



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:09 am BST

PDB ID : 3BNF  
Title : W. succinogenes NrfA Sulfite Complex  
Authors : Lukat, P.; Einsle, O.  
Deposited on : 2007-12-14  
Resolution : 1.70 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

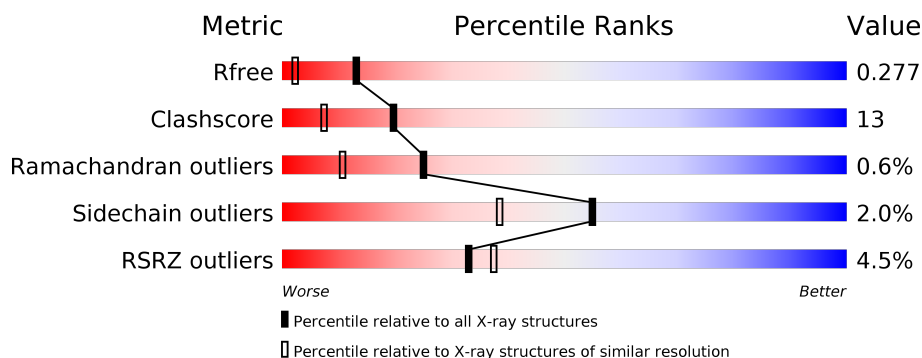
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	485	

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
5	ACT	A	5	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4685 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

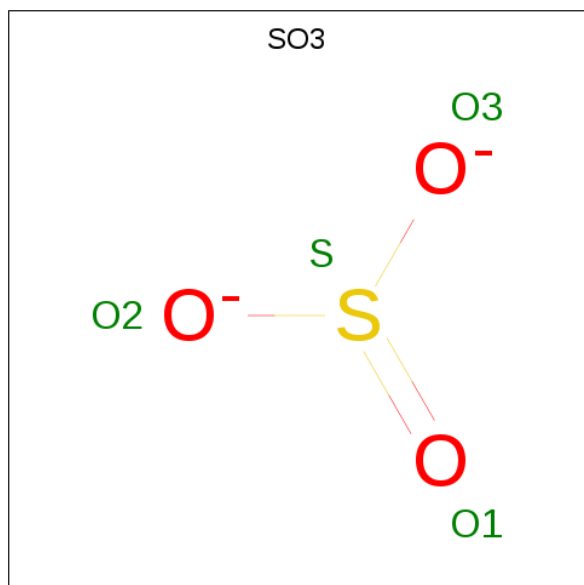
- Molecule 1 is a protein called Cytochrome c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	20	5	0
			3815	2414	656	724	21			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).

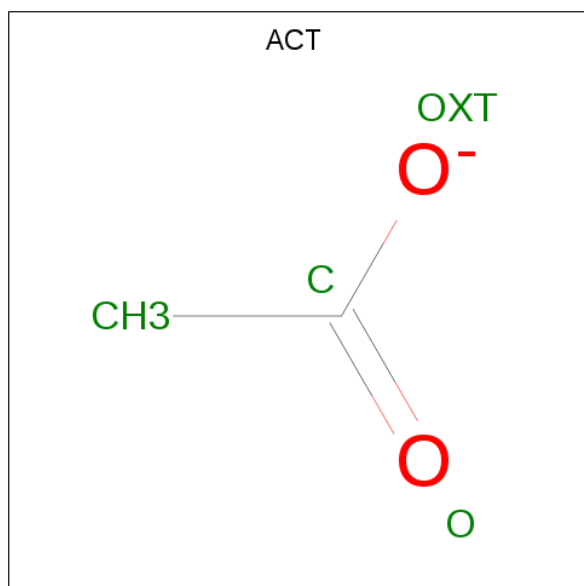


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			4	3	1		

- Molecule 4 is YTTRIUM ION (three-letter code: Y1) (formula: Y).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Y 3 3	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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



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

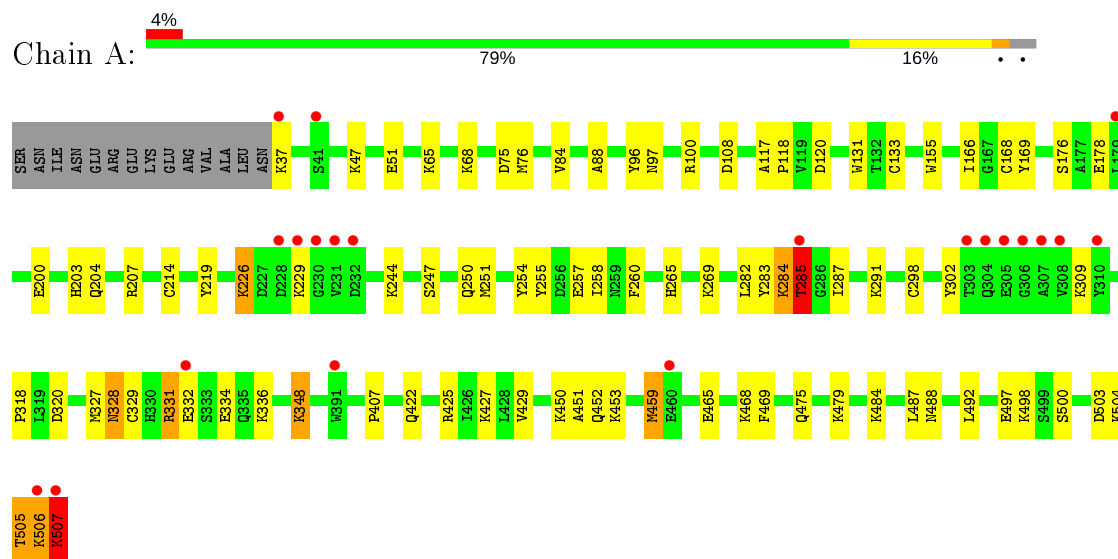
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	639	Total	O	0	0
			639	639		

### 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: Cytochrome c-552



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.50 Å 119.50 Å 186.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.31 – 1.70 22.31 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (22.31-1.70) 97.2 (22.31-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.233 , 0.280 0.232 , 0.277	Depositor DCC
$R_{free}$ test set	3660 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4685	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y1, HEM, CA, SO3, ACT

