



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:15 am BST

PDB ID : 2Z36  
Title : Crystal structure of cytochrome P450 MoxA from *Nonomuraea recticatena* (CYP105)  
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Deposited on : 2007-06-02  
Resolution : 2.80 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

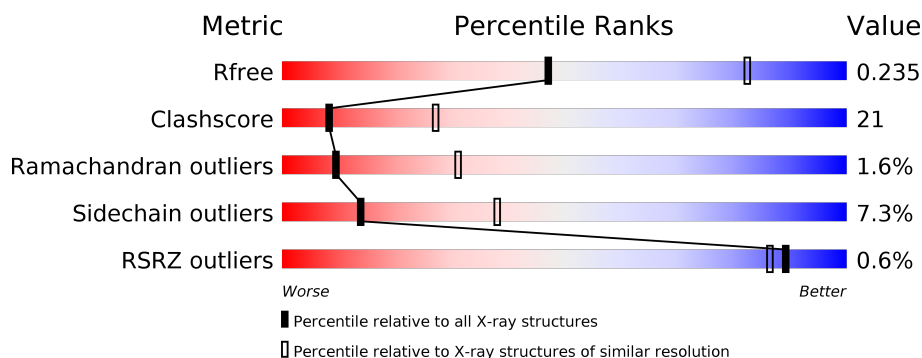
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	413	<div> <div></div> <div> <div></div> <div>57%</div> <div>35%</div> <div>5%</div> <div></div> </div> </div>
1	B	413	<div> <div></div> <div> <div></div> <div>60%</div> <div>33%</div> <div>5%</div> <div></div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6480 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 P450 type compactin 3",4"-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3146	1987	570	575	14			
1	B	404	Total	C	N	O	S	0	0	0
			3154	1993	571	576	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	HIS	-	EXPRESSION TAG	UNP Q2L6S8
A	409	HIS	-	EXPRESSION TAG	UNP Q2L6S8
A	410	HIS	-	EXPRESSION TAG	UNP Q2L6S8
A	411	HIS	-	EXPRESSION TAG	UNP Q2L6S8
A	412	HIS	-	EXPRESSION TAG	UNP Q2L6S8
A	413	HIS	-	EXPRESSION TAG	UNP Q2L6S8
B	408	HIS	-	EXPRESSION TAG	UNP Q2L6S8
B	409	HIS	-	EXPRESSION TAG	UNP Q2L6S8
B	410	HIS	-	EXPRESSION TAG	UNP Q2L6S8
B	411	HIS	-	EXPRESSION TAG	UNP Q2L6S8
B	412	HIS	-	EXPRESSION TAG	UNP Q2L6S8
B	413	HIS	-	EXPRESSION TAG	UNP Q2L6S8

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	27	Total	O	0	0
			27	27		



K392	
I397	
Y398	
G399	
V400	
H401	
E402	
L403	
P404	
V405	
T406	
H411	
B412	
HIS	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.56Å 83.26Å 175.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.80 47.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.4 (47.60-2.80) 93.3 (47.60-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.93 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.274 0.231 , 0.235	Depositor DCC
$R_{free}$ test set	1434 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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, FE, MES

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	0.28	0/3217	0.56	0/4368
1	B	0.29	0/3225	0.59	1/4379 (0.0%)
All	All	0.29	0/6442	0.57	1/8747 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	GLY	N-CA-C	-7.67	93.93	113.10

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	3146	0	3137	138	0
1	B	3154	0	3148	130	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	30	5	0
3	B	43	0	30	5	0
4	A	12	0	13	2	0
4	B	12	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	41	0	0	2	0
5	B	27	0	0	0	0
All	All	6480	0	6371	269	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 21.

