



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:14 pm BST

PDB ID : 3HOK  
Title : X-ray Crystal Structure of Human Heme Oxygenase-1 with (2R, 4S)-2-[2-(4-Chlorophenyl)ethyl]-2-[(1H-imidazol-1-yl)methyl]-4[[(5-trifluoromethylpyridin-2-yl)thio)methyl]-1,3-dioxolane: A Novel, Inducible Binding Mode  
Authors : Rahman, M.N.; Jia, Z.  
Deposited on : 2009-06-02  
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.11  
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) : 2.11

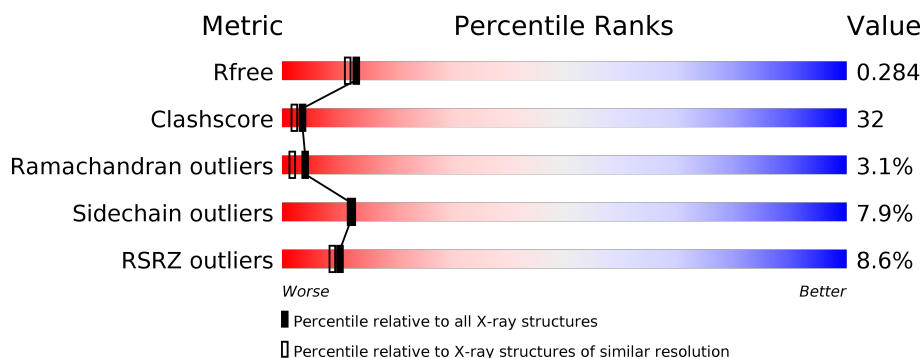
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\leq 5\%$ . 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	233	
1	B	233	

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	Q80	B	301	-	-	X	-

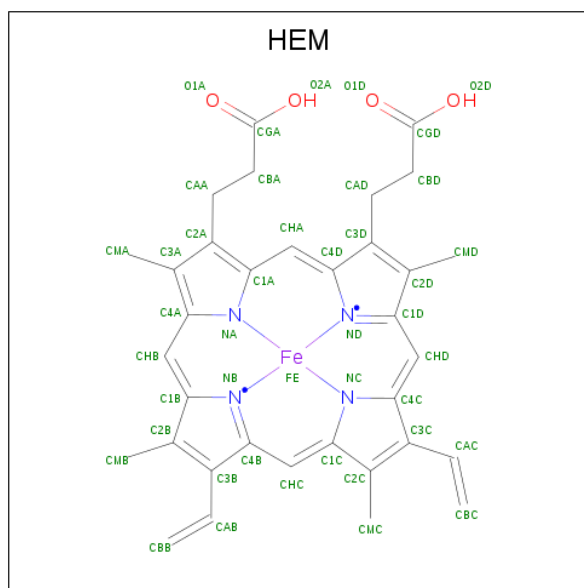


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Heme oxygenase 1.

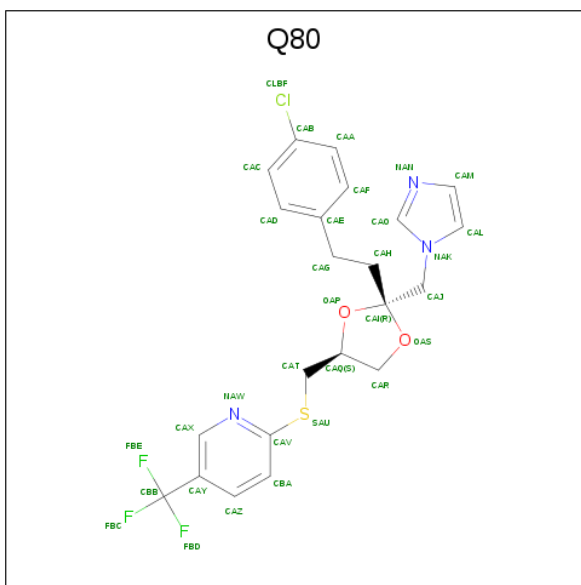
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total 1745	C 1121	N 299	O 320	S 5	0	0	0
1	B	215	Total 1753	C 1126	N 300	O 321	S 6	0	0	0

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



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

- Molecule 3 is 2-({[(2R,4S)-2-[2-(4-chlorophenyl)ethyl]-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methyl}sulfanyl)-5-(trifluoromethyl)pyridine (three-letter code: Q80) (formula: C<sub>22</sub>H<sub>21</sub>ClF<sub>3</sub>N<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	B	1	Total	C	Cl	F	N	O	S	0	0
			32	22	1	3	3	2	1		

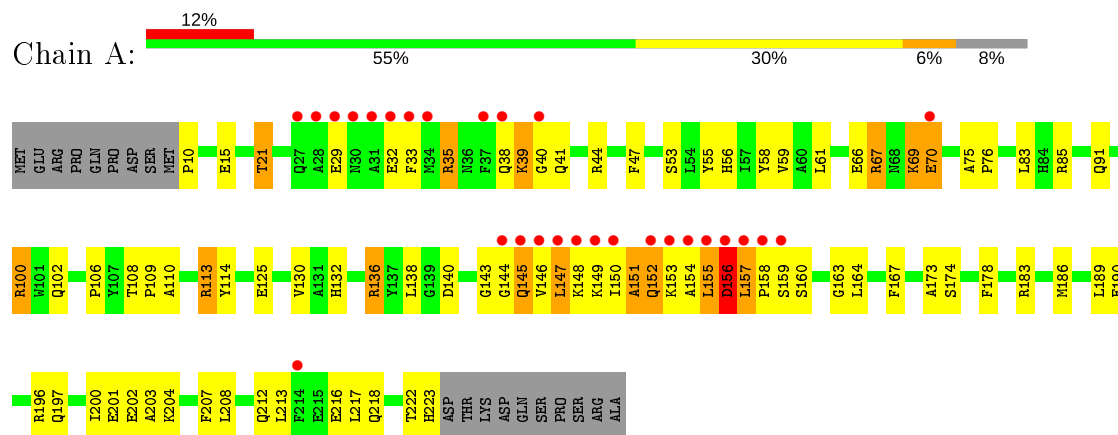
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	103	Total O 103 103	0	0
4	B	83	Total O 83 83	0	0