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	0.94	4/3906 (0.1%)	0.92	14/5258 (0.3%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	ARG	CA-CB	-13.55	1.24	1.53
1	A	229	LYS	CG-CD	13.08	1.97	1.52
1	A	168	CYS	CB-SG	-5.89	1.72	1.81
1	A	226	LYS	CB-CG	-5.38	1.38	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	LYS	CB-CG-CD	-13.59	76.26	111.60
1	A	336	LYS	CA-CB-CG	-9.81	91.81	113.40
1	A	331	ARG	CB-CA-C	-7.94	94.51	110.40
1	A	226	LYS	CA-CB-CG	7.72	130.38	113.40
1	A	331	ARG	N-CA-CB	7.02	123.24	110.60
1	A	285	THR	N-CA-CB	6.83	123.29	110.30
1	A	336	LYS	CB-CG-CD	-6.57	94.52	111.60
1	A	120	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	284	LYS	C-N-CA	5.99	136.69	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ARG	CA-CB-CG	-5.99	100.23	113.40
1	A	284	LYS	N-CA-C	5.87	126.85	111.00
1	A	507	LYS	N-CA-C	5.78	126.60	111.00
1	A	320	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	229	LYS	CG-CD-CE	-5.28	96.07	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	LYS	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	3815	0	3730	98	0
2	A	1	0	0	0	0
3	A	4	0	0	0	0
4	A	3	0	0	0	0
5	A	8	0	6	2	0
6	A	215	0	150	27	0
7	A	639	0	0	13	1
All	All	4685	0	3886	100	1

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 13.

All (100) 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:133:CYS:SG	6:A:508:HEM:CAC	2.09	1.39
1:A:214:CYS:SG	6:A:510:HEM:CAC	2.14	1.35
1:A:298:CYS:SG	6:A:511:HEM:CAC	2.16	1.31
5:A:5:ACT:H1	7:A:827:HOH:O	1.33	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:CYS:SG	6:A:512:HEM:CAC	2.34	1.15
1:A:214:CYS:SG	6:A:510:HEM:HAC	1.78	1.15
1:A:133:CYS:SG	6:A:508:HEM:HAC	1.83	1.11
1:A:331:ARG:O	1:A:332:GLU:HG3	1.51	1.09
1:A:133:CYS:HG	6:A:508:HEM:CAC	1.53	1.06
1:A:298:CYS:HG	6:A:511:HEM:CAC	1.62	1.04
1:A:497:GLU:HB2	1:A:507:LYS:HG2	1.36	1.03
1:A:329:CYS:SG	6:A:512:HEM:HAC	2.04	0.96
1:A:497:GLU:H	1:A:507:LYS:HE3	1.30	0.95
1:A:203:HIS:NE2	6:A:509:HEM:O2D	1.98	0.95
1:A:497:GLU:OE1	1:A:507:LYS:N	2.00	0.94
1:A:329:CYS:HG	6:A:512:HEM:CAC	1.77	0.94
1:A:51:GLU:HG3	7:A:923:HOH:O	1.71	0.89
1:A:506:LYS:HE3	1:A:506:LYS:HA	1.55	0.88
1:A:298:CYS:SG	6:A:511:HEM:CBC	2.63	0.85
1:A:100:ARG:HH22	1:A:507:LYS:NZ	1.74	0.84
1:A:298:CYS:SG	6:A:511:HEM:HAC	2.18	0.82
1:A:298:CYS:HG	6:A:511:HEM:CBC	1.93	0.81
1:A:100:ARG:HH12	1:A:507:LYS:HD2	1.48	0.78
1:A:133:CYS:SG	6:A:508:HEM:C3C	2.75	0.77
1:A:100:ARG:HH12	1:A:507:LYS:CD	1.97	0.77
1:A:100:ARG:HH22	1:A:507:LYS:HZ2	1.32	0.76
1:A:497:GLU:N	1:A:507:LYS:HE3	2.02	0.72
1:A:422:GLN:HE21	1:A:422:GLN:HA	1.56	0.71
1:A:328:ASN:HB2	7:A:975:HOH:O	1.91	0.69
1:A:298:CYS:SG	6:A:511:HEM:C3C	2.85	0.68
1:A:468[B]:LYS:HD3	1:A:468[B]:LYS:N	2.09	0.68
1:A:329:CYS:SG	6:A:512:HEM:C3C	2.86	0.68
1:A:331:ARG:O	1:A:332:GLU:CG	2.35	0.68
6:A:509:HEM:HBC1	6:A:510:HEM:HHC	1.76	0.67
1:A:133:CYS:SG	6:A:508:HEM:CBC	2.83	0.65
1:A:214:CYS:SG	6:A:510:HEM:C3C	2.90	0.64
1:A:488:ASN:OD1	7:A:917:HOH:O	2.16	0.61
1:A:497:GLU:OE1	1:A:507:LYS:HA	2.01	0.60
1:A:117:ALA:HB3	1:A:465:GLU:HG2	1.83	0.60
1:A:176:SER:OG	1:A:178:GLU:HG2	2.02	0.59
1:A:285:THR:O	7:A:1120:HOH:O	2.17	0.57
1:A:327:MET:CE	1:A:334:GLU:HA	2.34	0.57
1:A:51:GLU:OE2	1:A:488:ASN:HB3	2.04	0.57
1:A:285:THR:HG23	7:A:1120:HOH:O	2.05	0.56
1:A:117:ALA:CB	1:A:465:GLU:HG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:NH1	6:A:509:HEM:O1D	2.39	0.56
1:A:75:ASP:HA	1:A:97:ASN:HD22	1.70	0.56
1:A:506:LYS:HE3	1:A:506:LYS:CA	2.34	0.56
1:A:348:LYS:C	1:A:348:LYS:HD2	2.26	0.55
1:A:214:CYS:SG	6:A:510:HEM:CBC	2.88	0.55
1:A:503:ASP:OD1	1:A:505:THR:HA	2.07	0.55
1:A:204:GLN:HA	1:A:204:GLN:HE21	1.71	0.54
1:A:422:GLN:NE2	1:A:422:GLN:HA	2.22	0.53
1:A:68:LYS:HG2	1:A:68:LYS:O	2.08	0.52
1:A:452:GLN:HE22	1:A:459:MET:HE2	1.75	0.51
1:A:100:ARG:HH12	1:A:507:LYS:HD3	1.74	0.50
1:A:497:GLU:OE1	1:A:507:LYS:CA	2.60	0.50
1:A:200:GLU:HG2	7:A:1019:HOH:O	2.11	0.50
1:A:498:LYS:H	1:A:507:LYS:NZ	2.08	0.50
1:A:498:LYS:HB2	1:A:507:LYS:HD2	1.93	0.49
1:A:251:MET:O	1:A:254:TYR:HB3	2.12	0.49
1:A:318:PRO:HB2	6:A:512:HEM:HBB1	1.95	0.49
1:A:504:LYS:NZ	7:A:1054:HOH:O	2.45	0.49
1:A:118:PRO:HG2	1:A:469:PHE:CE1	2.48	0.49
1:A:247:SER:H	1:A:250:GLN:HE21	1.61	0.49
1:A:282:LEU:O	1:A:285:THR:HB	2.13	0.48
1:A:498:LYS:H	1:A:507:LYS:HZ1	1.60	0.48
1:A:450:LYS:HE3	7:A:1023:HOH:O	2.14	0.48
1:A:497:GLU:CB	1:A:507:LYS:HG2	2.26	0.48
1:A:265:HIS:O	1:A:269:LYS:HD3	2.14	0.47
1:A:291:LYS:NZ	6:A:512:HEM:O1D	2.48	0.46
1:A:487:LEU:HD21	1:A:492:LEU:HD11	1.98	0.46
1:A:427:LYS:HG2	7:A:850:HOH:O	2.16	0.46
1:A:287:ILE:O	1:A:291:LYS:HG2	2.16	0.46
1:A:453:LYS:HD3	7:A:799:HOH:O	2.14	0.45
1:A:484:LYS:HD2	7:A:811:HOH:O	2.16	0.45
1:A:498:LYS:HG3	1:A:507:LYS:HG3	1.98	0.45
1:A:407:PRO:HD2	5:A:5:ACT:OXT	2.17	0.44
1:A:97:ASN:HD21	1:A:500:SER:HB3	1.81	0.44
1:A:425:ARG:O	1:A:429:VAL:HG23	2.16	0.44
1:A:84:VAL:HB	1:A:451:ALA:HB1	2.00	0.44
1:A:76:MET:HB2	1:A:96:TYR:CD2	2.53	0.44
1:A:88:ALA:HB3	1:A:265:HIS:CE1	2.53	0.43
1:A:65:LYS:HE3	7:A:745:HOH:O	2.18	0.43
1:A:47:LYS:HE3	1:A:169:TYR:OH	2.18	0.43
1:A:505:THR:HG22	1:A:505:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TRP:NE1	1:A:155:TRP:O	2.46	0.43
1:A:47:LYS:HE3	1:A:169:TYR:CZ	2.54	0.43
1:A:214:CYS:CB	6:A:510:HEM:HAC	2.47	0.43
1:A:452:GLN:HE22	1:A:459:MET:CE	2.31	0.43
1:A:475:GLN:HB3	1:A:479:LYS:HE2	2.01	0.43
1:A:133:CYS:HB2	6:A:508:HEM:C4C	2.54	0.42
1:A:100:ARG:HH22	1:A:507:LYS:HZ3	1.58	0.42
1:A:108:ASP:OD2	6:A:510:HEM:O2D	2.38	0.41
1:A:219:TYR:HB3	1:A:255:TYR:OH	2.19	0.41
1:A:302:TYR:CE1	1:A:309:LYS:HE3	2.55	0.41
1:A:244:LYS:NZ	1:A:257:GLU:OE2	2.46	0.41
1:A:282:LEU:O	1:A:285:THR:CG2	2.69	0.41
1:A:497:GLU:OE1	1:A:506:LYS:HB3	2.21	0.41
1:A:258:ILE:HG13	1:A:260:PHE:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:634:HOH:O	7:A:850:HOH:O[10_565]	2.13	0.07

