



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 01:34 AM EDT

PDB ID : 1P0V  
Title : F393A mutant heme domain of flavocytochrome P450 BM3  
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Deposited on : 2003-04-11  
Resolution : 2.05 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

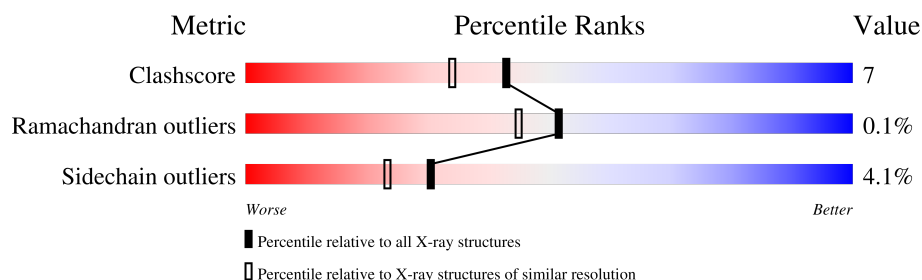
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	455	 80% 15% . .
1	B	455	 78% 16% . . .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8552 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
			3510	2249	595	649	17			
1	B	444	Total	C	N	O	S	0	0	0
			3547	2271	596	663	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	ALA	PHE	engineered mutation	UNP P14779
B	393	ALA	PHE	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.

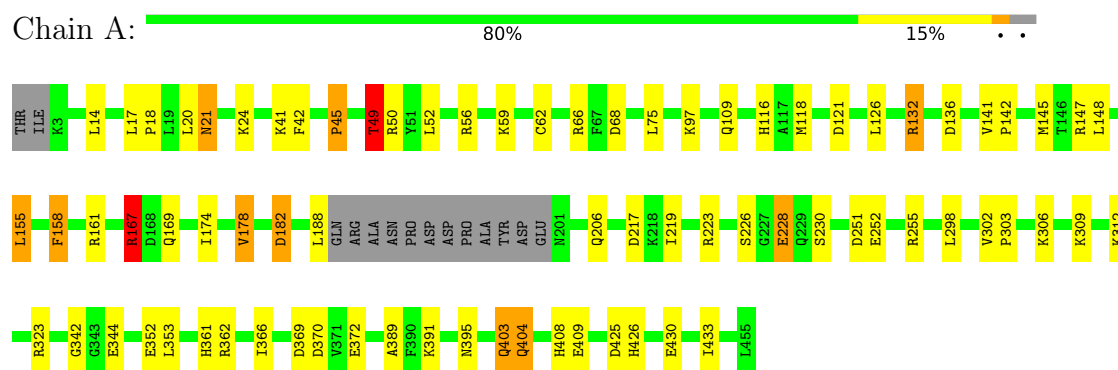
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	644	Total	O	0	0
			644	644		
3	B	765	Total	O	0	0
			765	765		

### 3 Residue-property plots

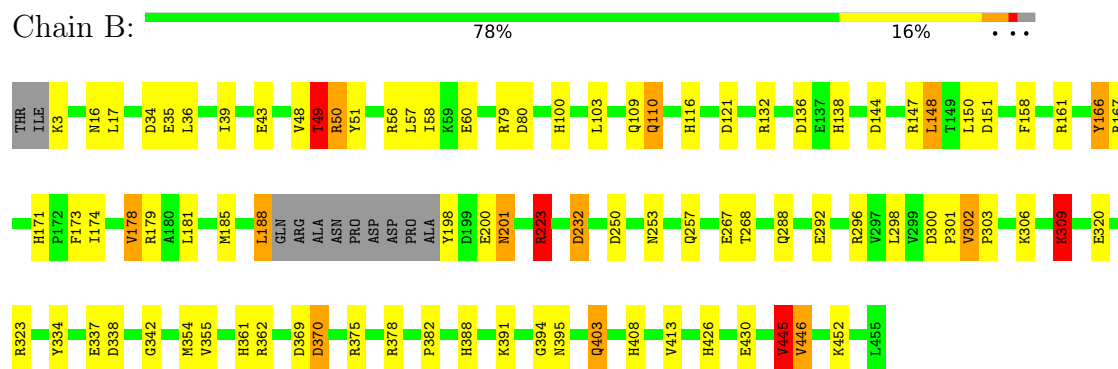
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