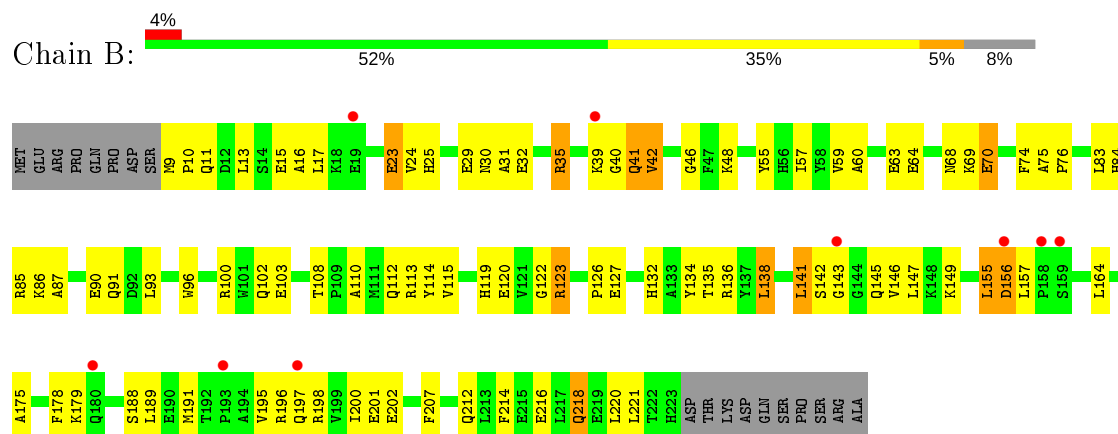
### 3 Residue-property plots [i](#)

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 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 1



#### • Molecule 1: Heme oxygenase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.07Å 54.59Å 71.88Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	43.42 – 2.19 43.42 – 2.19	Depositor EDS
% Data completeness (in resolution range)	88.4 (43.42-2.19) 88.3 (43.42-2.19)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.222 , 0.289 0.220 , 0.284	Depositor DCC
$R_{free}$ test set	1018 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.63% 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: HEM, Q80

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	0.36	0/1786	0.54	0/2414
1	B	0.38	0/1794	0.51	0/2425
All	All	0.37	0/3580	0.52	0/4839

