



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 08:01 AM EDT

PDB ID : 1YQO  
Title : T268A mutant heme domain of flavocytochrome P450 BM3  
Authors : Clark, J.P.; Miles, C.S.; Mowat, C.G.; Walkinshaw, M.D.; Reid, G.A.; Daff, S.N.; Chapman, S.K.  
Deposited on : 2005-02-02  
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

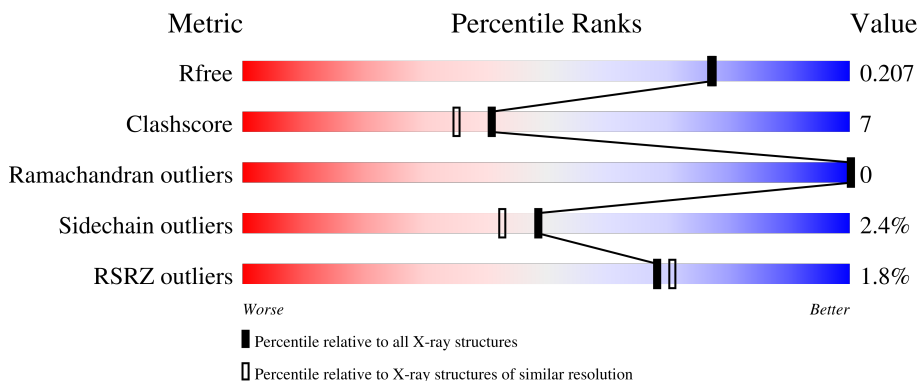
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of 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	455	 2% 85% 10% ..
1	B	455	 % 80% 15% ..

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8130 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 Bifunctional P-450:NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	441	Total 3531	C 2264	N 599	O 651	S 17	0	0	0
1	B	441	Total 3527	C 2261	N 595	O 654	S 17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	ALA	THR	engineered mutation	UNP P14779
B	268	ALA	THR	engineered mutation	UNP P14779

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

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

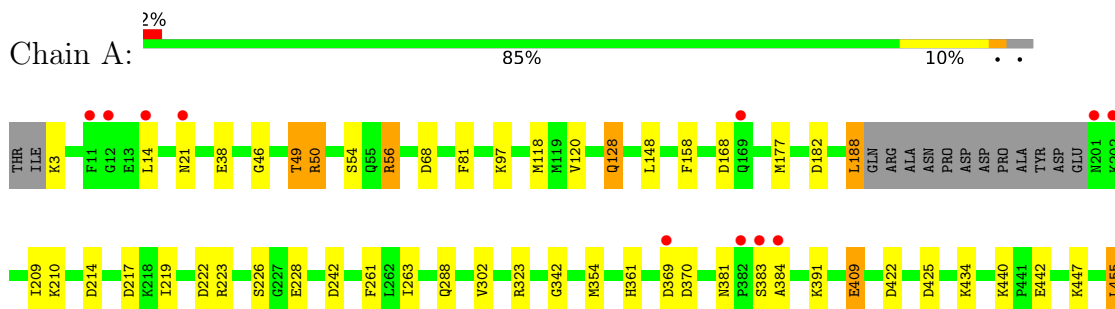
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	471	Total	O	0	0
			471	471		
3	B	515	Total	O	0	0
			515	515		

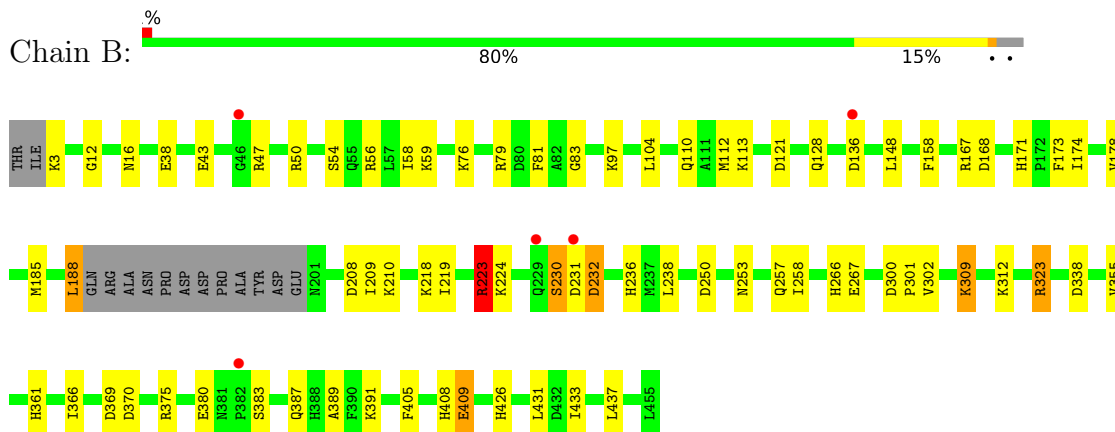
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Bifunctional P-450:NADPH-P450 reductase