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



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



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.69Å 152.91Å 61.20Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	20.00 – 2.05	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.05)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.169 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 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	0.66	0/3589	1.74	39/4856 (0.8%)
1	B	0.67	0/3628	1.52	45/4908 (0.9%)
All	All	0.67	0/7217	1.63	84/9764 (0.9%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	NE-CZ-NH2	41.98	141.29	120.30
1	A	132	ARG	NH1-CZ-NH2	-30.10	86.29	119.40
1	A	167	ARG	CG-CD-NE	29.92	174.63	111.80
1	A	132	ARG	NE-CZ-NH1	23.46	132.03	120.30
1	A	50	ARG	NE-CZ-NH1	-18.21	111.19	120.30
1	B	223	ARG	NE-CZ-NH2	-18.02	111.29	120.30
1	B	50	ARG	NE-CZ-NH2	-16.50	112.05	120.30
1	B	296	ARG	NE-CZ-NH1	15.64	128.12	120.30
1	A	132	ARG	CD-NE-CZ	-15.52	101.87	123.60
1	B	296	ARG	CD-NE-CZ	15.51	145.31	123.60
1	A	136	ASP	CB-CG-OD1	15.00	131.80	118.30
1	B	369	ASP	CB-CG-OD2	14.13	131.02	118.30
1	A	50	ARG	NE-CZ-NH2	13.65	127.13	120.30
1	A	323	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	255	ARG	NE-CZ-NH1	-11.83	114.38	120.30
1	A	323	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	B	50	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	A	161	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	50	ARG	CD-NE-CZ	10.09	137.72	123.60
1	B	430	GLU	OE1-CD-OE2	-9.92	111.39	123.30
1	B	223	ARG	CD-NE-CZ	9.80	137.33	123.60
1	A	182	ASP	CB-CG-OD1	-9.29	109.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ARG	NE-CZ-NH2	8.93	124.77	120.30
1	B	223	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	B	161	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	B	147	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	B	250	ASP	CB-CG-OD1	8.63	126.07	118.30
1	B	136	ASP	CB-CG-OD1	8.29	125.76	118.30
1	B	167	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	251	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	147	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	121	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	167	ARG	CA-CB-CG	7.74	130.42	113.40
1	B	362	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	378	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	370	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	79	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	68	ASP	CB-CG-OD1	7.15	124.73	118.30
1	B	34	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	161	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	56	ARG	CD-NE-CZ	7.07	133.50	123.60
1	B	56	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	A	136	ASP	OD1-CG-OD2	-6.83	110.33	123.30
1	A	182	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	80	ASP	CB-CG-OD1	6.45	124.10	118.30
1	B	445	VAL	N-CA-CB	-6.44	97.33	111.50
1	A	49	THR	N-CA-CB	6.44	122.53	110.30
1	B	166	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	B	232	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	21	ASN	CA-CB-CG	6.30	127.26	113.40
1	B	144	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	446	VAL	N-CA-CB	-6.18	97.90	111.50
1	B	151	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	445	VAL	CG1-CB-CG2	6.10	120.67	110.90
1	B	370	ASP	CB-CG-OD1	6.08	123.78	118.30
1	B	151	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	372	GLU	OE1-CD-OE2	-6.06	116.03	123.30
1	B	337	GLU	OE1-CD-OE2	-6.06	116.03	123.30
1	A	217	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	320	GLU	OE1-CD-OE2	-6.02	116.07	123.30
1	B	403	GLN	CG-CD-NE2	5.97	131.04	116.70
1	A	369	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	41	LYS	CA-CB-CG	5.75	126.04	113.40
1	B	338	ASP	CB-CG-OD2	5.74	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	49	THR	N-CA-CB	5.71	121.15	110.30
1	A	228	GLU	OE1-CD-OE2	5.71	130.15	123.30
1	B	446	VAL	CA-CB-CG1	5.65	119.38	110.90
1	B	362	ARG	CD-NE-CZ	5.59	131.43	123.60
1	A	425	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	362	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	252	GLU	OE1-CD-OE2	-5.57	116.61	123.30
1	B	179	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	296	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
1	A	66	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	147	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	145	MET	CG-SD-CE	5.25	108.60	100.20
1	B	121	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	334	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	200	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	B	267	GLU	OE1-CD-OE2	5.15	129.47	123.30
1	B	302	VAL	N-CA-CB	-5.13	100.20	111.50
1	A	404	GLN	N-CA-CB	5.08	119.75	110.60
1	B	309	LYS	CB-CG-CD	5.05	124.73	111.60

There are no chirality outliers.

