Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 08:46 PM EDT

PDB ID	:	1PHA
Title	:	INHIBITOR-INDUCED CONFORMATIONAL CHANGE IN CYTOCHROME P450-CAM
Authors	:	Poulos, T.L.
Deposited on	:	1992-07-27
Resolution	:	1.63 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

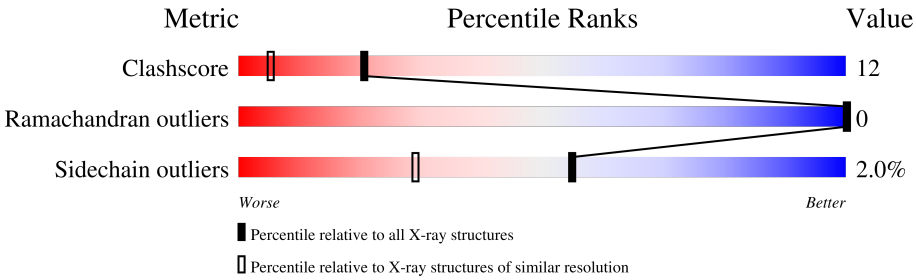
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	414	69% 24% • • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PFZ	A	422	X	-	X	-

2 Entry composition (i)

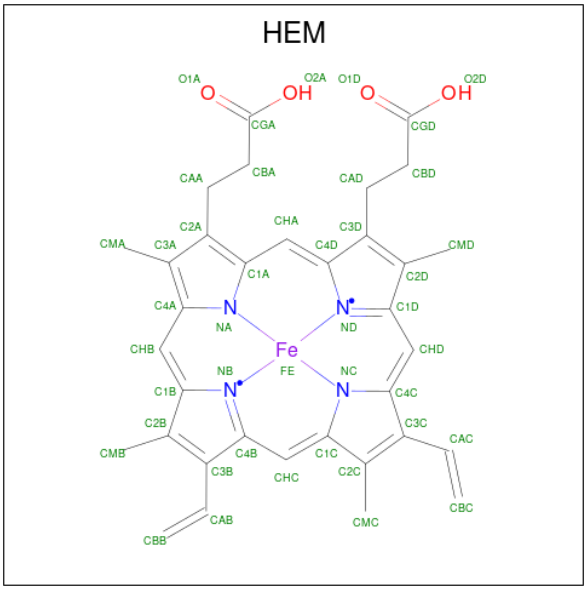
There are 4 unique types of molecules in this entry. The entry contains 3482 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-CAM.

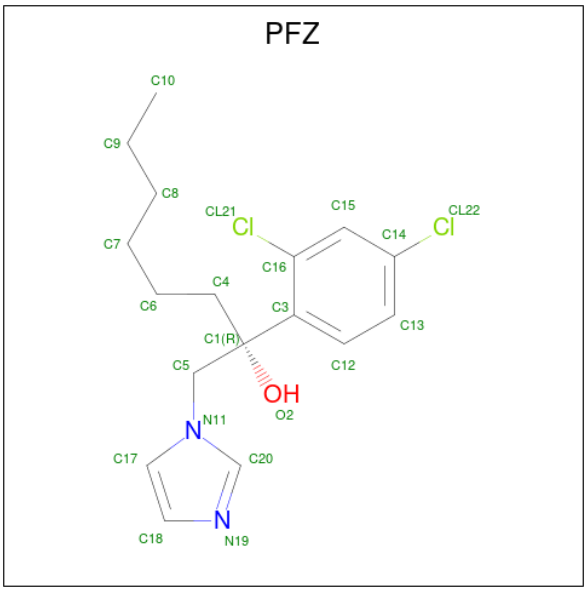
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3212	2035	560	598	19	0	2	0

- 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	43	34	1	4	4	0	0

- Molecule 3 is 1-(N-IMIDAZOLYL)-2-HYDROXY-2-(2,3-DICHLOROPHENYL)OCTANE (three-letter code: PFZ) (formula: $C_{17}H_{22}Cl_2N_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	22	17	2	2	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	205	205	205	0	0