All (269) 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:143:ARG:H	1:A:143:ARG:HD2	1.14	1.05
1:A:143:ARG:HB2	1:A:144:PRO:HD3	1.50	0.92
1:B:143:ARG:HB2	1:B:144:PRO:HD3	1.53	0.89
1:B:143:ARG:H	1:B:143:ARG:HD2	1.38	0.87
1:A:344:ARG:HB2	1:A:344:ARG:HH11	1.38	0.86
1:B:187:MET:HA	1:B:190:ARG:HD2	1.55	0.85
1:A:143:ARG:N	1:A:143:ARG:HD2	1.91	0.85
1:B:9:LEU:HD12	1:B:10:ALA:N	1.92	0.84
1:B:262:LEU:HD23	1:B:382:LEU:HD13	1.62	0.82
1:B:96:LEU:HD13	3:B:460:HEM:HAD2	1.61	0.81
1:B:295:VAL:HB	4:B:4575:MES:H71	1.63	0.80
1:B:14:LEU:HD23	1:B:16:VAL:HG23	1.64	0.79
1:B:373:LEU:HD11	1:B:380:LEU:HD22	1.66	0.78
1:A:143:ARG:HB2	1:A:144:PRO:CD	2.13	0.78
1:A:295:VAL:HB	4:A:4574:MES:H71	1.66	0.78
1:A:14:LEU:HD12	1:A:40:VAL:HG21	1.66	0.77
1:A:155:VAL:HB	1:A:156:PRO:HD3	1.66	0.76
1:B:18:ARG:HB2	1:B:18:ARG:HH11	1.49	0.76
1:A:96:LEU:HD13	3:A:450:HEM:HAD2	1.68	0.74
1:B:143:ARG:HB2	1:B:144:PRO:CD	2.17	0.74
1:B:108:ARG:HE	1:B:108:ARG:HA	1.52	0.74
1:A:147:LEU:HD21	1:A:151:LEU:HD12	1.70	0.73
1:B:210:SER:O	1:B:211:GLU:HB3	1.88	0.73
1:B:187:MET:HA	1:B:190:ARG:CD	2.19	0.73
1:A:153:LEU:HD23	1:A:179:THR:HG23	1.70	0.73
1:A:14:LEU:HD23	1:A:16:VAL:HG23	1.71	0.72
1:B:147:LEU:HD21	1:B:151:LEU:HD12	1.71	0.72
1:B:386:MET:O	1:B:389:VAL:HG12	1.90	0.71
1:B:143:ARG:HD2	1:B:143:ARG:N	2.05	0.71
1:A:181:MET:SD	1:A:197:LEU:HD12	2.31	0.70
1:A:284:GLU:OE2	1:A:341:ARG:HD3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD23	1:A:382:LEU:HD13	1.75	0.69
1:A:148:VAL:HA	1:A:152:SER:HB2	1.75	0.68
3:A:450:HEM:HHC	3:A:450:HEM:HBB2	1.76	0.68
1:B:148:VAL:HA	1:B:152:SER:HB2	1.77	0.67
3:B:460:HEM:HHC	3:B:460:HEM:HBB2	1.77	0.67
1:B:155:VAL:HB	1:B:156:PRO:HD3	1.77	0.66
1:A:267:GLN:HG3	1:A:337:LEU:HD12	1.77	0.66
1:B:14:LEU:CD2	1:B:16:VAL:HG23	2.25	0.66
1:B:255:SER:HB3	1:B:400:VAL:CG1	2.26	0.65
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.60	0.65
1:A:178:THR:HG22	1:A:247:HIS:CE1	2.32	0.65
1:B:230:LEU:HD23	1:B:231:ASP:H	1.62	0.65
1:B:291:ILE:HG22	1:B:398:TYR:HB3	1.78	0.65
1:B:157:SER:HB3	1:B:247:HIS:CE1	2.31	0.64
1:B:389:VAL:HG13	1:B:391:PHE:CE1	2.32	0.64
1:A:255:SER:HB3	1:A:400:VAL:HG13	1.80	0.64
1:B:123:ARG:HH22	1:B:367:GLN:HE22	1.46	0.64
1:A:54:HIS:CE1	1:A:58:ARG:HD2	2.33	0.63
1:B:198:ARG:HH21	1:B:236:VAL:HG23	1.63	0.63
1:B:387:GLU:CD	1:B:387:GLU:H	2.02	0.63
1:A:132:HIS:O	1:A:135:ASP:HB2	1.98	0.63
1:A:333:ASP:O	1:A:336:VAL:HG12	1.99	0.62
1:B:138:LEU:HD21	1:B:377:ILE:HG12	1.81	0.62
1:A:147:LEU:O	1:A:147:LEU:HD13	1.99	0.62
1:A:365:GLU:O	1:A:369:VAL:HG23	1.99	0.62
1:B:284:GLU:OE2	1:B:341:ARG:HD3	2.00	0.62
1:B:181:MET:SD	1:B:197:LEU:HD12	2.40	0.62
1:A:29:GLU:O	1:A:33:GLU:HG3	2.00	0.62
1:B:233:ALA:O	1:B:236:VAL:HG22	2.01	0.61
1:A:157:SER:CB	1:A:178:THR:HG21	2.30	0.61
1:B:153:LEU:HD23	1:B:179:THR:HG23	1.83	0.61
1:B:249:THR:HG22	1:B:397:ILE:HD13	1.83	0.60
1:B:255:SER:HB3	1:B:400:VAL:HG13	1.82	0.60
1:A:131:ASP:HA	1:A:376:ARG:NH2	2.15	0.60
1:B:12:LEU:HD21	1:B:14:LEU:HG	1.84	0.60
1:B:333:ASP:O	1:B:336:VAL:HG12	2.01	0.60
1:B:186:SER:O	1:B:190:ARG:HG3	2.00	0.60
1:A:113:GLU:OE2	1:A:216:LEU:HG	2.02	0.60
1:A:261:LEU:HD23	1:A:374:PHE:HE1	1.65	0.60
1:B:277:ARG:HH11	1:B:340:GLU:CD	2.05	0.59
1:A:261:LEU:HD23	1:A:374:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD21	1:A:85:LEU:HD12	1.85	0.59
1:B:232:HIS:O	1:B:236:VAL:HG13	2.03	0.59
1:A:253:MET:HE2	1:A:291:ILE:HG23	1.85	0.58
1:B:253:MET:HA	1:B:253:MET:HE2	1.85	0.58
1:A:131:ASP:HA	1:A:376:ARG:HH21	1.68	0.58
1:B:192:ARG:O	1:B:196:GLU:HG3	2.04	0.58
1:A:161:CYS:HB3	1:A:174:PHE:CD2	2.38	0.58
1:A:387:GLU:H	1:A:387:GLU:CD	2.06	0.58
1:A:60:VAL:HG13	1:A:66:PHE:CD1	2.38	0.58
1:A:181:MET:HG2	1:A:194:PHE:CD1	2.38	0.58
1:A:182:VAL:HG12	1:A:182:VAL:O	2.04	0.58
1:A:356:CYS:HB3	1:A:359:GLN:HB3	1.85	0.58
1:B:258:VAL:HG12	1:B:262:LEU:HD22	1.86	0.57
1:A:138:LEU:HD21	1:A:377:ILE:HG12	1.87	0.57
1:B:223:ARG:HG2	1:B:223:ARG:HH21	1.70	0.57
1:A:86:GLN:HG3	1:B:71:ARG:HD2	1.86	0.56
1:A:157:SER:HB3	1:A:178:THR:HG21	1.87	0.56