## 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	474/485 (98%)	456 (96%)	14 (3%)	4 (1%)	19 6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	THR
1	A	166[A]	ILE

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Mol	Chain	Res	Type
1	A	166[B]	ILE
1	A	285	THR

### 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	402/410 (98%)	394 (98%)	8 (2%)	55 38

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	226	LYS
1	A	283	TYR
1	A	328	ASN
1	A	348	LYS
1	A	459	MET
1	A	506	LYS
1	A	507	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	204	GLN
1	A	250	GLN
1	A	335	GLN
1	A	352	GLN
1	A	422	GLN
1	A	452	GLN
1	A	480	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
6	HEM	A	508	1,3	27,50,50	2.06	9 (33%)	17,82,82	1.84	4 (23%)
6	HEM	A	510	1	27,50,50	2.14	8 (29%)	17,82,82	2.38	6 (35%)
5	ACT	A	5	-	1,3,3	1.69	0	0,3,3	0.00	-
6	HEM	A	509	1	27,50,50	2.11	8 (29%)	17,82,82	1.74	4 (23%)
3	SO3	A	1	6	1,3,3	0.66	0	0,3,3	0.00	-
6	HEM	A	512	1	27,50,50	2.32	6 (22%)	17,82,82	2.38	4 (23%)
6	HEM	A	511	1	27,50,50	1.98	5 (18%)	17,82,82	2.20	8 (47%)
5	ACT	A	6	-	1,3,3	1.36	0	0,3,3	0.00	-