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ASP	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	1745	0	1738	107	0
1	B	1753	0	1746	104	0
2	A	43	0	30	15	0
2	B	43	0	30	20	0
3	B	32	0	21	19	0
4	A	103	0	0	3	0
4	B	83	0	0	0	0
All	All	3802	0	3565	227	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 32.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:HA	2:A:300:HEM:CBB	1.72	1.19
1:B:32:GLU:CB	2:B:300:HEM:HBB1	1.76	1.15
1:A:150:ILE:O	1:A:154:ALA:HB3	1.44	1.13
1:A:100:ARG:CG	1:A:100:ARG:HH11	1.56	1.13
1:A:67:ARG:HH21	1:A:67:ARG:CG	1.64	1.10
1:B:119:HIS:O	1:B:123:ARG:HD3	1.51	1.08
1:A:156:ASP:HB2	1:A:157:LEU:CA	1.86	1.04
1:A:156:ASP:HB2	1:A:157:LEU:HA	1.03	1.03
1:B:147:LEU:HD11	3:B:301:Q80:HAJ	1.36	1.03
1:B:110:ALA:HB3	1:B:216:GLU:OE1	1.61	1.01
1:A:113:ARG:HG2	1:A:113:ARG:HH21	1.22	1.00
3:B:301:Q80:HAO	3:B:301:Q80:OAS	1.60	1.00
1:A:67:ARG:HB2	1:A:67:ARG:NH2	1.77	0.99
1:A:156:ASP:CB	1:A:157:LEU:HA	1.93	0.99
1:A:100:ARG:NH1	1:A:100:ARG:HG2	1.54	0.98
2:B:300:HEM:CMC	3:B:301:Q80:SAU	2.51	0.98
1:A:67:ARG:HH21	1:A:67:ARG:HG3	1.24	0.97
1:B:32:GLU:HB2	2:B:300:HEM:HBB1	1.47	0.97
1:A:67:ARG:HH21	1:A:67:ARG:CB	1.78	0.96
3:B:301:Q80:CAO	3:B:301:Q80:OAS	2.13	0.95
2:B:300:HEM:HMC1	2:B:300:HEM:HBC2	1.49	0.95
2:B:300:HEM:HMC2	3:B:301:Q80:SAU	2.05	0.94
2:A:300:HEM:HBB2	2:A:300:HEM:HMB1	1.46	0.94
1:B:32:GLU:HB3	2:B:300:HEM:HBB1	1.54	0.89
1:A:100:ARG:HH11	1:A:100:ARG:HG2	0.72	0.86
1:A:69:LYS:O	1:A:70:GLU:HB2	1.75	0.85
1:A:55:TYR:O	1:A:59:VAL:HG23	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:HIS:HE1	1:B:202:GLU:OE2	1.60	0.84
1:B:23:GLU:HG2	1:B:24:VAL:N	1.90	0.84
1:A:149:LYS:HE3	1:A:153:LYS:NZ	1.94	0.82
1:B:147:LEU:CD1	3:B:301:Q80:HAJ	2.10	0.81
1:B:59:VAL:O	1:B:63:GLU:HG3	1.81	0.81
1:A:152:GLN:HG3	1:A:153:LYS:H	1.43	0.81
2:B:300:HEM:HMC3	3:B:301:Q80:SAU	2.19	0.80
1:A:67:ARG:NH2	1:A:67:ARG:HG3	1.96	0.80
1:B:75:ALA:HB3	1:B:76:PRO:HD3	1.67	0.75
1:A:67:ARG:CB	1:A:67:ARG:NH2	2.42	0.75
1:B:155:LEU:HD13	1:B:157:LEU:HD21	1.68	0.75
1:A:148:LYS:O	1:A:152:GLN:HG2	1.86	0.74
1:A:33:PHE:HB2	1:A:218:GLN:HG2	1.69	0.74
1:B:214:PHE:CE2	3:B:301:Q80:HATA	2.22	0.74
1:B:142:SER:OG	1:B:179:LYS:NZ	2.21	0.73
1:A:163:GLY:O	1:A:164:LEU:HD23	1.89	0.73
1:B:25:HIS:O	1:B:29:GLU:HG3	1.89	0.73
1:A:85:ARG:HH22	1:B:91:GLN:HE22	1.36	0.72
1:A:113:ARG:HH21	1:A:113:ARG:CG	1.97	0.72
1:A:100:ARG:CG	1:A:100:ARG:NH1	2.27	0.71
1:A:150:ILE:O	1:A:154:ALA:CB	2.31	0.71
1:A:149:LYS:HE3	1:A:153:LYS:HZ1	1.53	0.71
1:B:113:ARG:NH2	1:B:212:GLN:OE1	2.22	0.71
1:A:69:LYS:O	1:A:70:GLU:CB	2.37	0.71
1:B:86:LYS:NZ	1:B:90:GLU:OE2	2.23	0.70
1:B:46:GLY:HA2	1:B:221:LEU:HD11	1.72	0.70
1:B:55:TYR:HB2	1:B:93:LEU:HD11	1.71	0.70
1:B:69:LYS:O	1:B:70:GLU:HB2	1.92	0.69
1:B:32:GLU:OE2	1:B:35:ARG:NH1	2.25	0.69
1:A:146:VAL:O	1:A:150:ILE:HD13	1.93	0.68
1:B:155:LEU:HD13	1:B:157:LEU:CD2	2.23	0.68
1:A:38:GLN:C	1:A:40:GLY:H	1.97	0.67
1:A:113:ARG:HG2	1:A:113:ARG:NH2	2.03	0.66
1:A:33:PHE:HB2	1:A:218:GLN:CG	2.26	0.65
1:B:69:LYS:O	1:B:70:GLU:CB	2.44	0.65
1:A:108:THR:HB	1:A:109:PRO:HD2	1.79	0.64
1:A:152:GLN:HG3	1:A:153:LYS:N	2.12	0.64
1:B:32:GLU:HB3	2:B:300:HEM:CBB	2.28	0.64
1:B:127:GLU:CD	1:B:127:GLU:H	2.01	0.64
1:B:127:GLU:OE1	1:B:198:ARG:NH2	2.31	0.64
2:B:300:HEM:HHC	3:B:301:Q80:SAU	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:HB2	4:A:309:HOH:O	1.98	0.63
1:A:69:LYS:O	1:A:69:LYS:HG3	1.97	0.63
1:B:13:LEU:HD22	1:B:191:MET:HE2	1.81	0.63
1:B:32:GLU:OE1	1:B:35:ARG:NH1	2.32	0.63
1:B:132:HIS:CE1	1:B:202:GLU:OE2	2.48	0.63
1:B:32:GLU:CB	2:B:300:HEM:CBB	2.68	0.63
1:A:158:PRO:O	1:A:160:SER:N	2.31	0.62
1:B:149:LYS:HD3	1:B:149:LYS:C	2.19	0.62
1:A:158:PRO:HG2	1:A:160:SER:HB3	1.80	0.62
1:A:157:LEU:HD11	1:A:164:LEU:HD11	1.81	0.62
1:B:149:LYS:HD3	1:B:149:LYS:O	2.00	0.62
1:B:195:VAL:HG22	1:B:198:ARG:NH1	2.16	0.61
1:A:38:GLN:C	1:A:40:GLY:N	2.54	0.61
1:B:25:HIS:ND1	1:B:29:GLU:OE2	2.32	0.60
1:A:44:ARG:NH2	1:A:156:ASP:OD1	2.34	0.60
1:B:32:GLU:CD	1:B:35:ARG:NH1	2.55	0.60
1:B:13:LEU:HD22	1:B:191:MET:CE	2.31	0.60
1:B:110:ALA:CB	1:B:216:GLU:CD	2.71	0.60
1:A:29:GLU:HA	2:A:300:HEM:HBB2	1.81	0.59
1:B:110:ALA:CB	1:B:216:GLU:OE1	2.42	0.59
1:A:222:THR:O	1:A:223:HIS:ND1	2.35	0.59
1:B:55:TYR:O	1:B:59:VAL:HG23	2.01	0.59
1:A:29:GLU:OE1	2:A:300:HEM:CMB	2.51	0.59
1:B:41:GLN:O	1:B:42:VAL:HB	2.01	0.59
1:B:100:ARG:HD3	1:B:103:GLU:OE2	2.03	0.59
1:A:151:ALA:O	1:A:155:LEU:HB2	2.03	0.58
1:B:196:ARG:O	1:B:200:ILE:HG12	2.03	0.57
1:A:91:GLN:HE22	1:B:85:ARG:HH22	1.51	0.57
1:A:157:LEU:HB3	1:A:158:PRO:HD2	1.84	0.57
2:A:300:HEM:CMD	2:A:300:HEM:HBD1	2.35	0.57
1:A:218:GLN:O	1:A:222:THR:HG23	2.05	0.57
1:A:152:GLN:HB3	1:A:164:LEU:CD1	2.35	0.57
1:B:48:LYS:HG2	1:B:96:TRP:HB3	1.85	0.57
1:A:75:ALA:HB3	1:A:76:PRO:HD3	1.87	0.56
1:A:149:LYS:HE3	1:A:153:LYS:HZ3	1.68	0.56
2:B:300:HEM:HMC1	2:B:300:HEM:CBC	2.31	0.56
1:B:195:VAL:HA	1:B:198:ARG:HG3	1.88	0.56
1:A:132:HIS:CE1	1:A:202:GLU:OE2	2.59	0.55
1:B:84:HIS:CE1	1:B:87:ALA:H	2.23	0.55
1:A:132:HIS:HE1	1:A:202:GLU:OE2	1.87	0.55
1:A:153:LYS:C	1:A:153:LYS:HD2	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:HEM:C1C	3:B:301:Q80:HARA	2.40	0.55