1:A:392:LYS:HG2	1:A:401:HIS:CE1	2.41	0.56
1:B:384:VAL:HB	1:B:385:PRO:HD2	1.87	0.55
1:B:56:GLU:O	1:B:60:VAL:HG13	2.06	0.55
1:B:9:LEU:HD12	1:B:10:ALA:CA	2.37	0.55
1:A:157:SER:HB3	1:A:247:HIS:NE2	2.22	0.55
1:B:24:PRO:HB3	1:B:322:LEU:HD21	1.88	0.55
1:A:13:GLU:O	1:A:13:GLU:HG3	2.07	0.55
1:B:301:THR:HG22	1:B:302:GLU:HG3	1.89	0.55
1:A:127:GLN:NE2	1:A:131:ASP:OD1	2.38	0.55
1:A:21:PRO:HB3	1:A:398:TYR:OH	2.06	0.54
1:A:382:LEU:HD12	1:A:405:VAL:HG12	1.90	0.54
1:B:250:THR:HA	3:B:460:HEM:HBB1	1.90	0.54
1:B:318:ILE:N	1:B:318:ILE:HD12	2.23	0.54
1:B:373:LEU:HD11	1:B:380:LEU:CD2	2.36	0.54
1:A:277:ARG:NH1	1:A:277:ARG:HG3	2.23	0.54
1:B:284:GLU:CD	1:B:341:ARG:HD3	2.27	0.54
1:A:125:ARG:HD3	1:A:162:GLU:OE1	2.07	0.54
1:A:81:ASP:HB2	1:A:84:THR:OG1	2.08	0.54
1:A:15:PRO:HB3	1:A:78:PHE:CZ	2.43	0.53
1:A:18:ARG:HB2	1:A:18:ARG:HH11	1.73	0.53
1:B:125:ARG:HE	1:B:125:ARG:HA	1.73	0.53
1:B:285:LEU:HD23	1:B:337:LEU:HD21	1.91	0.53
1:B:392:LYS:HG2	1:B:401:HIS:CE1	2.43	0.53
1:A:108:ARG:N	1:A:109:PRO:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PHE:HA	1:B:119:LEU:HD13	1.91	0.52
1:B:326:TRP:CZ3	1:B:335:ALA:HA	2.45	0.52
1:B:356:CYS:HB3	1:B:359:GLN:HB3	1.92	0.52
1:A:256:LEU:HD21	1:A:398:TYR:CD2	2.45	0.52
1:B:186:SER:C	1:B:188:GLU:H	2.13	0.52
1:B:217:PHE:O	1:B:221:ILE:HG13	2.09	0.52
1:B:284:GLU:OE2	1:B:284:GLU:HA	2.10	0.52
1:A:41:ARG:NH1	1:A:45:GLY:O	2.40	0.51
1:A:96:LEU:HD21	4:A:4574:MES:HN4	1.75	0.51
1:A:178:THR:CG2	1:A:247:HIS:CE1	2.93	0.51
1:B:382:LEU:HD11	1:B:403:LEU:HD11	1.92	0.51
1:B:224:GLN:OE1	1:B:230:LEU:HD23	2.10	0.51
1:B:9:LEU:HD12	1:B:10:ALA:H	1.73	0.51
1:A:161:CYS:HB3	1:A:174:PHE:CE2	2.46	0.51
1:A:81:ASP:H	1:A:84:THR:HB	1.75	0.51
1:B:205:ILE:HD13	1:B:235:LEU:HG	1.93	0.51
1:B:255:SER:O	1:B:259:VAL:HG12	2.10	0.51
1:A:107:ARG:O	1:A:110:VAL:HG12	2.11	0.51
1:A:125:ARG:NH1	1:A:128:ASP:OD1	2.44	0.51
1:A:181:MET:HG3	1:A:193:ALA:HB1	1.93	0.50
1:A:390:PRO:HG3	1:A:402:GLU:HG2	1.93	0.50
1:B:183:SER:O	1:B:190:ARG:NH2	2.44	0.50
1:B:354:HIS:HA	3:B:460:HEM:O2D	2.11	0.50
1:B:156:PRO:HA	1:B:365:GLU:OE2	2.11	0.50
1:A:256:LEU:HD13	1:A:400:VAL:HG12	1.94	0.50
1:B:256:LEU:HA	1:B:259:VAL:HG13	1.93	0.50
1:B:278:THR:HB	1:B:279:PRO:HD3	1.92	0.50
1:A:157:SER:HB2	1:A:178:THR:HG21	1.93	0.50
1:A:326:TRP:CZ3	1:A:335:ALA:HA	2.47	0.50
1:A:384:VAL:HB	1:A:385:PRO:HD2	1.92	0.50
1:A:240:PHE:O	1:A:244:THR:HB	2.12	0.49
1:A:283:GLU:OE2	1:A:363:ARG:HD3	2.12	0.49
1:A:60:VAL:HG13	1:A:66:PHE:CG	2.48	0.49
1:B:148:VAL:HA	1:B:152:SER:CB	2.42	0.49
1:B:155:VAL:O	1:B:159:VAL:HG23	2.12	0.49
1:A:405:VAL:O	1:A:406:THR:HG23	2.12	0.49
1:B:123:ARG:HB3	1:B:124:PRO:HD3	1.93	0.49
1:B:182:VAL:HG12	1:B:182:VAL:O	2.11	0.49
1:A:250:THR:HA	3:A:450:HEM:HBB1	1.95	0.49
1:B:338:ASP:HB3	1:B:341:ARG:HD2	1.95	0.49
1:A:261:LEU:HG	1:A:268:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HG2	1:B:398:TYR:CE1	2.47	0.49
1:B:295:VAL:HG21	4:B:4575:MES:H52	1.95	0.49
1:A:32:ARG:NH1	1:A:32:ARG:HB3	2.27	0.49
1:B:174:PHE:O	1:B:178:THR:HG23	2.13	0.49
1:B:12:LEU:C	1:B:12:LEU:HD23	2.33	0.48
1:A:390:PRO:CG	1:A:402:GLU:HG2	2.43	0.48
1:A:201:ILE:HD12	1:A:240:PHE:CE1	2.48	0.48
1:B:118:ARG:NE	1:B:118:ARG:HA	2.28	0.48
1:B:54:HIS:CE1	1:B:58:ARG:HD2	2.48	0.48
1:A:282:VAL:O	1:A:286:LEU:HG	2.13	0.48
1:B:9:LEU:CD1	1:B:10:ALA:N	2.71	0.48
1:A:305:GLU:OE1	1:A:310:SER:HB3	2.14	0.48
1:A:156:PRO:HA	1:A:365:GLU:OE2	2.13	0.47
1:A:253:MET:HE2	1:A:291:ILE:CG2	2.43	0.47
1:B:256:LEU:HA	1:B:259:VAL:CG1	2.44	0.47
1:A:346:HIS:C	1:A:346:HIS:ND1	2.68	0.47
1:B:147:LEU:HD22	1:B:151:LEU:HB2	1.96	0.47
1:A:185:THR:O	1:A:186:SER:HB3	2.15	0.47
1:A:107:ARG:NH1	1:A:353:PRO:O	2.47	0.47
1:B:137:MET:C	1:B:139:ALA:H	2.18	0.47
1:B:253:MET:HA	1:B:253:MET:CE	2.45	0.47
1:A:344:ARG:HH11	1:A:344:ARG:CB	2.19	0.47
1:A:369:VAL:O	1:A:373:LEU:HB2	2.15	0.47
1:A:230:LEU:HD23	1:A:230:LEU:C	2.35	0.47
1:B:282:VAL:O	1:B:286:LEU:HG	2.15	0.47
1:A:192:ARG:O	1:A:196:GLU:HG3	2.14	0.47
1:A:281:ALA:HB2	1:A:339:VAL:HG13	1.97	0.47
