



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 02:18 AM EDT

PDB ID : 2NNB  
Title : The Q403K mutant heme domain of flavocytochrome P450 BM3  
Authors : Clark, J.P.; Anderson, J.L.R.; Miles, C.S.; Mowat, C.G.; Reid, G.A.; Chapman, S.K.  
Deposited on : 2006-10-24  
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.

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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	:	2.23.2
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)	:	2.23.2

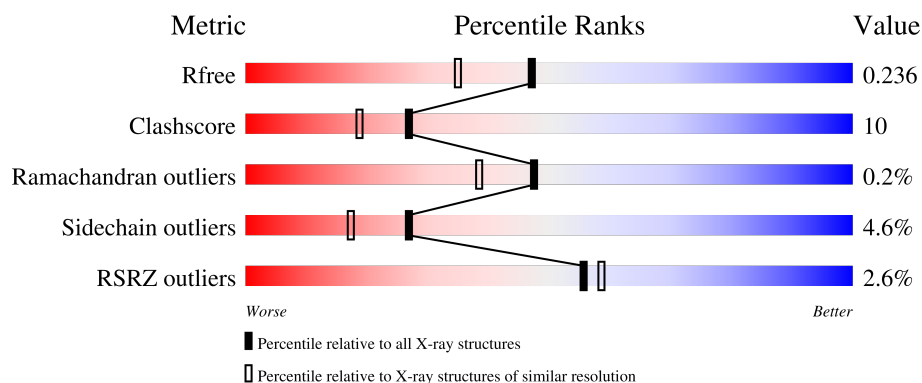
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

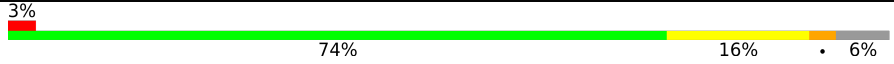

The reported resolution of this entry is 1.90 Å.

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	471	 3% 74% 16% • 6%
1	B	471	 0% 75% 16% • 6%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7898 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
1	A	441	Total	C	N	O	S	0	0	0
			3497	2245	593	642	17			
1	B	441	Total	C	N	O	S	0	0	0
			3515	2256	594	648	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	LYS	GLN	engineered mutation	UNP P14779
B	403	LYS	GLN	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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

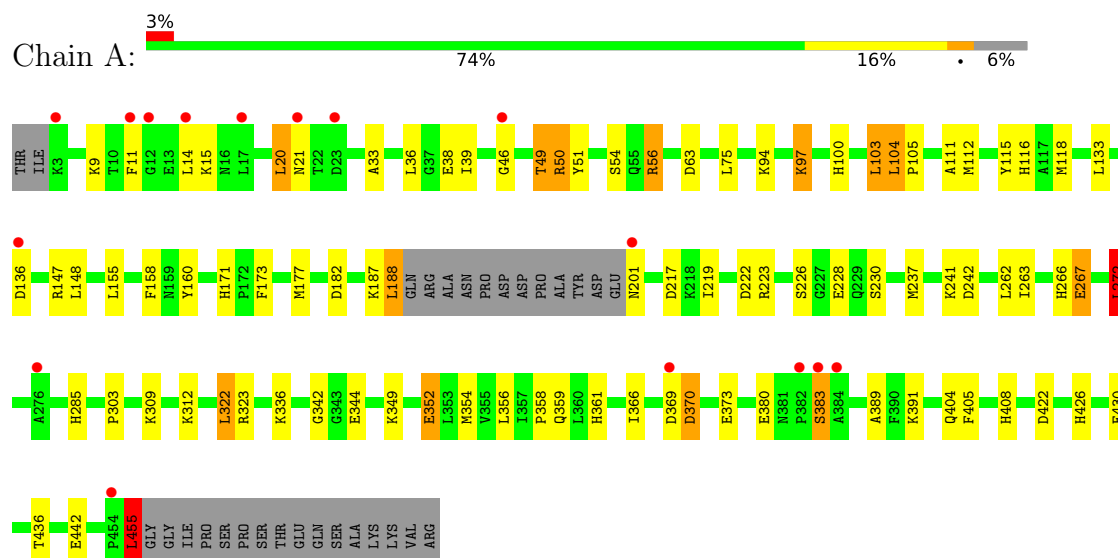
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	401	Total	O	0	0
			401	401		
3	B	399	Total	O	0	0
			399	399		

