



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:11 pm BST

PDB ID : 1SI8  
Title : Crystal structure of E. faecalis catalase  
Authors : Hakansson, K.O.; Brugna, M.; Tasse, L.  
Deposited on : 2004-02-28  
Resolution : 2.30 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

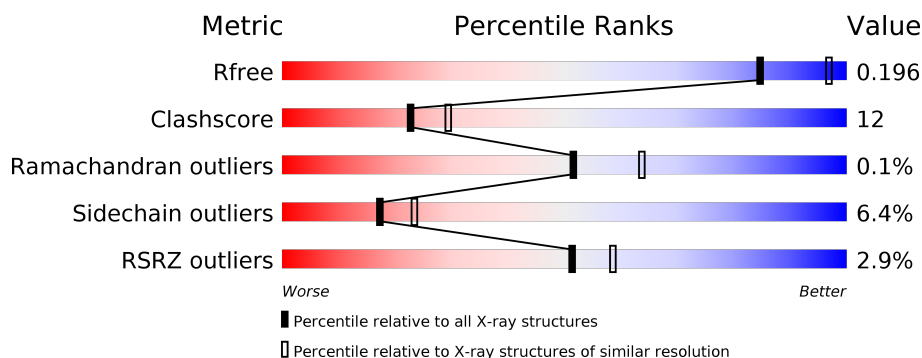
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	484	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	484	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
1	C	484	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	D	484	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16509 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 Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3775	2387	661	721	6			
1	B	474	Total	C	N	O	S	0	0	0
			3775	2387	661	721	6			
1	C	474	Total	C	N	O	S	0	0	0
			3775	2387	661	721	6			
1	D	474	Total	C	N	O	S	0	0	0
			3775	2387	661	721	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	479	HIS	-	EXPRESSION TAG	UNP Q834P5
A	480	HIS	-	EXPRESSION TAG	UNP Q834P5
A	481	HIS	-	EXPRESSION TAG	UNP Q834P5
A	482	HIS	-	EXPRESSION TAG	UNP Q834P5
A	483	HIS	-	EXPRESSION TAG	UNP Q834P5
A	484	HIS	-	EXPRESSION TAG	UNP Q834P5
B	479	HIS	-	EXPRESSION TAG	UNP Q834P5
B	480	HIS	-	EXPRESSION TAG	UNP Q834P5
B	481	HIS	-	EXPRESSION TAG	UNP Q834P5
B	482	HIS	-	EXPRESSION TAG	UNP Q834P5
B	483	HIS	-	EXPRESSION TAG	UNP Q834P5
B	484	HIS	-	EXPRESSION TAG	UNP Q834P5
C	479	HIS	-	EXPRESSION TAG	UNP Q834P5
C	480	HIS	-	EXPRESSION TAG	UNP Q834P5
C	481	HIS	-	EXPRESSION TAG	UNP Q834P5
C	482	HIS	-	EXPRESSION TAG	UNP Q834P5
C	483	HIS	-	EXPRESSION TAG	UNP Q834P5
C	484	HIS	-	EXPRESSION TAG	UNP Q834P5
D	479	HIS	-	EXPRESSION TAG	UNP Q834P5
D	480	HIS	-	EXPRESSION TAG	UNP Q834P5
D	481	HIS	-	EXPRESSION TAG	UNP Q834P5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	482	HIS	-	EXPRESSION TAG	UNP Q834P5
D	483	HIS	-	EXPRESSION TAG	UNP Q834P5
D	484	HIS	-	EXPRESSION TAG	UNP Q834P5

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

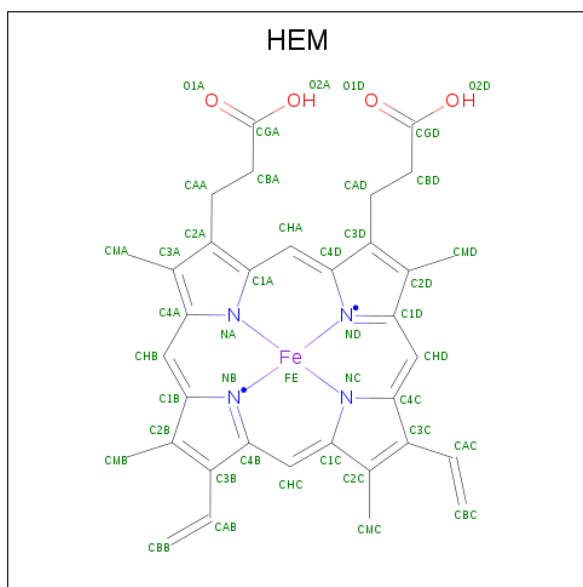


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	245	Total O 245 245	0	0
5	B	281	Total O 281 281	0	0
5	C	316	Total O 316 316	0	0

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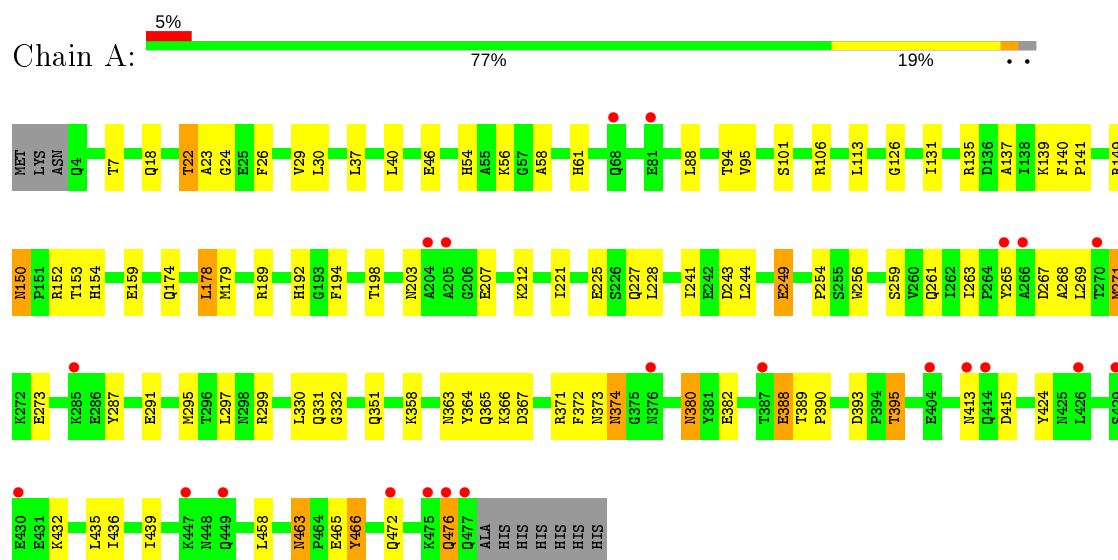
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	353	Total	O	0	0
			353	353		

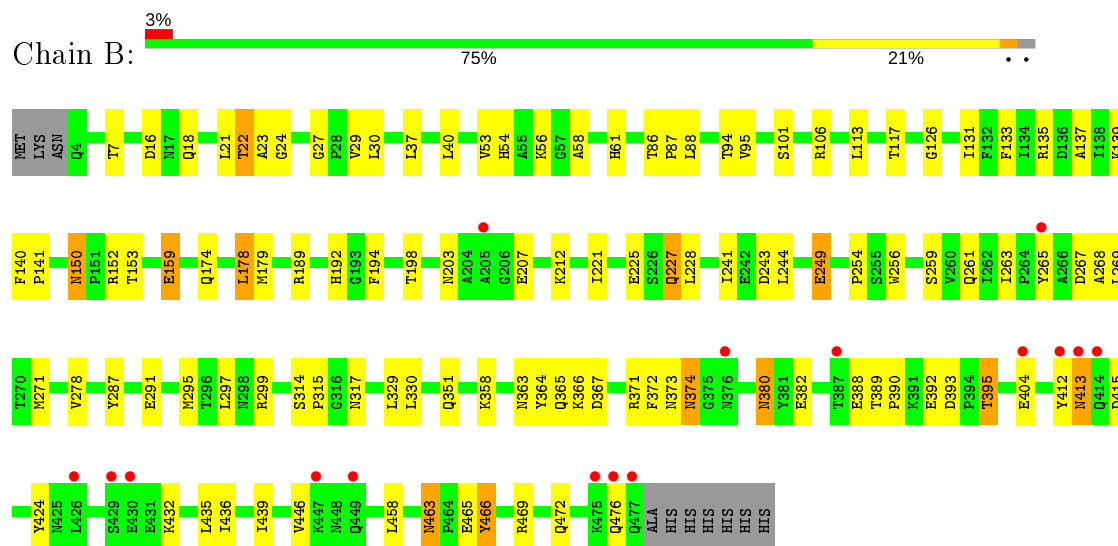
### 3 Residue-property plots [i](#)

