



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:38 am BST

PDB ID : 3NMJ  
Title : Crystal structure of a nickel mediated dimer for the phenanthroline-modified cytochrome cb562 variant, MBP-Phen2  
Authors : Radford, R.J.; Tezcan, F.A.  
Deposited on : 2010-06-22  
Resolution : 3.10 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.

---

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

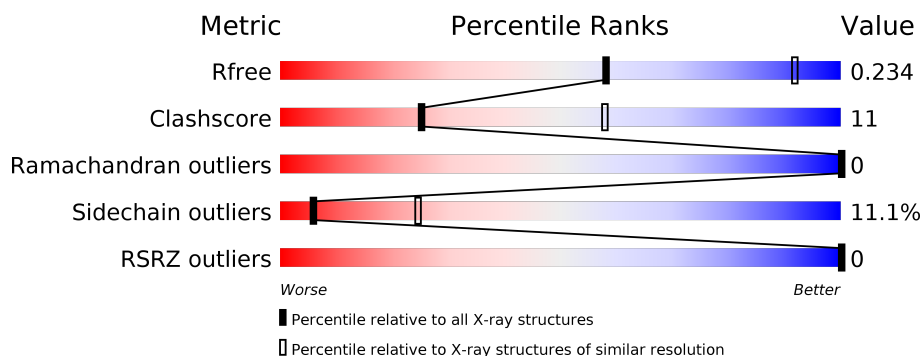
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	106	<div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	B	106	<div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	C	106	<div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	D	106	<div> <div>85%</div> <div>13%</div> <div>.</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3437 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 Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			798	489	138	165	6			
1	B	105	Total	C	N	O	S	0	0	0
			793	486	137	164	6			
1	C	106	Total	C	N	O	S	0	0	0
			798	489	138	165	6			
1	D	106	Total	C	N	O	S	0	0	0
			798	489	138	165	6			

There are 24 discrepancies between the modelled and reference sequences:

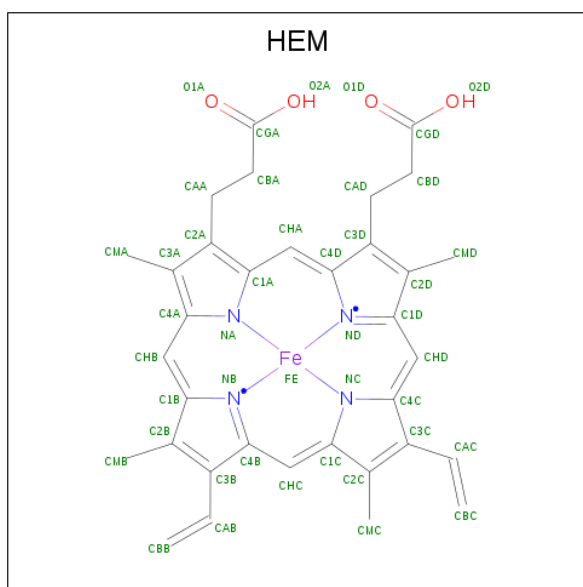
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	CYS	LYS	ENGINEERED MUTATION	UNP P0ABE7
A	62	ALA	ARG	ENGINEERED MUTATION	UNP P0ABE7
A	63	ALA	HIS	ENGINEERED MUTATION	UNP P0ABE7
A	66	ALA	ASP	ENGINEERED MUTATION	UNP P0ABE7
A	98	CYS	ARG	ENGINEERED MUTATION	UNP P0ABE7
A	101	CYS	TYR	ENGINEERED MUTATION	UNP P0ABE7
B	59	CYS	LYS	ENGINEERED MUTATION	UNP P0ABE7
B	62	ALA	ARG	ENGINEERED MUTATION	UNP P0ABE7
B	63	ALA	HIS	ENGINEERED MUTATION	UNP P0ABE7
B	66	ALA	ASP	ENGINEERED MUTATION	UNP P0ABE7
B	98	CYS	ARG	ENGINEERED MUTATION	UNP P0ABE7
B	101	CYS	TYR	ENGINEERED MUTATION	UNP P0ABE7
C	59	CYS	LYS	ENGINEERED MUTATION	UNP P0ABE7
C	62	ALA	ARG	ENGINEERED MUTATION	UNP P0ABE7
C	63	ALA	HIS	ENGINEERED MUTATION	UNP P0ABE7
C	66	ALA	ASP	ENGINEERED MUTATION	UNP P0ABE7
C	98	CYS	ARG	ENGINEERED MUTATION	UNP P0ABE7
C	101	CYS	TYR	ENGINEERED MUTATION	UNP P0ABE7
D	59	CYS	LYS	ENGINEERED MUTATION	UNP P0ABE7
D	62	ALA	ARG	ENGINEERED MUTATION	UNP P0ABE7
D	63	ALA	HIS	ENGINEERED MUTATION	UNP P0ABE7

*Continued on next page...*

*Continued from previous page...*

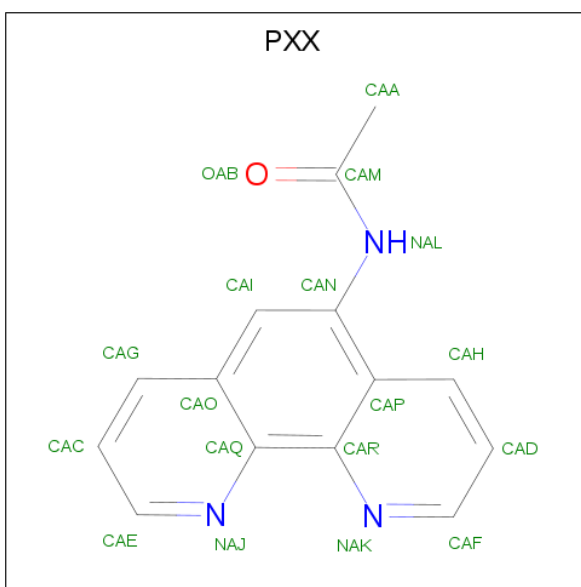
Chain	Residue	Modelled	Actual	Comment	Reference
D	66	ALA	ASP	ENGINEERED MUTATION	UNP P0ABE7
D	98	CYS	ARG	ENGINEERED MUTATION	UNP P0ABE7
D	101	CYS	TYR	ENGINEERED MUTATION	UNP P0ABE7

- 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
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is N-1,10-phenanthroline-5-ylacetamide (three-letter code: PXX) (formula:  $C_{14}H_{11}N_3O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 18	C 14	N 3	O 1	0	0
3	B	1	Total 18	C 14	N 3	O 1	0	0
3	C	1	Total 18	C 14	N 3	O 1	0	0
3	D	1	Total 18	C 14	N 3	O 1	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ni 1 1	0	0
4	C	1	Total Ni 1 1	0	0


- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	D	2	Total O 2 2	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.