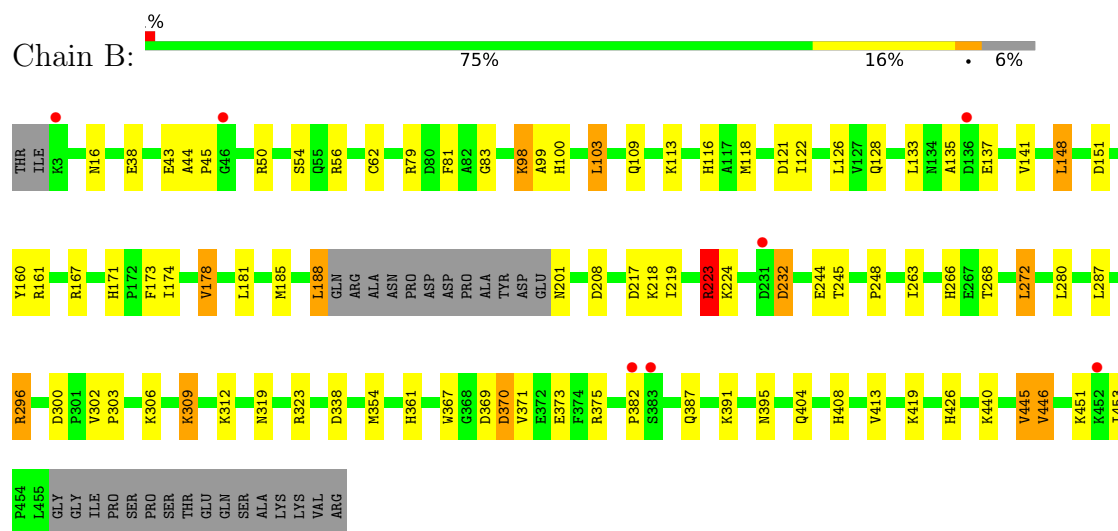
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	58.75Å 152.79Å 61.50Å 90.00° 94.67° 90.00°	Depositor
Resolution (Å)	24.00 – 1.90 23.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (24.00-1.90) 97.4 (23.52-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.182 , 0.233 0.186 , 0.236	Depositor DCC
$R_{free}$ test set	4118 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: 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	1.02	2/3577 (0.1%)	1.04	15/4841 (0.3%)
1	B	1.04	2/3596 (0.1%)	1.04	18/4863 (0.4%)
All	All	1.03	4/7173 (0.1%)	1.04	33/9704 (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	267	GLU	CD-OE1	7.75	1.34	1.25
1	B	141	VAL	CB-CG1	7.08	1.67	1.52
1	B	354	MET	SD-CE	-5.79	1.45	1.77
1	A	352	GLU	CD-OE1	5.30	1.31	1.25

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	ASP	CB-CG-OD2	12.34	129.41	118.30
1	B	223	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	B	223	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	370	ASP	CB-CG-OD2	8.53	125.97	118.30
1	A	50	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	B	445	VAL	CG1-CB-CG2	8.10	123.86	110.90
1	A	272	LEU	CB-CG-CD2	7.78	124.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	LEU	CB-CG-CD2	7.49	123.73	111.00
1	A	20	LEU	CA-CB-CG	7.45	132.43	115.30
1	B	300	ASP	CB-CG-OD2	7.43	124.99	118.30
1	B	446	VAL	CG1-CB-CG2	7.37	122.69	110.90
1	B	208	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	217	ASP	CB-CG-OD2	6.85	124.47	118.30
1	A	455	LEU	CA-CB-CG	6.76	130.86	115.30
1	B	338	ASP	CB-CG-OD2	6.69	124.32	118.30
1	B	151	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	148	LEU	CA-CB-CG	6.27	129.73	115.30
1	A	50	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	B	121	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	369	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	63	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	217	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	126	LEU	CB-CG-CD2	5.67	120.63	111.00
1	A	222	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	56	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	242	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	370	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	422	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	161	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	103	LEU	CB-CG-CD2	5.19	119.83	111.00
1	B	272	LEU	CB-CG-CD1	5.16	119.78	111.00
1	B	232	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	147	ARG	NE-CZ-NH2	-5.10	117.75	120.30

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

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	3497	0	3430	75	0
1	B	3515	0	3478	69	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	401	0	0	39	1
3	B	399	0	0	28	1
All	All	7898	0	6968	144	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 10.