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: Catalase

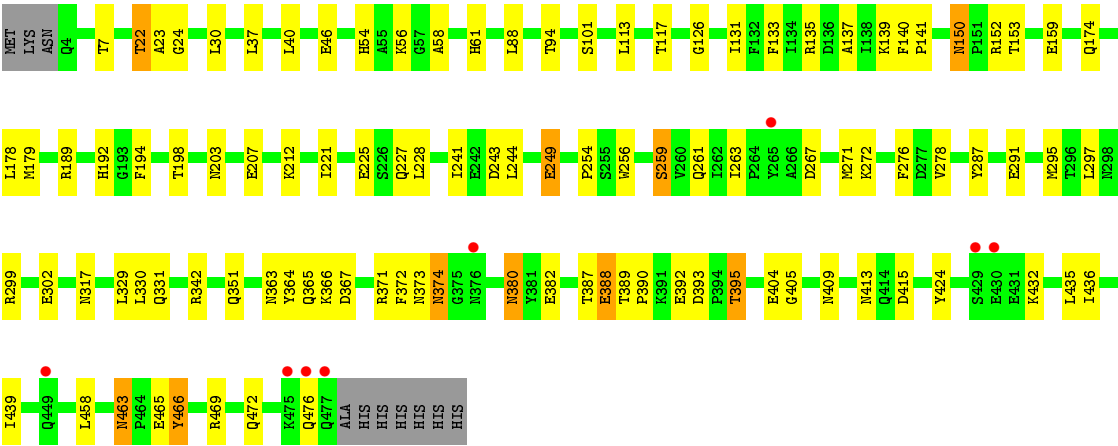


#### • Molecule 1: Catalase

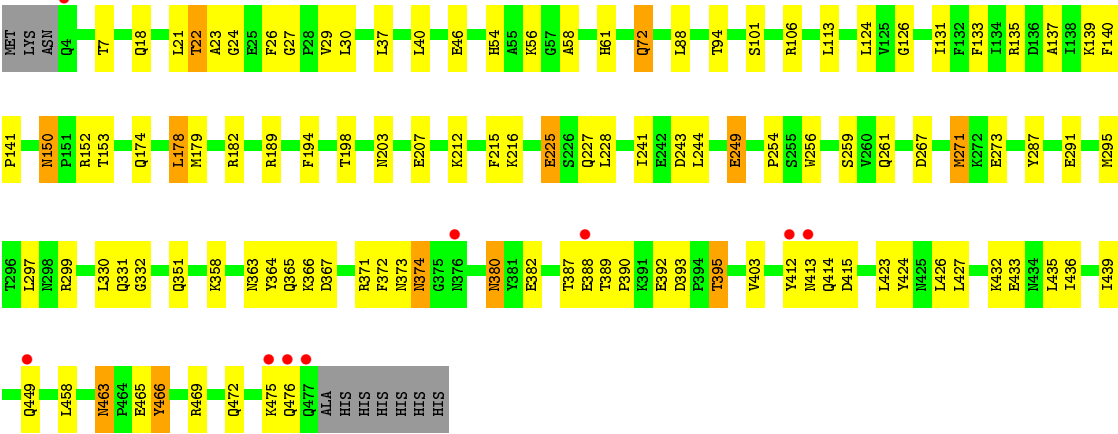
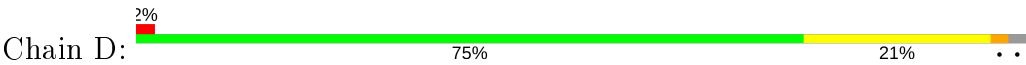


#### • Molecule 1: Catalase





• Molecule 1: Catalase





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	236.86Å 236.86Å 198.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.30) 99.8 (19.96-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.202 , 0.218 0.194 , 0.196	Depositor DCC
$R_{free}$ test set	9211 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, SO4, CL

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	0/3872	0.63	0/5254
1	B	0.37	0/3872	0.63	0/5254
1	C	0.37	0/3872	0.64	0/5254
1	D	0.38	0/3872	0.64	0/5254
All	All	0.37	0/15488	0.64	0/21016

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	A	3775	0	3623	87	0
1	B	3775	0	3623	87	0
1	C	3775	0	3623	77	0
1	D	3775	0	3623	94	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	43	0	30	9	0
4	B	43	0	30	7	0
4	C	43	0	30	7	0
4	D	43	0	30	7	0
5	A	245	0	0	3	0
5	B	281	0	0	6	0
5	C	316	0	0	5	0
5	D	353	0	0	11	0
All	All	16509	0	14612	345	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 12.