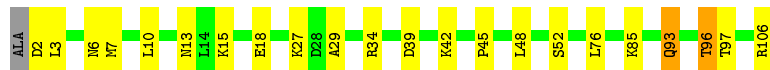
- Molecule 1: Soluble cytochrome b562

Chain A:  82% 15% .




- Molecule 1: Soluble cytochrome b562

Chain B:  78% 19% ..




- Molecule 1: Soluble cytochrome b562

Chain C:  77% 20% .



- Molecule 1: Soluble cytochrome b562

Chain D:  85% 13% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.29Å 99.29Å 109.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.99 – 3.10 85.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (85.99-3.10) 100.0 (85.99-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.38 (at 3.13Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.193 , 0.238 0.190 , 0.234	Depositor DCC
$R_{free}$ test set	776 reflections (6.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 20.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.457 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3437	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6786e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, PXX, NI

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	0.33	0/805	0.42	0/1083
1	B	0.32	0/800	0.42	0/1076
1	C	0.32	0/805	0.41	0/1083
1	D	0.33	0/805	0.42	0/1083
All	All	0.32	0/3215	0.42	0/4325

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	798	0	794	12	0
1	B	793	0	786	16	0
1	C	798	0	794	13	0
1	D	798	0	794	9	0
2	A	43	0	30	7	0
2	B	43	0	30	10	0
2	C	43	0	30	6	0
2	D	43	0	30	4	0
3	A	18	0	10	3	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	9	1	0
3	C	18	0	9	2	0
3	D	18	0	10	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	2	0
5	D	2	0	0	0	0
All	All	3437	0	3326	72	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 11.

All (72) 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)
2:A:150:HEM:HBA1	2:A:150:HEM:HHA	1.48	0.92
1:A:93:GLN:HA	1:A:93:GLN:HE21	1.49	0.77
1:C:6:ASN:HD21	1:C:39:ASP:HB3	1.52	0.74
1:B:6:ASN:HD21	1:B:39:ASP:HB3	1.53	0.71
2:B:150:HEM:CMC	2:B:150:HEM:HBC2	2.21	0.71
1:B:45:PRO:HG2	1:B:48:LEU:HB2	1.72	0.70
1:D:93:GLN:HA	1:D:93:GLN:HE21	1.55	0.70
2:A:150:HEM:HBA1	2:A:150:HEM:CHA	2.18	0.67
2:B:150:HEM:HMC2	2:B:150:HEM:HBC2	1.77	0.66
2:C:150:HEM:HMB2	2:C:150:HEM:HBB2	1.80	0.64
2:C:150:HEM:HBC2	2:C:150:HEM:CMC	2.28	0.64
2:A:150:HEM:HHA	2:A:150:HEM:CBA	2.27	0.64
2:C:150:HEM:HBB2	2:C:150:HEM:CMB	2.30	0.62
1:B:93:GLN:HE21	1:B:93:GLN:HA	1.65	0.62
2:C:150:HEM:HBC2	2:C:150:HEM:HMC2	1.82	0.61
1:B:6:ASN:ND2	1:B:39:ASP:HB3	2.15	0.61
2:B:150:HEM:HHA	2:B:150:HEM:CBA	2.30	0.60
1:C:45:PRO:HG2	1:C:48:LEU:HB2	1.82	0.60
1:C:6:ASN:ND2	1:C:39:ASP:HB3	2.15	0.60
1:A:45:PRO:HG2	1:A:48:LEU:HB2	1.83	0.59
2:A:150:HEM:HBC2	2:A:150:HEM:CMC	2.33	0.59
1:D:45:PRO:HG2	1:D:48:LEU:HB2	1.84	0.59
2:D:150:HEM:CMC	2:D:150:HEM:HBC2	2.34	0.58
1:B:39:ASP:OD2	5:B:107:HOH:O	2.16	0.57
1:C:1:ALA:N	1:C:39:ASP:OD2	2.31	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLN:HE21	1:C:93:GLN:HA	1.68	0.57
1:A:42:LYS:O	1:D:42:LYS:HE3	2.05	0.56
2:B:150:HEM:HHA	2:B:150:HEM:HBA1	1.89	0.54
1:A:2:ASP:HB3	1:D:2:ASP:HB3	1.91	0.52
1:A:42:LYS:O	1:D:42:LYS:CE	2.58	0.52
3:B:151:PXX:HAF	3:D:151:PXX:CAF	2.40	0.51
2:A:150:HEM:HMC2	2:A:150:HEM:HBC2	1.93	0.49
1:C:2:ASP:OD1	1:C:2:ASP:C	2.50	0.49
1:B:7:MET:HG3	2:B:150:HEM:C4D	2.48	0.49
1:A:91:ALA:O	1:A:94:LEU:HB2	2.13	0.49
1:B:2:ASP:C	1:B:2:ASP:OD1	2.51	0.49
1:D:91:ALA:O	1:D:94:LEU:HB2	2.14	0.48
2:B:150:HEM:CBC	2:B:150:HEM:HMC2	2.41	0.48
1:A:42:LYS:HE3	1:D:42:LYS:O	2.14	0.48
1:C:13:ASN:OD1	1:C:29:ALA:HA	2.14	0.48
2:D:150:HEM:HMC2	2:D:150:HEM:HBC2	1.95	0.47
1:B:96:THR:HG22	1:B:97:THR:N	2.30	0.47
1:C:96:THR:HG22	1:C:97:THR:N	2.29	0.47
2:B:150:HEM:CMC	2:B:150:HEM:CBC	2.92	0.46
2:C:150:HEM:CBC	2:C:150:HEM:HMC2	2.46	0.46
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.74	0.45
1:A:68:LEU:O	1:A:72:ILE:HG13	2.16	0.45
1:A:42:LYS:CE	1:D:42:LYS:O	2.64	0.45
1:A:106:ARG:HH11	2:A:150:HEM:HAA1	1.81	0.45
1:B:34:ARG:HH21	1:B:34:ARG:HG2	1.80	0.45
3:A:151:PXX:OAB	3:A:151:PXX:HAI	2.16	0.45
2:A:150:HEM:CBC	2:A:150:HEM:HMC2	2.47	0.45
3:A:151:PXX:CAF	3:C:151:PXX:HAF	2.46	0.44
1:C:84:VAL:O	1:C:88:GLN:HG3	2.17	0.44
2:C:150:HEM:HMB2	2:C:150:HEM:CBB	2.46	0.44
2:B:150:HEM:CHA	2:B:150:HEM:HBA1	2.48	0.44
1:A:84:VAL:O	1:A:88:GLN:HG3	2.18	0.43
3:A:151:PXX:NAK	3:C:151:PXX:HAF	2.34	0.43
1:B:39:ASP:O	1:B:42:LYS:HG2	2.18	0.43
1:B:13:ASN:OD1	1:B:29:ALA:HA	2.18	0.43
1:A:39:ASP:O	1:A:42:LYS:HG2	2.19	0.43
2:D:150:HEM:CBC	2:D:150:HEM:HMC2	2.48	0.43
1:C:92:GLU:O	1:C:95:LYS:HB2	2.18	0.42
1:B:10:LEU:HA	1:B:10:LEU:HD23	1.90	0.42
1:C:1:ALA:H3	1:C:39:ASP:CG	2.20	0.42
1:D:39:ASP:O	1:D:42:LYS:HG2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASP:N	5:B:107:HOH:O	2.53	0.41
1:B:7:MET:HG3	2:B:150:HEM:CHA	2.50	0.41
1:C:34:ARG:HG2	1:C:34:ARG:HH21	1.86	0.41
2:D:150:HEM:CBC	2:D:150:HEM:CMC	2.98	0.41
1:B:3:LEU:HD23	2:B:150:HEM:HBD2	2.03	0.40
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.75	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	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
1	B	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
1	C	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
1	D	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
All	All	415/424 (98%)	401 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	83/83 (100%)	74 (89%)	9 (11%)	6	25
1	B	83/83 (100%)	75 (90%)	8 (10%)	8	31
1	C	83/83 (100%)	73 (88%)	10 (12%)	5	20
1	D	83/83 (100%)	73 (88%)	10 (12%)	5	20
All	All	332/332 (100%)	295 (89%)	37 (11%)	6	24