All (144) 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:B:370:ASP:OD2	1:B:375:ARG:NH1	1.65	1.28
1:A:404:GLN:HG3	3:A:871:HOH:O	1.35	1.21
1:B:223:ARG:NH2	1:B:232:ASP:OD2	1.87	1.05
1:B:219:ILE:HD13	3:B:787:HOH:O	1.59	1.02
1:A:262:LEU:HA	3:A:792:HOH:O	1.61	1.00
1:A:111:ALA:O	3:A:846:HOH:O	1.78	0.99
1:A:356:LEU:HD13	1:A:358:PRO:HD2	1.47	0.94
1:A:201:ASN:N	3:A:517:HOH:O	2.01	0.93
1:A:33:ALA:HA	3:A:820:HOH:O	1.71	0.90
1:B:116:HIS:HD2	1:B:408:HIS:HE2	1.17	0.90
1:B:171:HIS:HD2	1:B:173:PHE:H	1.18	0.88
1:B:16:ASN:HD22	1:B:43:GLU:H	1.21	0.88
1:A:352:GLU:HB2	3:A:594:HOH:O	1.72	0.87
1:B:361:HIS:HE1	1:B:391:LYS:H	1.21	0.84
1:A:171:HIS:HD2	1:A:173:PHE:H	1.24	0.84
1:A:383:SER:HB2	3:A:827:HOH:O	1.77	0.83
1:A:361:HIS:HE1	1:A:391:LYS:H	1.27	0.82
1:A:97:LYS:HB2	3:A:689:HOH:O	1.82	0.79
1:B:404:GLN:HG3	3:B:766:HOH:O	1.81	0.79
1:B:201:ASN:N	3:B:598:HOH:O	2.16	0.79
1:A:158:PHE:CE2	1:A:219:ILE:HD13	2.18	0.78
1:A:373:GLU:HG3	3:A:686:HOH:O	1.83	0.77
1:A:118:MET:HG3	3:A:563:HOH:O	1.84	0.76
1:A:100:HIS:HD2	3:A:493:HOH:O	1.71	0.73
1:A:352:GLU:OE1	3:A:594:HOH:O	2.07	0.73
1:B:50:ARG:NH1	3:B:585:HOH:O	2.19	0.73
1:B:171:HIS:CD2	1:B:173:PHE:H	2.04	0.71
1:A:116:HIS:HD2	1:A:408:HIS:NE2	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:HE2	1:A:219:ILE:HD13	1.55	0.70
1:A:237:MET:CE	3:A:732:HOH:O	2.38	0.70
1:A:309:LYS:CB	3:A:629:HOH:O	2.39	0.69
1:B:223:ARG:HH22	1:B:232:ASP:CG	1.95	0.69
1:B:387:GLN:HB3	3:B:777:HOH:O	1.92	0.68
1:A:442:GLU:HG3	3:A:607:HOH:O	1.92	0.68
1:A:237:MET:HE3	3:A:732:HOH:O	1.94	0.67
1:A:188:LEU:C	3:A:670:HOH:O	2.34	0.67
1:A:285:HIS:HD2	3:A:802:HOH:O	1.77	0.66
1:B:426:HIS:H	1:B:426:HIS:CD2	2.14	0.64
1:A:49:THR:HG23	1:A:352:GLU:HG2	1.81	0.63
1:B:174:ILE:O	1:B:178:VAL:HG13	2.00	0.61
1:A:356:LEU:HD12	1:A:359:GLN:HG2	1.81	0.61
1:B:98:LYS:NZ	1:B:248:PRO:O	2.30	0.61
1:B:361:HIS:CE1	1:B:391:LYS:H	2.12	0.61
1:A:36:LEU:HB2	3:A:820:HOH:O	2.00	0.60
1:B:100:HIS:HE1	3:B:601:HOH:O	1.84	0.60
1:B:223:ARG:HD3	3:B:675:HOH:O	2.03	0.59
1:A:136:ASP:HA	3:A:675:HOH:O	2.02	0.59
1:A:171:HIS:CD2	1:A:173:PHE:H	2.13	0.59
1:B:100:HIS:HD2	3:B:495:HOH:O	1.86	0.59
1:B:116:HIS:CD2	1:B:408:HIS:HE2	2.08	0.58
1:B:137:GLU:CG	3:B:705:HOH:O	2.51	0.58
1:B:171:HIS:HD2	1:B:173:PHE:N	1.96	0.58
1:A:49:THR:HG23	1:A:352:GLU:CG	2.32	0.58
1:B:280:LEU:HB3	1:B:287:LEU:HD23	1.84	0.58
1:A:160:TYR:OH	1:A:171:HIS:HE1	1.87	0.57
1:B:137:GLU:HG3	3:B:705:HOH:O	2.05	0.57
1:B:306:LYS:HE2	3:B:600:HOH:O	2.04	0.57
1:B:373:GLU:HG3	3:B:795:HOH:O	2.05	0.56
1:B:160:TYR:OH	1:B:171:HIS:HE1	1.88	0.56
1:B:128:GLN:HG2	3:B:836:HOH:O	2.06	0.55
1:A:228:GLU:HB3	3:A:751:HOH:O	2.07	0.55
1:B:218:LYS:HE3	3:B:787:HOH:O	2.05	0.55
1:A:112:MET:C	3:A:846:HOH:O	2.46	0.54
1:B:296:ARG:HD2	3:B:701:HOH:O	2.07	0.54
1:A:380:GLU:CB	3:A:771:HOH:O	2.56	0.54
1:A:49:THR:CG2	1:A:352:GLU:HG2	2.38	0.53
1:A:361:HIS:CE1	1:A:391:LYS:H	2.18	0.53
1:A:226:SER:OG	1:A:228:GLU:HG2	2.08	0.53
1:B:56:ARG:HD2	3:B:602:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:HIS:HE1	1:B:303:PRO:O	1.91	0.53
1:B:81:PHE:HE1	1:B:263:ILE:HG21	1.74	0.52
1:A:112:MET:CA	3:A:846:HOH:O	2.56	0.52