All (345) 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:D:413:ASN:HD21	1:D:415:ASP:HB3	1.01	1.11
1:D:413:ASN:HD21	1:D:415:ASP:CB	1.67	1.06
1:B:413:ASN:HD21	1:B:415:ASP:HB3	1.14	1.04
1:A:413:ASN:HD21	1:A:415:ASP:HB3	1.22	1.03
1:D:413:ASN:ND2	1:D:415:ASP:HB3	1.78	0.98
4:B:501:HEM:HMB2	4:B:501:HEM:HBB2	1.49	0.95
4:D:501:HEM:HMB2	4:D:501:HEM:HBB2	1.48	0.95
4:A:501:HEM:HMB2	4:A:501:HEM:HBB2	1.48	0.95
1:A:413:ASN:ND2	1:A:415:ASP:H	1.68	0.91
1:A:413:ASN:HD21	1:A:415:ASP:CB	1.84	0.90
4:C:501:HEM:HBB2	4:C:501:HEM:HMB2	1.54	0.90
1:D:72:GLN:HG3	5:D:2055:HOH:O	1.76	0.85
1:B:413:ASN:HD21	1:B:415:ASP:CB	1.92	0.82
1:A:137:ALA:HA	4:A:501:HEM:HBB1	1.64	0.78
1:A:22:THR:HG23	1:A:24:GLY:O	1.83	0.77
1:B:22:THR:HG23	1:B:24:GLY:O	1.84	0.77
1:B:413:ASN:ND2	1:B:415:ASP:H	1.82	0.77
1:B:137:ALA:HA	4:B:501:HEM:HBB1	1.66	0.77
1:D:182:ARG:HG3	5:D:2257:HOH:O	1.85	0.77
1:D:22:THR:HG23	1:D:24:GLY:O	1.84	0.76
4:A:501:HEM:HBC2	4:A:501:HEM:HMC2	1.68	0.76
1:C:22:THR:HG23	1:C:24:GLY:O	1.85	0.75
1:C:56:LYS:HE3	1:C:101:SER:O	1.87	0.75
1:A:413:ASN:ND2	1:A:415:ASP:HB3	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:501:HEM:HMC2	4:B:501:HEM:HBC2	1.69	0.74
1:C:137:ALA:HA	4:C:501:HEM:HBB1	1.70	0.73
1:C:413:ASN:HD21	1:C:415:ASP:HB3	1.52	0.73
1:A:363:ASN:ND2	1:C:7:THR:O	2.20	0.73
1:D:137:ALA:HA	4:D:501:HEM:HBB1	1.70	0.73
1:A:56:LYS:HE3	1:A:101:SER:O	1.88	0.72
1:B:413:ASN:ND2	1:B:415:ASP:HB3	1.98	0.72
1:D:56:LYS:HE3	1:D:101:SER:O	1.89	0.72
1:B:56:LYS:HE3	1:B:101:SER:O	1.90	0.72
4:B:501:HEM:HBB2	4:B:501:HEM:CMB	2.20	0.72
1:D:413:ASN:ND2	1:D:415:ASP:H	1.88	0.71
4:D:501:HEM:CMB	4:D:501:HEM:HBB2	2.19	0.71
1:B:150:ASN:ND2	1:B:152:ARG:H	1.89	0.70
4:A:501:HEM:HBC2	4:A:501:HEM:CMC	2.21	0.70
1:B:150:ASN:HD22	1:B:152:ARG:H	1.39	0.70
4:D:501:HEM:HBC2	4:D:501:HEM:HMC2	1.74	0.70
1:C:150:ASN:ND2	1:C:152:ARG:H	1.89	0.70
4:C:501:HEM:HBC2	4:C:501:HEM:HMC2	1.74	0.70
1:B:263:ILE:HG21	1:B:271:MET:HE3	1.74	0.69
4:A:501:HEM:CMB	4:A:501:HEM:HBB2	2.20	0.69
1:C:413:ASN:ND2	1:C:415:ASP:H	1.90	0.69
1:C:259:SER:HB3	1:C:291:GLU:HA	1.74	0.69
1:B:256:TRP:HB2	1:B:295:MET:HE2	1.75	0.68
1:D:150:ASN:ND2	1:D:152:ARG:H	1.92	0.68
4:C:501:HEM:HBC2	4:C:501:HEM:CMC	2.23	0.68
4:D:501:HEM:HBC2	4:D:501:HEM:CMC	2.23	0.68
1:D:256:TRP:HB2	1:D:295:MET:HE2	1.74	0.68
1:A:256:TRP:HB2	1:A:295:MET:HE2	1.75	0.68
1:C:256:TRP:HB2	1:C:295:MET:HE2	1.75	0.68
1:B:363:ASN:ND2	1:D:7:THR:O	2.22	0.68
1:A:150:ASN:HD22	1:A:152:ARG:H	1.42	0.68
1:A:150:ASN:ND2	1:A:152:ARG:H	1.91	0.68
1:C:150:ASN:HD22	1:C:152:ARG:H	1.40	0.68
4:B:501:HEM:HBC2	4:B:501:HEM:CMC	2.23	0.67
1:A:424:TYR:O	1:A:432:LYS:HE2	1.95	0.67
4:C:501:HEM:HBB2	4:C:501:HEM:CMB	2.24	0.67
1:B:268:ALA:HA	1:B:271:MET:HE2	1.77	0.67
1:A:259:SER:HB3	1:A:291:GLU:HA	1.77	0.66
1:B:259:SER:HB3	1:B:291:GLU:HA	1.76	0.66
1:D:150:ASN:HD22	1:D:152:ARG:H	1.43	0.65
1:C:424:TYR:O	1:C:432:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:O	1:C:363:ASN:ND2	2.22	0.64
1:B:393:ASP:OD2	1:B:395:THR:HB	1.97	0.64
1:B:424:TYR:O	1:B:432:LYS:HE2	1.97	0.64
1:C:393:ASP:OD2	1:C:395:THR:HB	1.98	0.64
1:D:267:ASP:HB3	1:D:271:MET:CE	2.28	0.63
1:A:263:ILE:HG21	1:A:271:MET:HE3	1.80	0.63
1:D:424:TYR:O	1:D:432:LYS:HE2	1.99	0.63
1:B:263:ILE:HG21	1:B:271:MET:CE	2.30	0.62
1:D:393:ASP:OD2	1:D:395:THR:HB	2.00	0.62
1:A:393:ASP:OD2	1:A:395:THR:HB	1.99	0.62
1:C:415:ASP:HB2	5:C:2238:HOH:O	1.99	0.61
1:D:367:ASP:H	1:D:374:ASN:HD21	1.48	0.61
1:A:263:ILE:HG21	1:A:271:MET:CE	2.30	0.61
1:D:259:SER:HB3	1:D:291:GLU:HA	1.83	0.60
1:B:367:ASP:H	1:B:374:ASN:HD21	1.49	0.60
1:D:426:LEU:HD12	1:D:426:LEU:C	2.21	0.60
1:A:139:LYS:HZ3	1:D:18:GLN:HE22	1.50	0.60
1:A:367:ASP:H	1:A:374:ASN:HD21	1.48	0.59
1:B:203:ASN:HD21	1:B:207:GLU:HB2	1.67	0.59
1:A:203:ASN:HD21	1:A:207:GLU:HB2	1.65	0.59
1:C:363:ASN:HB3	1:C:365:GLN:H	1.68	0.59
1:C:367:ASP:H	1:C:374:ASN:HD21	1.50	0.59
1:A:380:ASN:HD22	1:A:380:ASN:H	1.51	0.58
1:D:414:GLN:HG2	5:D:2230:HOH:O	2.03	0.58
1:B:380:ASN:HD22	1:B:380:ASN:H	1.51	0.58
1:A:363:ASN:HB3	1:A:365:GLN:H	1.68	0.58
1:D:351:GLN:NE2	1:D:372:PHE:H	2.02	0.58
1:A:203:ASN:ND2	1:A:207:GLU:HB2	2.19	0.58
1:C:380:ASN:H	1:C:380:ASN:HD22	1.50	0.57
1:B:363:ASN:HB3	1:B:365:GLN:H	1.68	0.57
1:D:413:ASN:ND2	1:D:415:ASP:CB	2.50	0.57
1:D:351:GLN:HE22	1:D:372:PHE:H	1.53	0.57
1:B:203:ASN:ND2	1:B:207:GLU:HB2	2.20	0.57
1:C:203:ASN:HD21	1:C:207:GLU:HB2	1.69	0.57
1:B:358:LYS:HE3	5:B:2135:HOH:O	2.05	0.56
1:B:351:GLN:HE22	1:B:372:PHE:H	1.53	0.56
1:D:469:ARG:NH2	5:D:2274:HOH:O	2.38	0.56
1:A:131:ILE:HG13	1:A:174:GLN:HE21	1.68	0.56
1:A:351:GLN:NE2	1:A:372:PHE:H	2.03	0.56
1:D:363:ASN:HB3	1:D:365:GLN:H	1.69	0.56
1:C:22:THR:CG2	1:C:24:GLY:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:GLU:HG3	1:B:446:VAL:HG13	1.86	0.56
1:D:131:ILE:HG13	1:D:174:GLN:HE21	1.71	0.56
1:C:351:GLN:HE22	1:C:372:PHE:H	1.54	0.55
1:A:351:GLN:HE22	1:A:372:PHE:H	1.54	0.55
1:A:472:GLN:O	1:A:476:GLN:HG3	2.07	0.55
1:A:18:GLN:HE22	1:D:139:LYS:HZ3	1.54	0.55
1:D:225:GLU:HB3	5:D:2221:HOH:O	2.04	0.55
1:A:331:GLN:NE2	1:D:29:VAL:H	2.05	0.55
1:A:413:ASN:ND2	1:A:415:ASP:N	2.47	0.54
1:B:22:THR:CG2	1:B:24:GLY:O	2.53	0.54
1:C:203:ASN:ND2	1:C:207:GLU:HB2	2.22	0.54
1:C:351:GLN:NE2	1:C:372:PHE:H	2.05	0.54
1:B:131:ILE:HG13	1:B:174:GLN:HE21	1.72	0.54
1:B:351:GLN:NE2	1:B:372:PHE:H	2.05	0.54
1:D:22:THR:CG2	1:D:24:GLY:O	2.54	0.54
1:D:380:ASN:H	1:D:380:ASN:HD22	1.55	0.54
1:B:29:VAL:H	1:C:331:GLN:NE2	2.05	0.54
1:D:198:THR:OG1	1:D:212:LYS:HE3	2.07	0.54
1:D:358:LYS:HE3	5:D:2177:HOH:O	2.07	0.54
1:C:189:ARG:HD3	1:C:243:ASP:OD1	2.09	0.53
1:D:203:ASN:ND2	1:D:207:GLU:HB2	2.24	0.53
1:B:7:THR:O	1:D:363:ASN:ND2	2.28	0.53
1:B:472:GLN:HG3	5:B:2205:HOH:O	2.07	0.53
1:C:150:ASN:HD22	1:C:152:ARG:N	2.05	0.53
1:C:131:ILE:HG13	1:C:174:GLN:HE21	1.73	0.53
1:A:22:THR:CG2	1:A:24:GLY:O	2.55	0.53
1:D:203:ASN:HD21	1:D:207:GLU:HB2	1.73	0.52
1:D:189:ARG:HD3	1:D:243:ASP:OD1	2.09	0.52
1:B:371:ARG:HD2	1:B:373:ASN:O	2.10	0.52
1:D:150:ASN:HD22	1:D:152:ARG:N	2.08	0.52
1:A:432:LYS:O	1:A:436:ILE:HG12	2.10	0.51
1:B:140:PHE:HB3	1:B:141:PRO:HD3	1.92	0.51
1:B:189:ARG:HD3	1:B:243:ASP:OD1	2.10	0.51
1:A:371:ARG:HD2	1:A:373:ASN:O	2.11	0.51
1:C:342:ARG:HD3	5:C:2145:HOH:O	2.11	0.51
1:A:268:ALA:HA	1:A:271:MET:HE2	1.91	0.51
1:B:227:GLN:HB2	5:B:2249:HOH:O	2.09	0.51
1:A:140:PHE:HB3	1:A:141:PRO:HD3	1.92	0.51
1:C:263:ILE:HG21	1:C:271:MET:CE	2.40	0.51
1:A:150:ASN:HD22	1:A:152:ARG:N	2.08	0.51
1:B:278:VAL:HG11	1:B:329:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:GLU:HG2	5:D:2077:HOH:O	2.11	0.50
1:C:54:HIS:HA	1:C:94:THR:O	2.12	0.50
4:A:501:HEM:HMB2	4:A:501:HEM:CBB	2.33	0.50
1:A:189:ARG:HD3	1:A:243:ASP:OD1	2.10	0.50
1:C:432:LYS:O	1:C:436:ILE:HG12	2.12	0.50
1:A:395:THR:HG22	5:A:2204:HOH:O	2.11	0.50
1:B:265:TYR:CE2	1:B:269:LEU:HD21	2.47	0.49
1:B:432:LYS:O	1:B:436:ILE:HG12	2.12	0.49
1:C:472:GLN:O	1:C:476:GLN:HG3	2.12	0.49
1:B:351:GLN:HE22	1:B:372:PHE:N	2.10	0.49
1:D:351:GLN:HE22	1:D:372:PHE:N	2.10	0.49
1:D:371:ARG:HD2	1:D:373:ASN:O	2.13	0.49
1:A:150:ASN:HD22	1:A:153:THR:H	1.59	0.49
1:A:351:GLN:HE22	1:A:372:PHE:N	2.10	0.49
1:C:371:ARG:HD2	1:C:373:ASN:O	2.11	0.49
1:D:463:ASN:HD22	1:D:465:GLU:H	1.61	0.49
1:B:469:ARG:HD2	5:B:2138:HOH:O	2.12	0.49
1:B:198:THR:OG1	1:B:212:LYS:HE3	2.12	0.48
1:C:351:GLN:HE22	1:C:372:PHE:N	2.11	0.48
1:C:58:ALA:HB2	1:C:241:ILE:HG12	1.96	0.48
1:D:432:LYS:O	1:D:436:ILE:HG12	2.13	0.48
1:A:382:GLU:O	1:B:139:LYS:NZ	2.46	0.48
1:B:463:ASN:HB3	1:B:466:TYR:HB2	1.95	0.48
1:B:54:HIS:HA	1:B:94:THR:O	2.13	0.48
1:B:159:GLU:OE1	1:B:446:VAL:HA	2.14	0.48