2:A:300:HEM:HBA2	2:A:300:HEM:HHA	1.89	0.55
1:B:110:ALA:HB3	1:B:216:GLU:CD	2.27	0.55
3:B:301:Q80:CAR	3:B:301:Q80:CAO	2.86	0.54
2:B:300:HEM:C2C	3:B:301:Q80:HARA	2.42	0.54
1:B:32:GLU:CD	1:B:35:ARG:HH12	2.10	0.54
1:A:156:ASP:C	1:A:157:LEU:HG	2.28	0.54
1:A:222:THR:O	1:A:223:HIS:CG	2.61	0.54
1:B:175:ALA:O	1:B:179:LYS:HG3	2.08	0.54
1:B:96:TRP:HH2	1:B:157:LEU:HD21	1.73	0.53
1:A:203:ALA:O	1:A:207:PHE:HD2	1.91	0.53
1:B:35:ARG:HD2	1:B:218:GLN:HG3	1.89	0.53
1:A:108:THR:HB	1:A:109:PRO:CD	2.37	0.53
1:A:157:LEU:C	1:A:158:PRO:O	2.44	0.53
1:B:195:VAL:HG22	1:B:198:ARG:HH12	1.72	0.53
1:B:84:HIS:HE1	1:B:87:ALA:CB	2.21	0.53
1:A:39:LYS:HG3	1:A:39:LYS:O	2.09	0.53
1:A:56:HIS:HE1	1:A:106:PRO:O	1.91	0.52
1:B:123:ARG:HH11	1:B:123:ARG:HB2	1.74	0.52
1:B:83:LEU:O	1:B:84:HIS:C	2.48	0.51
1:A:113:ARG:CG	1:A:113:ARG:NH2	2.63	0.51
1:A:58:TYR:OH	1:A:140:ASP:OD2	2.23	0.51
1:A:29:GLU:OE1	2:A:300:HEM:HMB1	2.11	0.51
1:B:68:ASN:ND2	1:B:126:PRO:HB3	2.26	0.51
1:A:32:GLU:H	1:A:32:GLU:CD	2.14	0.51
2:A:300:HEM:HBB2	2:A:300:HEM:CMB	2.28	0.51
1:B:143:GLY:HA3	3:B:301:Q80:HAL	1.93	0.51
1:B:120:GLU:HA	1:B:123:ARG:NH1	2.25	0.50
1:B:11:GLN:O	1:B:196:ARG:NH1	2.45	0.50
1:B:10:PRO:HG2	1:B:16:ALA:N	2.27	0.50
1:B:110:ALA:HB2	1:B:216:GLU:CD	2.31	0.50
1:B:96:TRP:HH2	1:B:157:LEU:CD2	2.25	0.50
1:A:183:ARG:HA	1:A:186:MET:HE2	1.94	0.49
1:B:155:LEU:O	1:B:156:ASP:C	2.51	0.49
1:A:83:LEU:HD21	1:A:178:PHE:CE2	2.48	0.49
1:B:214:PHE:HE2	3:B:301:Q80:HATA	1.73	0.49
1:A:47:PHE:CG	1:A:155:LEU:HD11	2.48	0.48
1:A:183:ARG:HA	1:A:186:MET:CE	2.43	0.48
1:A:39:LYS:HG2	1:A:41:GLN:NE2	2.28	0.48
1:A:143:GLY:C	1:A:145:GLN:H	2.16	0.48
1:A:47:PHE:CD1	1:A:155:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:O	1:B:39:LYS:O	2.31	0.48
1:B:143:GLY:HA3	3:B:301:Q80:CAL	2.44	0.48
1:B:207:PHE:HA	2:B:300:HEM:CBC	2.44	0.47
1:B:32:GLU:CG	2:B:300:HEM:HBB1	2.43	0.47
1:A:143:GLY:O	1:A:145:GLN:N	2.47	0.47
1:A:157:LEU:HD11	1:A:164:LEU:CD1	2.45	0.47
1:B:42:VAL:O	1:B:42:VAL:CG1	2.63	0.47
1:A:66:GLU:O	1:A:69:LYS:HG2	2.16	0.46
1:B:42:VAL:O	1:B:42:VAL:HG13	2.15	0.46
1:A:213:LEU:O	1:A:217:LEU:HG	2.16	0.46
1:A:29:GLU:CA	2:A:300:HEM:CBB	2.67	0.46
1:B:191:MET:HB2	1:B:195:VAL:CG1	2.45	0.46
1:A:157:LEU:O	1:A:158:PRO:C	2.52	0.46
1:A:56:HIS:HD2	4:A:0:HOH:O	1.97	0.46
1:A:85:ARG:NH2	1:B:91:GLN:HE22	2.11	0.46
1:B:84:HIS:HE1	1:B:87:ALA:HB3	1.80	0.45
1:A:197:GLN:O	1:A:201:GLU:HG2	2.16	0.45
1:B:83:LEU:HD21	1:B:178:PHE:CE2	2.51	0.45
1:A:143:GLY:C	1:A:145:GLN:N	2.70	0.45
1:B:55:TYR:CB	1:B:93:LEU:HD11	2.45	0.45
1:B:138:LEU:HB3	2:B:300:HEM:HBD2	1.99	0.45
1:A:61:LEU:HD22	1:A:136:ARG:HG3	1.99	0.45
1:B:57:ILE:HG21	1:B:136:ARG:HD2	1.99	0.45
1:A:44:ARG:HH21	1:A:156:ASP:CG	2.20	0.45
2:A:300:HEM:CHA	2:A:300:HEM:HBA2	2.47	0.45
1:B:108:THR:HG21	1:B:220:LEU:HD11	1.99	0.45
1:B:10:PRO:HB2	1:B:15:GLU:HB2	1.99	0.45
1:B:31:ALA:HB1	3:B:301:Q80:FBC	2.06	0.45
1:B:64:GLU:OE1	1:B:122:GLY:HA3	2.16	0.44
1:B:17:LEU:HD23	1:B:200:ILE:HD13	2.00	0.44
1:B:214:PHE:CE2	3:B:301:Q80:CAT	2.98	0.44
1:B:74:PHE:O	1:B:75:ALA:C	2.55	0.44
1:A:10:PRO:HG2	1:A:15:GLU:CB	2.48	0.44
1:A:10:PRO:HG2	1:A:15:GLU:HB2	1.98	0.44
2:A:300:HEM:CBA	2:A:300:HEM:HHA	2.48	0.44
1:B:135:THR:CG2	2:B:300:HEM:HAC	2.48	0.44
1:A:157:LEU:O	1:A:158:PRO:O	2.36	0.44
1:A:138:LEU:HB3	2:A:300:HEM:HBD2	2.00	0.44
1:A:174:SER:HB2	4:A:314:HOH:O	2.17	0.44
1:B:147:LEU:HD11	3:B:301:Q80:CAJ	2.26	0.43
1:B:155:LEU:CD1	1:B:157:LEU:HD21	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:HG3	1:B:218:GLN:NE2	2.34	0.43
1:A:196:ARG:O	1:A:200:ILE:HG12	2.17	0.43
2:A:300:HEM:HMD2	2:A:300:HEM:CBD	2.49	0.43
1:A:147:LEU:HD13	1:A:167:PHE:HE1	1.83	0.43
1:B:75:ALA:HB3	1:B:76:PRO:CD	2.44	0.43
1:A:110:ALA:HB3	1:A:216:GLU:CD	2.39	0.42
1:A:130:VAL:O	1:A:130:VAL:HG22	2.19	0.42
1:B:207:PHE:HA	2:B:300:HEM:HBC1	2.01	0.42
1:A:190:GLU:HA	1:A:190:GLU:OE1	2.19	0.42
1:A:173:ALA:HB1	1:B:100:ARG:HG2	2.01	0.42
1:B:135:THR:HG22	2:B:300:HEM:HAC	2.01	0.42
1:B:141:LEU:HD13	1:B:141:LEU:HA	1.89	0.42
2:B:300:HEM:HBC2	2:B:300:HEM:CMC	2.33	0.42
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.95	0.42
1:B:197:GLN:O	1:B:201:GLU:HG2	2.19	0.42
1:A:85:ARG:HH22	1:B:91:GLN:NE2	2.12	0.41
3:B:301:Q80:CAR	3:B:301:Q80:HAO	2.45	0.41
2:A:300:HEM:CBD	2:A:300:HEM:CMD	2.98	0.41
1:A:29:GLU:OE1	2:A:300:HEM:HMB2	2.21	0.41
1:B:60:ALA:HB2	1:B:115:VAL:HG13	2.02	0.41
1:B:84:HIS:NE2	1:B:86:LYS:HB3	2.36	0.41
1:B:119:HIS:O	1:B:123:ARG:CD	2.42	0.41
1:A:153:LYS:HE2	1:A:153:LYS:HB3	1.89	0.41
1:A:35:ARG:O	1:A:39:LYS:CB	2.69	0.41
1:B:157:LEU:HD11	1:B:164:LEU:HG	2.02	0.41
1:A:21:THR:HG21	1:A:203:ALA:HB1	2.03	0.41
1:B:134:TYR:CD1	1:B:138:LEU:CD2	3.04	0.41
1:B:134:TYR:CD1	1:B:138:LEU:HD22	2.56	0.41
1:A:158:PRO:C	1:A:160:SER:N	2.75	0.40
1:A:208:LEU:O	1:A:212:GLN:HG3	2.22	0.40
1:B:108:THR:O	1:B:112:GLN:HG3	2.21	0.40
1:A:149:LYS:O	1:A:150:ILE:C	2.59	0.40
1:B:96:TRP:CH2	1:B:157:LEU:CD2	3.04	0.40
1:A:151:ALA:O	1:A:152:GLN:C	2.60	0.40
1:A:148:LYS:HB2	1:A:167:PHE:HB3	2.04	0.40
1:A:53:SER:HB3	1:A:213:LEU:HD21	2.03	0.40