1:A:223:ARG:HD3	1:A:228:GLU:HG3	1.90	0.52
1:B:122:ILE:HG22	1:B:148:LEU:HD22	1.92	0.52
1:A:267:GLU:CG	3:A:574:HOH:O	2.58	0.51
1:A:38:GLU:HB2	1:A:54:SER:HB3	1.92	0.51
1:A:455:LEU:C	3:A:640:HOH:O	2.49	0.51
1:B:118:MET:HG2	3:B:578:HOH:O	2.10	0.51
1:A:436:THR:HG21	3:A:819:HOH:O	2.10	0.51
1:B:309:LYS:N	1:B:309:LYS:HD2	2.25	0.51
1:B:109:GLN:HE22	1:B:309:LYS:HZ1	1.59	0.50
1:B:245:THR:HB	3:B:826:HOH:O	2.11	0.50
1:B:99:ALA:O	1:B:103:LEU:HB2	2.12	0.49
1:A:116:HIS:HE1	1:A:303:PRO:O	1.96	0.49
1:B:50:ARG:NE	3:B:572:HOH:O	2.26	0.49
1:A:158:PHE:HE2	1:A:219:ILE:CD1	2.24	0.49
1:B:109:GLN:HE22	1:B:309:LYS:NZ	2.12	0.48
1:B:323:ARG:HA	1:B:361:HIS:CD2	2.49	0.48
1:A:112:MET:HA	3:A:846:HOH:O	2.14	0.48
1:B:62:CYS:SG	1:B:391:LYS:HE2	2.54	0.48
1:B:268:THR:HB	2:B:472:HEM:C3B	2.49	0.47
1:B:382:PRO:HD2	3:B:688:HOH:O	2.13	0.47
1:A:223:ARG:CD	1:A:228:GLU:HG3	2.44	0.47
1:A:187:LYS:HE2	3:A:847:HOH:O	2.15	0.47
1:B:408:HIS:CD2	3:B:794:HOH:O	2.66	0.47
1:B:137:GLU:N	3:B:705:HOH:O	2.48	0.47
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.80	0.47
1:B:309:LYS:NZ	1:B:408:HIS:ND1	2.63	0.47
1:A:267:GLU:OE2	3:A:819:HOH:O	2.21	0.46
1:A:112:MET:SD	1:A:405:PHE:HA	2.55	0.46
1:A:104:LEU:N	1:A:105:PRO:HD2	2.30	0.46
1:B:44:ALA:HB1	1:B:45:PRO:HD2	1.97	0.46
1:B:391:LYS:HZ3	1:B:395:ASN:HD22	1.64	0.46
1:B:419:LYS:HE2	1:B:453:ILE:HG21	1.97	0.46
1:B:167:ARG:NH2	3:B:680:HOH:O	2.37	0.46
1:A:158:PHE:CD2	1:A:219:ILE:HD13	2.51	0.45
1:A:21:ASN:HB3	3:A:742:HOH:O	2.16	0.45
1:A:49:THR:HG22	1:A:50:ARG:H	1.81	0.45
1:B:185:MET:O	1:B:188:LEU:HB2	2.17	0.45
1:B:244:GLU:HG2	3:B:776:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MET:HG3	1:A:263:ILE:HD11	1.99	0.44
1:B:426:HIS:CD2	1:B:426:HIS:N	2.83	0.44
1:A:39:ILE:HA	1:A:51:TYR:O	2.16	0.44
1:A:373:GLU:CG	3:A:686:HOH:O	2.56	0.44
1:A:94:LYS:NZ	3:A:831:HOH:O	2.51	0.43
1:A:267:GLU:HB2	3:A:552:HOH:O	2.18	0.43
1:A:115:TYR:N	3:A:846:HOH:O	2.09	0.43
1:A:160:TYR:OH	1:A:171:HIS:CE1	2.69	0.43
1:B:160:TYR:OH	1:B:171:HIS:CE1	2.70	0.43
1:A:223:ARG:HD2	3:A:617:HOH:O	2.18	0.43
1:A:223:ARG:HD3	1:A:228:GLU:CG	2.49	0.43
1:A:56:ARG:NH2	1:A:342:GLY:O	2.52	0.43
1:A:266:HIS:HE1	3:A:773:HOH:O	2.02	0.43
1:A:342:GLY:O	1:A:344:GLU:HG3	2.18	0.42
1:A:366:ILE:HG21	1:A:389:ALA:HB1	2.01	0.42
1:B:312:LYS:HB2	3:B:801:HOH:O	2.19	0.42
1:B:113:LYS:HE2	3:B:758:HOH:O	2.18	0.42
1:B:266:HIS:HE1	3:B:562:HOH:O	2.01	0.42
1:B:287:LEU:C	1:B:287:LEU:HD13	2.39	0.42
1:A:9:LYS:HG2	1:A:11:PHE:CE1	2.55	0.42
1:A:426:HIS:CD2	1:A:426:HIS:H	2.38	0.42
1:B:38:GLU:HB2	1:B:54:SER:HB3	2.01	0.42
1:A:323:ARG:HA	1:A:361:HIS:CD2	2.54	0.42
1:A:354:MET:HE3	1:A:354:MET:HB2	1.77	0.42
1:A:336:LYS:O	1:A:349:LYS:HG3	2.19	0.42
1:A:182:ASP:CB	3:A:768:HOH:O	2.68	0.42
1:B:319:ASN:HD22	1:B:319:ASN:HA	1.61	0.41
1:B:79:ARG:HG3	1:B:83:GLY:O	2.20	0.41
1:B:148:LEU:HD11	1:B:413:VAL:HG21	2.01	0.41
1:B:223:ARG:HH11	1:B:223:ARG:CG	2.32	0.41
1:B:440:LYS:HB3	3:B:584:HOH:O	2.19	0.41
1:A:241:LYS:HE3	3:A:621:HOH:O	2.21	0.41
1:B:367:TRP:HB2	1:B:371:VAL:HG12	2.03	0.41
1:A:272:LEU:HG	1:A:322:LEU:HD13	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)
3:A:766:HOH:O	3:B:827:HOH:O[2_656]	2.11	0.09