- Molecule 1: Bifunctional P-450:NADPH-P450 reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.73Å 152.96Å 61.73Å 90.00° 94.37° 90.00°	Depositor
Resolution (Å)	24.00 – 1.90 23.55 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (24.00-1.90) 99.4 (23.55-1.90)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.15 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.166 , 0.206 0.167 , 0.207	Depositor DCC
$R_{free}$ test set	4224 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.014 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8130	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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

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	0.89	0/3612	0.93	13/4883 (0.3%)
1	B	0.88	0/3608	0.92	12/4878 (0.2%)
All	All	0.89	0/7220	0.92	25/9761 (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

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	ASP	CB-CG-OD2	10.46	127.71	118.30
1	A	50	ARG	NE-CZ-NH1	-7.99	116.30	120.30
1	A	369	ASP	CB-CG-OD2	7.65	125.18	118.30
1	A	455	LEU	CA-CB-CG	7.53	132.62	115.30
1	A	370	ASP	CB-CG-OD2	7.06	124.66	118.30
1	A	50	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	B	338	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	217	ASP	CB-CG-OD2	6.69	124.32	118.30
1	B	208	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	242	ASP	CB-CG-OD2	6.22	123.89	118.30
1	B	232	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	148	LEU	CA-CB-CG	5.89	128.86	115.30
1	B	250	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	56	ARG	NE-CZ-NH2	-5.74	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	56	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	425	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	223	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	148	LEU	CB-CG-CD2	5.33	120.07	111.00
1	B	121	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	222	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	50	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	422	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	323	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	68	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	GLY	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	3531	0	3502	36	0
1	B	3527	0	3490	64	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	471	0	0	19	1
3	B	515	0	0	31	1
All	All	8130	0	7052	101	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 7.