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	18	GLU
1	A	19	LYS
1	A	27	LYS
1	A	42	LYS
1	A	54	ASP
1	A	85	LYS
1	A	93	GLN
1	A	106	ARG
1	B	15	LYS
1	B	18	GLU
1	B	27	LYS
1	B	52	SER
1	B	85	LYS
1	B	93	GLN
1	B	96	THR
1	B	106	ARG
1	C	2	ASP
1	C	15	LYS
1	C	18	GLU
1	C	25	GLN
1	C	27	LYS
1	C	52	SER
1	C	85	LYS
1	C	93	GLN
1	C	96	THR
1	C	106	ARG
1	D	15	LYS
1	D	18	GLU
1	D	19	LYS
1	D	27	LYS
1	D	42	LYS
1	D	54	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	85	LYS
1	D	93	GLN
1	D	96	THR
1	D	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	99	ASN
1	B	6	ASN
1	B	93	GLN
1	B	99	ASN
1	C	6	ASN
1	C	93	GLN
1	C	99	ASN
1	D	88	GLN
1	D	93	GLN
1	D	99	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 10 ligands modelled in this entry, 2 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
3	PXX	A	151	4	20,20,20	1.17	1 (5%)	27,28,28	1.30	2 (7%)
2	HEM	D	150	1	27,50,50	2.17	6 (22%)	17,82,82	1.47	3 (17%)
2	HEM	A	150	1	27,50,50	2.18	6 (22%)	17,82,82	1.34	2 (11%)
3	PXX	D	151	4	20,20,20	1.15	1 (5%)	27,28,28	1.26	2 (7%)
2	HEM	C	150	1	27,50,50	2.18	5 (18%)	17,82,82	1.53	3 (17%)
3	PXX	C	151	4	20,20,20	1.16	1 (5%)	27,28,28	1.32	5 (18%)
3	PXX	B	151	4	20,20,20	1.17	1 (5%)	27,28,28	1.31	5 (18%)
2	HEM	B	150	1	27,50,50	2.18	5 (18%)	17,82,82	1.51	3 (17%)