1:C:140:PHE:HB3	1:C:141:PRO:HD3	1.94	0.48
1:A:198:THR:OG1	1:A:212:LYS:HE3	2.13	0.48
1:B:150:ASN:HD22	1:B:153:THR:H	1.61	0.48
1:B:58:ALA:HB2	1:B:241:ILE:HG12	1.95	0.48
1:B:463:ASN:HD22	1:B:465:GLU:H	1.62	0.48
1:C:463:ASN:HB3	1:C:466:TYR:HB2	1.95	0.48
1:D:58:ALA:HB2	1:D:241:ILE:HG12	1.95	0.48
1:D:389:THR:HB	1:D:390:PRO:HD2	1.96	0.48
1:A:366:LYS:O	1:C:46:GLU:HG2	2.14	0.48
1:B:150:ASN:HD22	1:B:152:ARG:N	2.07	0.48
1:C:380:ASN:H	1:C:380:ASN:ND2	2.12	0.48
1:A:273:GLU:HG2	1:D:26:PHE:HZ	1.78	0.47
1:A:380:ASN:HD22	1:A:380:ASN:N	2.11	0.47
1:B:24:GLY:HA3	1:C:404:GLU:O	2.14	0.47
1:A:265:TYR:CE2	1:A:269:LEU:HD21	2.50	0.47
4:D:501:HEM:HMB2	4:D:501:HEM:CBB	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:GLN:HG3	5:C:2032:HOH:O	2.14	0.47
1:C:389:THR:HB	1:C:390:PRO:HD2	1.97	0.47
1:D:463:ASN:HB3	1:D:466:TYR:HB2	1.96	0.47
1:A:58:ALA:HB2	1:A:241:ILE:HG12	1.97	0.47
1:C:263:ILE:HG21	1:C:271:MET:HE3	1.96	0.47
1:B:366:LYS:O	1:D:46:GLU:HG2	2.15	0.47
1:A:46:GLU:HG2	1:C:366:LYS:O	2.15	0.47
1:B:261:GLN:HG2	1:B:287:TYR:O	2.15	0.47
1:A:463:ASN:HB3	1:A:466:TYR:HB2	1.97	0.47
1:B:380:ASN:N	1:B:380:ASN:HD22	2.11	0.47
1:C:150:ASN:ND2	1:C:153:THR:H	2.13	0.47
1:D:124:LEU:HD23	1:D:215:PHE:CZ	2.50	0.47
1:A:18:GLN:HE22	1:D:139:LYS:NZ	2.12	0.47
1:B:150:ASN:ND2	1:B:153:THR:H	2.13	0.47
1:C:463:ASN:ND2	1:C:465:GLU:H	2.14	0.46
1:D:56:LYS:HA	5:D:2229:HOH:O	2.15	0.46
1:A:150:ASN:ND2	1:A:153:THR:H	2.13	0.46
1:A:389:THR:HB	1:A:390:PRO:HD2	1.97	0.46
1:B:472:GLN:O	1:B:476:GLN:HG3	2.15	0.46
1:A:29:VAL:H	1:D:331:GLN:NE2	2.13	0.46
1:C:413:ASN:HD21	1:C:415:ASP:H	1.64	0.46
1:D:426:LEU:HD12	1:D:427:LEU:N	2.30	0.46
1:B:380:ASN:H	1:B:380:ASN:ND2	2.13	0.46
1:D:150:ASN:HD22	1:D:153:THR:H	1.62	0.46
1:A:463:ASN:HD22	1:A:465:GLU:H	1.63	0.46
1:A:88:LEU:C	1:A:88:LEU:HD12	2.36	0.46
1:C:463:ASN:HD22	1:C:465:GLU:H	1.62	0.46
4:B:501:HEM:CMB	4:B:501:HEM:CBB	2.93	0.46
1:C:126:GLY:HA3	1:C:194:PHE:O	2.16	0.46
1:D:140:PHE:HB3	1:D:141:PRO:HD3	1.98	0.46
1:D:54:HIS:HA	1:D:94:THR:O	2.16	0.46
1:D:271:MET:HE1	1:D:287:TYR:OH	2.15	0.46
1:D:449:GLN:HG2	5:D:2206:HOH:O	2.15	0.46
1:A:380:ASN:H	1:A:380:ASN:ND2	2.12	0.45
4:A:501:HEM:CBC	4:A:501:HEM:CMC	2.94	0.45
1:B:374:ASN:HA	1:B:374:ASN:HD22	1.53	0.45
1:B:88:LEU:HD12	1:B:88:LEU:C	2.36	0.45
1:C:469:ARG:HD2	5:C:2274:HOH:O	2.15	0.45
1:D:463:ASN:ND2	1:D:465:GLU:H	2.14	0.45
1:A:139:LYS:NZ	1:D:18:GLN:HE22	2.12	0.45
1:C:150:ASN:HD22	1:C:153:THR:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:501:HEM:CMB	4:D:501:HEM:CBB	2.93	0.45
1:C:413:ASN:HD21	1:C:415:ASP:CB	2.24	0.45
1:D:126:GLY:HA3	1:D:194:PHE:O	2.16	0.45
1:A:388:GLU:HG3	1:A:388:GLU:H	1.35	0.45
1:A:463:ASN:ND2	1:A:465:GLU:H	2.14	0.45
1:C:267:ASP:O	1:C:271:MET:HE2	2.16	0.45
1:C:88:LEU:HD12	1:C:88:LEU:C	2.37	0.45
1:B:126:GLY:HA3	1:B:194:PHE:O	2.17	0.45
1:C:23:ALA:HB2	1:C:30:LEU:HD21	1.99	0.45
1:C:249:GLU:HA	1:C:249:GLU:OE1	2.17	0.45
1:A:126:GLY:HA3	1:A:194:PHE:O	2.16	0.45
1:A:106:ARG:HG2	1:A:178:LEU:HD22	1.99	0.45
1:B:23:ALA:O	1:B:27:GLY:HA3	2.17	0.45
1:B:372:PHE:HB2	5:B:2281:HOH:O	2.16	0.45
1:B:463:ASN:ND2	1:B:465:GLU:H	2.14	0.45
1:C:392:GLU:HG2	5:C:2052:HOH:O	2.16	0.45
1:D:88:LEU:C	1:D:88:LEU:HD12	2.36	0.45
1:A:23:ALA:HB2	1:A:30:LEU:HD21	1.99	0.44
1:A:249:GLU:OE1	1:A:249:GLU:HA	2.18	0.44
1:D:150:ASN:ND2	1:D:153:THR:H	2.14	0.44
1:B:463:ASN:ND2	1:B:465:GLU:HB3	2.32	0.44
1:C:261:GLN:HG2	1:C:287:TYR:O	2.17	0.44
1:B:54:HIS:CE1	1:B:95:VAL:HG22	2.52	0.44
4:C:501:HEM:CBC	4:C:501:HEM:CMC	2.95	0.44
1:A:268:ALA:HA	1:A:271:MET:CE	2.47	0.44
1:C:198:THR:OG1	1:C:212:LYS:HE3	2.18	0.44
1:D:267:ASP:C	1:D:271:MET:HE3	2.38	0.44
1:D:124:LEU:HD23	1:D:215:PHE:CE1	2.52	0.44
1:B:189:ARG:HG2	1:B:254:PRO:HB3	1.99	0.43
1:B:463:ASN:HD22	1:B:465:GLU:N	2.16	0.43
1:C:278:VAL:HG11	1:C:329:LEU:HD22	1.99	0.43
1:D:475:LYS:HE3	5:D:2358:HOH:O	2.18	0.43
1:A:463:ASN:ND2	1:A:465:GLU:HB3	2.33	0.43
1:D:366:LYS:NZ	1:D:374:ASN:O	2.47	0.43
1:D:380:ASN:ND2	1:D:380:ASN:H	2.16	0.43
1:D:472:GLN:O	1:D:476:GLN:HG3	2.17	0.43
1:B:16:ASP:OD2	1:C:409:ASN:HB3	2.18	0.43
1:B:249:GLU:HA	1:B:249:GLU:OE1	2.17	0.43
1:B:389:THR:HB	1:B:390:PRO:HD2	1.99	0.43
4:B:501:HEM:CMC	4:B:501:HEM:CBC	2.95	0.43
1:B:86:THR:HA	1:B:87:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:TYR:CE2	1:A:382:GLU:HB2	2.53	0.43
1:A:131:ILE:HG13	1:A:174:GLN:NE2	2.34	0.43
1:A:189:ARG:HG2	1:A:254:PRO:HB3	1.99	0.43
1:A:137:ALA:HA	4:A:501:HEM:CBB	2.44	0.43
1:B:413:ASN:ND2	1:B:415:ASP:N	2.58	0.43
1:D:249:GLU:HA	1:D:249:GLU:OE1	2.19	0.43
1:C:380:ASN:HD22	1:C:380:ASN:N	2.11	0.43
4:C:501:HEM:HMC2	4:C:501:HEM:CBC	2.47	0.43
1:D:463:ASN:HD22	1:D:465:GLU:N	2.16	0.43
1:B:106:ARG:HG2	1:B:178:LEU:HD22	2.01	0.42
1:D:106:ARG:HG2	1:D:178:LEU:HD22	2.01	0.42
4:A:501:HEM:HMC2	4:A:501:HEM:CBC	2.42	0.42
1:A:54:HIS:HA	1:A:94:THR:O	2.19	0.42
1:B:364:TYR:CE2	1:B:382:GLU:HB2	2.54	0.42
1:C:364:TYR:CE2	1:C:382:GLU:HB2	2.55	0.42
1:C:463:ASN:ND2	1:C:465:GLU:HB3	2.33	0.42
1:A:263:ILE:CG2	1:A:271:MET:HE1	2.50	0.42
1:A:358:LYS:HE3	5:A:2230:HOH:O	2.19	0.42
1:A:463:ASN:HD22	1:A:465:GLU:N	2.17	0.42
1:C:133:PHE:CE2	1:C:174:GLN:HG3	2.55	0.42
1:C:463:ASN:HD22	1:C:465:GLU:N	2.17	0.42
1:A:26:PHE:CZ	1:D:273:GLU:HG2	2.54	0.42
1:A:54:HIS:CE1	1:A:95:VAL:HG22	2.55	0.42
1:B:317:ASN:HD22	1:B:317:ASN:HA	1.71	0.42
1:D:133:PHE:CE2	1:D:174:GLN:HG3	2.55	0.42
1:B:268:ALA:HA	1:B:271:MET:CE	2.46	0.42
1:A:150:ASN:HD21	1:A:152:ARG:HB3	1.85	0.42
1:C:317:ASN:HD22	1:C:317:ASN:HA	1.70	0.42
1:C:61:HIS:HB2	1:C:299:ARG:HB3	2.01	0.41
1:B:21:LEU:HA	1:B:21:LEU:HD23	1.93	0.41
1:A:331:GLN:HG3	5:A:2097:HOH:O	2.20	0.41
1:A:366:LYS:NZ	1:A:374:ASN:O	2.49	0.41
1:B:150:ASN:HD21	1:B:152:ARG:HB3	1.85	0.41
1:C:192:HIS:CD2	1:C:221:ILE:HD11	2.55	0.41
1:C:189:ARG:HG2	1:C:254:PRO:HB3	2.01	0.41
1:A:26:PHE:HZ	1:D:273:GLU:HG2	1.86	0.41
1:D:23:ALA:O	1:D:27:GLY:HA3	2.21	0.41
1:A:331:GLN:HE21	1:D:29:VAL:H	1.67	0.41
1:D:364:TYR:CE2	1:D:382:GLU:HB2	2.55	0.41
1:A:61:HIS:HB2	1:A:299:ARG:HB3	2.02	0.41
1:B:392:GLU:HG2	5:B:2168:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:O	1:B:54:HIS:HB2	2.21	0.41
1:A:139:LYS:HD2	1:D:18:GLN:NE2	2.35	0.41
1:A:261:GLN:HG2	1:A:287:TYR:O	2.20	0.41
1:B:61:HIS:HB2	1:B:299:ARG:HB3	2.03	0.41
1:D:150:ASN:HD21	1:D:152:ARG:HB3	1.86	0.41
1:D:216:LYS:HD2	5:D:2190:HOH:O	2.20	0.41
1:D:423:LEU:O	1:D:426:LEU:HG	2.21	0.41
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.92	0.41
1:D:426:LEU:CD1	1:D:426:LEU:C	2.88	0.41
1:D:463:ASN:ND2	1:D:465:GLU:HB3	2.35	0.41
1:A:137:ALA:CB	1:A:332:GLY:HA3	2.51	0.41
1:B:18:GLN:NE2	1:C:139:LYS:HD2	2.36	0.41
1:B:192:HIS:CD2	1:B:221:ILE:HD11	2.56	0.41
1:C:272:LYS:HD3	1:C:276:PHE:HE2	1.85	0.41
1:D:61:HIS:HB2	1:D:299:ARG:HB3	2.03	0.41
1:B:314:SER:HA	1:B:315:PRO:HD3	1.97	0.41
1:D:23:ALA:HB2	1:D:30:LEU:HD21	2.03	0.41
1:D:380:ASN:N	1:D:380:ASN:HD22	2.14	0.41
1:A:149:ARG:HD3	1:A:154:HIS:CE1	2.56	0.41
1:B:133:PHE:CE2	1:B:174:GLN:HG3	2.56	0.41
1:B:179:MET:HG3	1:B:439:ILE:HG12	2.02	0.41
1:D:189:ARG:HG2	1:D:254:PRO:HB3	2.02	0.41
1:C:405:GLY:O	1:D:403:VAL:HG12	2.21	0.41
1:A:192:HIS:CD2	1:A:221:ILE:HD11	2.56	0.41
1:B:23:ALA:HB2	1:B:30:LEU:HD21	2.03	0.41
1:C:374:ASN:HD22	1:C:374:ASN:HA	1.51	0.41
1:B:404:GLU:O	1:C:24:GLY:HA3	2.21	0.40
1:C:388:GLU:HG3	1:C:388:GLU:H	1.35	0.40
1:D:137:ALA:CB	1:D:332:GLY:HA3	2.51	0.40
1:D:261:GLN:HG2	1:D:287:TYR:O	2.20	0.40
1:A:179:MET:HG3	1:A:439:ILE:HG12	2.02	0.40
1:C:179:MET:HG3	1:C:439:ILE:HG12	2.03	0.40
1:C:413:ASN:ND2	1:C:415:ASP:N	2.64	0.40
1:D:179:MET:HG3	1:D:439:ILE:HG12	2.04	0.40