1:A:66:PHE:O	1:A:298:ARG:HD2	2.15	0.47
1:B:145:VAL:O	1:B:405:VAL:HG22	2.15	0.47
1:A:78:PHE:CG	1:A:318:ILE:HD13	2.49	0.46
1:A:330:VAL:HG23	1:A:331:PHE:CD2	2.50	0.46
1:A:291:ILE:HG22	1:A:398:TYR:HB3	1.97	0.46
1:A:165:GLY:HA3	1:A:215:ASP:CB	2.45	0.46
1:B:216:LEU:C	1:B:216:LEU:HD23	2.36	0.46
1:A:212:PRO:HB3	1:A:218:SER:CB	2.45	0.46
1:A:278:THR:HB	1:A:279:PRO:HD3	1.97	0.46
1:B:130:VAL:O	1:B:134:ILE:HG12	2.16	0.46
1:A:18:ARG:CZ	1:A:322:LEU:HD22	2.46	0.46
1:B:81:ASP:HB2	1:B:84:THR:H	1.81	0.46
1:A:123:ARG:HB3	1:A:124:PRO:HD3	1.98	0.46
1:B:387:GLU:CD	1:B:387:GLU:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:CD1	1:B:27:ALA:HB1	2.46	0.46
1:A:137:MET:C	1:A:139:ALA:H	2.20	0.46
1:A:107:ARG:HH21	1:A:357:LEU:HA	1.81	0.45
1:B:143:ARG:O	1:B:406:THR:HG22	2.16	0.45
1:A:354:HIS:HA	3:A:450:HEM:O2D	2.16	0.45
1:B:21:PRO:HB3	1:B:398:TYR:OH	2.17	0.45
1:A:96:LEU:HD11	3:A:450:HEM:HBA1	1.99	0.45
1:A:151:LEU:HD11	1:A:373:LEU:HG	1.97	0.45
1:A:77:LEU:HD22	1:A:81:ASP:O	2.17	0.45
1:A:299:LEU:C	1:A:299:LEU:HD13	2.38	0.45
1:A:36:PRO:HB3	1:A:56:GLU:CD	2.37	0.45
1:B:108:ARG:N	1:B:109:PRO:HD2	2.32	0.45
1:A:332:LYS:O	1:A:341:ARG:NH2	2.50	0.44
1:B:274:ASN:ND2	1:B:277:ARG:HG2	2.32	0.44
1:B:320:SER:OG	1:B:323:SER:HB2	2.18	0.44
1:A:204:LEU:HD12	1:A:217:PHE:CE1	2.52	0.44
1:A:290:THR:HA	5:A:533:HOH:O	2.17	0.44
1:B:110:VAL:HG22	1:B:110:VAL:O	2.18	0.44
1:B:223:ARG:HG3	1:B:224:GLN:N	2.33	0.44
1:B:185:THR:HG22	1:B:186:SER:N	2.33	0.44
1:A:157:SER:HB3	1:A:247:HIS:CD2	2.53	0.44
1:A:81:ASP:HB2	1:A:84:THR:CB	2.48	0.43
1:B:253:MET:HE3	1:B:291:ILE:HG23	1.99	0.43
1:A:87:GLN:NE2	1:A:87:GLN:HA	2.33	0.43
1:B:209:GLU:O	1:B:225:ARG:NH2	2.43	0.43
1:B:69:ASP:OD2	1:B:71:ARG:HB2	2.19	0.43
1:A:110:VAL:HG13	1:A:357:LEU:HD11	2.01	0.43
1:B:178:THR:HG22	1:B:243:LEU:HD21	2.00	0.43
1:A:148:VAL:HA	1:A:152:SER:CB	2.46	0.43
1:A:408:HIS:CD2	1:A:408:HIS:C	2.91	0.43
1:B:354:HIS:O	1:B:355:GLN:C	2.57	0.43
1:B:283:GLU:OE1	1:B:363:ARG:NH1	2.52	0.43
1:A:29:GLU:CD	1:A:32:ARG:HH22	2.22	0.43
1:A:255:SER:CB	1:A:400:VAL:HG13	2.47	0.42
1:B:281:ALA:HB2	1:B:339:VAL:CG1	2.49	0.42
1:B:49:TRP:CD1	1:B:311:ILE:HG23	2.54	0.42
1:A:156:PRO:O	1:A:160:ILE:HG13	2.20	0.42
1:B:14:LEU:HA	1:B:14:LEU:HD23	1.86	0.42
1:A:255:SER:HB3	1:A:400:VAL:CG1	2.48	0.42
1:A:81:ASP:HB2	1:A:84:THR:H	1.85	0.42
1:B:223:ARG:CG	1:B:223:ARG:HH21	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:OE1	1:A:226:GLN:HA	2.20	0.42
1:A:290:THR:O	1:A:290:THR:HG22	2.20	0.42
1:B:96:LEU:HD11	3:B:460:HEM:HBA1	2.01	0.42
1:B:174:PHE:CE2	1:B:178:THR:HG21	2.55	0.42
1:B:125:ARG:HA	1:B:125:ARG:NE	2.35	0.41
1:B:268:LEU:HD11	1:B:374:PHE:CD2	2.55	0.41
5:A:528:HOH:O	1:B:71:ARG:HD3	2.19	0.41
1:A:188:GLU:OE2	1:A:188:GLU:HA	2.20	0.41
1:A:244:THR:HG22	1:A:245:ALA:N	2.35	0.41
1:A:49:TRP:CZ3	1:A:309:VAL:HG11	2.55	0.41
1:B:210:SER:O	1:B:211:GLU:CB	2.60	0.41
1:A:145:VAL:O	1:A:405:VAL:HG22	2.21	0.41
1:A:347:LEU:HD22	1:A:351:PHE:HB2	2.00	0.41
1:B:121:ALA:O	1:B:124:PRO:HD2	2.21	0.41
1:A:204:LEU:HA	1:A:207:ARG:HD2	2.02	0.41
1:A:376:ARG:NH1	1:A:376:ARG:HG2	2.36	0.41
1:B:389:VAL:HG13	1:B:391:PHE:HE1	1.85	0.41
1:A:14:LEU:HD13	1:A:50:TRP:CE3	2.56	0.41
1:A:262:LEU:HD12	1:A:262:LEU:HA	1.89	0.41
1:A:66:PHE:CE2	1:A:317:VAL:HG21	2.56	0.41
1:A:331:PHE:O	1:A:334:PRO:HD3	2.20	0.41
1:B:205:ILE:HG21	1:B:235:LEU:HD23	2.03	0.41
1:B:230:LEU:HD23	1:B:231:ASP:N	2.33	0.41
1:B:256:LEU:HD12	1:B:256:LEU:HA	1.87	0.41
1:A:39:LYS:HE3	1:A:49:TRP:CH2	2.56	0.40
1:B:143:ARG:H	1:B:143:ARG:CD	2.21	0.40
1:A:257:GLY:O	1:A:261:LEU:HB2	2.22	0.40
1:A:330:VAL:HG23	1:A:331:PHE:CG	2.56	0.40
1:A:12:LEU:HD21	1:A:16:VAL:HG21	2.03	0.40
1:B:108:ARG:HE	1:B:108:ARG:CA	2.27	0.40
1:B:113:GLU:OE1	1:B:219:ARG:NH1	2.46	0.40
1:B:113:GLU:C	1:B:118:ARG:HG2	2.42	0.40
1:B:212:PRO:HB3	1:B:218:SER:HB3	2.04	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	401/413 (97%)	364 (91%)	29 (7%)	8 (2%)	7	24
1	B	402/413 (97%)	361 (90%)	36 (9%)	5 (1%)	13	39
All	All	803/826 (97%)	725 (90%)	65 (8%)	13 (2%)	9	31