All (101) 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:182:ASP:HB3	3:A:839:HOH:O	1.42	1.19
1:A:384:ALA:HB3	3:A:883:HOH:O	1.51	1.07
1:A:354:MET:HE3	3:A:840:HOH:O	1.55	1.05
1:B:219:ILE:HD13	3:B:887:HOH:O	1.62	0.97
1:A:56:ARG:HD3	3:A:692:HOH:O	1.70	0.90
1:A:97:LYS:HB2	3:A:665:HOH:O	1.72	0.88
1:B:361:HIS:HE1	1:B:391:LYS:H	1.21	0.88
1:A:188:LEU:C	3:A:723:HOH:O	2.13	0.85
1:A:288:GLN:HG3	3:A:866:HOH:O	1.76	0.84
1:B:16:ASN:HD22	1:B:43:GLU:H	1.26	0.84
1:B:309:LYS:HE3	3:B:604:HOH:O	1.79	0.83
1:A:361:HIS:HE1	1:A:391:LYS:H	1.32	0.78
1:B:309:LYS:CE	3:B:604:HOH:O	2.32	0.77
1:A:447:LYS:HE2	3:A:856:HOH:O	1.85	0.76
1:B:56:ARG:NH1	3:B:920:HOH:O	2.19	0.75
1:B:236:HIS:CE1	3:B:974:HOH:O	2.39	0.74
1:B:210:LYS:CB	3:B:880:HOH:O	2.34	0.74
1:B:158:PHE:HD2	1:B:219:ILE:HG21	1.53	0.74
1:B:3:LYS:NZ	3:B:653:HOH:O	2.20	0.74
1:B:174:ILE:O	1:B:178:VAL:HG13	1.89	0.73
1:B:171:HIS:HD2	1:B:173:PHE:H	1.36	0.70
1:B:223:ARG:HD2	3:B:866:HOH:O	1.92	0.69
1:B:409:GLU:OE1	3:B:779:HOH:O	2.10	0.69
1:B:380:GLU:OE1	3:B:898:HOH:O	2.11	0.68
1:A:168:ASP:HB2	3:A:752:HOH:O	1.95	0.67
1:A:56:ARG:CD	3:A:692:HOH:O	2.34	0.65
1:A:128:GLN:HA	1:A:128:GLN:HE21	1.61	0.65
1:A:158:PHE:CE2	1:A:219:ILE:HD13	2.32	0.65
1:B:370:ASP:OD2	1:B:375:ARG:NH1	2.31	0.64
1:A:354:MET:HB2	3:A:840:HOH:O	1.98	0.64
1:A:158:PHE:HE2	1:A:219:ILE:HD13	1.62	0.64
1:B:76:LYS:HE2	3:B:820:HOH:O	1.98	0.63
1:B:59:LYS:NZ	1:B:387:GLN:HE22	1.98	0.60
1:A:442:GLU:HG3	3:A:639:HOH:O	2.04	0.57
1:A:409:GLU:HG2	3:A:920:HOH:O	2.05	0.56
1:A:3:LYS:N	3:A:886:HOH:O	2.38	0.56
1:A:226:SER:OG	1:A:228:GLU:HG2	2.05	0.56
1:B:370:ASP:OD2	1:B:375:ARG:NH2	2.37	0.56
1:B:409:GLU:HG2	3:B:779:HOH:O	2.06	0.54
1:B:47:ARG:N	3:B:914:HOH:O	2.41	0.54
1:B:409:GLU:CG	3:B:779:HOH:O	2.55	0.54
1:A:120:VAL:HG11	1:A:302:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:HIS:CD2	1:B:173:PHE:H	2.23	0.52
1:B:223:ARG:HH22	1:B:230:SER:HB2	1.74	0.52
1:A:210:LYS:HE3	3:A:829:HOH:O	2.10	0.52
1:B:223:ARG:NH2	1:B:230:SER:HB2	2.25	0.51
1:B:266:HIS:NE2	1:B:267:GLU:HG3	2.25	0.51
1:A:210:LYS:HE2	1:A:214:ASP:OD2	2.11	0.51
1:B:167:ARG:NH2	3:B:741:HOH:O	2.39	0.50
1:B:38:GLU:HB2	1:B:54:SER:HB3	1.94	0.50
1:B:361:HIS:CE1	1:B:391:LYS:H	2.13	0.50
1:A:118:MET:HG2	3:A:889:HOH:O	2.11	0.49
1:B:323:ARG:HA	1:B:361:HIS:CD2	2.48	0.49
1:B:110:GLN:HE22	1:B:113:LYS:NZ	2.11	0.49
1:A:177:MET:HG3	1:A:263:ILE:HD11	1.96	0.48
1:A:381:ASN:O	3:A:883:HOH:O	2.20	0.48
1:A:361:HIS:CE1	1:A:391:LYS:H	2.22	0.48
1:A:409:GLU:CG	3:A:920:HOH:O	2.62	0.48
1:B:309:LYS:NZ	1:B:408:HIS:ND1	2.59	0.47
1:A:434:LYS:HD3	1:A:440:LYS:HE2	1.97	0.46
1:A:56:ARG:NH2	1:A:342:GLY:O	2.49	0.46
1:A:261:PHE:CE1	3:A:595:HOH:O	2.56	0.46
1:A:158:PHE:HD2	1:A:219:ILE:HG21	1.80	0.45
1:B:97:LYS:HE3	3:B:883:HOH:O	2.15	0.45
1:A:223:ARG:HD3	1:A:228:GLU:HG3	1.97	0.45
1:A:38:GLU:HB2	1:A:54:SER:HB3	1.99	0.45
1:B:223:ARG:NH2	1:B:232:ASP:OD2	2.49	0.45
1:B:81:PHE:HB3	1:B:209:ILE:HG12	1.99	0.45
1:B:185:MET:O	1:B:188:LEU:HB2	2.17	0.44
1:B:128:GLN:NE2	3:B:494:HOH:O	2.50	0.44
1:B:218:LYS:HE2	3:B:827:HOH:O	2.17	0.43
1:B:231:ASP:HB2	3:B:790:HOH:O	2.18	0.43
1:B:3:LYS:N	3:B:961:HOH:O	2.51	0.43
1:B:366:ILE:HG21	1:B:389:ALA:HB1	2.00	0.43
1:B:12:GLY:HA2	3:B:863:HOH:O	2.18	0.43
1:A:49:THR:HG22	1:A:50:ARG:H	1.84	0.43
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.92	0.43
1:B:59:LYS:HZ3	1:B:387:GLN:HE22	1.62	0.43
1:B:312:LYS:HB2	3:B:691:HOH:O	2.19	0.43
1:B:59:LYS:HZ2	1:B:387:GLN:NE2	2.17	0.42
1:B:300:ASP:HB3	1:B:301:PRO:HD2	2.01	0.42
1:B:387:GLN:HG3	3:B:708:HOH:O	2.20	0.42
1:B:409:GLU:CD	3:B:779:HOH:O	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:HIS:HE1	3:B:533:HOH:O	2.01	0.42
1:A:323:ARG:HA	1:A:361:HIS:CD2	2.54	0.42
1:B:258:ILE:HG12	3:B:788:HOH:O	2.20	0.41
1:B:59:LYS:NZ	1:B:387:GLN:NE2	2.67	0.41
1:B:58:ILE:HD13	1:B:355:VAL:HG13	2.01	0.41
1:B:370:ASP:HB3	3:B:958:HOH:O	2.20	0.41
1:B:253:ASN:O	1:B:257:GLN:HG2	2.21	0.41
1:B:185:MET:CE	1:B:437:LEU:HD13	2.51	0.41
1:B:59:LYS:HE3	3:B:963:HOH:O	2.20	0.41
1:B:309:LYS:NZ	3:B:604:HOH:O	2.53	0.41
1:B:370:ASP:OD2	1:B:375:ARG:CZ	2.69	0.41
1:B:431:LEU:HD21	1:B:433:ILE:HD11	2.03	0.41
1:A:81:PHE:HB3	1:A:209:ILE:HG12	2.02	0.41
1:B:136:ASP:N	3:B:868:HOH:O	2.53	0.40
1:B:178:VAL:HG22	3:B:755:HOH:O	2.22	0.40
1:B:79:ARG:HG3	1:B:83:GLY:O	2.21	0.40
1:B:112:MET:SD	1:B:405:PHE:HA	2.61	0.40
2:B:460:HEM:CMC	2:B:460:HEM:HBC2	2.51	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)
3:A:491:HOH:O	3:B:900:HOH:O[2_656]	2.02	0.18