## 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	437/471 (93%)	428 (98%)	8 (2%)	1 (0%)	47	38
1	B	437/471 (93%)	418 (96%)	18 (4%)	1 (0%)	47	38
All	All	874/942 (93%)	846 (97%)	26 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	ASP
1	B	135	ALA

### 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	369/412 (90%)	350 (95%)	19 (5%)	24	14
1	B	377/412 (92%)	362 (96%)	15 (4%)	31	22
All	All	746/824 (90%)	712 (95%)	34 (5%)	27	17

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	15	LYS
1	A	20	LEU
1	A	49	THR

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Mol	Chain	Res	Type
1	A	75	LEU
1	A	97	LYS
1	A	103	LEU
1	A	104	LEU
1	A	133	LEU
1	A	148	LEU
1	A	155	LEU
1	A	188	LEU
1	A	230	SER
1	A	272	LEU
1	A	312	LYS
1	A	322	LEU
1	A	383	SER
1	A	430	GLU
1	A	455	LEU
1	B	98	LYS
1	B	103	LEU
1	B	133	LEU
1	B	178	VAL
1	B	181	LEU
1	B	188	LEU
1	B	223	ARG
1	B	224	LYS
1	B	272	LEU
1	B	296	ARG
1	B	302	VAL
1	B	309	LYS
1	B	445	VAL
1	B	446	VAL
1	B	451	LYS

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	100	HIS
1	A	110	GLN
1	A	116	HIS
1	A	159	ASN
1	A	171	HIS

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Mol	Chain	Res	Type
1	A	266	HIS
1	A	319	ASN
1	A	361	HIS
1	A	395	ASN
1	A	426	HIS
1	B	7	GLN
1	B	16	ASN
1	B	92	HIS
1	B	95	ASN
1	B	100	HIS
1	B	109	GLN
1	B	116	HIS
1	B	171	HIS
1	B	266	HIS
1	B	319	ASN
1	B	361	HIS
1	B	387	GLN
1	B	388	HIS
1	B	395	ASN
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 [i](#)

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	472	1,3	27,50,50	2.30	10 (37%)	17,82,82	2.24	6 (35%)
2	HEM	A	472	1,3	27,50,50	2.05	7 (25%)	17,82,82	1.87	4 (23%)

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	472	1,3	-	0/6/54/54	-
2	HEM	A	472	1,3	-	0/6/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	HEM	C3B-C2B	-5.95	1.32	1.40
2	A	472	HEM	C3B-C2B	-5.47	1.32	1.40
2	A	472	HEM	C3C-C2C	-5.10	1.33	1.40
2	B	472	HEM	C3D-C2D	4.37	1.50	1.37
2	B	472	HEM	C3C-C2C	-3.62	1.35	1.40
2	B	472	HEM	C3B-CAB	3.52	1.55	1.47
2	B	472	HEM	C3C-CAC	3.41	1.54	1.47
2	B	472	HEM	CAA-C2A	3.15	1.56	1.52
2	A	472	HEM	C3B-CAB	3.09	1.54	1.47
2	B	472	HEM	CMB-C2B	2.75	1.58	1.51
2	B	472	HEM	C1A-NA	2.62	1.41	1.36
2	A	472	HEM	C3D-C2D	2.59	1.45	1.37
2	A	472	HEM	CMC-C2C	2.36	1.57	1.51
2	A	472	HEM	C4B-NB	2.23	1.40	1.36
2	B	472	HEM	CMD-C2D	2.17	1.56	1.51
2	A	472	HEM	C3C-CAC	2.09	1.52	1.47
2	B	472	HEM	CMC-C2C	2.05	1.56	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	472	HEM	CBD-CAD-C3D	-4.29	104.58	112.48
2	B	472	HEM	CBD-CAD-C3D	-4.17	104.80	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	472	HEM	C1D-C2D-C3D	-4.09	104.15	107.00
2	B	472	HEM	C4C-C3C-C2C	3.72	109.50	106.90
2	B	472	HEM	CBA-CAA-C2A	-3.72	105.62	112.49
2	A	472	HEM	CBA-CAA-C2A	-2.88	107.17	112.49
2	B	472	HEM	C4A-C3A-C2A	2.72	108.89	107.00
2	A	472	HEM	CMA-C3A-C4A	-2.43	124.73	128.46
2	A	472	HEM	C4C-C3C-C2C	2.42	108.59	106.90
2	B	472	HEM	CMA-C3A-C4A	-2.19	125.09	128.46

There are no chirality outliers.