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	472/484 (98%)	456 (97%)	15 (3%)	1 (0%)	47	58
1	B	472/484 (98%)	456 (97%)	15 (3%)	1 (0%)	47	58
1	C	472/484 (98%)	457 (97%)	15 (3%)	0	100	100
1	D	472/484 (98%)	456 (97%)	16 (3%)	0	100	100
All	All	1888/1936 (98%)	1825 (97%)	61 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	413	ASN
1	A	476	GLN

### 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	408/417 (98%)	383 (94%)	25 (6%)	18	25
1	B	408/417 (98%)	382 (94%)	26 (6%)	17	23
1	C	408/417 (98%)	381 (93%)	27 (7%)	16	22
1	D	408/417 (98%)	381 (93%)	27 (7%)	16	22
All	All	1632/1668 (98%)	1527 (94%)	105 (6%)	17	23

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	37	LEU
1	A	40	LEU
1	A	113	LEU
1	A	135	ARG
1	A	150	ASN
1	A	159	GLU
1	A	178	LEU
1	A	225	GLU
1	A	227	GLN
1	A	228	LEU
1	A	244	LEU
1	A	249	GLU
1	A	267	ASP
1	A	271	MET
1	A	297	LEU
1	A	330	LEU
1	A	374	ASN
1	A	380	ASN
1	A	388	GLU
1	A	395	THR
1	A	435	LEU
1	A	458	LEU
1	A	463	ASN
1	A	466	TYR
1	B	22	THR
1	B	37	LEU
1	B	40	LEU
1	B	113	LEU
1	B	117	THR
1	B	135	ARG
1	B	150	ASN
1	B	159	GLU
1	B	178	LEU
1	B	225	GLU
1	B	227	GLN
1	B	228	LEU
1	B	244	LEU
1	B	249	GLU
1	B	267	ASP
1	B	297	LEU
1	B	330	LEU
1	B	374	ASN

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Mol	Chain	Res	Type
1	B	380	ASN
1	B	388	GLU
1	B	395	THR
1	B	412	TYR
1	B	435	LEU
1	B	458	LEU
1	B	463	ASN
1	B	466	TYR
1	C	22	THR
1	C	37	LEU
1	C	40	LEU
1	C	113	LEU
1	C	117	THR
1	C	135	ARG
1	C	150	ASN
1	C	159	GLU
1	C	178	LEU
1	C	225	GLU
1	C	227	GLN
1	C	228	LEU
1	C	244	LEU
1	C	249	GLU
1	C	259	SER
1	C	297	LEU
1	C	302	GLU
1	C	330	LEU
1	C	374	ASN
1	C	380	ASN
1	C	387	THR
1	C	388	GLU
1	C	395	THR
1	C	435	LEU
1	C	458	LEU
1	C	463	ASN
1	C	466	TYR
1	D	22	THR
1	D	37	LEU
1	D	40	LEU
1	D	72	GLN
1	D	113	LEU
1	D	135	ARG
1	D	150	ASN

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Mol	Chain	Res	Type
1	D	178	LEU
1	D	225	GLU
1	D	227	GLN
1	D	228	LEU
1	D	244	LEU
1	D	249	GLU
1	D	271	MET
1	D	297	LEU
1	D	330	LEU
1	D	374	ASN
1	D	380	ASN
1	D	387	THR
1	D	388	GLU
1	D	395	THR
1	D	412	TYR
1	D	433	GLU
1	D	435	LEU
1	D	458	LEU
1	D	463	ASN
1	D	466	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	32	GLN
1	A	68	GLN
1	A	121	ASN
1	A	150	ASN
1	A	174	GLN
1	A	190	HIS
1	A	245	HIS
1	A	300	ASN
1	A	317	ASN
1	A	331	GLN
1	A	351	GLN
1	A	373	ASN
1	A	374	ASN
1	A	380	ASN
1	A	413	ASN
1	A	463	ASN
1	B	18	GLN

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Mol	Chain	Res	Type
1	B	32	GLN
1	B	121	ASN
1	B	150	ASN
1	B	174	GLN
1	B	190	HIS
1	B	300	ASN
1	B	317	ASN
1	B	331	GLN
1	B	351	GLN
1	B	373	ASN
1	B	374	ASN
1	B	380	ASN
1	B	413	ASN
1	B	463	ASN
1	C	18	GLN
1	C	32	GLN
1	C	68	GLN
1	C	121	ASN
1	C	150	ASN
1	C	174	GLN
1	C	190	HIS
1	C	300	ASN
1	C	317	ASN
1	C	331	GLN
1	C	351	GLN
1	C	373	ASN
1	C	374	ASN
1	C	380	ASN
1	C	413	ASN
1	C	463	ASN
1	D	18	GLN
1	D	32	GLN
1	D	121	ASN
1	D	150	ASN
1	D	174	GLN
1	D	190	HIS
1	D	300	ASN
1	D	317	ASN
1	D	331	GLN
1	D	351	GLN
1	D	373	ASN
1	D	374	ASN

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Mol	Chain	Res	Type
1	D	380	ASN
1	D	413	ASN
1	D	437	ASN
1	D	463	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	D	2004	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	A	2005	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	A	2001	-	4,4,4	0.23	0	6,6,6	0.08	0
4	HEM	A	501	1	27,50,50	1.29	4 (14%)	17,82,82	2.15	6 (35%)
2	SO4	B	2006	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SO4	B	2002	-	4,4,4	0.26	0	6,6,6	0.11	0
4	HEM	D	501	1	27,50,50	1.29	2 (7%)	17,82,82	2.11	6 (35%)
2	SO4	D	2008	-	4,4,4	0.20	0	6,6,6	0.14	0
2	SO4	C	2007	-	4,4,4	0.23	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HEM	B	501	1	27,50,50	1.33	3 (11%)	17,82,82	2.14	6 (35%)
2	SO4	C	2003	-	4,4,4	0.24	0	6,6,6	0.07	0
4	HEM	C	501	1	27,50,50	1.33	4 (14%)	17,82,82	2.16	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
4	HEM	B	501	1	-	0/6/54/54	-
4	HEM	A	501	1	-	0/6/54/54	-
4	HEM	D	501	1	-	0/6/54/54	-
4	HEM	C	501	1	-	0/6/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	HEM	C3B-CAB	-3.04	1.41	1.47
4	C	501	HEM	C3B-CAB	-3.03	1.41	1.47
4	D	501	HEM	C3B-CAB	-3.00	1.41	1.47
4	A	501	HEM	C3B-CAB	-2.96	1.41	1.47
4	A	501	HEM	C3C-CAC	-2.74	1.42	1.47
4	B	501	HEM	C3C-CAC	-2.64	1.42	1.47
4	C	501	HEM	C3C-CAC	-2.62	1.42	1.47
4	D	501	HEM	C3C-CAC	-2.42	1.42	1.47
4	C	501	HEM	C3C-C2C	-2.21	1.37	1.40
4	C	501	HEM	CAA-C2A	2.20	1.55	1.52
4	A	501	HEM	C3B-C2B	-2.09	1.37	1.40
4	A	501	HEM	C3C-C2C	-2.09	1.37	1.40
4	B	501	HEM	CAA-C2A	2.05	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	HEM	C4A-C3A-C2A	4.96	110.45	107.00
4	A	501	HEM	C4A-C3A-C2A	4.81	110.34	107.00
4	B	501	HEM	C4A-C3A-C2A	4.81	110.34	107.00
4	D	501	HEM	C4A-C3A-C2A	4.61	110.20	107.00
4	B	501	HEM	C1D-C2D-C3D	4.47	110.10	107.00
4	C	501	HEM	C1D-C2D-C3D	4.41	110.07	107.00
4	A	501	HEM	C1D-C2D-C3D	4.36	110.03	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	HEM	C1D-C2D-C3D	4.24	109.94	107.00
4	D	501	HEM	C3B-C4B-NB	-3.04	105.29	109.21
4	B	501	HEM	C3B-C4B-NB	-3.03	105.30	109.21
4	A	501	HEM	C3C-C4C-NC	-2.96	105.35	110.94
4	A	501	HEM	C3B-C4B-NB	-2.95	105.39	109.21
4	B	501	HEM	C3C-C4C-NC	-2.82	105.61	110.94
4	D	501	HEM	C3C-C4C-NC	-2.78	105.70	110.94
4	C	501	HEM	C3B-C4B-NB	-2.76	105.64	109.21
4	C	501	HEM	C3C-C4C-NC	-2.72	105.81	110.94
4	C	501	HEM	CMD-C2D-C1D	-2.35	124.85	128.46
4	A	501	HEM	CMD-C2D-C1D	-2.28	124.96	128.46
4	C	501	HEM	CMA-C3A-C4A	-2.25	125.00	128.46
4	A	501	HEM	CMA-C3A-C4A	-2.25	125.01	128.46
4	B	501	HEM	CMA-C3A-C4A	-2.21	125.07	128.46
4	B	501	HEM	CMD-C2D-C1D	-2.19	125.10	128.46
4	D	501	HEM	CMA-C3A-C4A	-2.15	125.17	128.46
4	D	501	HEM	C4C-C3C-C2C	2.05	108.33	106.90