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
6	HEM	A	511	1	-	1/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	A	512	1	-	1/6/54/54	-
6	HEM	A	508	1,3	-	0/6/54/54	-
6	HEM	A	510	1	-	0/6/54/54	-
6	HEM	A	509	1	-	0/6/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	512	HEM	C3D-C2D	5.50	1.54	1.37
6	A	509	HEM	C3D-C2D	5.13	1.52	1.37
6	A	510	HEM	C3D-C2D	5.09	1.52	1.37
6	A	511	HEM	C3C-C2C	-4.86	1.33	1.40
6	A	510	HEM	C3B-CAB	4.66	1.57	1.47
6	A	508	HEM	C3D-C2D	4.64	1.51	1.37
6	A	512	HEM	C3C-CAC	4.60	1.57	1.47
6	A	511	HEM	C3D-C2D	4.48	1.51	1.37
6	A	512	HEM	C3B-CAB	4.45	1.57	1.47
6	A	508	HEM	C3C-C2C	-4.23	1.34	1.40
6	A	510	HEM	C3C-C2C	-4.08	1.34	1.40
6	A	509	HEM	C3C-C2C	-4.01	1.34	1.40
6	A	509	HEM	C3C-CAC	4.01	1.56	1.47
6	A	512	HEM	C3C-C2C	-3.95	1.34	1.40
6	A	511	HEM	C3C-CAC	3.87	1.55	1.47
6	A	512	HEM	C3B-C2B	-3.80	1.35	1.40
6	A	509	HEM	C3B-CAB	3.77	1.55	1.47
6	A	508	HEM	C3B-C2B	-3.51	1.35	1.40
6	A	510	HEM	C3C-CAC	3.40	1.54	1.47
6	A	511	HEM	C3B-C2B	-3.32	1.35	1.40
6	A	509	HEM	C3B-C2B	-3.23	1.35	1.40
6	A	508	HEM	C3C-CAC	3.00	1.54	1.47
6	A	510	HEM	C3B-C2B	-2.79	1.36	1.40
6	A	508	HEM	C3B-CAB	2.75	1.53	1.47
6	A	508	HEM	C4A-NA	2.71	1.41	1.36
6	A	508	HEM	C1D-CHD	-2.59	1.33	1.41
6	A	511	HEM	CAA-C2A	2.59	1.55	1.52
6	A	512	HEM	C1C-C2C	2.55	1.48	1.42
6	A	510	HEM	CAA-C2A	2.49	1.55	1.52
6	A	508	HEM	C1B-C2B	2.46	1.48	1.42
6	A	510	HEM	CMD-C2D	2.46	1.56	1.51
6	A	508	HEM	CAA-C2A	2.43	1.55	1.52
6	A	509	HEM	CAA-C2A	2.40	1.55	1.52
6	A	509	HEM	C1C-C2C	2.39	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	510	HEM	C1C-C2C	2.31	1.47	1.42
6	A	509	HEM	C1B-C2B	2.02	1.47	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	512	HEM	C1D-C2D-C3D	-5.47	103.19	107.00
6	A	510	HEM	C1D-C2D-C3D	-5.01	103.51	107.00
6	A	508	HEM	C4A-C3A-C2A	4.88	110.39	107.00
6	A	512	HEM	CAD-CBD-CGD	-4.45	105.21	112.67
6	A	512	HEM	CBA-CAA-C2A	-4.18	104.77	112.49
6	A	511	HEM	CAA-CBA-CGA	-4.09	105.81	112.67
6	A	510	HEM	CMA-C3A-C4A	-3.97	122.37	128.46
6	A	508	HEM	CMA-C3A-C4A	-3.76	122.68	128.46
6	A	510	HEM	CBA-CAA-C2A	-3.56	105.92	112.49
6	A	510	HEM	CMA-C3A-C2A	3.44	131.43	124.94
6	A	510	HEM	CBD-CAD-C3D	-3.35	106.30	112.48
6	A	509	HEM	C4C-C3C-C2C	3.14	109.09	106.90
6	A	511	HEM	CAD-CBD-CGD	-3.11	107.46	112.67
6	A	510	HEM	CMD-C2D-C3D	3.05	130.69	124.94
6	A	512	HEM	CMD-C2D-C3D	2.97	130.54	124.94
6	A	509	HEM	CBD-CAD-C3D	-2.95	107.03	112.48
6	A	511	HEM	C4C-C3C-C2C	2.95	108.96	106.90
6	A	511	HEM	CMC-C2C-C3C	2.94	130.18	124.68
6	A	509	HEM	C1D-C2D-C3D	-2.92	104.97	107.00
6	A	511	HEM	C1D-C2D-C3D	-2.90	104.98	107.00
6	A	508	HEM	C1D-C2D-C3D	-2.73	105.10	107.00
6	A	509	HEM	C4A-C3A-C2A	2.58	108.79	107.00
6	A	511	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
6	A	511	HEM	CBD-CAD-C3D	-2.52	107.83	112.48
6	A	511	HEM	C3C-C4C-NC	-2.43	106.35	110.94
6	A	508	HEM	CMB-C2B-C3B	2.13	128.67	124.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	512	HEM	C2A-CAA-CBA-CGA
6	A	511	HEM	C3D-CAD-CBD-CGD

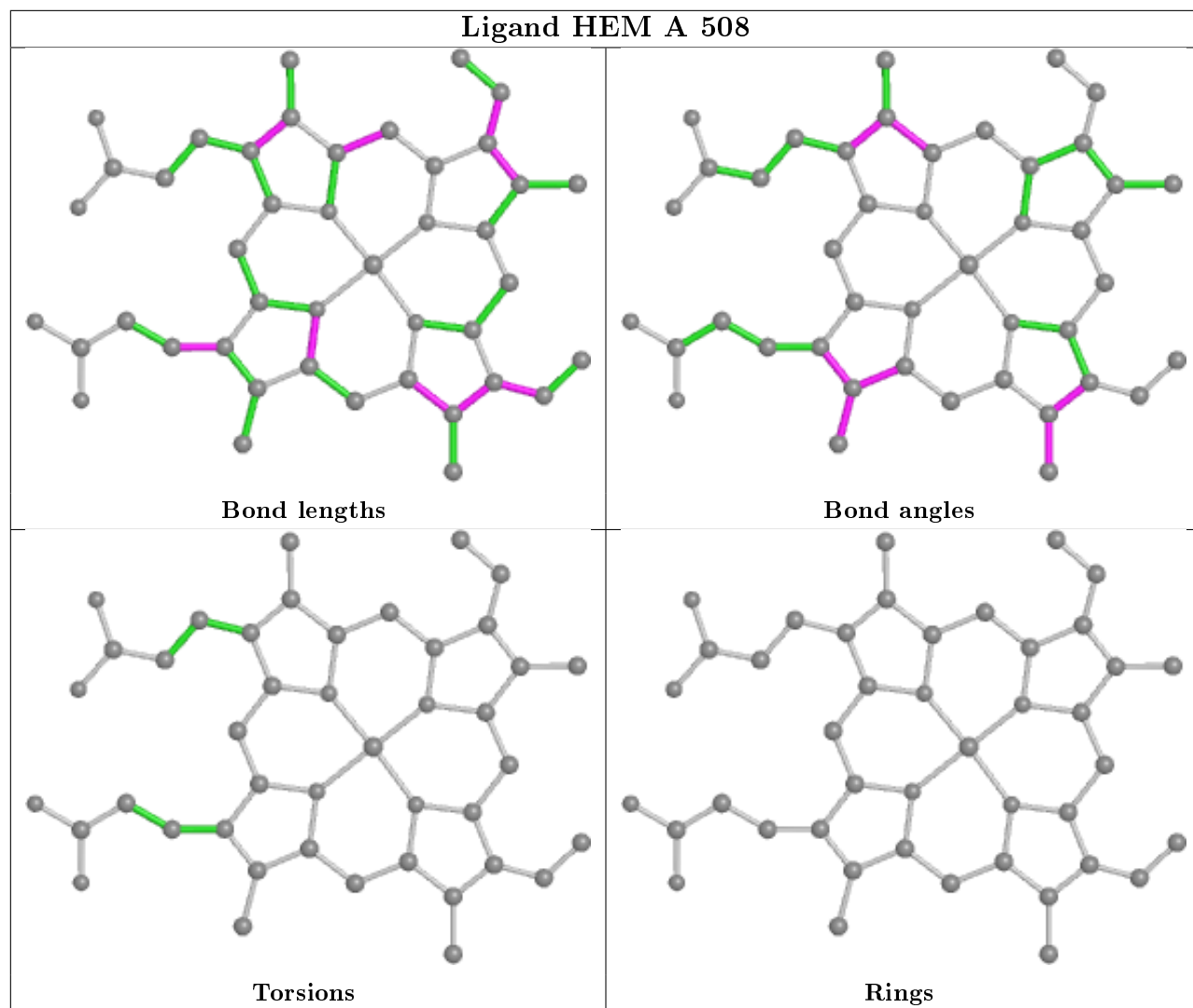
There are no ring outliers.