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
3	PXX	A	151	4	-	0/4/4/4	0/3/3/3
2	HEM	D	150	1	-	0/6/54/54	-
2	HEM	A	150	1	-	3/6/54/54	-
3	PXX	D	151	4	-	0/4/4/4	0/3/3/3
2	HEM	C	150	1	-	2/6/54/54	-
3	PXX	C	151	4	-	1/4/4/4	0/3/3/3
3	PXX	B	151	4	-	2/4/4/4	0/3/3/3
2	HEM	B	150	1	-	3/6/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	150	HEM	C3D-C2D	5.30	1.53	1.37
2	B	150	HEM	C3D-C2D	5.23	1.53	1.37
2	C	150	HEM	C3D-C2D	5.19	1.53	1.37
2	D	150	HEM	C3D-C2D	5.18	1.53	1.37
2	B	150	HEM	C3C-C2C	-4.74	1.33	1.40
2	D	150	HEM	C3B-C2B	-4.74	1.33	1.40
2	D	150	HEM	C3C-C2C	-4.65	1.33	1.40
2	C	150	HEM	C3C-C2C	-4.61	1.34	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	150	HEM	C3C-C2C	-4.54	1.34	1.40
2	C	150	HEM	C3B-C2B	-4.53	1.34	1.40
2	A	150	HEM	C3B-C2B	-4.52	1.34	1.40
2	B	150	HEM	C3B-C2B	-4.44	1.34	1.40
2	A	150	HEM	C3B-CAB	3.65	1.55	1.47
2	D	150	HEM	C3B-CAB	3.60	1.55	1.47
2	A	150	HEM	C3C-CAC	3.45	1.54	1.47
2	B	150	HEM	C3B-CAB	3.45	1.55	1.47
2	C	150	HEM	C3C-CAC	3.44	1.54	1.47
2	C	150	HEM	C3B-CAB	3.42	1.54	1.47
2	B	150	HEM	C3C-CAC	3.37	1.54	1.47
2	D	150	HEM	C3C-CAC	3.36	1.54	1.47
3	A	151	PXX	CAI-CAN	3.04	1.39	1.36
3	D	151	PXX	CAI-CAN	2.83	1.39	1.36
3	C	151	PXX	CAI-CAN	2.82	1.39	1.36
3	B	151	PXX	CAI-CAN	2.77	1.39	1.36
2	A	150	HEM	CAA-C2A	2.19	1.55	1.52
2	D	150	HEM	CAA-C2A	2.04	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	150	HEM	C1D-C2D-C3D	-3.19	104.78	107.00
2	B	150	HEM	CAA-CBA-CGA	-2.92	107.76	112.67
2	B	150	HEM	C1D-C2D-C3D	-2.88	105.00	107.00
2	D	150	HEM	CMA-C3A-C4A	-2.80	124.17	128.46
2	B	150	HEM	CAD-CBD-CGD	-2.79	108.00	112.67
2	C	150	HEM	CAA-CBA-CGA	-2.73	108.09	112.67
3	B	151	PXX	CAN-CAP-CAR	2.46	120.64	118.02
2	C	150	HEM	CAD-CBD-CGD	-2.40	108.65	112.67
3	C	151	PXX	CAN-NAL-CAM	-2.36	119.65	126.84
3	B	151	PXX	CAD-CAF-NAK	-2.29	120.43	123.94
3	C	151	PXX	CAN-CAP-CAR	2.29	120.45	118.02
3	D	151	PXX	CAN-CAP-CAR	2.21	120.37	118.02
3	C	151	PXX	CAD-CAF-NAK	-2.16	120.64	123.94
2	D	150	HEM	CBA-CAA-C2A	-2.14	108.54	112.49
3	A	151	PXX	CAN-CAP-CAR	2.14	120.30	118.02
3	B	151	PXX	CAN-NAL-CAM	-2.13	120.36	126.84
2	A	150	HEM	C1D-C2D-C3D	-2.12	105.52	107.00
3	A	151	PXX	CAH-CAP-CAN	-2.10	119.65	123.00
3	C	151	PXX	CAF-NAK-CAR	2.09	120.86	117.12
3	B	151	PXX	CAC-CAE-NAJ	-2.04	120.81	123.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	150	HEM	C1D-C2D-C3D	-2.03	105.58	107.00
3	B	151	PXX	CAF-NAK-CAR	2.03	120.75	117.12
2	A	150	HEM	CAA-CBA-CGA	-2.03	109.27	112.67
3	C	151	PXX	CAC-CAE-NAJ	-2.02	120.84	123.94
3	D	151	PXX	CAH-CAP-CAN	-2.02	119.79	123.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	150	HEM	C1A-C2A-CAA-CBA
2	A	150	HEM	C3A-C2A-CAA-CBA
2	A	150	HEM	C2A-CAA-CBA-CGA
2	C	150	HEM	C1A-C2A-CAA-CBA
2	C	150	HEM	C3A-C2A-CAA-CBA
2	B	150	HEM	C1A-C2A-CAA-CBA
2	B	150	HEM	C3A-C2A-CAA-CBA
2	B	150	HEM	C2A-CAA-CBA-CGA
3	B	151	PXX	CAI-CAN-NAL-CAM
3	C	151	PXX	CAI-CAN-NAL-CAM
3	B	151	PXX	CAP-CAN-NAL-CAM

There are no ring outliers.