There are no planarity outliers.

## 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	3510	0	3453	39	4
1	B	3547	0	3491	56	1
2	A	43	0	30	0	0
2	B	43	0	30	2	0
3	A	644	0	0	11	0
3	B	765	0	0	11	3
All	All	8552	0	7004	96	4

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 (96) 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:59:LYS:CE	1:A:59:LYS:CG	2.50	0.90
1:B:116:HIS:HD2	1:B:408:HIS:HE2	1.20	0.88
1:A:116:HIS:HD2	1:A:408:HIS:HE2	1.22	0.85
1:B:361:HIS:HE1	1:B:391:LYS:H	1.28	0.82
1:B:16:ASN:HD22	1:B:43:GLU:H	1.28	0.82
1:A:361:HIS:HE1	1:A:391:LYS:H	1.26	0.81
1:A:118:MET:HG3	3:A:694:HOH:O	1.82	0.80
1:B:49:THR:HG21	1:B:354:MET:HG2	1.68	0.74
1:B:171:HIS:HD2	1:B:173:PHE:H	1.34	0.74
1:B:174:ILE:O	1:B:178:VAL:HG13	1.95	0.67
1:B:223:ARG:NH2	1:B:232:ASP:OD2	2.28	0.66
1:A:141:VAL:HB	1:A:142:PRO:HD3	1.77	0.66
1:B:100:HIS:HD2	3:B:560:HOH:O	1.80	0.65
1:B:370:ASP:OD2	1:B:375:ARG:NH2	2.28	0.62
1:B:43:GLU:HG2	1:B:48:VAL:HG22	1.81	0.62
1:B:35:GLU:HG2	1:B:36:LEU:HD23	1.82	0.61
1:B:201:ASN:HD22	1:B:201:ASN:H	1.49	0.61
1:B:391:LYS:NZ	1:B:395:ASN:HD22	1.99	0.60
1:A:167:ARG:HG3	1:A:169:GLN:O	2.00	0.60
1:A:17:LEU:HB3	1:A:18:PRO:HD3	1.84	0.60
1:B:3:LYS:HD2	3:B:1119:HOH:O	2.02	0.60
1:A:109:GLN:NE2	1:A:309:LYS:HZ2	2.01	0.59
1:B:57:LEU:HD21	3:B:1013:HOH:O	2.02	0.59
1:B:388:HIS:HD2	1:B:391:LYS:HZ3	1.52	0.57
1:B:16:ASN:ND2	1:B:43:GLU:H	2.00	0.57
1:A:404:GLN:HG2	3:A:862:HOH:O	2.05	0.57
1:B:116:HIS:CD2	1:B:408:HIS:HE2	2.12	0.57
1:A:109:GLN:HE22	1:A:309:LYS:NZ	2.02	0.56
1:B:171:HIS:CD2	1:B:173:PHE:H	2.20	0.56
1:B:223:ARG:HD3	3:B:730:HOH:O	2.04	0.56
1:A:126:LEU:C	1:A:126:LEU:HD13	2.27	0.55
1:A:109:GLN:HE22	1:A:309:LYS:HZ2	1.52	0.55
1:A:97:LYS:HB2	3:A:857:HOH:O	2.07	0.54
1:A:158:PHE:CE2	1:A:219:ILE:HD13	2.41	0.54
1:A:174:ILE:O	1:A:178:VAL:HG13	2.08	0.53
1:A:118:MET:SD	1:A:155:LEU:HD13	2.47	0.53
1:A:391:LYS:NZ	1:A:395:ASN:HD22	2.07	0.53
1:B:391:LYS:HE3	1:B:394:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ARG:HA	1:B:361:HIS:CD2	2.44	0.52
1:B:300:ASP:HB3	1:B:301:PRO:HD2	1.92	0.52
1:B:198:TYR:HA	1:B:201:ASN:ND2	2.23	0.52
1:A:62:CYS:HB3	1:A:395:ASN:ND2	2.26	0.51
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.93	0.51
1:B:116:HIS:HE1	1:B:303:PRO:O	1.94	0.51
