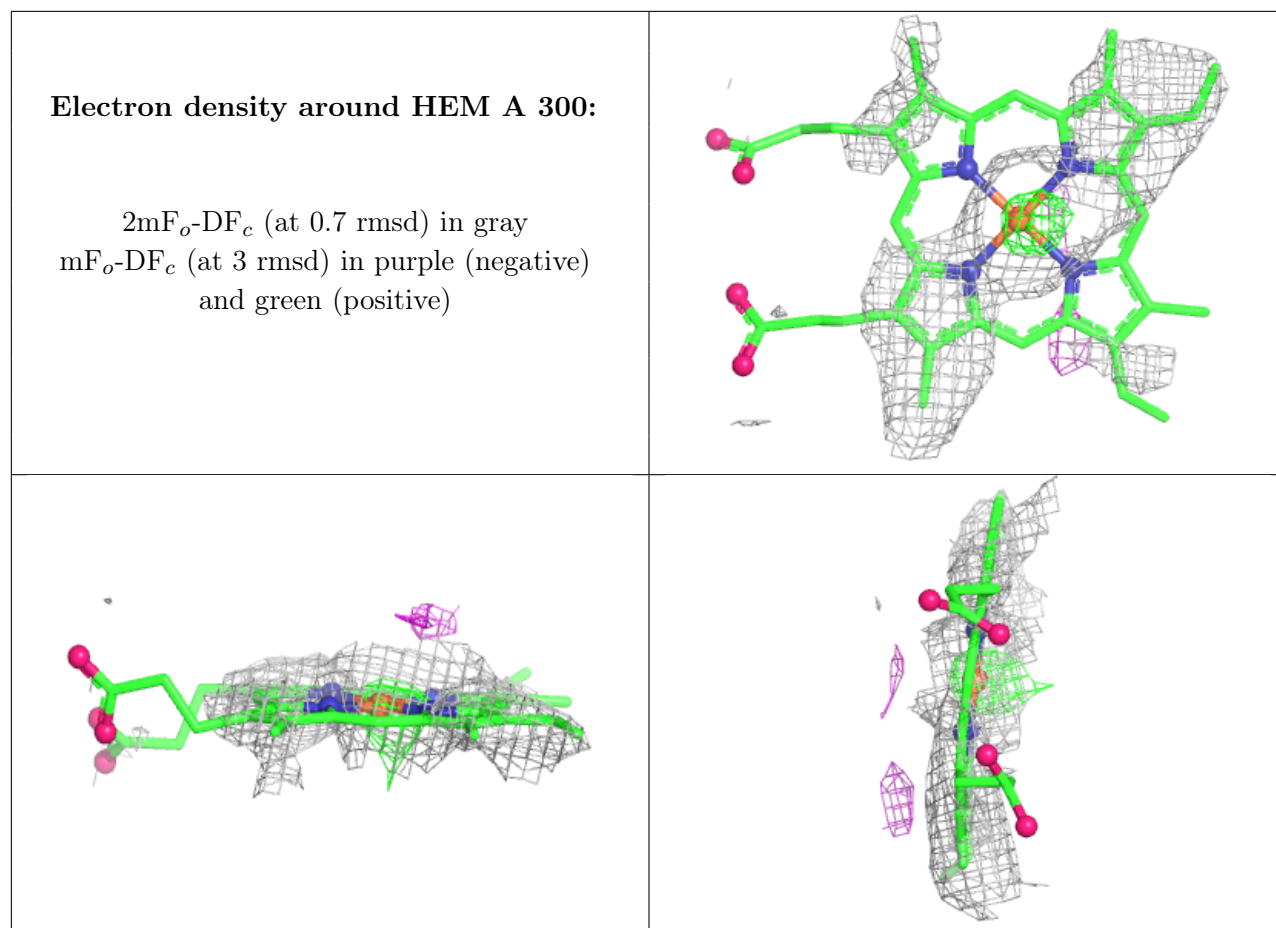
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	14-A	300	43/43	-	-	44,50,53,56	43
2	HEM	15-A	300	43/43	-	-	41,51,59,62	43
2	HEM	16-A	300	43/43	-	-	44,51,55,56	43
2	HEM	1-A	300	43/43	0.62	0.61	47,53,59,60	43
2	HEM	2-B	265	43/43	-	-	57,62,64,64	43
2	HEM	3-B	265	43/43	-	-	44,62,64,65	43
2	HEM	4-B	265	43/43	-	-	59,63,65,66	43
2	HEM	5-B	265	43/43	-	-	56,64,66,67	43
2	HEM	6-B	265	43/43	-	-	57,64,66,68	43
2	HEM	7-B	265	43/43	-	-	58,64,65,66	43
2	HEM	8-B	265	43/43	-	-	55,64,65,66	43
2	HEM	9-B	265	43/43	-	-	54,63,65,65	43
2	HEM	10-B	265	43/43	-	-	59,64,66,67	43
2	HEM	11-B	265	43/43	-	-	57,62,64,65	43
2	HEM	12-B	265	43/43	-	-	56,62,65,65	43
2	HEM	13-B	265	43/43	-	-	56,63,65,67	43
2	HEM	14-B	265	43/43	-	-	50,60,64,66	43
2	HEM	15-B	265	43/43	-	-	54,63,65,66	43
2	HEM	16-B	265	43/43	-	-	54,61,63,64	43

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 B 265:

$2mF_o-DF_c$ (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.