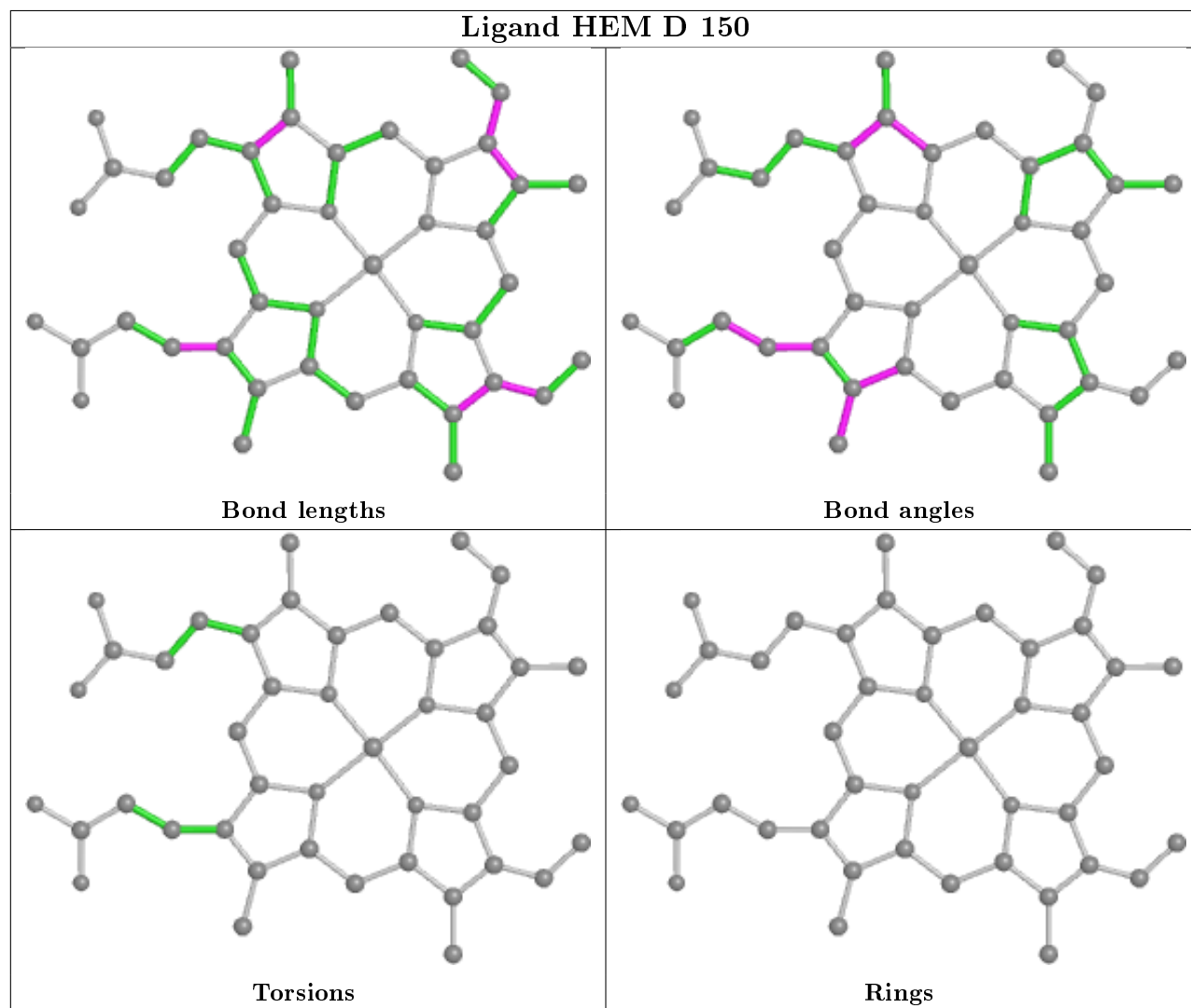
8 monomers are involved in 31 short contacts:

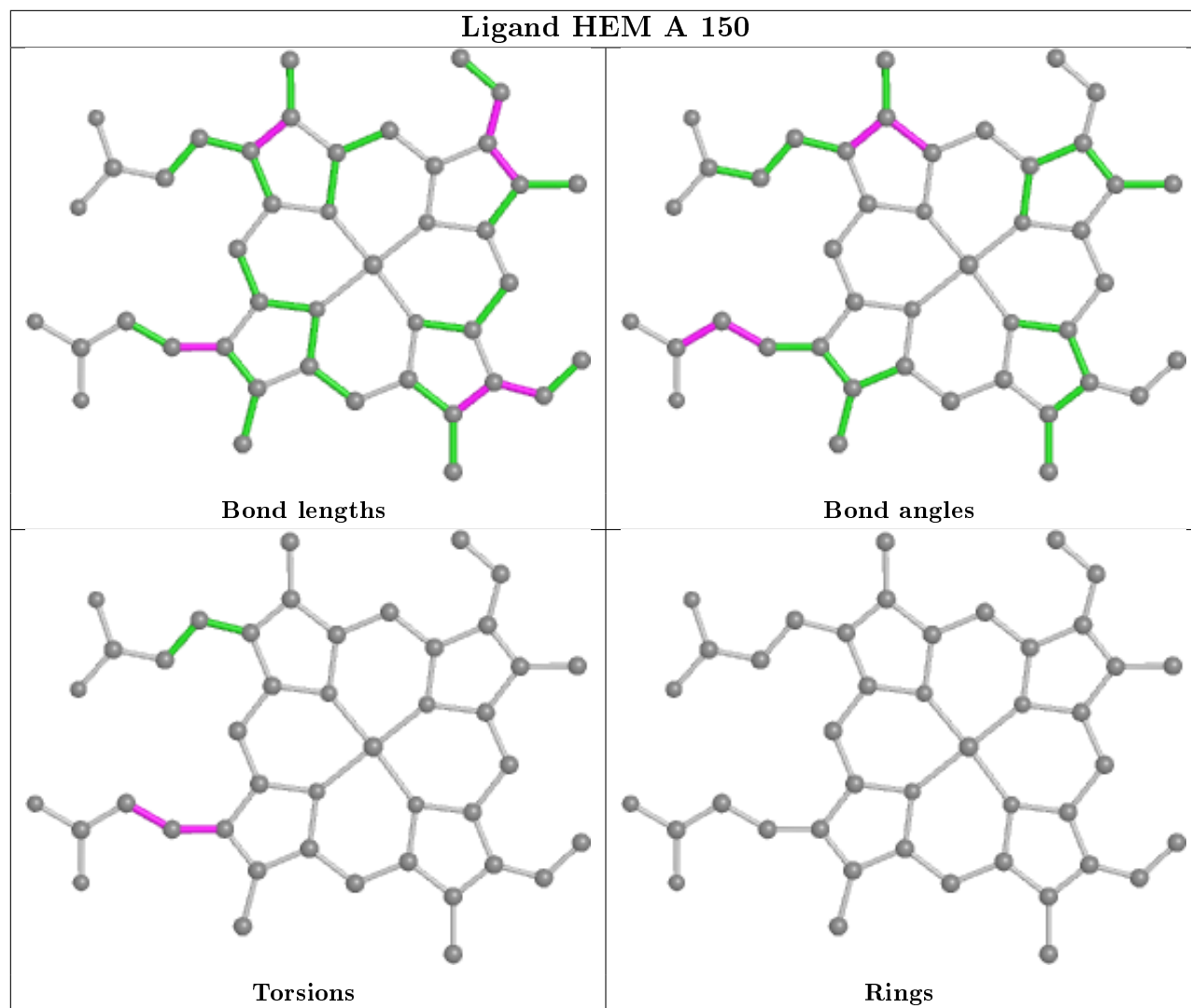
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	151	PXX	3	0
2	D	150	HEM	4	0
2	A	150	HEM	7	0
3	D	151	PXX	1	0
2	C	150	HEM	6	0
3	C	151	PXX	2	0
3	B	151	PXX	1	0
2	B	150	HEM	10	0