There are no chirality outliers.

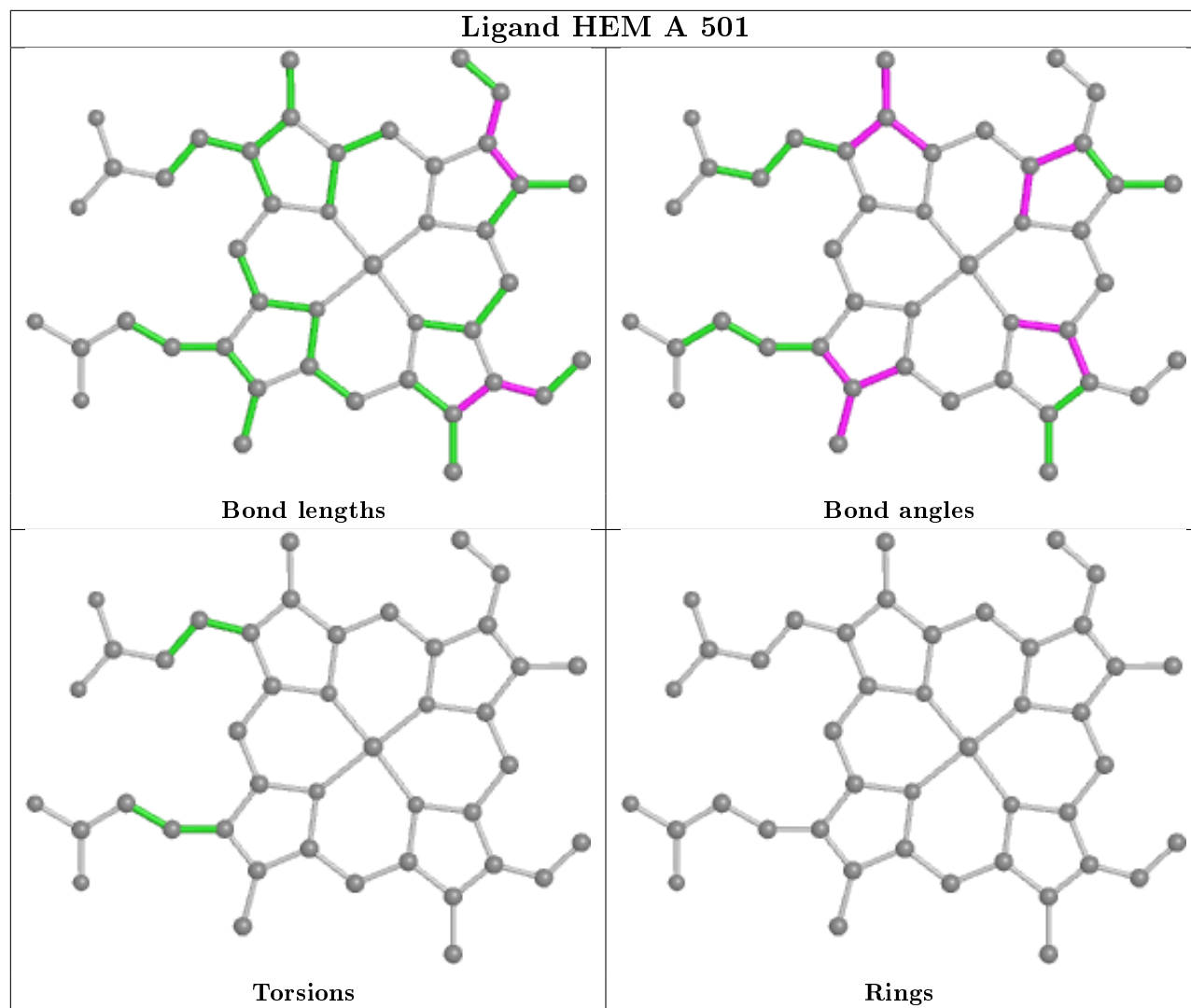
There are no torsion outliers.

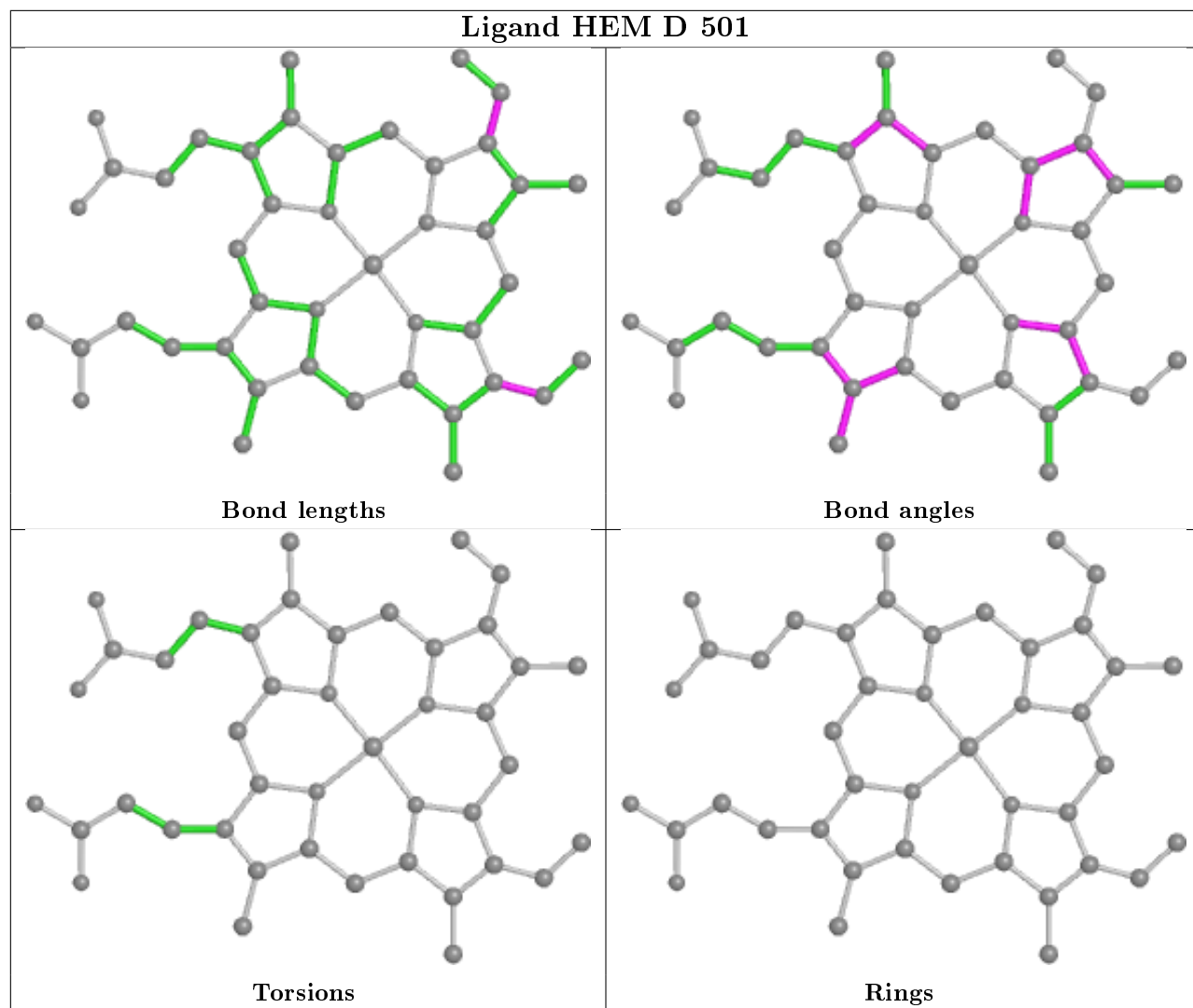
There are no ring outliers.