## 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	437/455 (96%)	429 (98%)	8 (2%)	0	100	100
1	B	437/455 (96%)	425 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	874/910 (96%)	854 (98%)	20 (2%)	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	380/398 (96%)	371 (98%)	9 (2%)	49	43
1	B	380/398 (96%)	371 (98%)	9 (2%)	49	43
All	All	760/796 (96%)	742 (98%)	18 (2%)	49	43

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	21	ASN
1	A	49	THR
1	A	128	GLN
1	A	148	LEU
1	A	188	LEU
1	A	383	SER
1	A	409	GLU
1	A	455	LEU
1	B	104	LEU
1	B	188	LEU
1	B	223	ARG
1	B	224	LYS
1	B	230	SER
1	B	302	VAL
1	B	309	LYS
1	B	383	SER
1	B	409	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	21	ASN
1	A	95	ASN
1	A	109	GLN
1	A	110	GLN
1	A	128	GLN
1	A	159	ASN
1	A	236	HIS
1	A	288	GLN
1	A	319	ASN
1	A	361	HIS
1	A	395	ASN
1	A	403	GLN
1	B	7	GLN
1	B	16	ASN
1	B	95	ASN
1	B	109	GLN
1	B	110	GLN
1	B	128	GLN
1	B	171	HIS
1	B	288	GLN
1	B	319	ASN
1	B	361	HIS
1	B	387	GLN
1	B	388	HIS
1	B	395	ASN
1	B	403	GLN
1	B	426	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	460	1,3	41,50,50	1.96	9 (21%)	45,82,82	2.16	16 (35%)
2	HEM	A	460	1,3	41,50,50	1.77	9 (21%)	45,82,82	1.71	11 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	460	1,3	-	2/12/54/54	-
2	HEM	A	460	1,3	-	2/12/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	460	HEM	C3D-C2D	6.72	1.51	1.36
2	A	460	HEM	C3C-C2C	-5.25	1.33	1.40
2	A	460	HEM	C3D-C2D	4.86	1.47	1.36
2	B	460	HEM	C3C-C2C	-3.54	1.35	1.40
2	B	460	HEM	FE-ND	3.18	2.12	1.96
2	B	460	HEM	C3C-CAC	3.12	1.54	1.47
2	A	460	HEM	CMB-C2B	2.89	1.56	1.50
2	A	460	HEM	C3C-CAC	2.83	1.53	1.47
2	B	460	HEM	CMB-C2B	2.77	1.56	1.50
2	A	460	HEM	FE-ND	2.75	2.10	1.96
2	B	460	HEM	C1A-NA	2.66	1.41	1.36
2	A	460	HEM	CAA-C2A	2.63	1.55	1.52
2	B	460	HEM	CMC-C2C	2.56	1.57	1.51
2	B	460	HEM	CAA-C2A	2.56	1.55	1.52
2	A	460	HEM	CMD-C2D	2.45	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	460	HEM	CMC-C2C	2.33	1.57	1.51
2	A	460	HEM	CMA-C3A	2.18	1.56	1.51
2	B	460	HEM	CAB-C3B	2.17	1.53	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	460	HEM	C4D-ND-C1D	6.99	112.29	105.07
2	B	460	HEM	C2C-C3C-C4C	5.49	110.73	106.90
2	A	460	HEM	C4D-ND-C1D	5.30	110.55	105.07
2	A	460	HEM	C4B-C3B-C2B	3.48	109.88	107.11
2	B	460	HEM	CHC-C4B-NB	3.44	128.17	124.43
2	B	460	HEM	C1B-NB-C4B	3.29	108.47	105.07
2	A	460	HEM	CHC-C4B-NB	3.28	127.99	124.43
2	B	460	HEM	CHB-C1B-NB	3.17	128.30	124.38
2	B	460	HEM	CBD-CAD-C3D	-3.08	104.07	112.63
2	B	460	HEM	C4C-CHD-C1D	2.91	126.40	122.56
2	A	460	HEM	CBD-CAD-C3D	-2.88	104.64	112.63
2	A	460	HEM	C1B-NB-C4B	2.80	107.97	105.07
2	B	460	HEM	CBA-CAA-C2A	-2.70	108.01	112.62
2	B	460	HEM	CAD-CBD-CGD	-2.69	107.82	113.60
2	B	460	HEM	C4A-C3A-C2A	2.56	108.78	107.00
2	A	460	HEM	CMA-C3A-C4A	-2.53	124.57	128.46
2	B	460	HEM	CMA-C3A-C4A	-2.46	124.68	128.46
2	A	460	HEM	C2C-C3C-C4C	2.39	108.56	106.90
2	B	460	HEM	C4B-C3B-C2B	2.38	109.00	107.11
2	A	460	HEM	CHA-C4D-ND	2.31	127.23	124.38
2	A	460	HEM	C4A-C3A-C2A	2.30	108.60	107.00
2	A	460	HEM	C3D-C4D-ND	-2.23	107.69	110.17
2	B	460	HEM	C3D-C4D-ND	-2.20	107.72	110.17
2	A	460	HEM	C4C-CHD-C1D	2.18	125.44	122.56
2	B	460	HEM	CMD-C2D-C1D	2.15	128.32	125.04
2	B	460	HEM	C1D-C2D-C3D	-2.12	104.72	106.96
2	B	460	HEM	CHA-C4D-ND	2.08	126.95	124.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	460	HEM	CAD-CBD-CGD-O1D
2	B	460	HEM	CAD-CBD-CGD-O1D
2	A	460	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	B	460	HEM	CAD-CBD-CGD-O2D