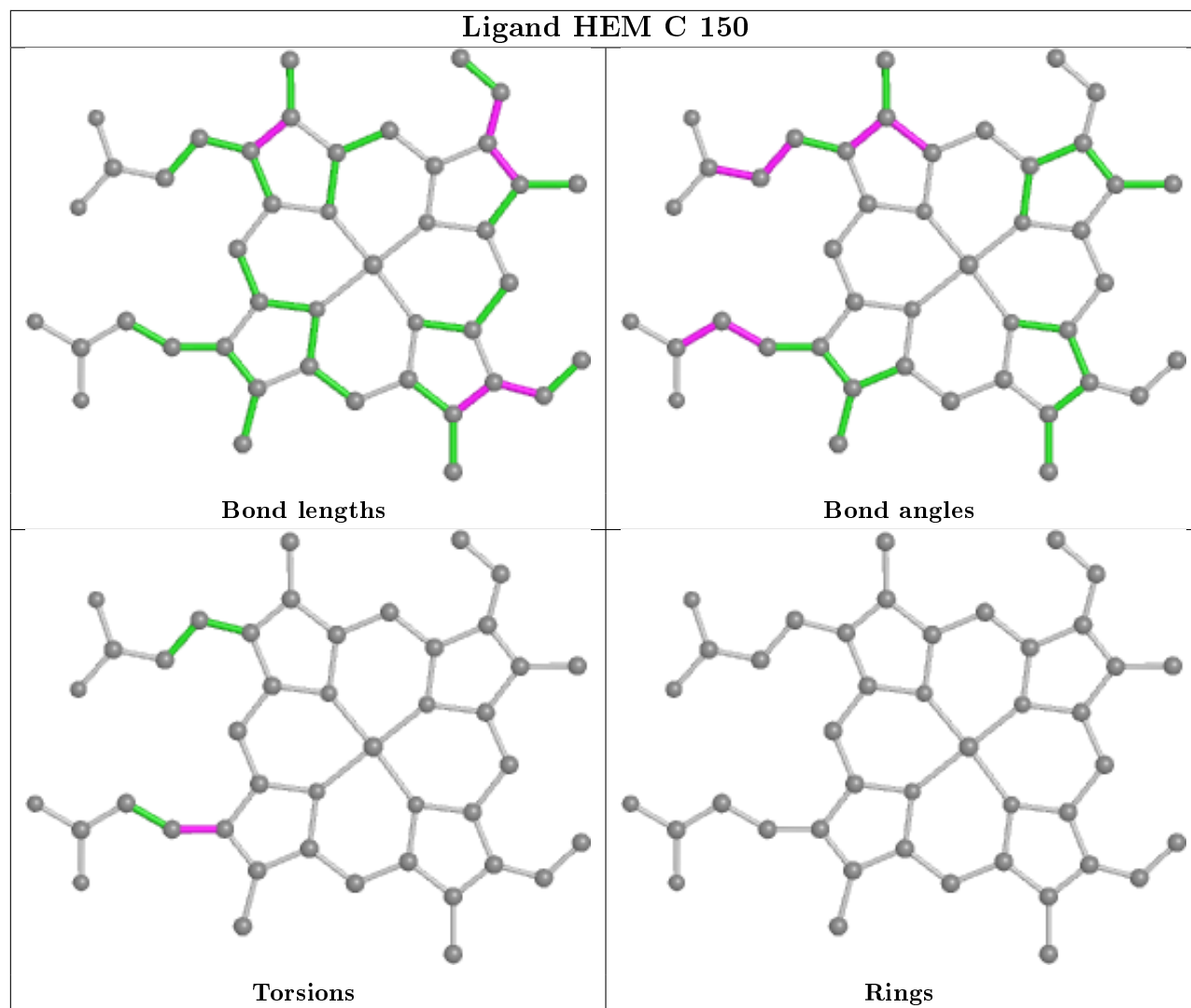
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