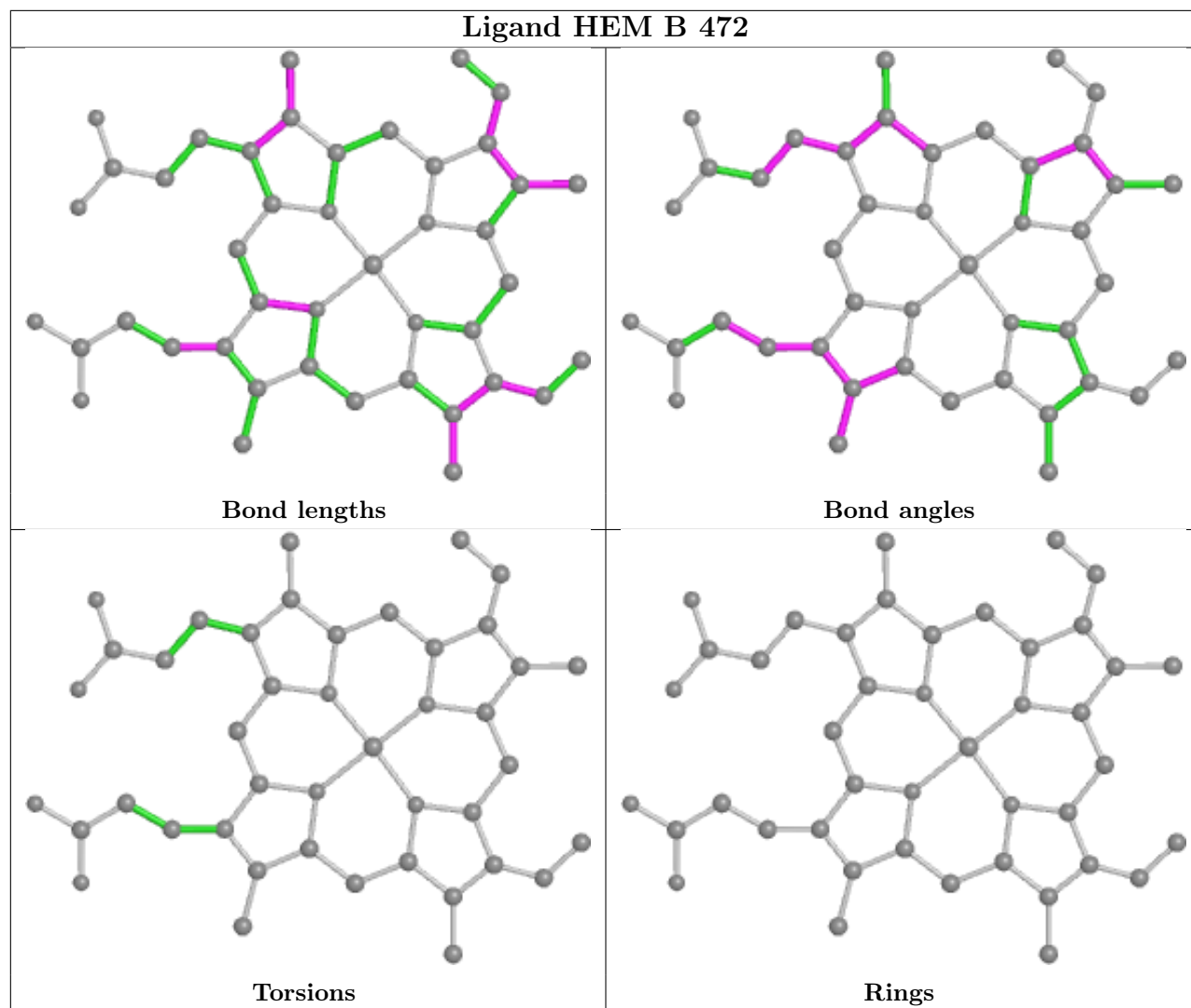
There are no torsion outliers.