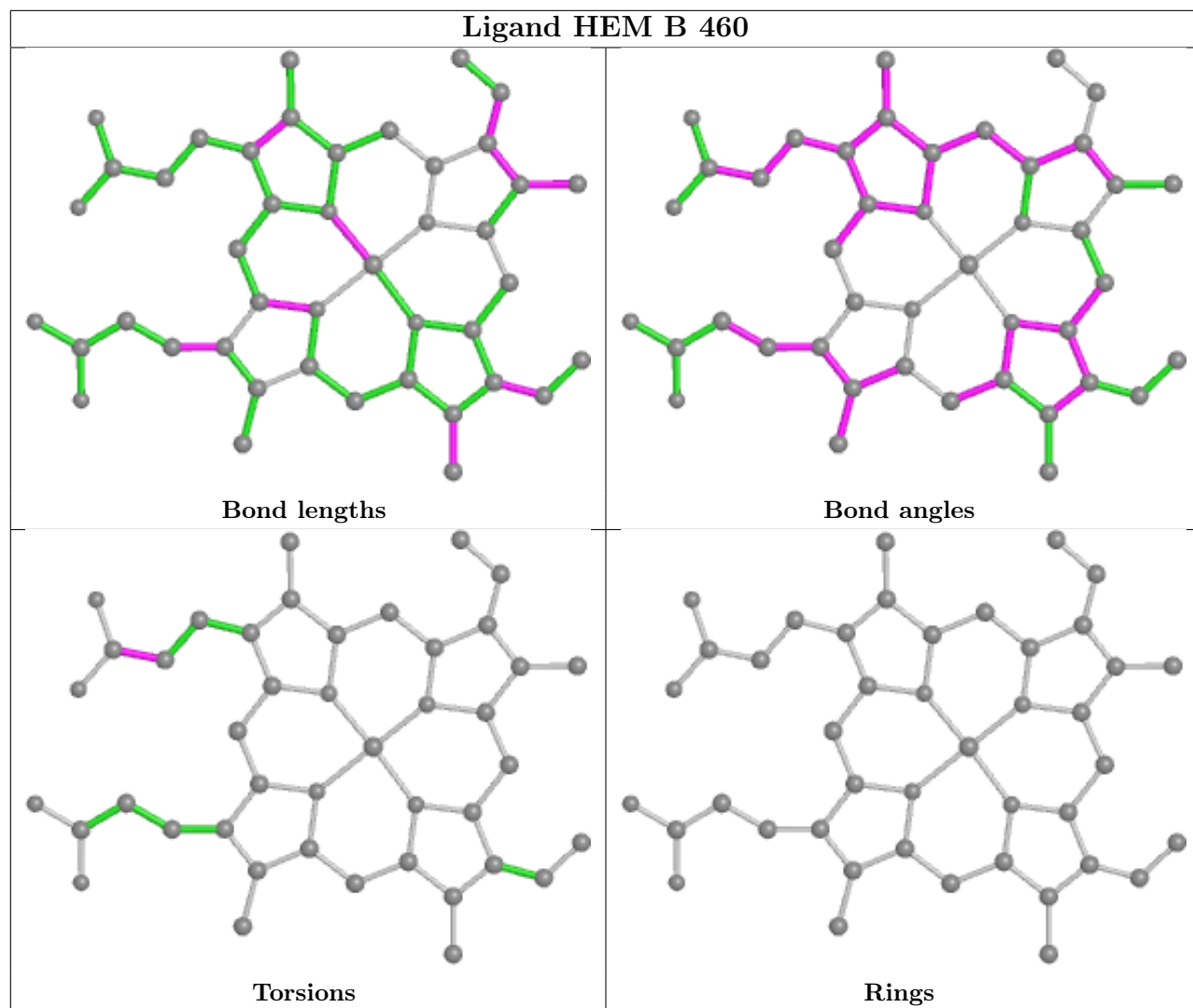
There are no ring outliers.