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	212/233 (91%)	190 (90%)	14 (7%)	8 (4%)	3	1
1	B	213/233 (91%)	198 (93%)	10 (5%)	5 (2%)	6	3
All	All	425/466 (91%)	388 (91%)	24 (6%)	13 (3%)	4	2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	151	ALA
1	B	42	VAL
1	A	159	SER
1	B	40	GLY
1	B	41	GLN
1	B	156	ASP
1	B	70	GLU
1	A	70	GLU
1	A	21	THR
1	A	39	LYS
1	A	144	GLY
1	A	152	GLN

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/202 (91%)	170 (92%)	14 (8%)	13	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	185/202 (92%)	170 (92%)	15 (8%)	11	12
All	All	369/404 (91%)	340 (92%)	29 (8%)	12	12

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	69	LYS
1	A	100	ARG
1	A	102	GLN
1	A	113	ARG
1	A	114	TYR
1	A	125	GLU
1	A	136	ARG
1	A	145	GLN
1	A	147	LEU
1	A	155	LEU
1	A	156	ASP
1	A	157	LEU
1	A	204	LYS
1	B	9	MET
1	B	23	GLU
1	B	30	ASN
1	B	35	ARG
1	B	102	GLN
1	B	114	TYR
1	B	123	ARG
1	B	138	LEU
1	B	141	LEU
1	B	145	GLN
1	B	146	VAL
1	B	155	LEU
1	B	188	SER
1	B	189	LEU
1	B	218	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	56	HIS

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Mol	Chain	Res	Type
1	A	84	HIS
1	A	132	HIS
1	A	171	ASN
1	A	180	GLN
1	B	30	ASN
1	B	38	GLN
1	B	56	HIS
1	B	68	ASN
1	B	132	HIS
1	B	152	GLN
1	B	171	ASN
1	B	180	GLN
1	B	197	GLN
1	B	218	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	A	300	1	27,50,50	2.20	6 (22%)	17,82,82	1.57	3 (17%)
2	HEM	B	300	1	27,50,50	2.13	5 (18%)	17,82,82	1.62	3 (17%)
3	Q80	B	301	-	33,35,35	1.22	3 (9%)	39,50,50	1.88	8 (20%)