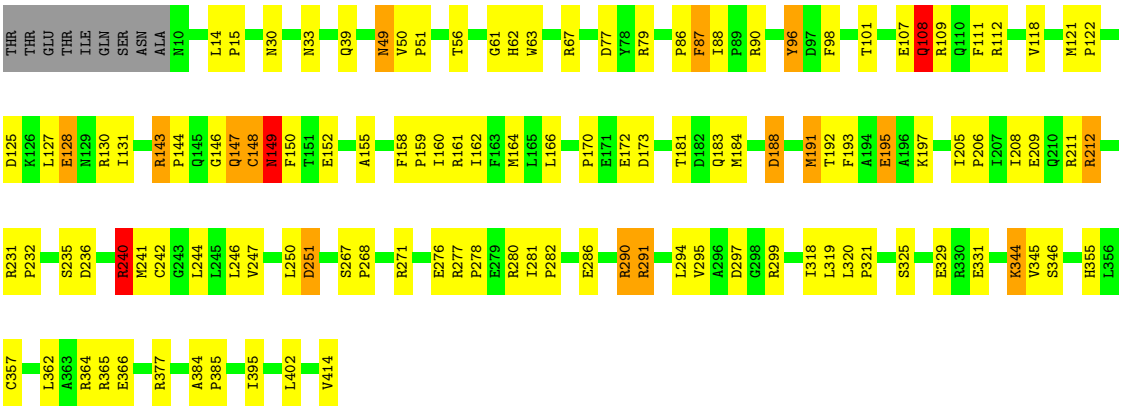
3 Residue-property plots (i)

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. 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: CYTOCHROME P450-CAM

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.67Å 103.90Å 36.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.63	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.63)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3482	wwPDB-VP
Average B, all atoms ($Å^2$)	19.0	wwPDB-VP

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: PFZ, 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	1.15	8/3298 (0.2%)	1.57	57/4481 (1.3%)

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	1	9

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	GLU	CD-OE1	8.67	1.35	1.25
1	A	109	ARG	CZ-NH2	6.32	1.41	1.33
1	A	212	ARG	NE-CZ	-5.60	1.25	1.33
1	A	212	ARG	CZ-NH2	5.35	1.40	1.33
1	A	286	GLU	CD-OE1	-5.28	1.19	1.25
1	A	251	ASP	C-O	5.02	1.32	1.23
1	A	414	VAL	C-O	5.02	1.32	1.23
1	A	212	ARG	CZ-NH1	-5.02	1.26	1.33

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	ARG	NE-CZ-NH2	-13.37	113.62	120.30
1	A	79	ARG	NE-CZ-NH1	10.67	125.63	120.30
1	A	109	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	A	280	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	A	90	ARG	NE-CZ-NH1	10.15	125.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	A	195	GLU	CA-CB-CG	9.16	133.55	113.40
1	A	271	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	A	192[A]	THR	N-CA-CB	8.47	126.40	110.30
1	A	192[B]	THR	N-CA-CB	8.47	126.40	110.30
1	A	365	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	A	280	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	A	96	TYR	CB-CG-CD2	-7.52	116.49	121.00
1	A	112	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	67	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	112	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	290	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	365	ARG	CD-NE-CZ	6.90	133.27	123.60
1	A	291	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	A	148	CYS	C-N-CA	6.74	138.56	121.70
1	A	191[A]	MET	C-N-CA	6.64	138.31	121.70
1	A	191[B]	MET	C-N-CA	6.64	138.31	121.70
1	A	109	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	143	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	211	ARG	CD-NE-CZ	6.44	132.62	123.60
1	A	152	GLU	CA-CB-CG	6.21	127.06	113.40
1	A	33	ASN	CB-CA-C	6.11	122.62	110.40
1	A	357	CYS	CB-CA-C	-6.10	98.19	110.40
1	A	161	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	188	ASP	N-CA-CB	-5.96	99.87	110.60
1	A	364	ARG	CD-NE-CZ	5.93	131.90	123.60
1	A	67	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	130	ARG	CD-NE-CZ	5.86	131.80	123.60
1	A	149	ASN	CA-C-O	-5.78	107.97	120.10
1	A	96	TYR	CB-CA-C	5.73	121.86	110.40
1	A	128	GLU	CG-CD-OE1	5.71	129.72	118.30
1	A	125	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	161	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	299	ARG	NH1-CZ-NH2	5.60	125.56	119.40
1	A	240	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	148	CYS	O-C-N	-5.50	113.90	122.70
1	A	277	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	149	ASN	N-CA-CB	5.43	120.38	110.60
1	A	329	GLU	CA-CB-CG	5.43	125.36	113.40
1	A	291	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
1	A	96	TYR	CB-CG-CD1	5.37	124.22	121.00
1	A	172	GLU	CG-CD-OE2	5.37	129.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	87	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	A	195	GLU	CB-CG-CD	5.30	128.53	114.20
1	A	33	ASN	N-CA-CB	5.22	119.99	110.60
1	A	191[A]	MET	N-CA-C	5.19	125.02	111.00
1	A	191[B]	MET	N-CA-C	5.19	125.02	111.00
1	A	108	GLN	CB-CG-CD	5.18	125.07	111.60
1	A	251	ASP	O-C-N	-5.12	114.52	122.70
1	A	107	GLU	CA-CB-CG	5.11	124.64	113.40
1	A	251	ASP	CB-CA-C	5.03	120.45	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	96	TYR	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	VAL	Mainchain
1	A	147	GLN	Mainchain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	377	ARG	Sidechain
1	A	77	ASP	Mainchain

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	3212	0	3149	70	0
2	A	43	0	30	7	0
3	A	22	0	22	27	0
4	A	205	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3482	0	3201	80	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 12.