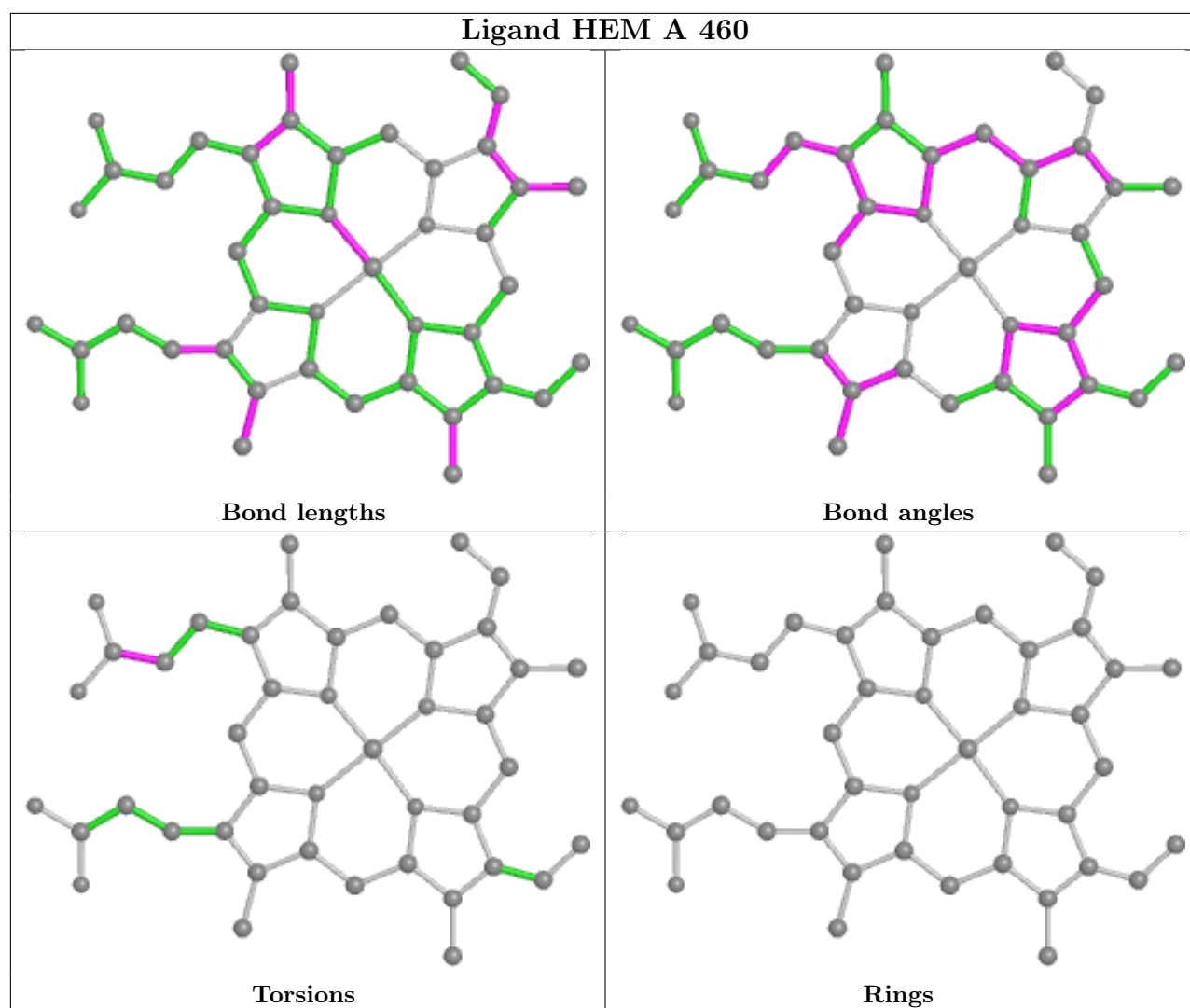
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	460	HEM	1	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	441/455 (96%)	-0.23	11 (2%) 57 60	12, 21, 38, 50	0
1	B	441/455 (96%)	-0.27	5 (1%) 80 82	13, 23, 38, 55	0
All	All	882/910 (96%)	-0.25	16 (1%) 68 71	12, 22, 38, 55	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	ASP	4.3
1	B	46	GLY	4.1
1	A	382	PRO	3.7
1	A	383	SER	3.3
1	A	12	GLY	3.2
1	A	384	ALA	3.0
1	A	14	LEU	2.9
1	A	169	GLN	2.8
1	A	201	ASN	2.8
1	A	369	ASP	2.6
1	B	382	PRO	2.4
1	A	11	PHE	2.3
1	B	229	GLN	2.3
1	B	136	ASP	2.3
1	A	202	LYS	2.2
1	A	21	ASN	2.2