1:B:388:HIS:HD2	1:B:391:LYS:NZ	2.09	0.51
1:B:109:GLN:HE22	1:B:309:LYS:HZ3	1.58	0.51
1:A:302:VAL:HG22	3:A:917:HOH:O	2.11	0.50
1:A:118:MET:HE1	3:A:912:HOH:O	2.10	0.50
2:B:460:HEM:HBC2	2:B:460:HEM:HMC2	1.93	0.50
1:B:109:GLN:HE22	1:B:309:LYS:NZ	2.10	0.50
1:B:201:ASN:H	1:B:201:ASN:ND2	2.09	0.50
1:B:452:LYS:HE2	3:B:807:HOH:O	2.11	0.50
1:B:391:LYS:HZ3	1:B:395:ASN:HD22	1.59	0.49
1:B:132:ARG:NH2	3:B:517:HOH:O	2.46	0.49
1:B:39:ILE:HA	1:B:51:TYR:O	2.12	0.49
1:B:49:THR:HG22	1:B:50:ARG:H	1.77	0.49
1:A:14:LEU:HD12	3:A:955:HOH:O	2.12	0.48
1:B:3:LYS:HD3	1:B:3:LYS:HA	1.79	0.47
1:A:403:GLN:HG2	3:A:1098:HOH:O	2.15	0.47
1:B:60:GLU:OE2	1:B:342:GLY:HA2	2.16	0.46
1:B:298:LEU:HD22	1:B:303:PRO:HB3	1.98	0.46
1:B:58:ILE:HD13	1:B:355:VAL:HG13	1.97	0.46
1:B:300:ASP:HB3	1:B:301:PRO:CD	2.46	0.46
1:B:185:MET:O	1:B:188:LEU:HB2	2.16	0.46
1:B:253:ASN:O	1:B:257:GLN:HG2	2.16	0.46
1:A:118:MET:HB3	1:A:155:LEU:HD13	1.98	0.45
1:B:178:VAL:HG22	3:B:732:HOH:O	2.16	0.45
1:B:306:LYS:HE3	3:B:1171:HOH:O	2.17	0.44
1:B:110:GLN:HG2	3:B:1069:HOH:O	2.16	0.44
1:A:24:LYS:HE2	1:A:433:ILE:O	2.17	0.44
1:B:150:LEU:HD13	1:B:174:ILE:HD13	1.99	0.44
1:A:361:HIS:HE1	1:A:391:LYS:N	2.03	0.44
1:A:116:HIS:CD2	1:A:408:HIS:HE2	2.14	0.43
1:A:342:GLY:O	1:A:344:GLU:HG3	2.18	0.43
1:A:409:GLU:HG2	3:A:1095:HOH:O	2.18	0.42
1:B:17:LEU:HD23	3:B:1057:HOH:O	2.19	0.42
1:A:52:LEU:HD11	1:A:353:LEU:HD13	2.01	0.42
1:A:426:HIS:HE1	3:A:520:HOH:O	2.01	0.42
1:B:138:HIS:CD2	1:B:445:VAL:HG22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLN:O	1:B:292:GLU:HG3	2.19	0.42
1:B:138:HIS:HD2	1:B:445:VAL:HG22	1.85	0.42
1:A:206:GLN:HG2	3:A:877:HOH:O	2.20	0.41
1:A:366:ILE:HG21	1:A:389:ALA:HB1	2.03	0.41
1:B:382:PRO:HD2	3:B:744:HOH:O	2.20	0.41
1:B:268:THR:HB	2:B:460:HEM:C3B	2.55	0.41
1:A:298:LEU:HD22	1:A:303:PRO:HB3	2.03	0.41
1:A:49:THR:HG23	1:A:352:GLU:HB2	2.02	0.41
1:A:141:VAL:HB	1:A:142:PRO:CD	2.49	0.41
1:A:223:ARG:HG3	3:A:544:HOH:O	2.21	0.41
1:A:116:HIS:HE1	1:A:303:PRO:O	2.04	0.41
1:B:426:HIS:CE1	1:B:445:VAL:HG13	2.56	0.41
1:B:370:ASP:OD2	1:B:375:ARG:NH1	2.49	0.40
1:A:20:LEU:HG	1:A:42:PHE:HZ	1.86	0.40
1:A:226:SER:OG	1:A:228:GLU:HG2	2.21	0.40
1:B:109:GLN:NE2	1:B:309:LYS:HZ3	2.19	0.40
1:B:391:LYS:HE2	1:B:395:ASN:HB2	2.03	0.40