All (80) 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:297:ASP:CG	3:A:422:PFZ:CL22	2.50	0.87
1:A:295:VAL:HG13	3:A:422:PFZ:H13	1.56	0.85
2:A:417:HEM:C4A	3:A:422:PFZ:H18	2.14	0.83
1:A:247:VAL:HG11	3:A:422:PFZ:H41	1.64	0.80
1:A:96:TYR:CE2	3:A:422:PFZ:H102	2.18	0.78
1:A:247:VAL:CG1	3:A:422:PFZ:H41	2.23	0.68
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.76	0.67
1:A:101:THR:HG21	3:A:422:PFZ:CL21	2.32	0.67
1:A:297:ASP:OD2	3:A:422:PFZ:CL22	2.50	0.66
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.79	0.65
2:A:417:HEM:HBA1	3:A:422:PFZ:H15	1.79	0.65
3:A:422:PFZ:C12	3:A:422:PFZ:H17	2.28	0.64
1:A:181:THR:HG23	1:A:247:VAL:HG13	1.80	0.63
1:A:87:PHE:HE2	4:A:709:HOH:O	1.81	0.63
1:A:87:PHE:CE2	3:A:422:PFZ:H92	2.37	0.60
2:A:417:HEM:C1B	3:A:422:PFZ:H18	2.36	0.59
3:A:422:PFZ:C17	3:A:422:PFZ:C3	2.80	0.59
3:A:422:PFZ:CL21	3:A:422:PFZ:O2	2.55	0.59
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.84	0.58
1:A:149:ASN:ND2	1:A:402:LEU:H	2.03	0.57
1:A:96:TYR:HE2	3:A:422:PFZ:H102	1.70	0.56
1:A:49:ASN:HD22	1:A:49:ASN:H	1.53	0.56
1:A:395:ILE:HD13	3:A:422:PFZ:H103	1.89	0.55
1:A:183:GLN:HE22	1:A:188:ASP:HB2	1.71	0.55
2:A:417:HEM:CHB	3:A:422:PFZ:H18	2.28	0.54
1:A:395:ILE:HD13	3:A:422:PFZ:C9	2.37	0.54
1:A:170:PRO:HG2	1:A:173:ASP:OD2	2.07	0.54
2:A:417:HEM:HBA2	3:A:422:PFZ:CL22	2.45	0.54
1:A:362:LEU:O	1:A:366:GLU:HG3	2.08	0.53
1:A:295:VAL:CG1	3:A:422:PFZ:CL22	2.94	0.53
1:A:208:ILE:O	1:A:212:ARG:HG3	2.10	0.52
1:A:295:VAL:HG13	3:A:422:PFZ:C13	2.34	0.51
3:A:422:PFZ:H17	3:A:422:PFZ:C3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:HD13	1:A:320:LEU:HD21	1.93	0.51
1:A:242:CYS:O	1:A:246:LEU:HD23	2.12	0.50
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.94	0.49
1:A:30:ASN:ND2	4:A:555:HOH:O	2.43	0.49
1:A:131:ILE:HG12	1:A:162:ILE:HD13	1.93	0.49
1:A:395:ILE:HD13	3:A:422:PFZ:C10	2.43	0.49
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.95	0.49
1:A:395:ILE:HD13	3:A:422:PFZ:H91	1.93	0.48
1:A:184:MET:CE	1:A:197:LYS:HA	2.42	0.48
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.47	0.48
1:A:127:LEU:CD1	1:A:166:LEU:HD13	2.43	0.47
1:A:160:ILE:O	1:A:164:MET:HG2	2.14	0.47
1:A:56:THR:O	1:A:61:GLY:HA2	2.13	0.47
1:A:108:GLN:HG3	1:A:355:HIS:CE1	2.49	0.47
1:A:111:PHE:HB3	1:A:241:MET:HE2	1.97	0.47
1:A:30:ASN:ND2	4:A:556:HOH:O	2.49	0.46
1:A:14:LEU:HA	1:A:15:PRO:HD3	1.86	0.46
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.85	0.46
1:A:325:SER:O	1:A:331:GLU:HG3	2.15	0.46
1:A:276:GLU:C	1:A:278:PRO:HD3	2.36	0.45
1:A:290:ARG:HD3	1:A:345:VAL:HG13	1.96	0.45
2:A:417:HEM:CBA	3:A:422:PFZ:H15	2.46	0.45
1:A:209:GLU:HG2	4:A:603:HOH:O	2.16	0.44
1:A:150:PHE:CE2	1:A:155:ALA:HB2	2.53	0.44
1:A:297:ASP:OD1	3:A:422:PFZ:CL22	2.72	0.44
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.90	0.44
1:A:149:ASN:HD21	1:A:402:LEU:H	1.65	0.44
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.48	0.43
1:A:236:ASP:O	1:A:240:ARG:HG3	2.18	0.43
1:A:295:VAL:HG11	2:A:417:HEM:HMA2	1.99	0.43
1:A:344:LYS:HE3	1:A:346:SER:HB2	2.00	0.43
1:A:319:LEU:HG	1:A:321:PRO:HG3	2.01	0.43
1:A:294:LEU:HD23	1:A:294:LEU:H	1.84	0.42
1:A:39:GLN:NE2	1:A:39:GLN:H	2.17	0.42
1:A:281:ILE:N	1:A:282:PRO:CD	2.83	0.42
1:A:184:MET:HB3	3:A:422:PFZ:H81	2.01	0.42
1:A:191[A]:MET:O	1:A:195:GLU:HG3	2.20	0.41
1:A:86:PRO:HG2	1:A:87:PHE:CD2	2.55	0.41
1:A:63:TRP:HB2	1:A:318:ILE:HG13	2.02	0.41
1:A:98:PHE:HB3	1:A:244:LEU:HB2	2.03	0.41
1:A:146:GLY:O	1:A:147:GLN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD23	1:A:294:LEU:N	2.36	0.41
1:A:267:SER:HA	1:A:268:PRO:HD2	1.94	0.41
1:A:39:GLN:HG2	1:A:291:ARG:O	2.21	0.41
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.46	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	405/414 (98%)	388 (96%)	17 (4%)	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	351/358 (98%)	344 (98%)	7 (2%)	55 29