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	A	300	1	-	6/6/54/54	-
2	HEM	B	300	1	-	3/6/54/54	-
3	Q80	B	301	-	-	13/22/33/33	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	HEM	C3D-C2D	5.45	1.53	1.37
2	B	300	HEM	C3D-C2D	5.37	1.53	1.37
2	A	300	HEM	C3C-C2C	-4.76	1.33	1.40
2	B	300	HEM	C3B-C2B	-4.40	1.34	1.40
2	B	300	HEM	C3C-C2C	-4.39	1.34	1.40
2	A	300	HEM	C3B-C2B	-4.38	1.34	1.40
3	B	301	Q80	CAV-SAU	-4.18	1.69	1.76
3	B	301	Q80	CAL-NAK	3.98	1.45	1.37
2	A	300	HEM	C3B-CAB	3.53	1.55	1.47
2	B	300	HEM	C3C-CAC	3.51	1.55	1.47
2	A	300	HEM	C3C-CAC	3.46	1.54	1.47
2	B	300	HEM	C3B-CAB	3.46	1.55	1.47
3	B	301	Q80	CAB-CLBF	2.74	1.80	1.74
2	A	300	HEM	CAA-C2A	2.23	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	Q80	CAJ-NAK-CAO	-6.85	111.53	125.79
2	B	300	HEM	CAA-CBA-CGA	-3.66	106.53	112.67
3	B	301	Q80	CAY-CAX-NAW	-3.45	120.05	123.34
3	B	301	Q80	FBE-CBB-CAY	-3.24	105.81	112.93
3	B	301	Q80	CAX-NAW-CAV	3.17	120.63	117.06
2	A	300	HEM	CAD-CBD-CGD	-3.01	107.63	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	HEM	C1D-C2D-C3D	-2.90	104.97	107.00
2	B	300	HEM	C1D-C2D-C3D	-2.62	105.17	107.00
3	B	301	Q80	CAT-SAU-CAV	2.58	107.94	102.76
3	B	301	Q80	CAL-NAK-CAO	-2.43	105.82	108.21
2	A	300	HEM	CAA-CBA-CGA	-2.42	108.61	112.67
3	B	301	Q80	CAZ-CAY-CAX	2.33	120.36	117.69
3	B	301	Q80	CAH-CAG-CAE	-2.32	106.77	112.85
2	B	300	HEM	CBD-CAD-C3D	-2.05	108.70	112.48

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	HEM	C1A-C2A-CAA-CBA
2	A	300	HEM	C3A-C2A-CAA-CBA
2	A	300	HEM	C2A-CAA-CBA-CGA
2	A	300	HEM	C2D-C3D-CAD-CBD
2	A	300	HEM	C4D-C3D-CAD-CBD
2	B	300	HEM	C2D-C3D-CAD-CBD
2	B	300	HEM	C4D-C3D-CAD-CBD
2	B	300	HEM	C3D-CAD-CBD-CGD
3	B	301	Q80	CAG-CAH-CAI-CAJ
3	B	301	Q80	CAG-CAH-CAI-OAS
3	B	301	Q80	CAH-CAI-CAJ-NAK
3	B	301	Q80	OAP-CAI-CAJ-NAK
3	B	301	Q80	OAS-CAI-CAJ-NAK
3	B	301	Q80	CAI-CAJ-NAK-CAO
3	B	301	Q80	CAQ-CAT-SAU-CAV
3	B	301	Q80	NAW-CAV-SAU-CAT
3	B	301	Q80	CBA-CAV-SAU-CAT
3	B	301	Q80	CAG-CAH-CAI-OAP
3	B	301	Q80	CAE-CAG-CAH-CAI
3	B	301	Q80	CAI-CAJ-NAK-CAL
2	A	300	HEM	C3D-CAD-CBD-CGD
3	B	301	Q80	CAR-CAQ-CAT-SAU

There are no ring outliers.

3 monomers are involved in 48 short contacts:

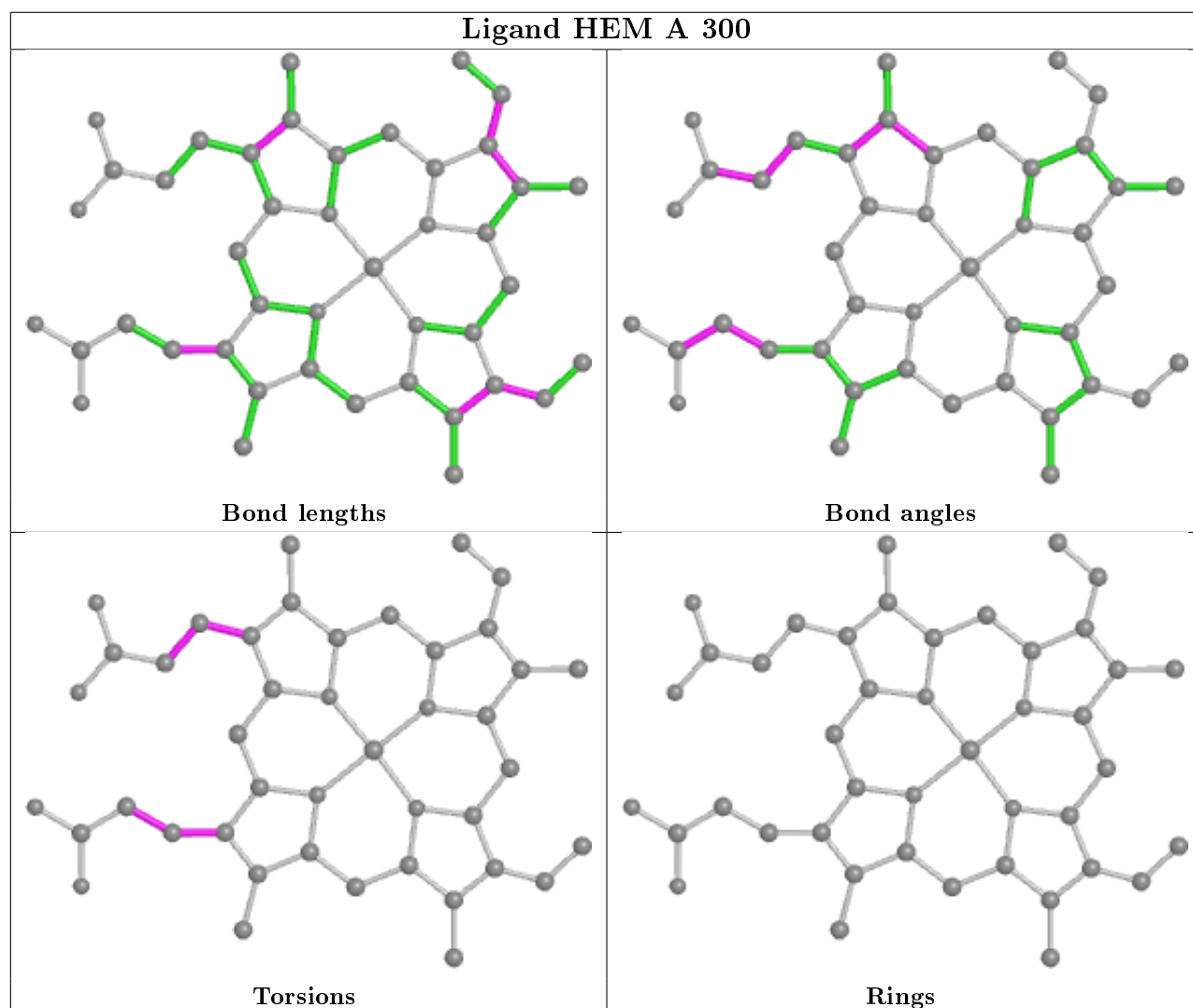
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	HEM	15	0