All (4) 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)
1:A:132:ARG:NH1	3:B:485:HOH:O[2_656]	1.86	0.34
1:A:132:ARG:NH2	1:B:166:TYR:OH[2_656]	1.96	0.24
1:A:132:ARG:NE	3:B:485:HOH:O[2_656]	1.99	0.21
1:A:132:ARG:CZ	3:B:485:HOH:O[2_656]	2.01	0.19

## 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	437/455 (96%)	426 (98%)	10 (2%)	1 (0%)	47 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	440/455 (97%)	428 (97%)	12 (3%)	0	100	100
All	All	877/910 (96%)	854 (97%)	22 (2%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PRO

### 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	373/398 (94%)	357 (96%)	16 (4%)	29	22
1	B	381/398 (96%)	366 (96%)	15 (4%)	32	25
All	All	754/796 (95%)	723 (96%)	31 (4%)	30	23

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	45	PRO
1	A	49	THR
1	A	75	LEU
1	A	148	LEU
1	A	155	LEU
1	A	158	PHE
1	A	167	ARG
1	A	178	VAL
1	A	182	ASP
1	A	188	LEU
1	A	230	SER
1	A	306	LYS
1	A	312	LYS
1	A	403	GLN

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Mol	Chain	Res	Type
1	A	430	GLU
1	B	49	THR
1	B	103	LEU
1	B	110	GLN
1	B	148	LEU
1	B	158	PHE
1	B	178	VAL
1	B	181	LEU
1	B	188	LEU
1	B	201	ASN
1	B	223	ARG
1	B	302	VAL
1	B	309	LYS
1	B	403	GLN
1	B	445	VAL
1	B	446	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	95	ASN
1	A	109	GLN
1	A	110	GLN
1	A	116	HIS
1	A	266	HIS
1	A	319	ASN
1	A	361	HIS
1	A	395	ASN
1	A	403	GLN
1	A	404	GLN
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	110	GLN
1	B	116	HIS
1	B	128	GLN
1	B	171	HIS

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Mol	Chain	Res	Type
1	B	201	ASN
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	404	GLN

### 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	A	460	1,3	27,50,50	1.96	8 (29%)	17,82,82	1.52	4 (23%)
2	HEM	B	460	1	27,50,50	2.12	7 (25%)	17,82,82	1.32	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
2	HEM	A	460	1,3	-	0/6/54/54	-
2	HEM	B	460	1	-	0/6/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	460	HEM	C3B-C2B	-5.47	1.32	1.40
2	A	460	HEM	C3C-C2C	-5.06	1.33	1.40
2	A	460	HEM	C3B-C2B	-5.01	1.33	1.40
2	B	460	HEM	C3C-C2C	-4.71	1.33	1.40
2	B	460	HEM	CAA-C2A	4.09	1.58	1.52
2	A	460	HEM	C3C-CAC	2.97	1.53	1.47
2	B	460	HEM	C3B-CAB	2.90	1.53	1.47
2	B	460	HEM	C3C-CAC	2.85	1.53	1.47
2	A	460	HEM	CMC-C2C	2.25	1.56	1.51
2	A	460	HEM	CAA-C2A	2.19	1.55	1.52
2	B	460	HEM	CMD-C2D	2.14	1.56	1.51
2	A	460	HEM	C3B-CAB	2.12	1.52	1.47
2	B	460	HEM	C1A-NA	2.08	1.40	1.36
2	A	460	HEM	CMD-C2D	2.06	1.55	1.51
2	A	460	HEM	C4B-NB	2.02	1.40	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	460	HEM	CMA-C3A-C4A	-2.96	123.91	128.46
2	A	460	HEM	CMC-C2C-C3C	2.60	129.55	124.68
2	B	460	HEM	CMD-C2D-C1D	-2.50	124.62	128.46
2	A	460	HEM	CMD-C2D-C1D	-2.23	125.04	128.46
2	A	460	HEM	CMA-C3A-C2A	2.13	128.96	124.94
2	B	460	HEM	CMD-C2D-C3D	2.01	128.73	124.94
2	B	460	HEM	CMB-C2B-C3B	2.00	128.42	124.68

There are no chirality outliers.