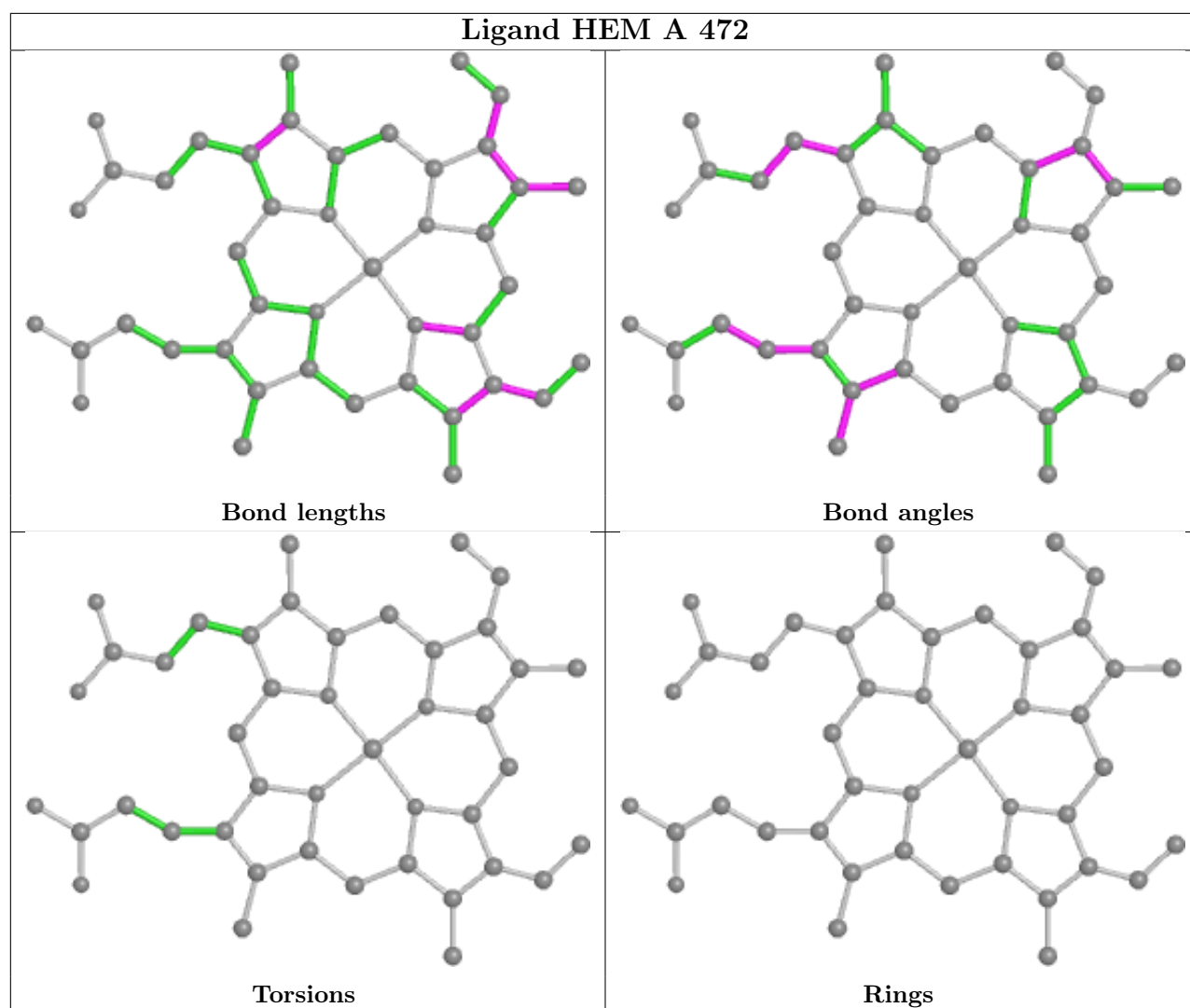
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	472	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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	441/471 (93%)	-0.20	16 (3%) 42 45	16, 26, 41, 58	0
1	B	441/471 (93%)	-0.24	7 (1%) 72 74	18, 28, 41, 52	0
All	All	882/942 (93%)	-0.22	23 (2%) 56 58	16, 27, 42, 58	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	GLY	4.4
1	A	383	SER	4.1
1	A	21	ASN	3.6
1	A	3	LYS	3.5
1	A	382	PRO	3.3
1	A	384	ALA	3.1
1	A	12	GLY	2.9
1	B	231	ASP	2.7
1	A	14	LEU	2.7
1	B	383	SER	2.7
1	B	382	PRO	2.7
1	A	23	ASP	2.5
1	A	136	ASP	2.5
1	B	136	ASP	2.4
1	A	46	GLY	2.3
1	A	369	ASP	2.3
1	A	201	ASN	2.2
1	B	452	LYS	2.2
1	A	17	LEU	2.2
1	A	276	ALA	2.2
1	B	3	LYS	2.2
1	A	11	PHE	2.2
1	A	454	PRO	2.1

## 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](#)

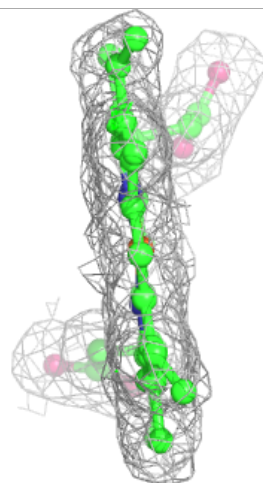
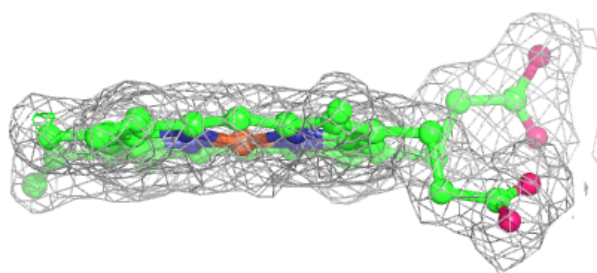
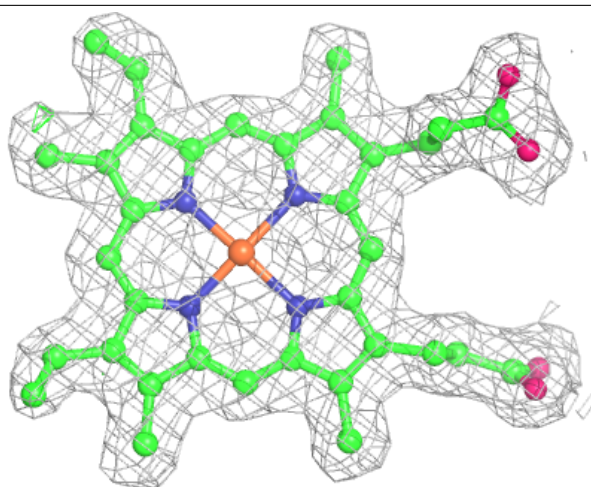
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