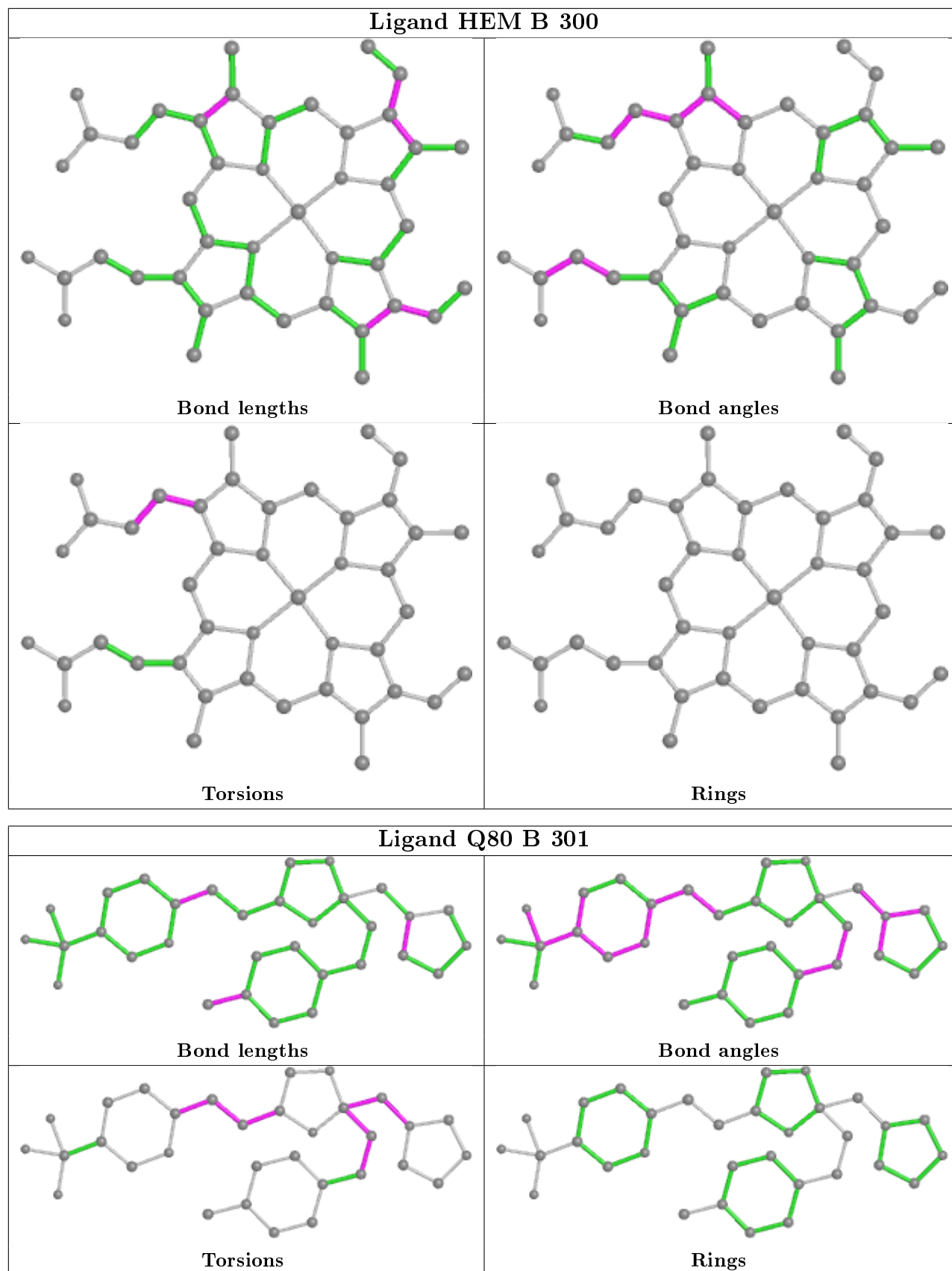
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	300	HEM	20	0
3	B	301	Q80	19	0

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

### 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, 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	214/233 (91%)	0.82	28 (13%) <b>3</b> <b>3</b>	22, 36, 67, 71	0
1	B	215/233 (92%)	0.48	9 (4%) 36 34	20, 34, 54, 60	0
All	All	429/466 (92%)	0.65	37 (8%) <b>10</b> <b>9</b>	20, 35, 63, 71	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	LEU	6.9
1	A	154	ALA	5.4
1	A	29	GLU	5.2
1	A	155	LEU	4.9
1	A	159	SER	4.9
1	A	156	ASP	4.8
1	A	33	PHE	4.4
1	A	153	LYS	4.3
1	A	37	PHE	4.2
1	A	158	PRO	4.1
1	A	40	GLY	4.1
1	A	152	GLN	4.0
1	A	28	ALA	3.6
1	A	30	ASN	3.6
1	A	146	VAL	3.5
1	A	150	ILE	3.5
1	A	34	MET	3.4
1	A	38	GLN	3.1
1	B	39	LYS	3.0
1	A	149	LYS	2.9
1	A	214	PHE	2.9
1	B	180	GLN	2.8
1	B	156	ASP	2.8
1	B	143	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	159	SER	2.6
1	A	32	GLU	2.6
1	A	147	LEU	2.6
1	A	144	GLY	2.5
1	A	31	ALA	2.5
1	B	193	PRO	2.5
1	A	148	LYS	2.5
1	A	27	GLN	2.4
1	A	145	GLN	2.4
1	B	197	GLN	2.3
1	A	70	GLU	2.3
1	B	19	GLU	2.1
1	B	158	PRO	2.0

## 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 carbohydrates 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.