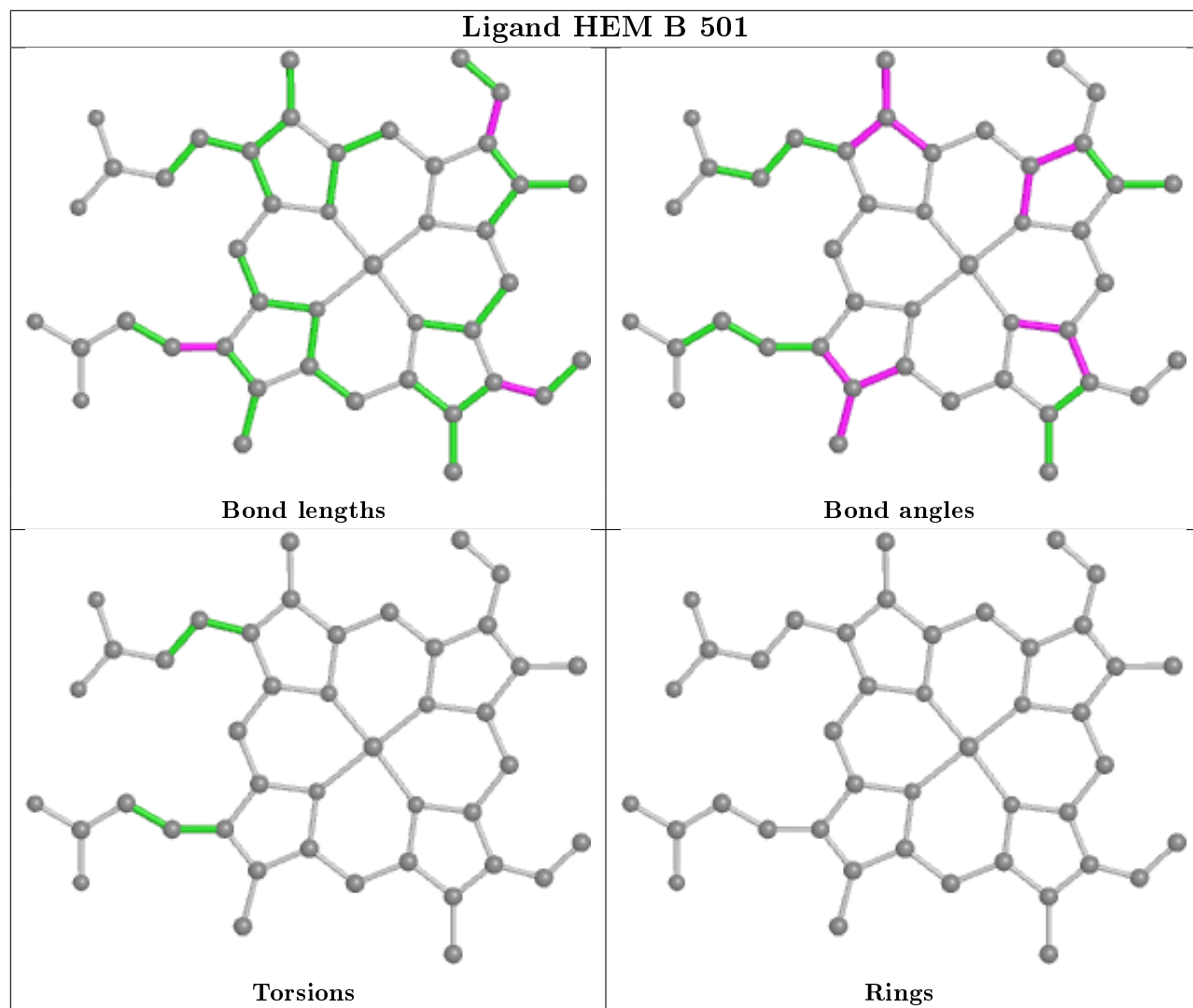
4 monomers are involved in 30 short contacts:

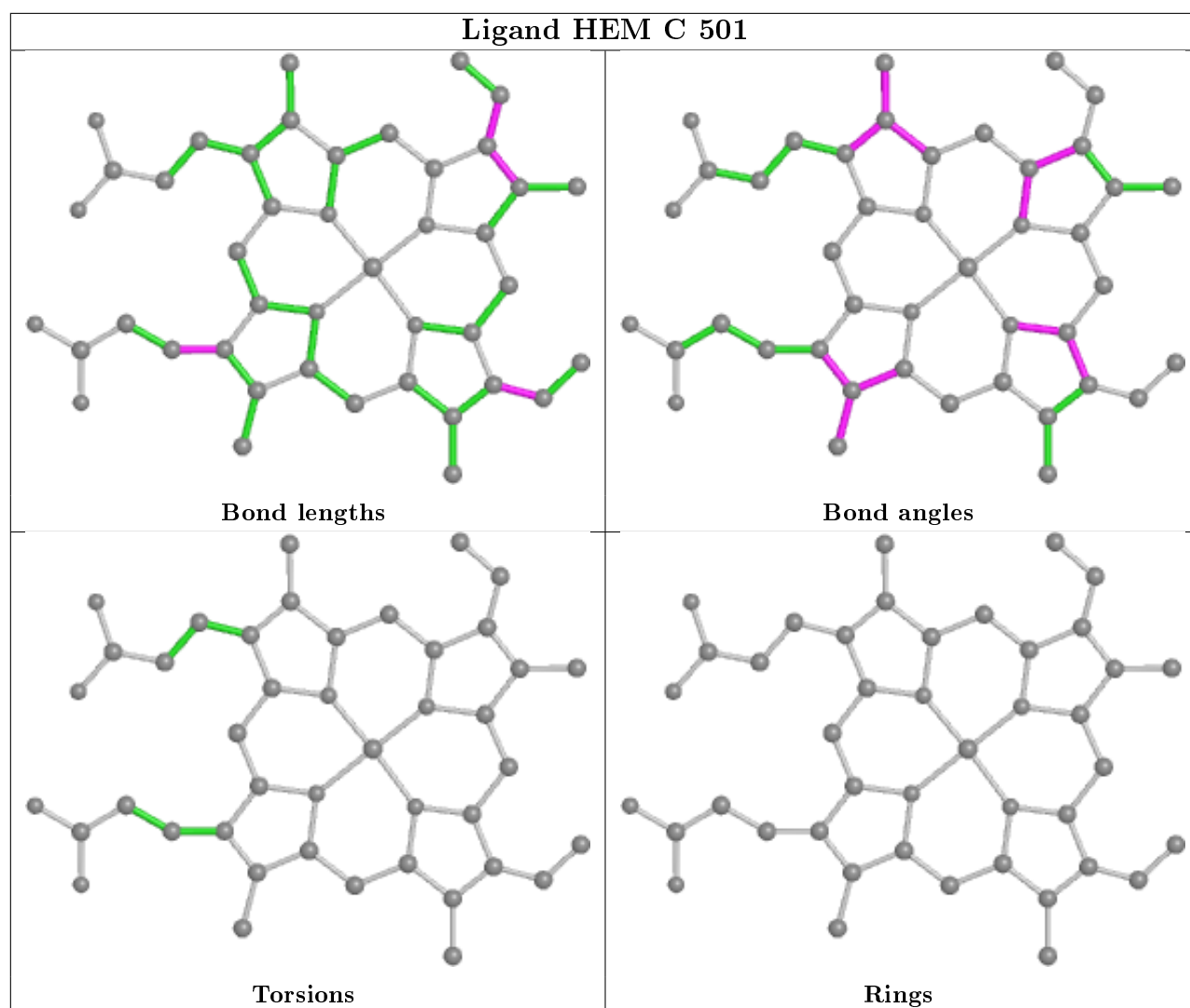
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	HEM	9	0
4	D	501	HEM	7	0
4	B	501	HEM	7	0
4	C	501	HEM	7	0

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	474/484 (97%)	-0.18	22 (4%) 32 39	15, 29, 45, 57	0
1	B	474/484 (97%)	-0.32	16 (3%) 45 52	15, 27, 43, 57	0
1	C	474/484 (97%)	-0.38	8 (1%) 70 76	16, 26, 40, 57	0
1	D	474/484 (97%)	-0.37	9 (1%) 66 73	14, 25, 39, 53	0
All	All	1896/1936 (97%)	-0.31	55 (2%) 51 58	14, 27, 42, 57	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	LYS	4.5
1	B	475	LYS	4.1
1	A	426	LEU	4.1
1	A	265	TYR	4.0
1	C	477	GLN	4.0
1	B	477	GLN	3.9
1	A	477	GLN	3.9
1	A	475	LYS	3.7
1	A	429	SER	3.6
1	A	376	ASN	3.6
1	D	4	GLN	3.5
1	A	476	GLN	3.5
1	C	475	LYS	3.5
1	B	476	GLN	3.4
1	D	413	ASN	3.4
1	A	413	ASN	3.3
1	A	449	GLN	3.3
1	B	265	TYR	3.2
1	C	476	GLN	3.1
1	A	205	ALA	3.1
1	A	430	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	270	THR	3.1
1	C	449	GLN	3.1
1	B	447	LYS	3.0
1	B	430	GLU	3.0
1	B	387	THR	2.9
1	D	376	ASN	2.9
1	A	447	LYS	2.8
1	B	376	ASN	2.8
1	D	412	TYR	2.8
1	B	449	GLN	2.8
1	B	412	TYR	2.7
1	A	404	GLU	2.6
1	B	404	GLU	2.6
1	C	430	GLU	2.6
1	C	376	ASN	2.6
1	B	426	LEU	2.5
1	B	205	ALA	2.5
1	D	449	GLN	2.5
1	D	476	GLN	2.5
1	C	429	SER	2.5
1	C	265	TYR	2.5
1	B	413	ASN	2.4
1	B	429	SER	2.3
1	A	68	GLN	2.3
1	D	475	LYS	2.3
1	D	477	GLN	2.2
1	A	81	GLU	2.2
1	A	266	ALA	2.2
1	B	414	GLN	2.1
1	A	204	ALA	2.1
1	A	387	THR	2.1
1	A	414	GLN	2.1
1	A	472	GLN	2.1
1	D	388	GLU	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