### 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](#)

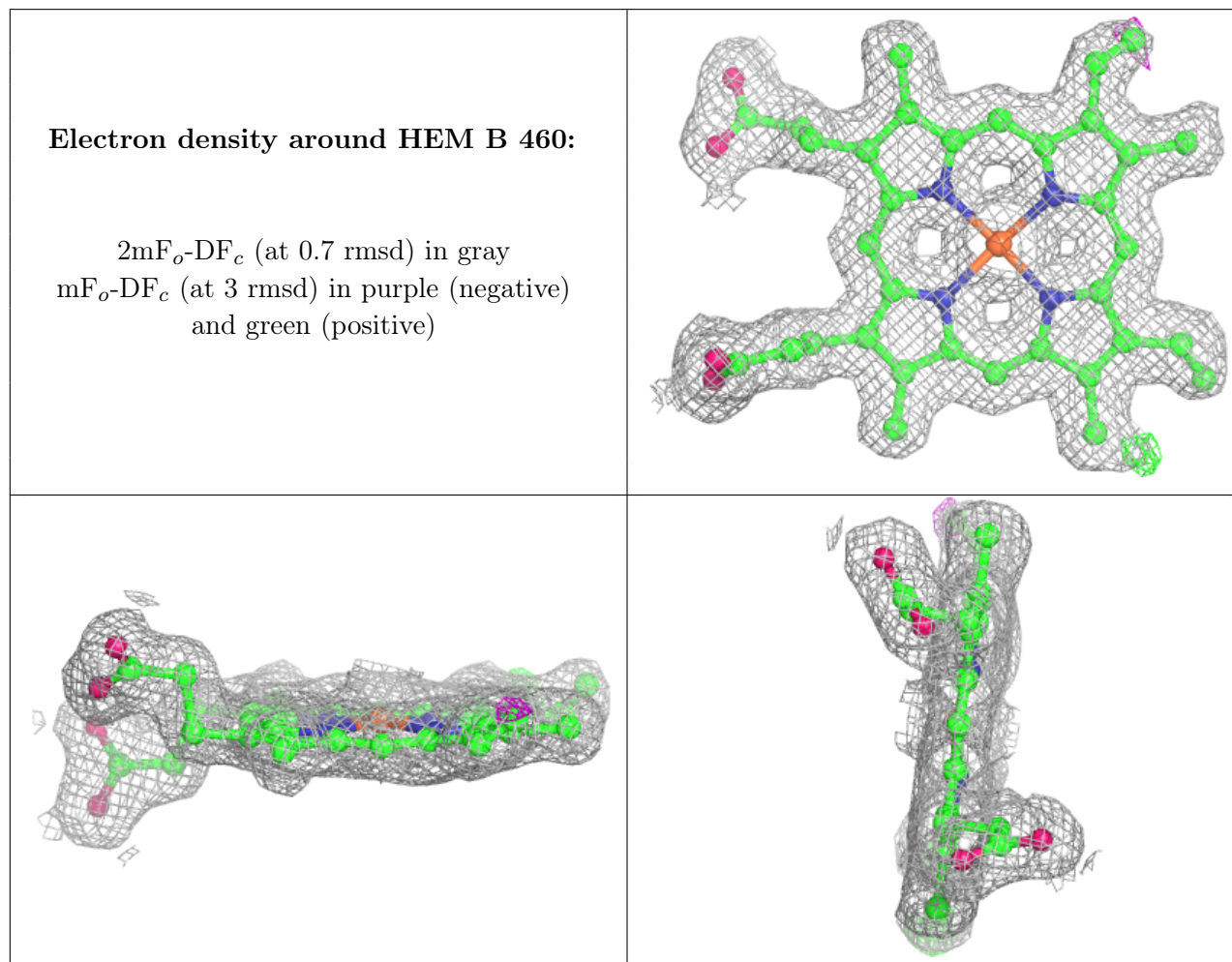
There are no monosaccharides in this entry.