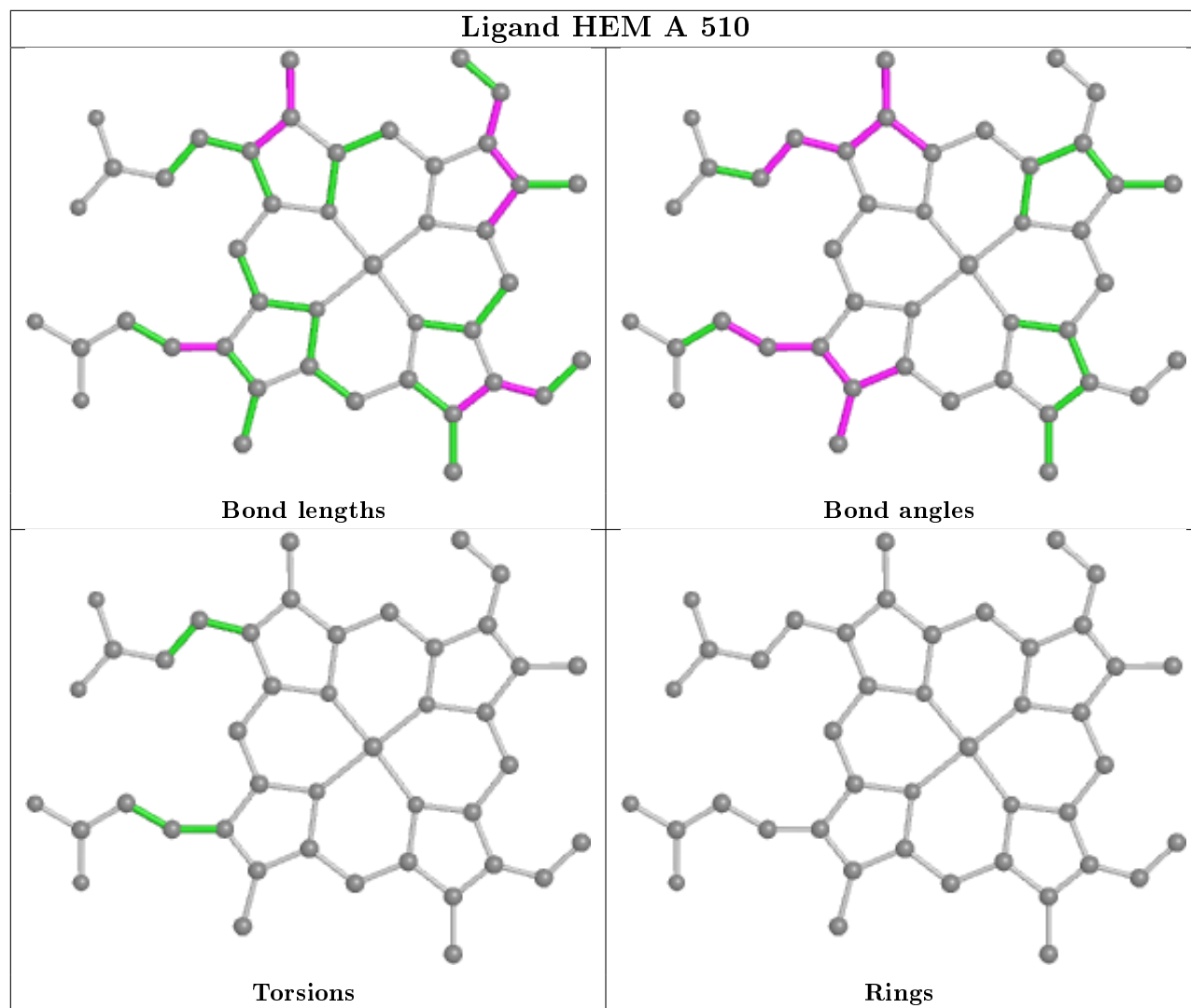


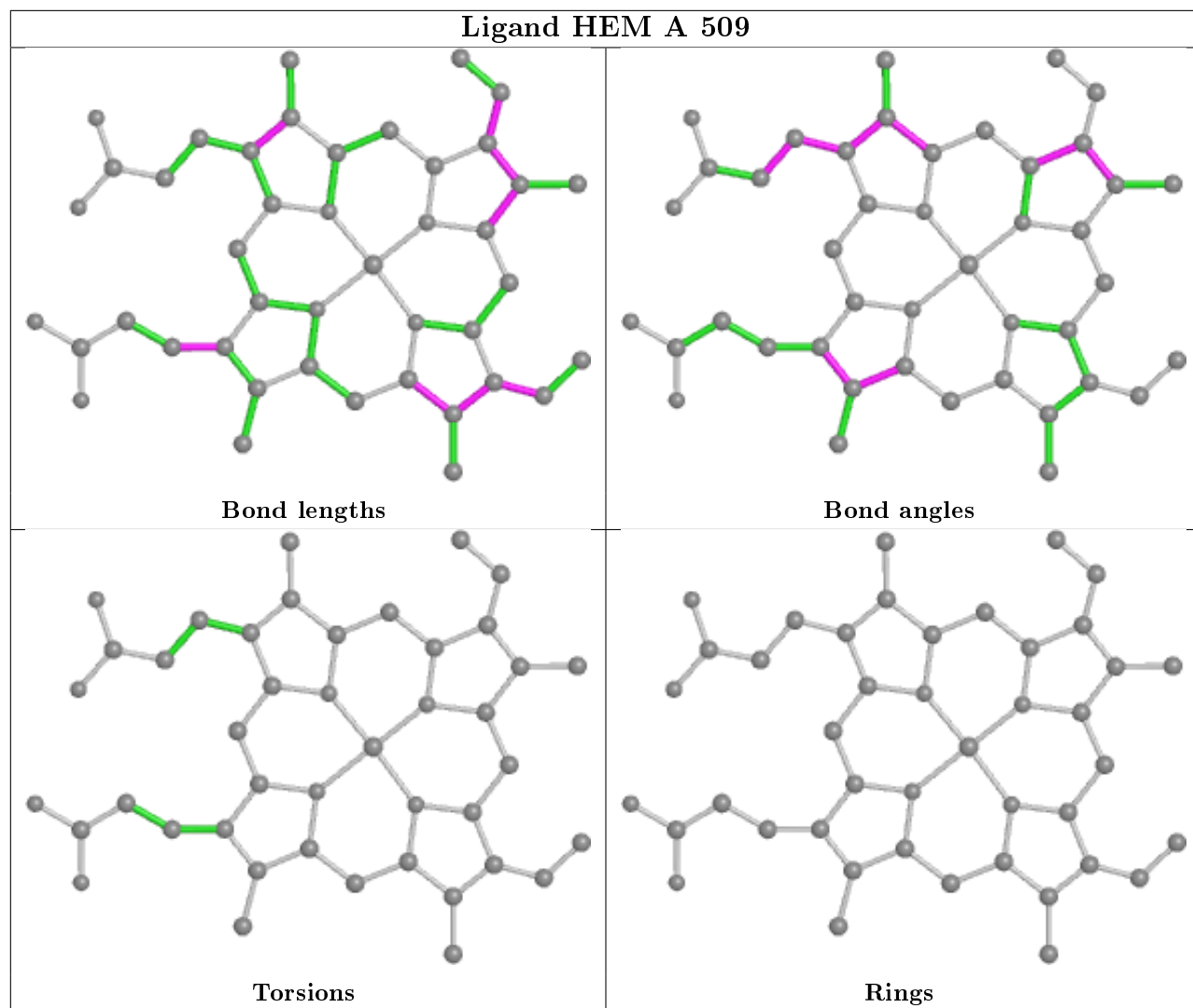
6 monomers are involved in 29 short contacts:

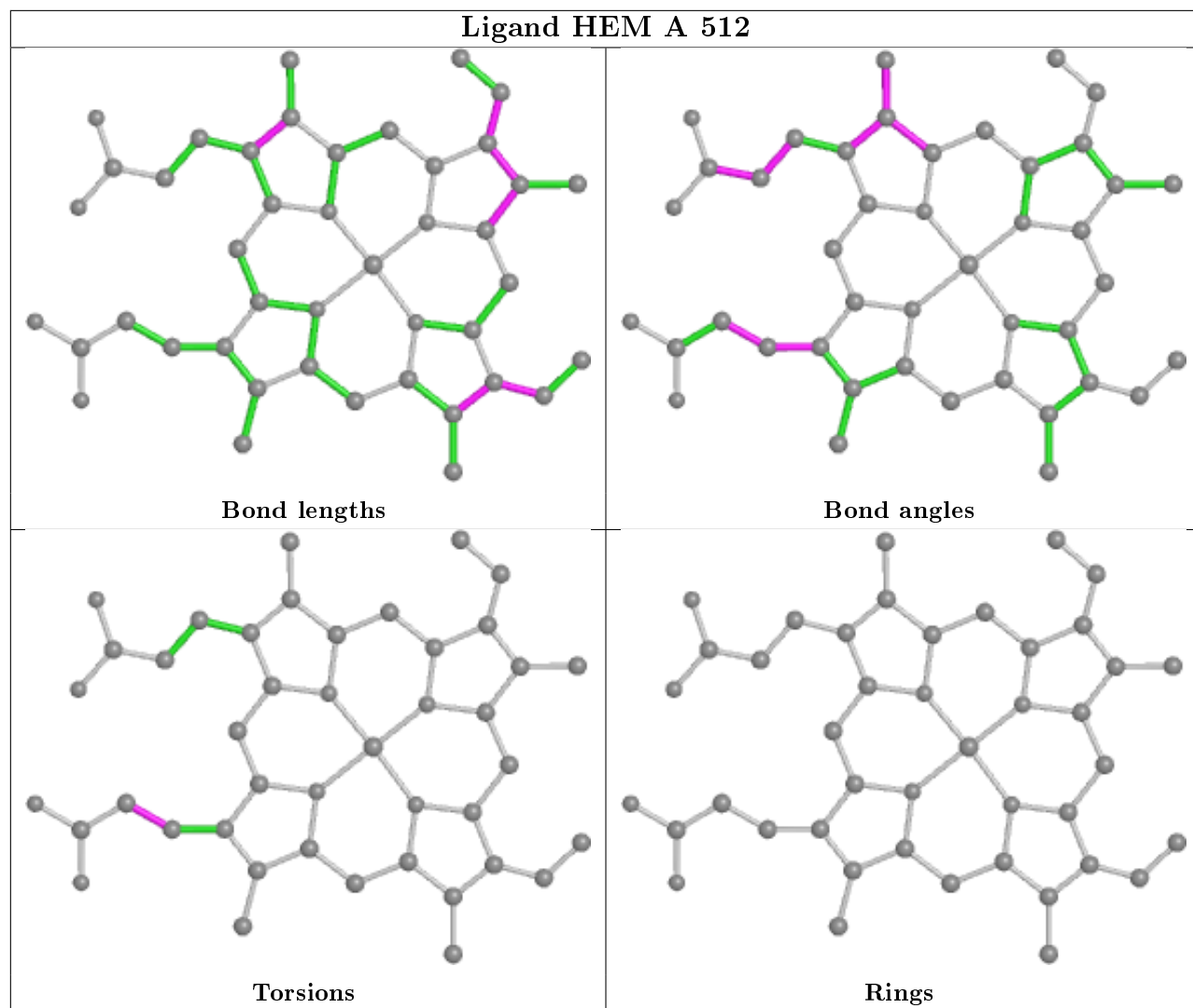
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	508	HEM	6	0
6	A	510	HEM	7	0
5	A	5	ACT	2	0
6	A	509	HEM	3	0
6	A	512	HEM	6	0
6	A	511	HEM	6	0