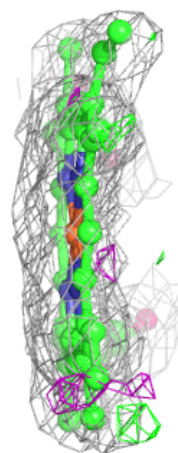
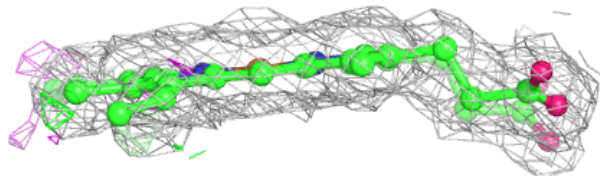
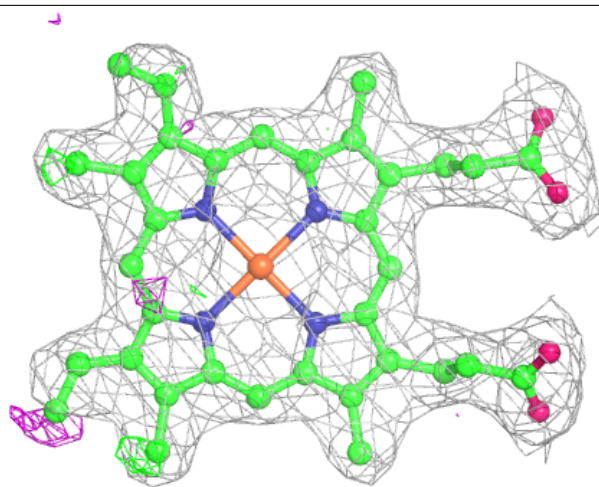
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	SO4	A	2005	5/5	0.96	0.21	62,62,63,63	0
2	SO4	B	2006	5/5	0.96	0.12	55,55,56,56	0
4	HEM	A	501	43/43	0.97	0.11	18,28,34,36	0
4	HEM	D	501	43/43	0.97	0.11	12,17,21,28	0
2	SO4	C	2007	5/5	0.97	0.16	54,55,56,56	0
4	HEM	B	501	43/43	0.97	0.10	19,23,27,33	0
2	SO4	D	2004	5/5	0.98	0.08	42,42,44,44	0
4	HEM	C	501	43/43	0.98	0.10	13,17,21,27	0
2	SO4	D	2008	5/5	0.98	0.10	54,55,56,56	0
2	SO4	C	2003	5/5	0.98	0.08	50,51,51,52	0
3	CL	C	2010	1/1	0.98	0.04	31,31,31,31	0
3	CL	A	2009	1/1	0.99	0.05	25,25,25,25	0
2	SO4	B	2002	5/5	0.99	0.07	31,32,33,33	0
2	SO4	A	2001	5/5	0.99	0.05	31,32,34,34	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.

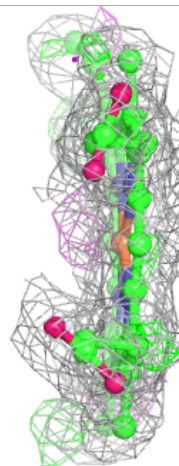
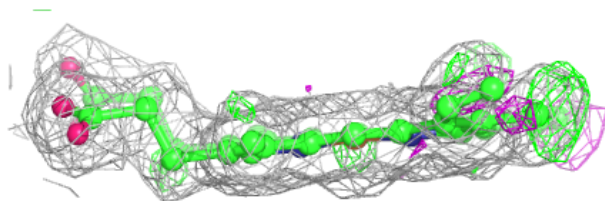
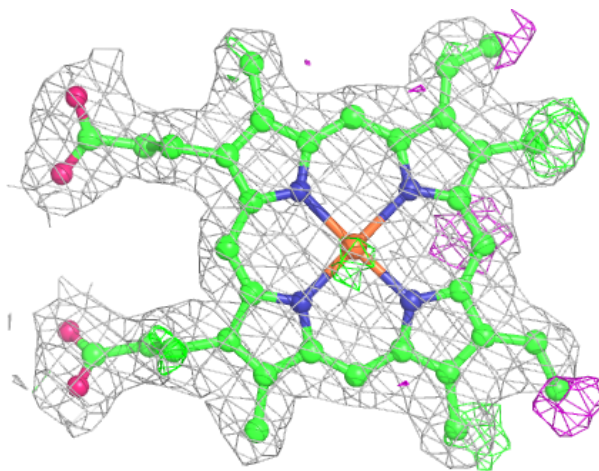
**Electron density around HEM A 501:**

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



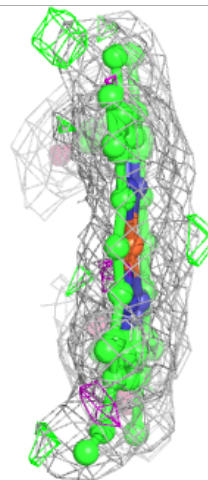
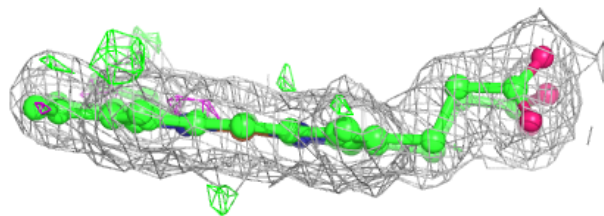
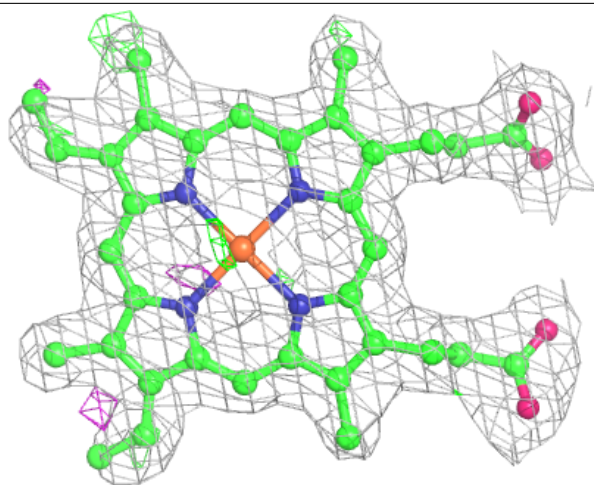
**Electron density around HEM D 501:**

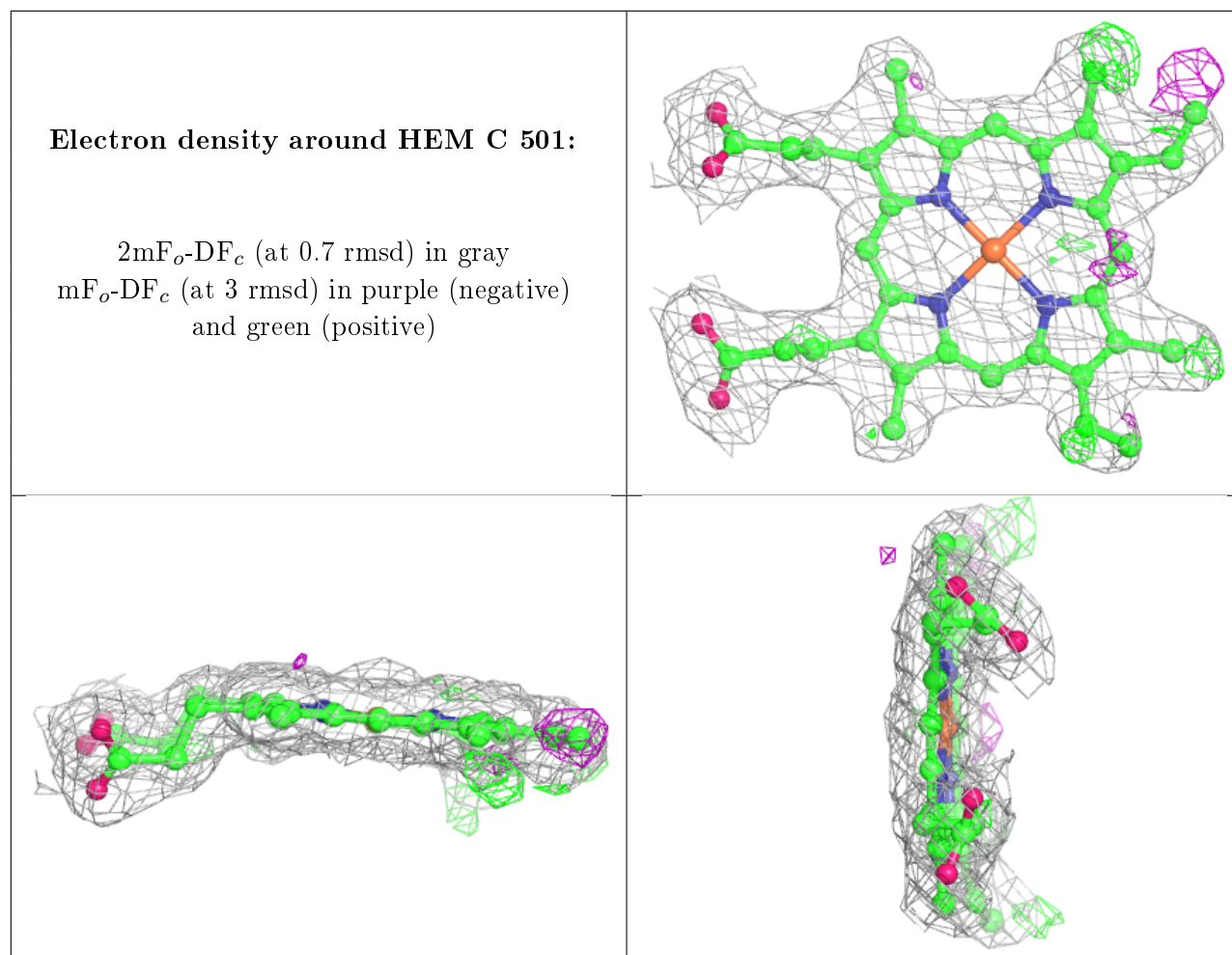
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM B 501:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.