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	293	ASP
1	B	293	ASP
1	B	343	ALA
1	A	100	GLY
1	B	100	GLY
1	A	138	LEU
1	A	343	ALA
1	B	138	LEU
1	B	211	GLU
1	A	211	GLU
1	A	212	PRO
1	A	344	ARG

### 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	336/345 (97%)	311 (93%)	25 (7%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	337/345 (98%)	313 (93%)	24 (7%)	14	39
All	All	673/690 (98%)	624 (93%)	49 (7%)	14	38

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	41	ARG
1	A	73	ASP
1	A	85	LEU
1	A	119	LEU
1	A	127	GLN
1	A	143	ARG
1	A	153	LEU
1	A	172	ASP
1	A	215	ASP
1	A	229	THR
1	A	242	LEU
1	A	244	THR
1	A	256	LEU
1	A	262	LEU
1	A	277	ARG
1	A	340	GLU
1	A	344	ARG
1	A	346	HIS
1	A	357	LEU
1	A	373	LEU
1	A	376	ARG
1	A	382	LEU
1	A	400	VAL
1	A	410	HIS
1	B	12	LEU
1	B	18	ARG
1	B	41	ARG
1	B	60	VAL
1	B	85	LEU
1	B	108	ARG
1	B	125	ARG
1	B	127	GLN
1	B	141	ASP
1	B	161	CYS
1	B	187	MET