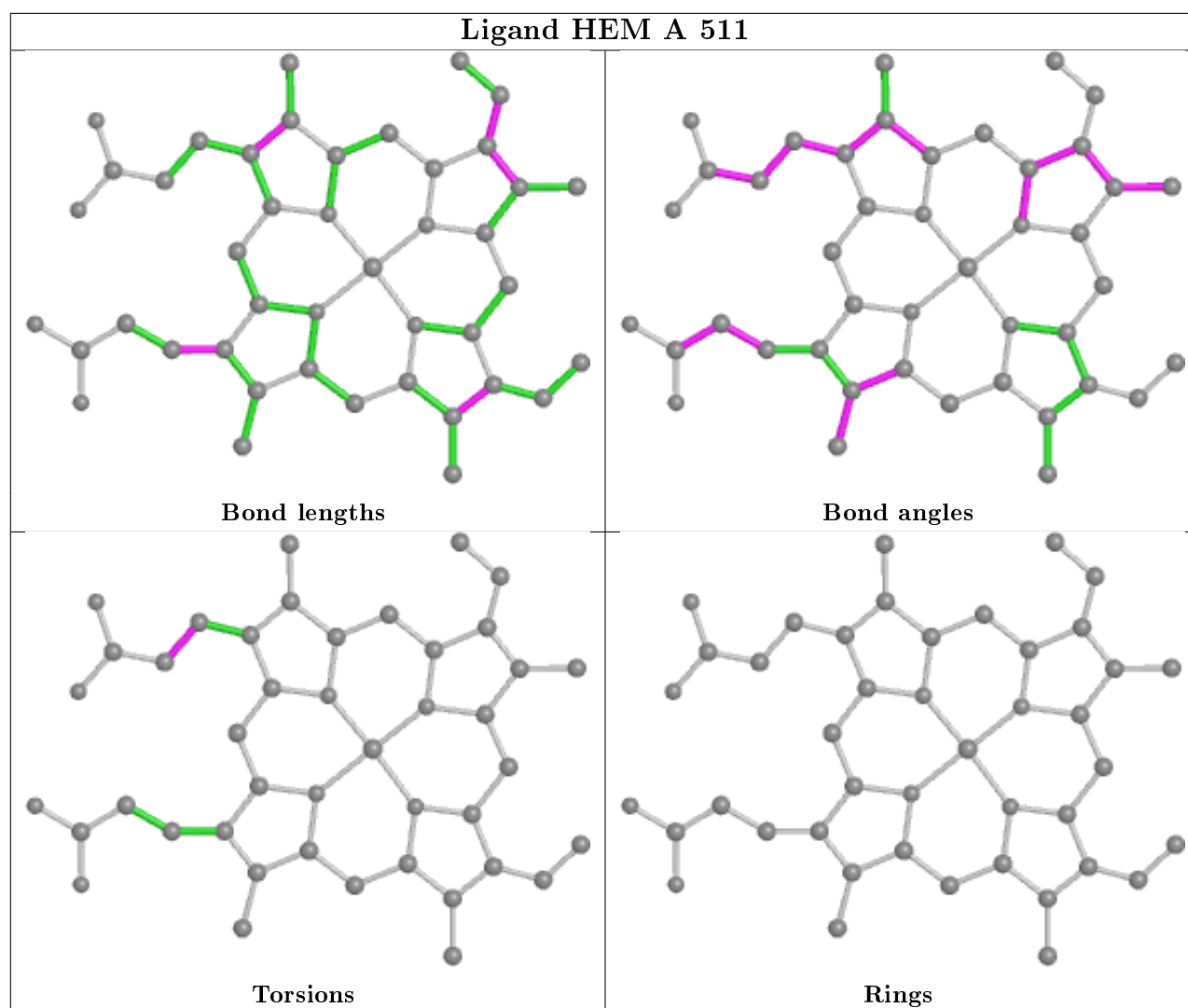
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	471/485 (97%)	0.30	21 (4%)	33 37	19, 27, 44, 53	5 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	ALA	6.2
1	A	308	VAL	6.1
1	A	231	VAL	6.0
1	A	506	LYS	4.7
1	A	507	LYS	3.5
1	A	306	GLY	3.4
1	A	230	GLY	3.4
1	A	232	ASP	3.2
1	A	228	ASP	3.0
1	A	310	TYR	2.9
1	A	229	LYS	2.8
1	A	332	GLU	2.7
1	A	304	GLN	2.6
1	A	37	LYS	2.5
1	A	460	GLU	2.4
1	A	285	THR	2.3
1	A	303	THR	2.3
1	A	305	GLU	2.3
1	A	41	SER	2.2
1	A	179	LEU	2.1
1	A	391	TRP	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 ⓘ

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.

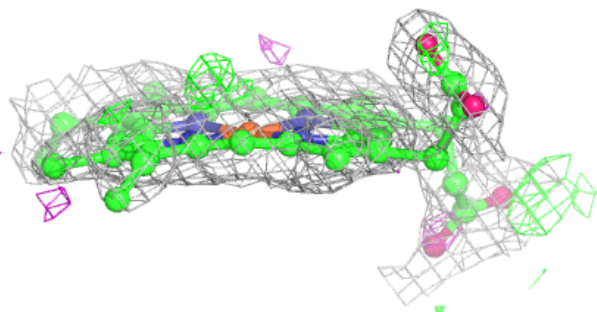
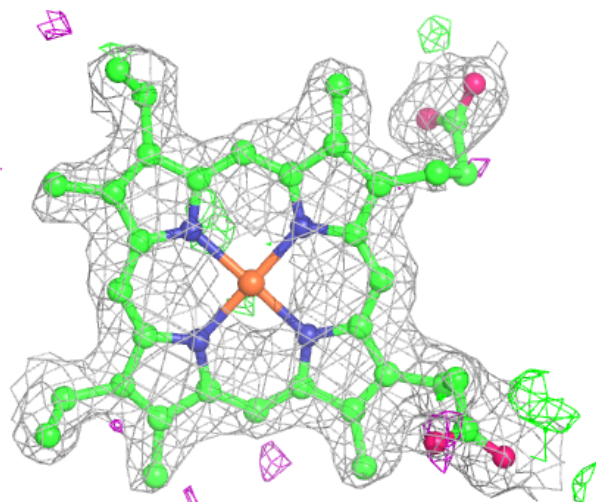
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ACT	A	5	4/4	0.50	0.36	45,46,46,46	0
5	ACT	A	6	4/4	0.78	0.22	40,40,40,40	0
4	Y1	A	3	1/1	0.94	0.15	54,54,54,54	1
6	HEM	A	512	43/43	0.95	0.13	25,30,44,47	0
6	HEM	A	509	43/43	0.95	0.13	21,26,33,43	0
6	HEM	A	510	43/43	0.96	0.10	16,21,26,31	0
6	HEM	A	511	43/43	0.96	0.11	19,22,37,41	0
6	HEM	A	508	43/43	0.97	0.09	16,21,24,25	0
4	Y1	A	4	1/1	0.97	0.04	32,32,32,32	1
4	Y1	A	2	1/1	0.99	0.03	29,29,29,29	0
3	SO3	A	1	4/4	0.99	0.04	23,26,28,29	0
2	CA	A	513	1/1	0.99	0.07	29,29,29,29	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.