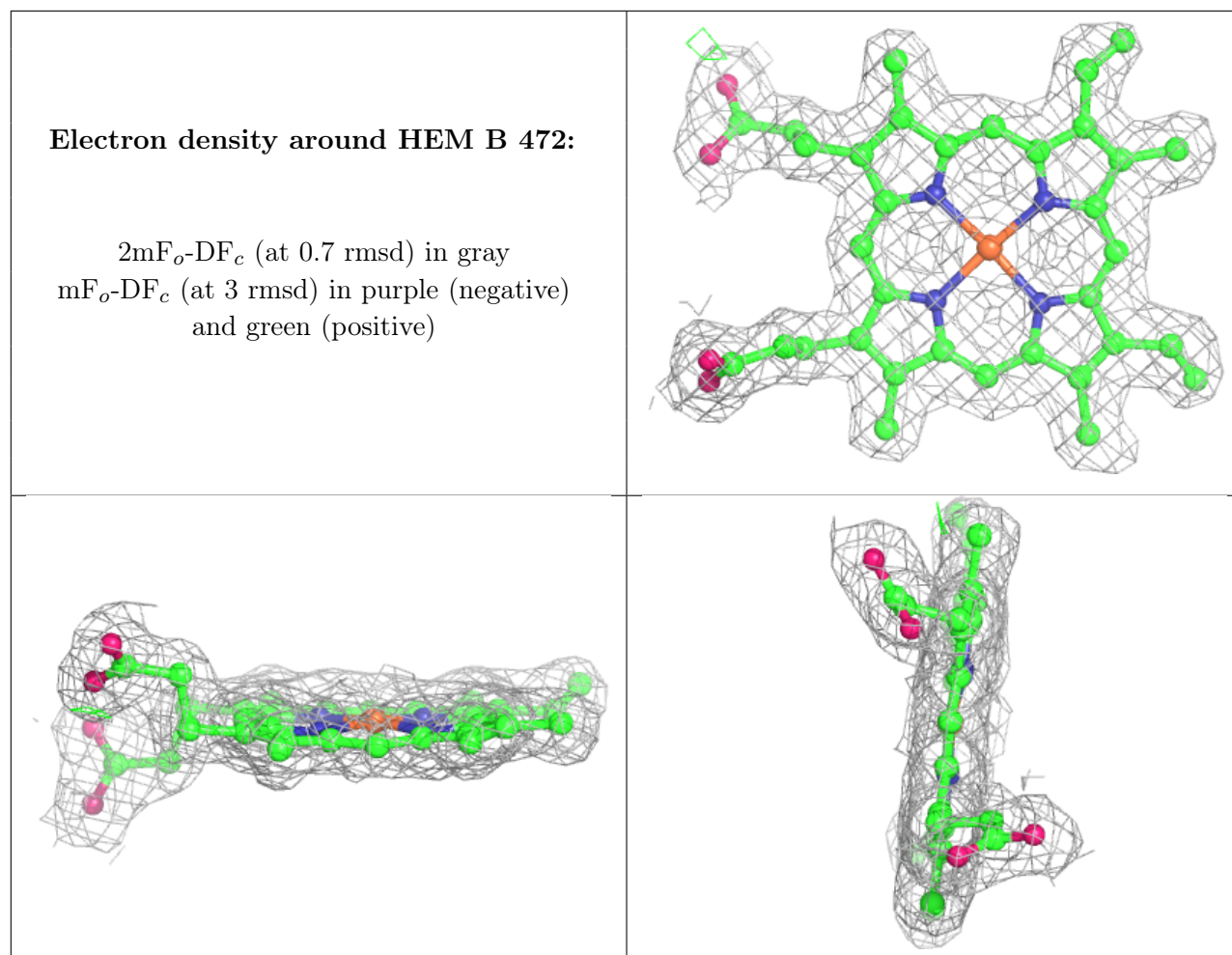
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	472	43/43	0.98	0.08	13,17,20,26	0
2	HEM	B	472	43/43	0.99	0.07	14,19,22,30	0

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 472:**

$2mF_o-DF_c$  (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.