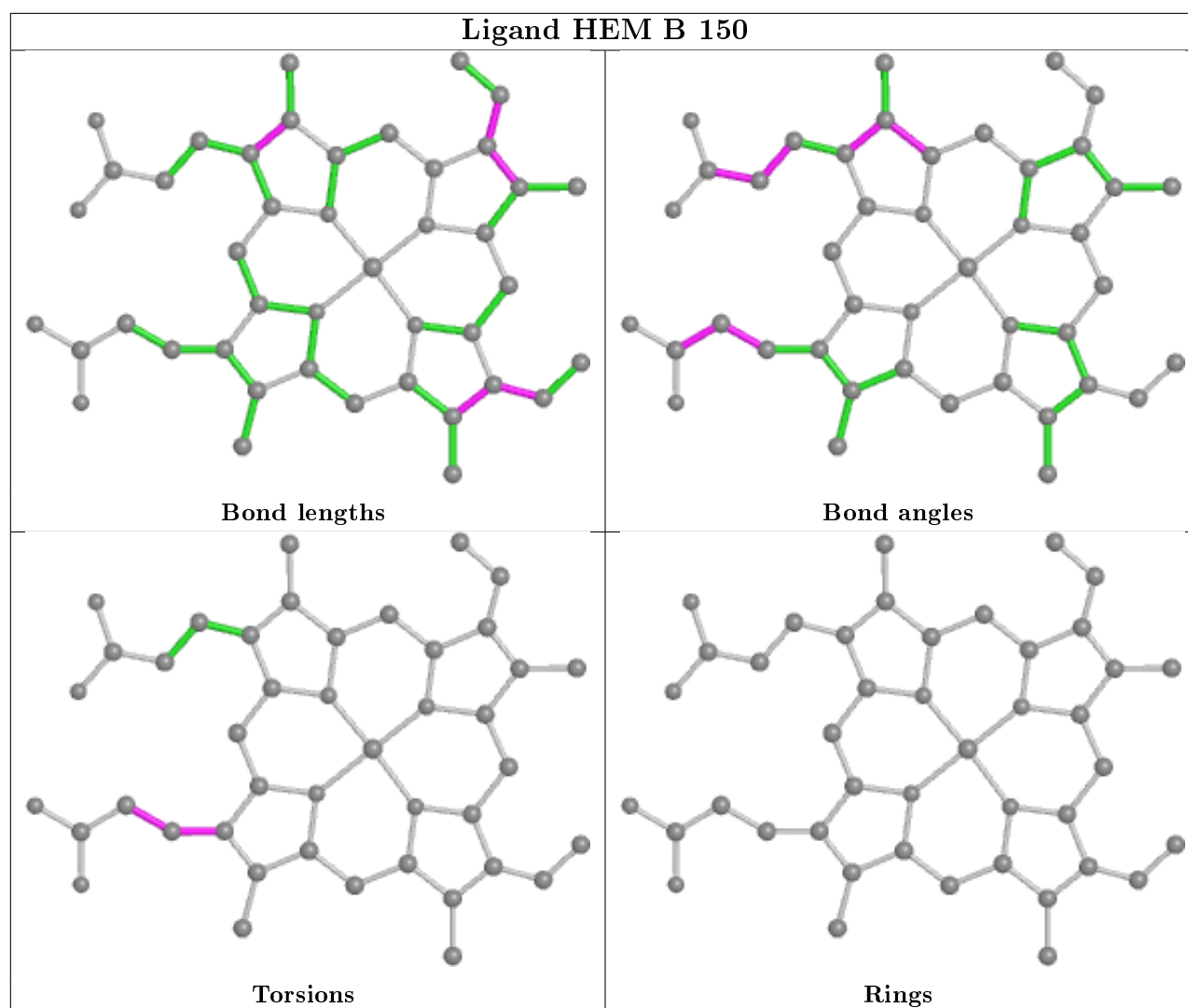


in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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	106/106 (100%)	-0.11	0 100 100	36, 53, 67, 70	0
1	B	105/106 (99%)	-0.14	0 100 100	37, 53, 66, 70	0
1	C	106/106 (100%)	-0.09	0 100 100	37, 53, 66, 70	0
1	D	106/106 (100%)	-0.14	0 100 100	36, 53, 67, 70	0
All	All	423/424 (99%)	-0.12	0 100 100	36, 53, 67, 70	0

There are no RSRZ outliers to report.

### 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(Å <sup>2</sup> )	Q<0.9
3	PXX	A	151	18/18	0.96	0.22	46,60,66,72	0
4	NI	B	152	1/1	0.97	0.18	44,44,44,44	0
3	PXX	C	151	18/18	0.98	0.18	34,39,50,55	0
3	PXX	D	151	18/18	0.98	0.20	49,61,67,73	0

*Continued on next page...*

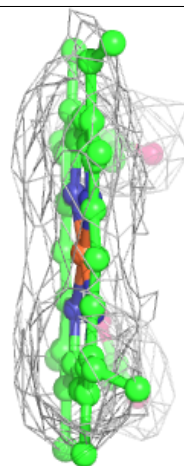
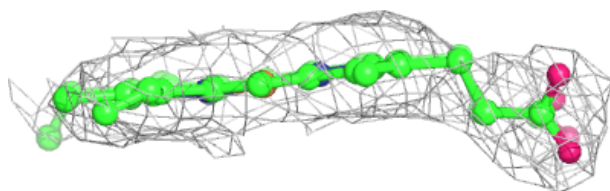
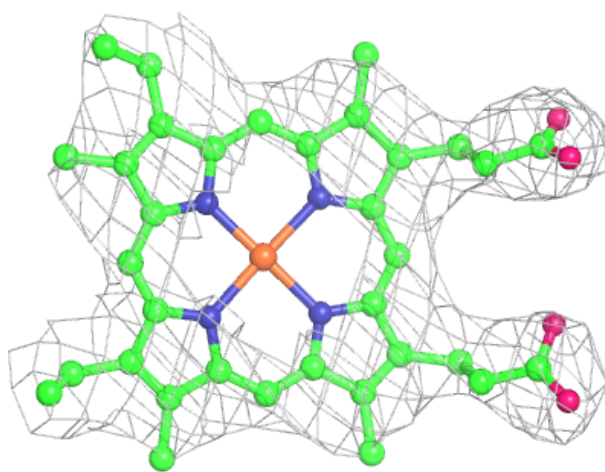
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	D	150	43/43	0.98	0.23	38,44,61,71	0
3	PXX	B	151	18/18	0.98	0.17	31,35,48,56	0
2	HEM	C	150	43/43	0.99	0.22	33,48,69,79	0
4	NI	C	152	1/1	0.99	0.17	44,44,44,44	0
2	HEM	A	150	43/43	0.99	0.23	32,44,62,68	0
2	HEM	B	150	43/43	0.99	0.22	34,50,69,78	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.

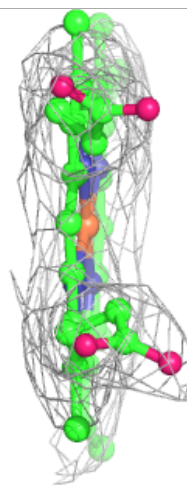
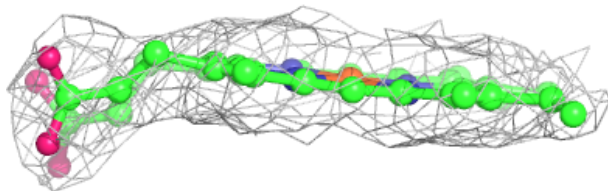
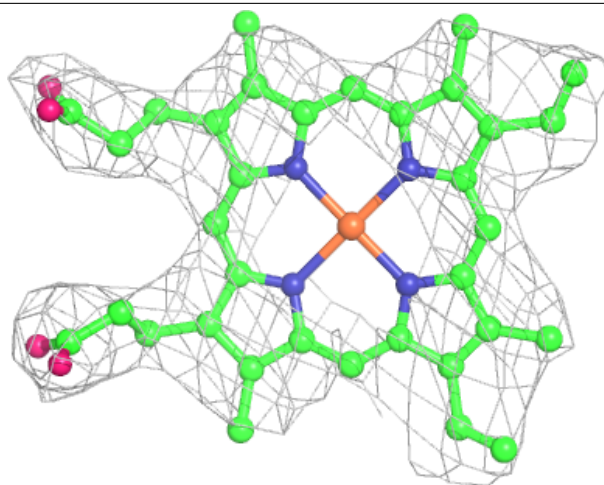
**Electron density around HEM D 150:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