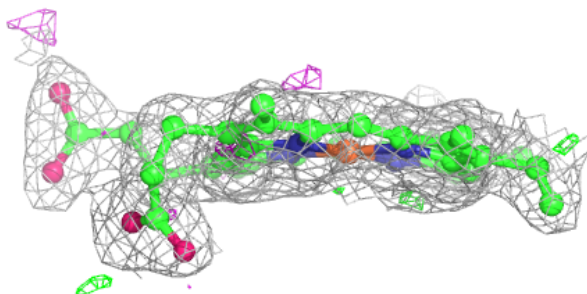
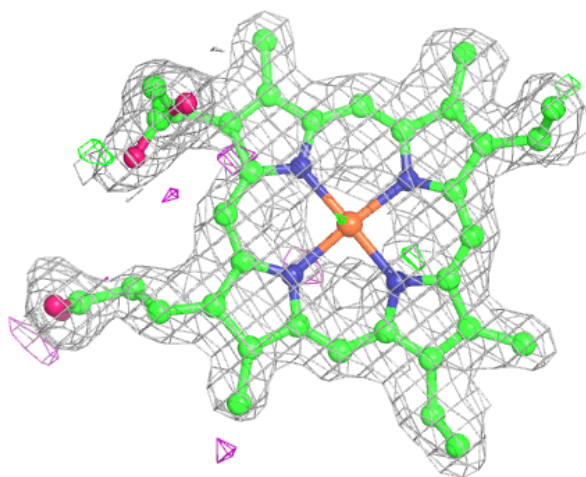
**Electron density around HEM A 512:**

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



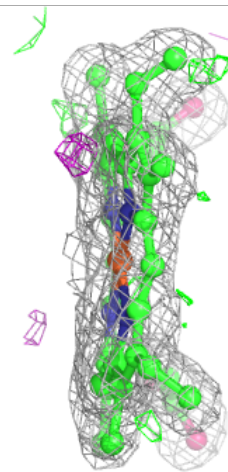
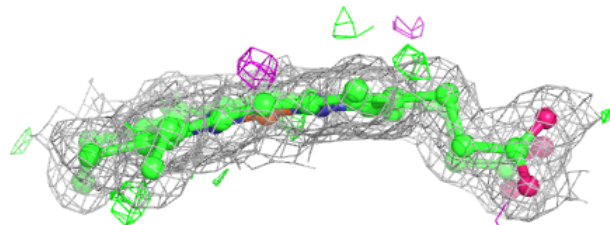
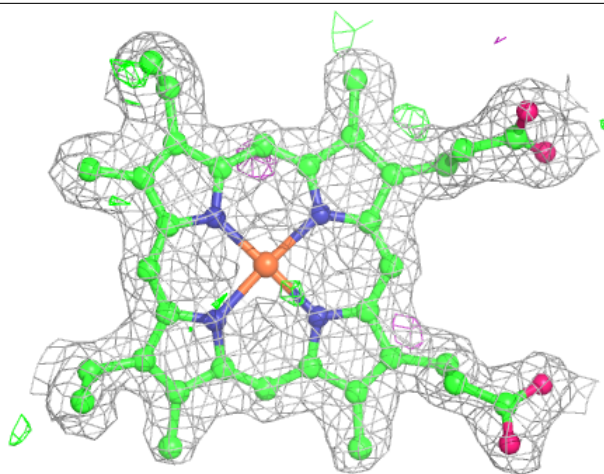
**Electron density around HEM A 509:**

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



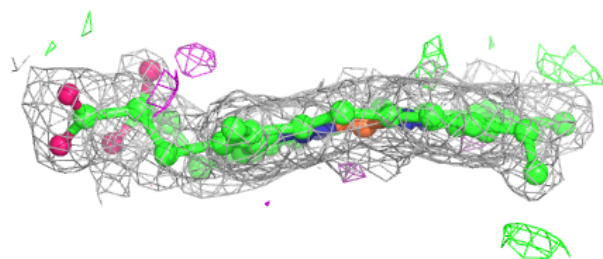
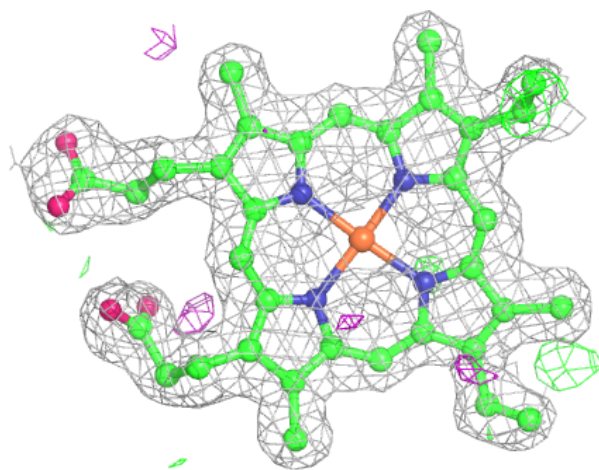
**Electron density around HEM A 510:**

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



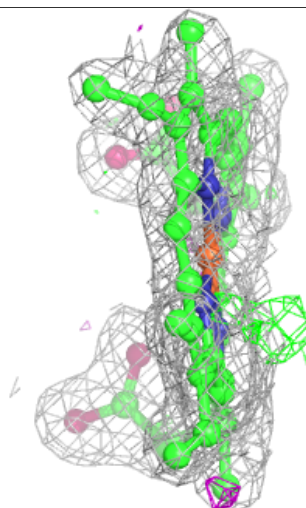
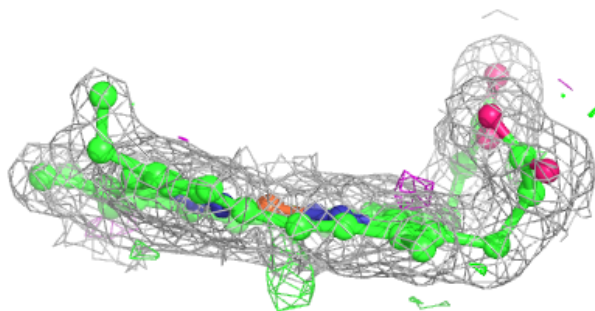
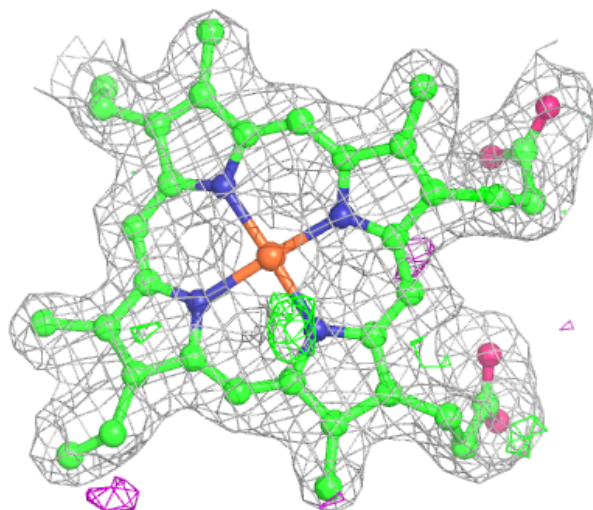
**Electron density around HEM A 511:**

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



**Electron density around HEM A 508:**

$2mF_o-DF_c$  (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.