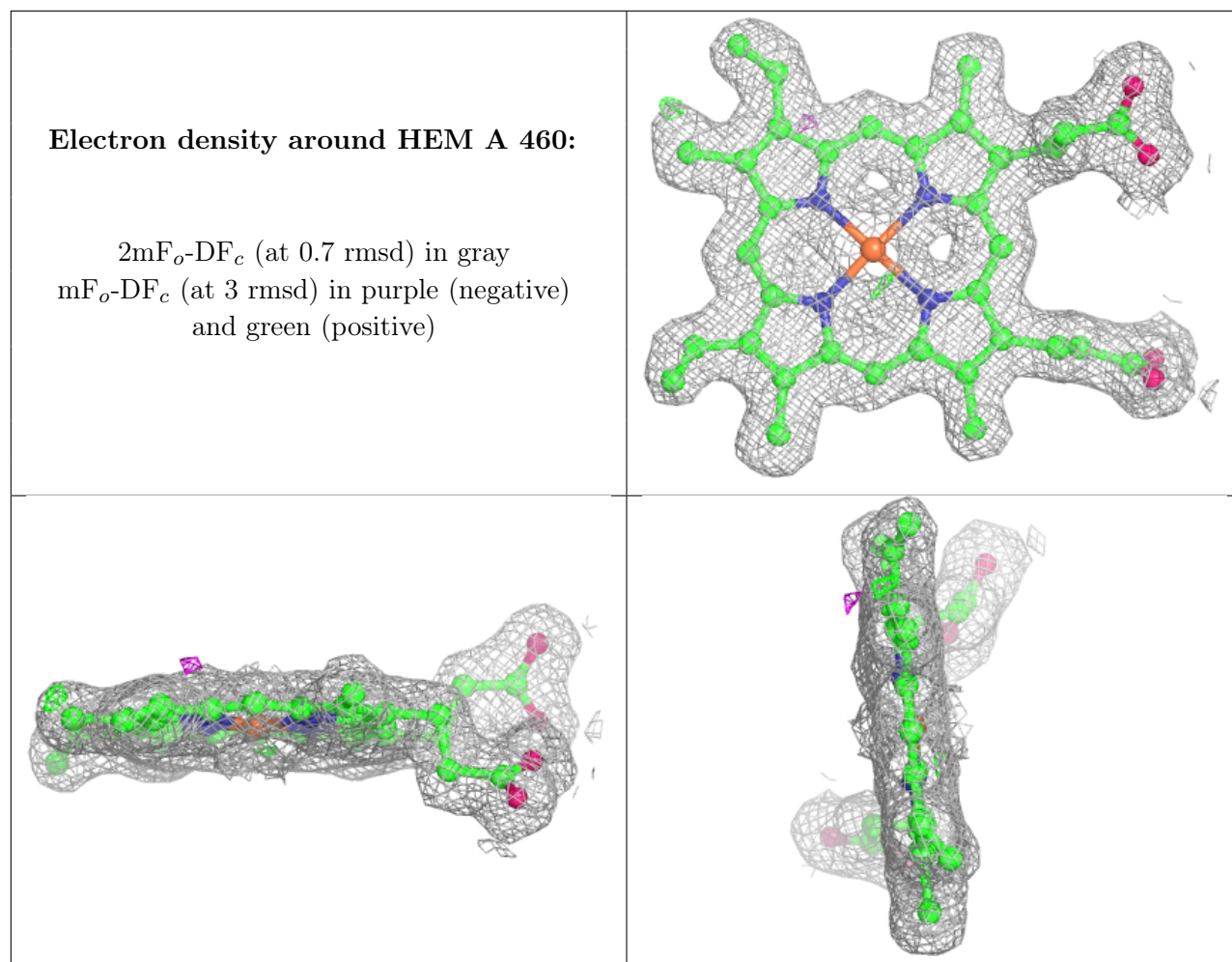
### 6.4 Ligands [i](#)

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
2	HEM	B	460	43/43	0.98	0.07	12,15,21,26	0
2	HEM	A	460	43/43	0.99	0.07	8,12,15,23	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.