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Mol	Chain	Res	Type
1	B	194	PHE
1	B	223	ARG
1	B	230	LEU
1	B	256	LEU
1	B	259	VAL
1	B	262	LEU
1	B	301	THR
1	B	337	LEU
1	B	340	GLU
1	B	367	GLN
1	B	382	LEU
1	B	400	VAL
1	B	411	HIS

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	87	GLN
1	A	91	GLN
1	A	127	GLN
1	A	149	GLN
1	A	408	HIS
1	A	409	HIS
1	B	87	GLN
1	B	91	GLN
1	B	127	GLN
1	B	149	GLN
1	B	367	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	HEM	A	450	1	27,50,50	1.57	5 (18%)	17,82,82	0.99	0
4	MES	B	4575	-	12,12,12	1.68	2 (16%)	14,16,16	1.43	2 (14%)
3	HEM	B	460	1	27,50,50	1.60	4 (14%)	17,82,82	0.94	0
4	MES	A	4574	-	12,12,12	1.67	2 (16%)	14,16,16	1.40	3 (21%)

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	HEM	A	450	1	-	0/6/54/54	-
4	MES	B	4575	-	-	4/6/14/14	0/1/1/1
3	HEM	B	460	1	-	0/6/54/54	-
4	MES	A	4574	-	-	3/6/14/14	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	460	HEM	C3B-C2B	-5.34	1.33	1.40
3	A	450	HEM	C3B-C2B	-5.22	1.33	1.40
4	B	4575	MES	C8-S	3.94	1.83	1.77
4	A	4574	MES	C8-S	3.87	1.83	1.77
4	A	4574	MES	C7-C8	-3.40	1.43	1.52
4	B	4575	MES	C7-C8	-3.35	1.43	1.52
3	B	460	HEM	C4D-C3D	2.84	1.49	1.42
3	A	450	HEM	C4D-C3D	2.50	1.48	1.42
3	B	460	HEM	C1A-CHA	-2.49	1.34	1.41
3	A	450	HEM	C4A-CHB	-2.45	1.34	1.41
3	B	460	HEM	C4A-CHB	-2.44	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	HEM	C1A-CHA	-2.15	1.35	1.41
3	A	450	HEM	C3C-C2C	-2.12	1.37	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4575	MES	O2S-S-C8	3.10	110.65	106.92
4	A	4574	MES	O1S-S-C8	2.56	109.99	106.92
4	A	4574	MES	C7-N4-C3	-2.54	104.75	111.23
4	B	4575	MES	C7-N4-C3	-2.54	104.75	111.23
4	A	4574	MES	O3S-S-C8	2.12	109.20	105.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	4575	MES	C8-C7-N4-C3
4	B	4575	MES	C7-C8-S-O2S
4	A	4574	MES	C8-C7-N4-C3
4	B	4575	MES	C7-C8-S-O3S
4	B	4575	MES	C7-C8-S-O1S
4	A	4574	MES	C7-C8-S-O2S
4	A	4574	MES	C7-C8-S-O3S

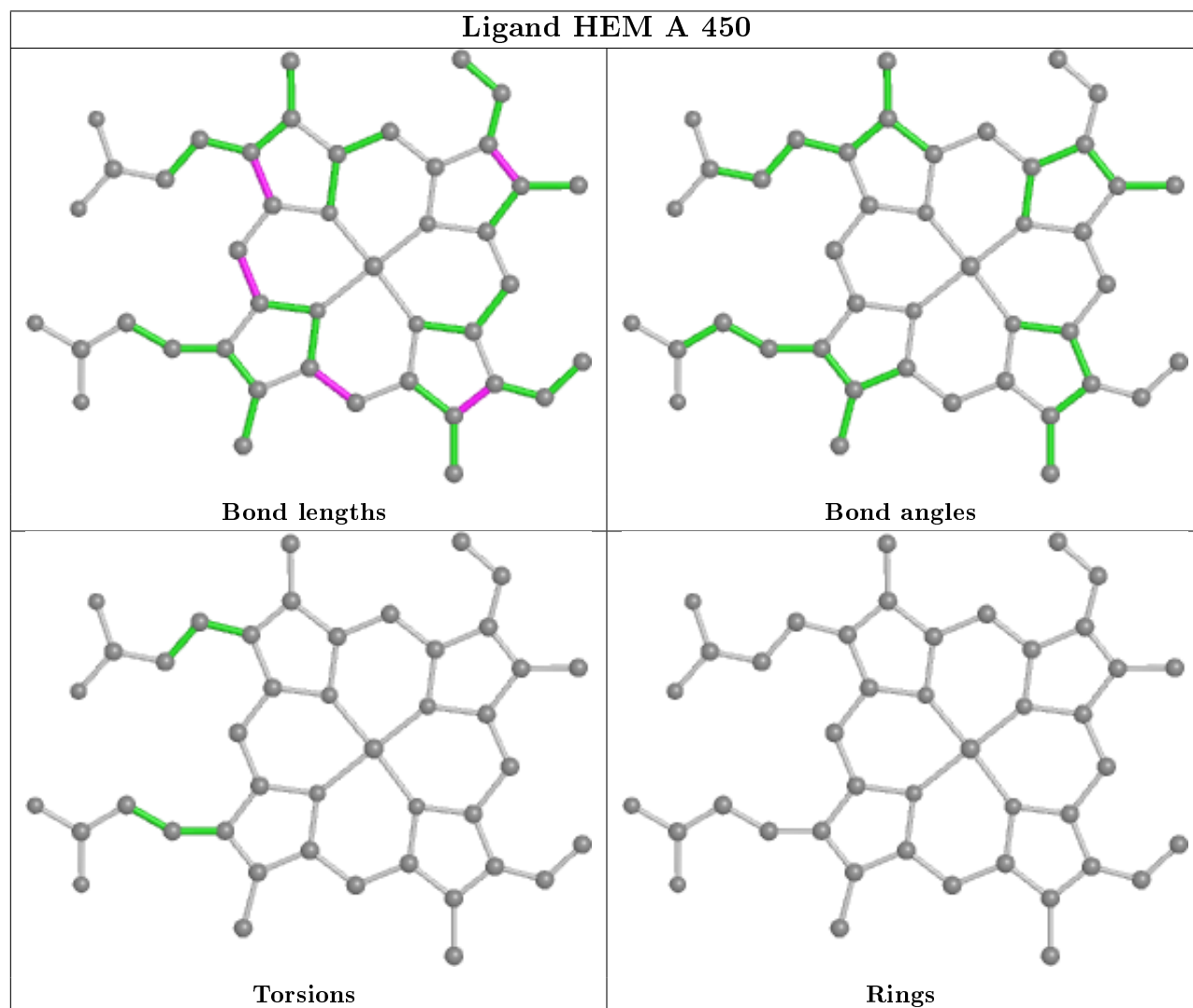
There are no ring outliers.