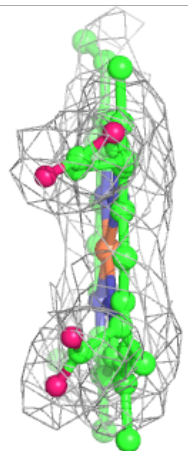
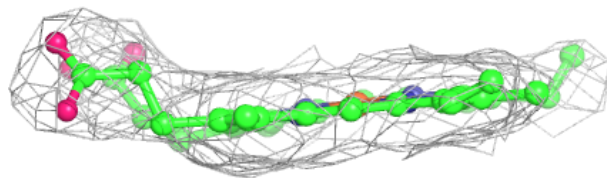
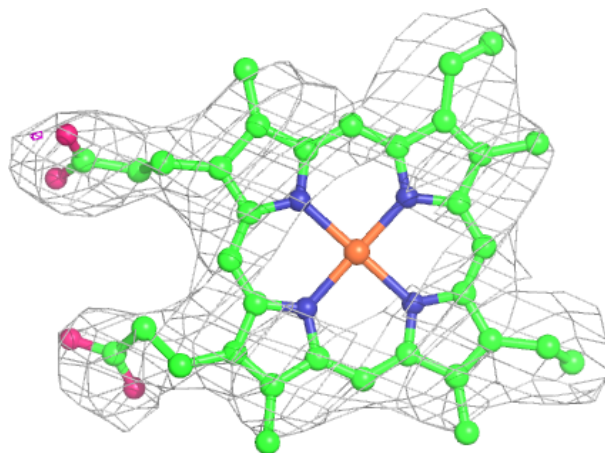
**Electron density around HEM C 150:**

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

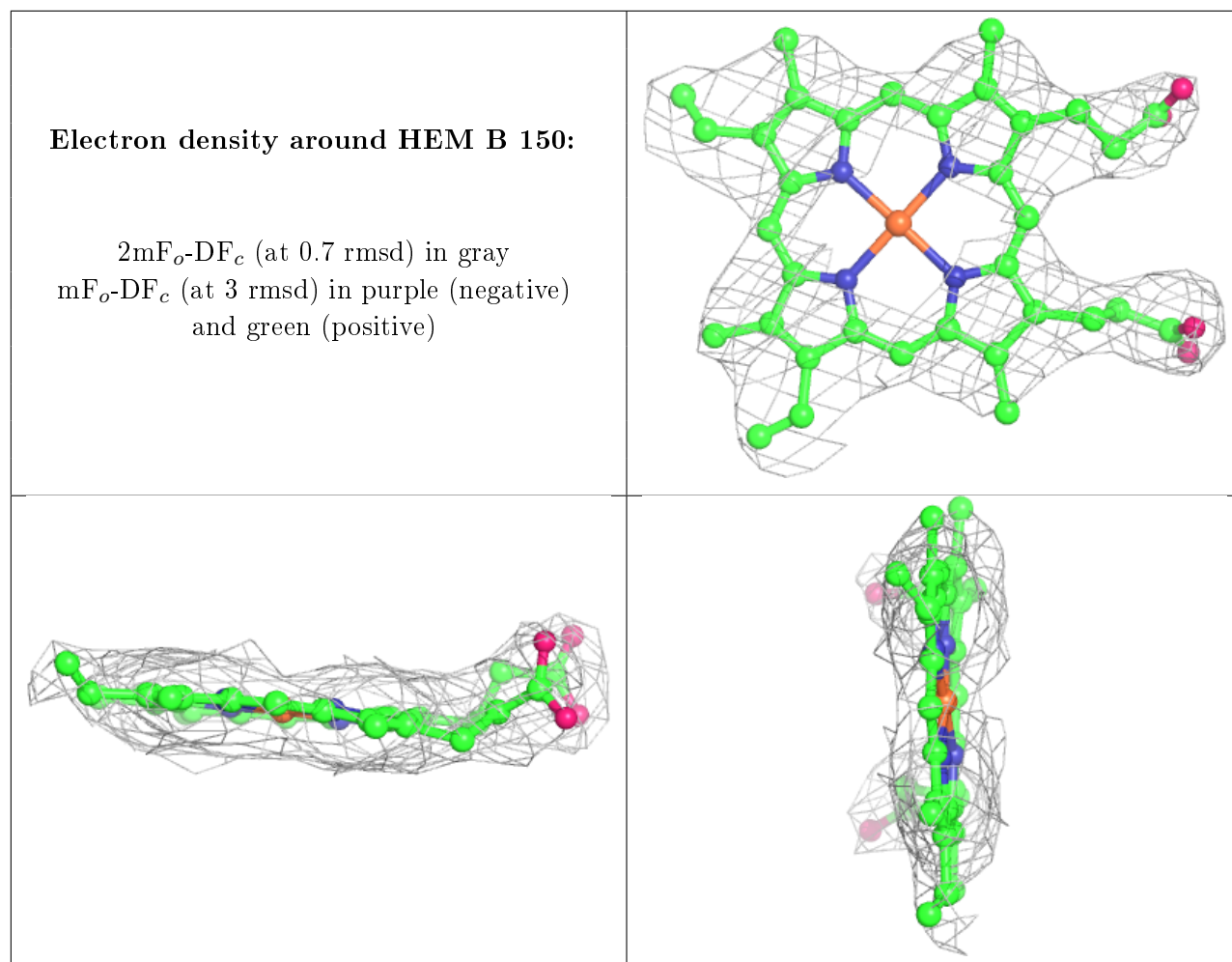


**Electron density around HEM A 150:**

$2mF_o-DF_c$  (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.