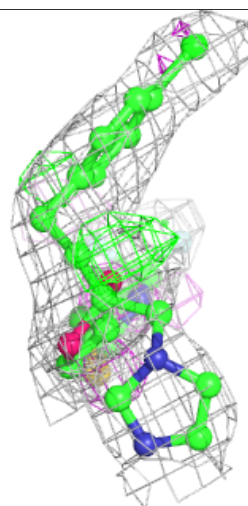
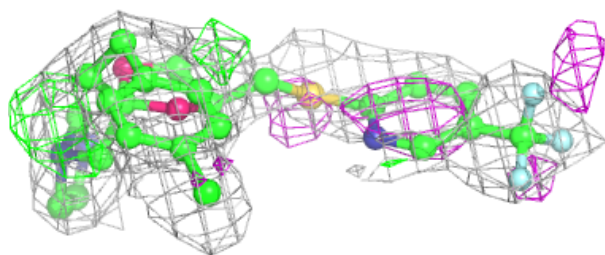
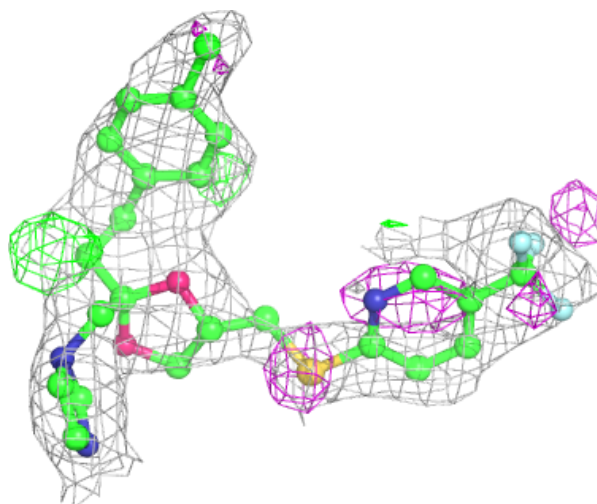
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	Q80	B	301	32/32	0.69	0.25	47,55,61,61	0
2	HEM	A	300	43/43	0.91	0.24	53,54,58,59	0
2	HEM	B	300	43/43	0.95	0.17	34,37,44,47	0

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.



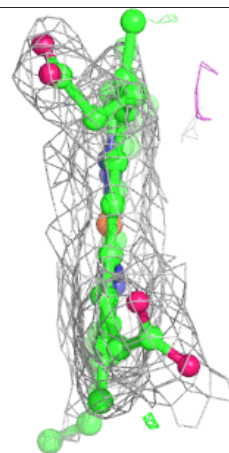
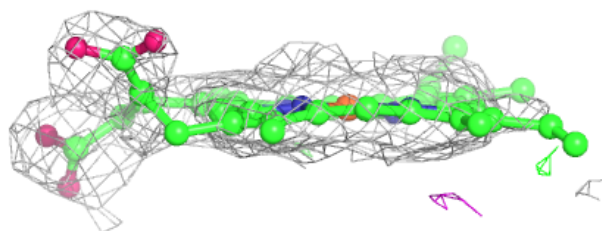
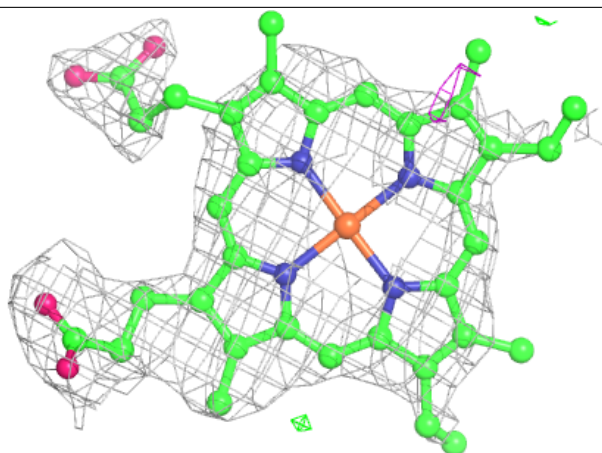
**Electron density around Q80 B 301:**

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



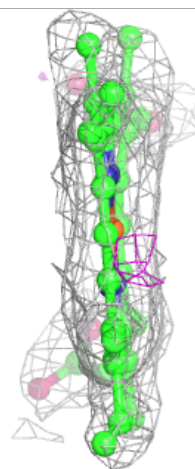
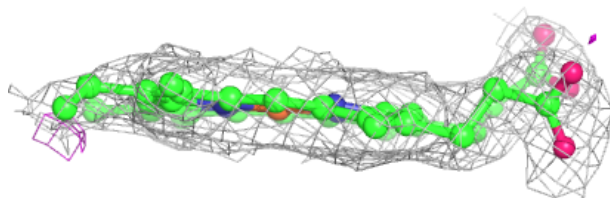
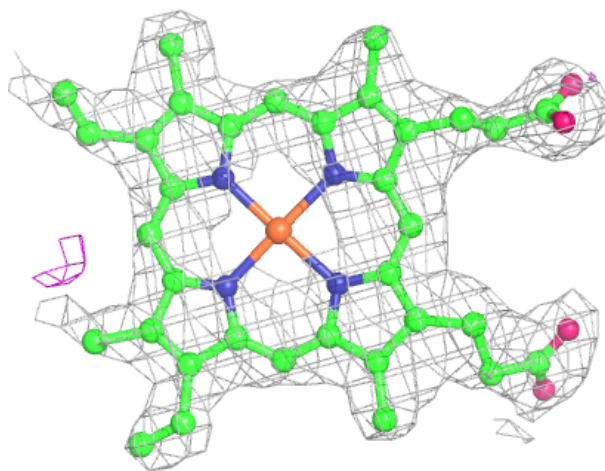
**Electron density around HEM A 300:**

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



**Electron density around HEM B 300:**

$2mF_o-DF_c$  (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.