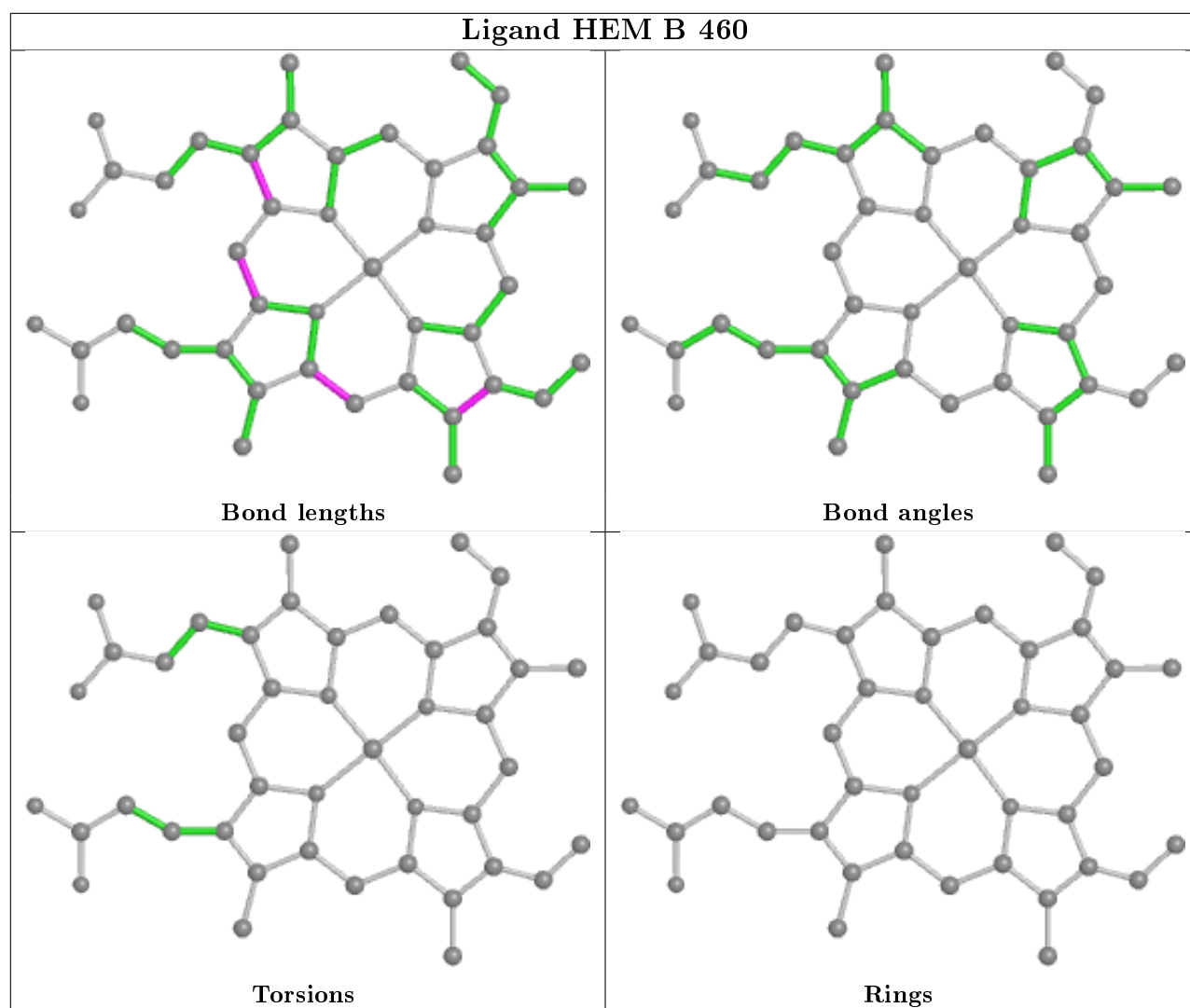
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	HEM	5	0
4	B	4575	MES	2	0
3	B	460	HEM	5	0
4	A	4574	MES	2	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	403/413 (97%)	-0.14	4 (0%) 82 77	24, 46, 83, 101	0
1	B	404/413 (97%)	-0.24	1 (0%) 95 94	18, 44, 84, 102	0
All	All	807/826 (97%)	-0.19	5 (0%) 89 86	18, 45, 84, 102	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	ASP	4.1
1	A	143	ARG	3.6
1	B	143	ARG	3.5
1	A	230	LEU	2.7
1	A	345	HIS	2.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