There are no torsion outliers.

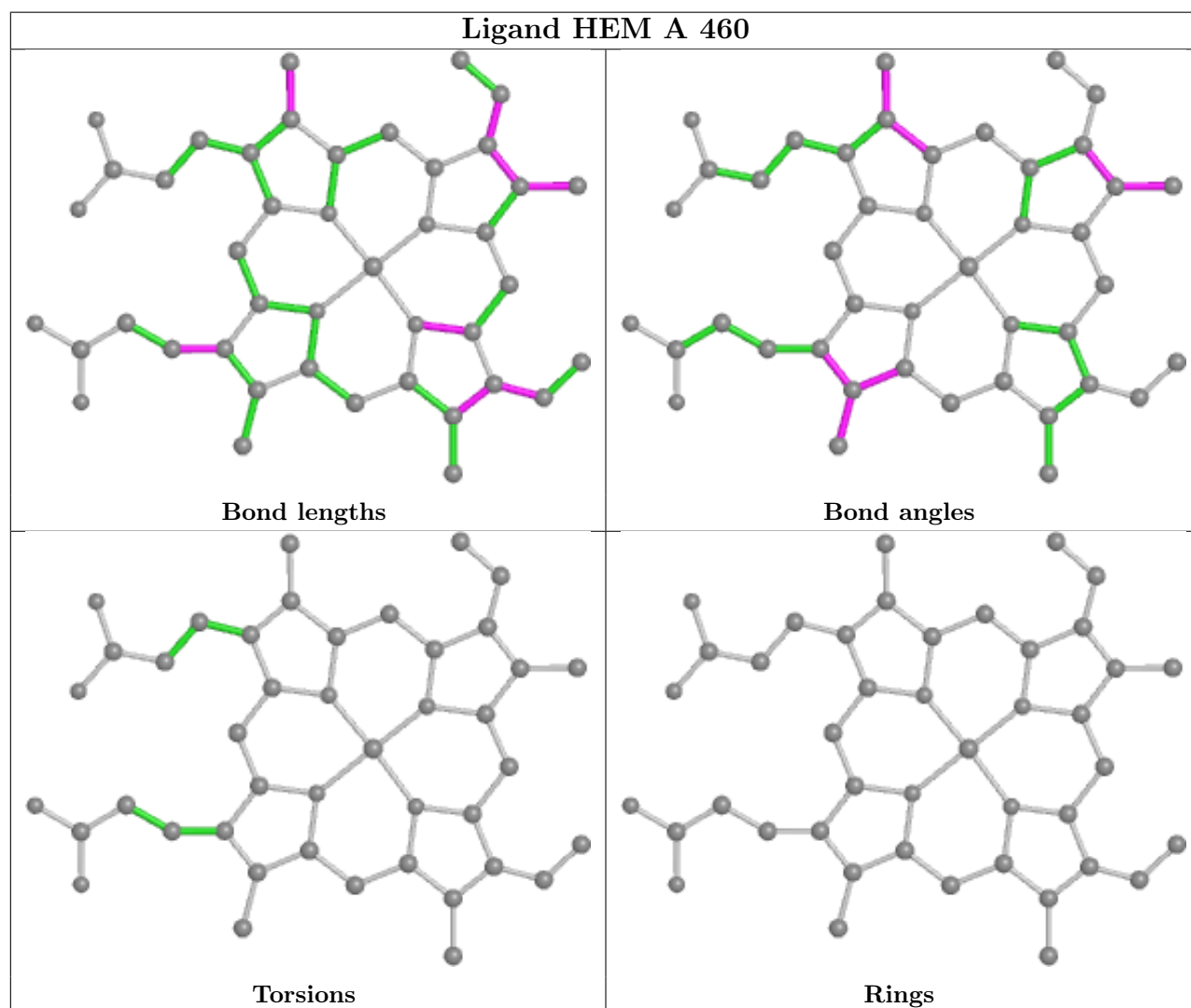
There are no ring outliers.