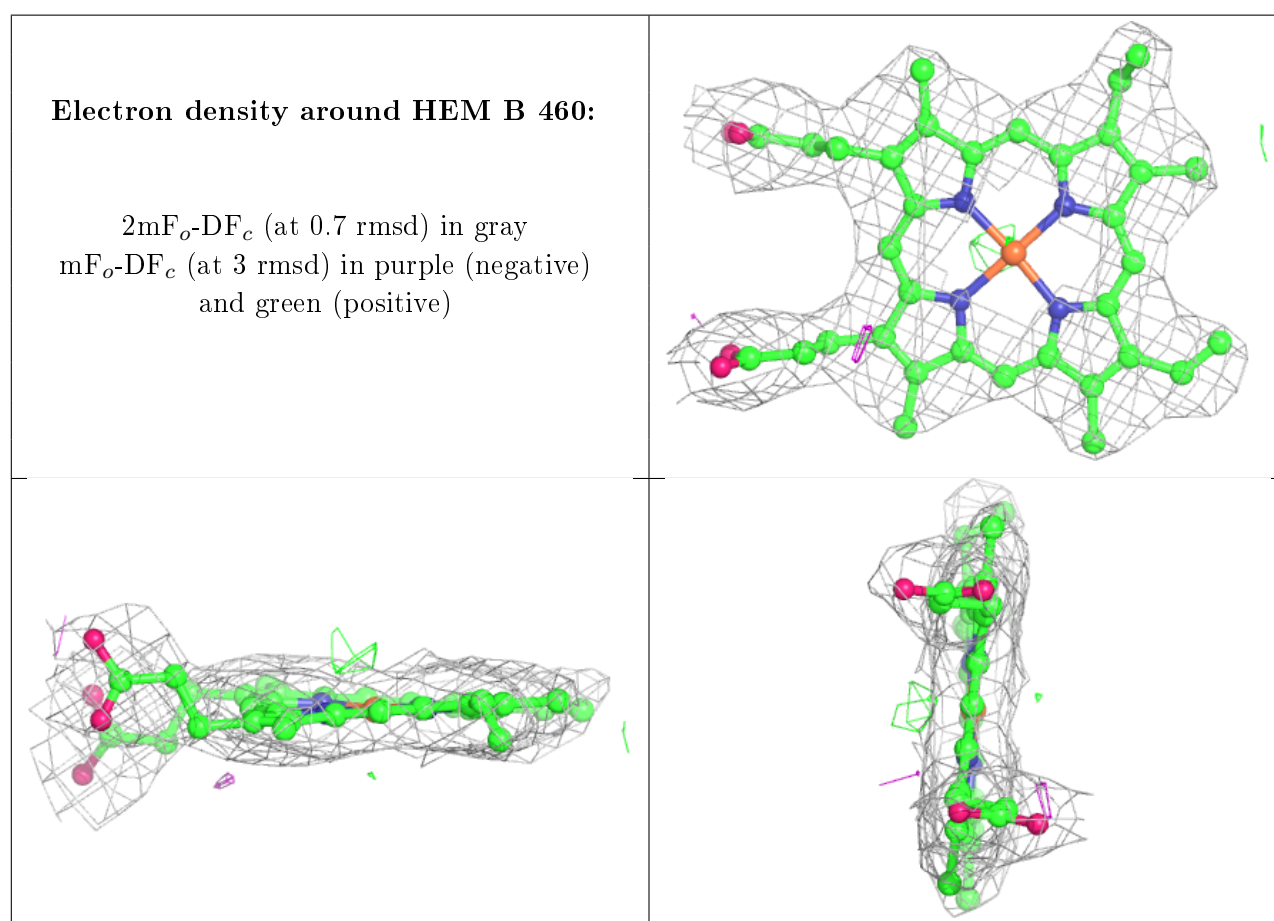
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.



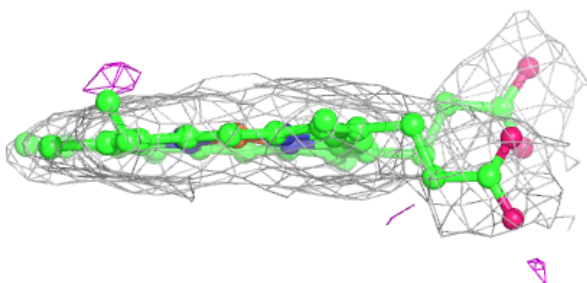
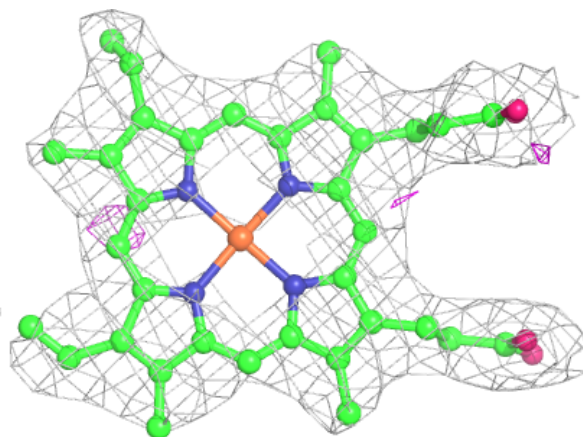
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MES	B	4575	12/12	0.81	0.30	85,98,111,111	0
4	MES	A	4574	12/12	0.89	0.24	79,93,108,108	0
3	HEM	B	460	43/43	0.98	0.16	14,25,33,38	0
3	HEM	A	450	43/43	0.98	0.17	19,29,40,53	0
2	FE	B	601	1/1	0.99	0.09	51,51,51,51	0
2	FE	A	602	1/1	0.99	0.12	43,43,43,43	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 450:**

$2mF_o-DF_c$  (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.