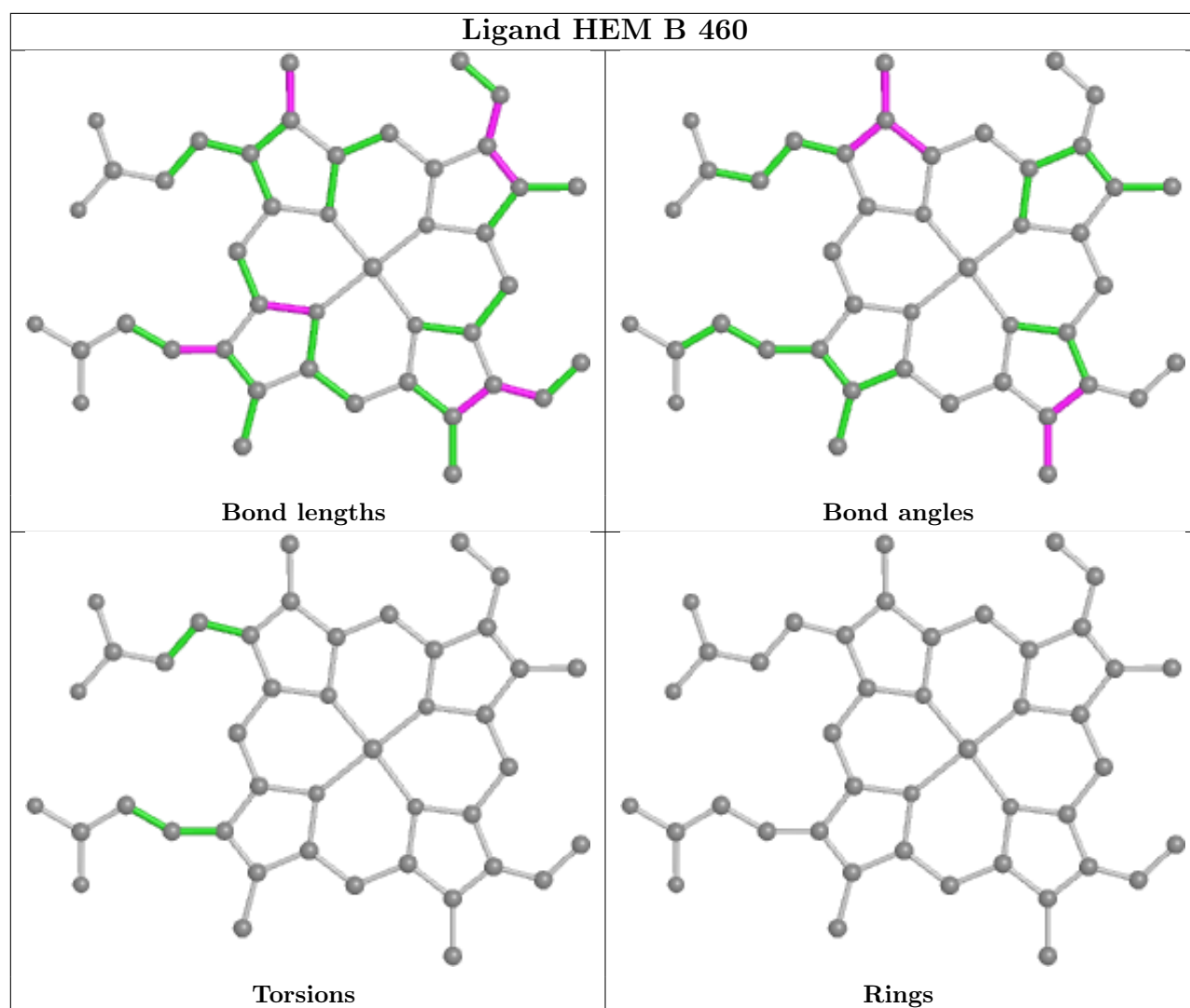
1 monomer is involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	460	HEM	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.