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	128	GLU
1	A	149	ASN
1	A	193	PHE
1	A	235	SER
1	A	344	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	69	GLN
1	A	108	GLN
1	A	149	ASN
1	A	225	ASN
1	A	388	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	$\#\|Z\| > 2$
3	PFZ	A	422	2	21,23,23	0.95	0	25,31,31	2.48	4 (16%)
2	HEM	A	417	3,1	42,50,50	1.41	4 (9%)	46,82,82	1.49	11 (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
3	PFZ	A	422	2	1/1/1/1	14/18/18/18	0/2/2/2
2	HEM	A	417	3,1	-	2/12/54/54	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	HEM	C3C-C2C	-4.81	1.33	1.40
2	A	417	HEM	C3C-C4C	3.41	1.46	1.41
2	A	417	HEM	C3C-CAC	2.83	1.54	1.47
2	A	417	HEM	CAB-C3B	2.21	1.53	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	422	PFZ	O2-C1-C5	-9.18	87.01	108.20
3	A	422	PFZ	C5-C1-C3	5.76	125.38	110.86
2	A	417	HEM	CMA-C3A-C4A	-3.56	123.24	128.46
2	A	417	HEM	C4C-CHD-C1D	3.28	126.89	122.56
2	A	417	HEM	O1D-CGD-CBD	-3.07	113.37	123.09
3	A	422	PFZ	C6-C4-C1	-2.87	112.33	116.01
2	A	417	HEM	O2A-CGA-O1A	2.82	130.59	123.33
2	A	417	HEM	C4B-CHC-C1C	2.76	126.20	122.56
2	A	417	HEM	CMA-C3A-C2A	2.66	129.96	124.94
2	A	417	HEM	C3B-C2B-C1B	2.51	108.30	106.41
2	A	417	HEM	CBD-CAD-C3D	2.36	119.06	112.53
2	A	417	HEM	O2D-CGD-O1D	2.12	128.78	123.33
2	A	417	HEM	O1A-CGA-CBA	-2.11	116.42	123.09
3	A	422	PFZ	C15-C16-C3	-2.05	119.92	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	417	HEM	CMC-C2C-C3C	2.03	128.74	124.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	422	PFZ	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	422	PFZ	C5-C1-C4-C6
3	A	422	PFZ	C3-C1-C5-N11
3	A	422	PFZ	C1-C5-N11-C17
3	A	422	PFZ	C1-C5-N11-C20
3	A	422	PFZ	O2-C1-C5-N11
3	A	422	PFZ	C4-C1-C3-C12
3	A	422	PFZ	C4-C1-C3-C16
3	A	422	PFZ	O2-C1-C3-C16
3	A	422	PFZ	C4-C6-C7-C8
3	A	422	PFZ	O2-C1-C3-C12
3	A	422	PFZ	C4-C1-C5-N11
3	A	422	PFZ	C7-C8-C9-C10
3	A	422	PFZ	C1-C4-C6-C7
3	A	422	PFZ	C5-C1-C3-C16
2	A	417	HEM	CAD-CBD-CGD-O2D
2	A	417	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

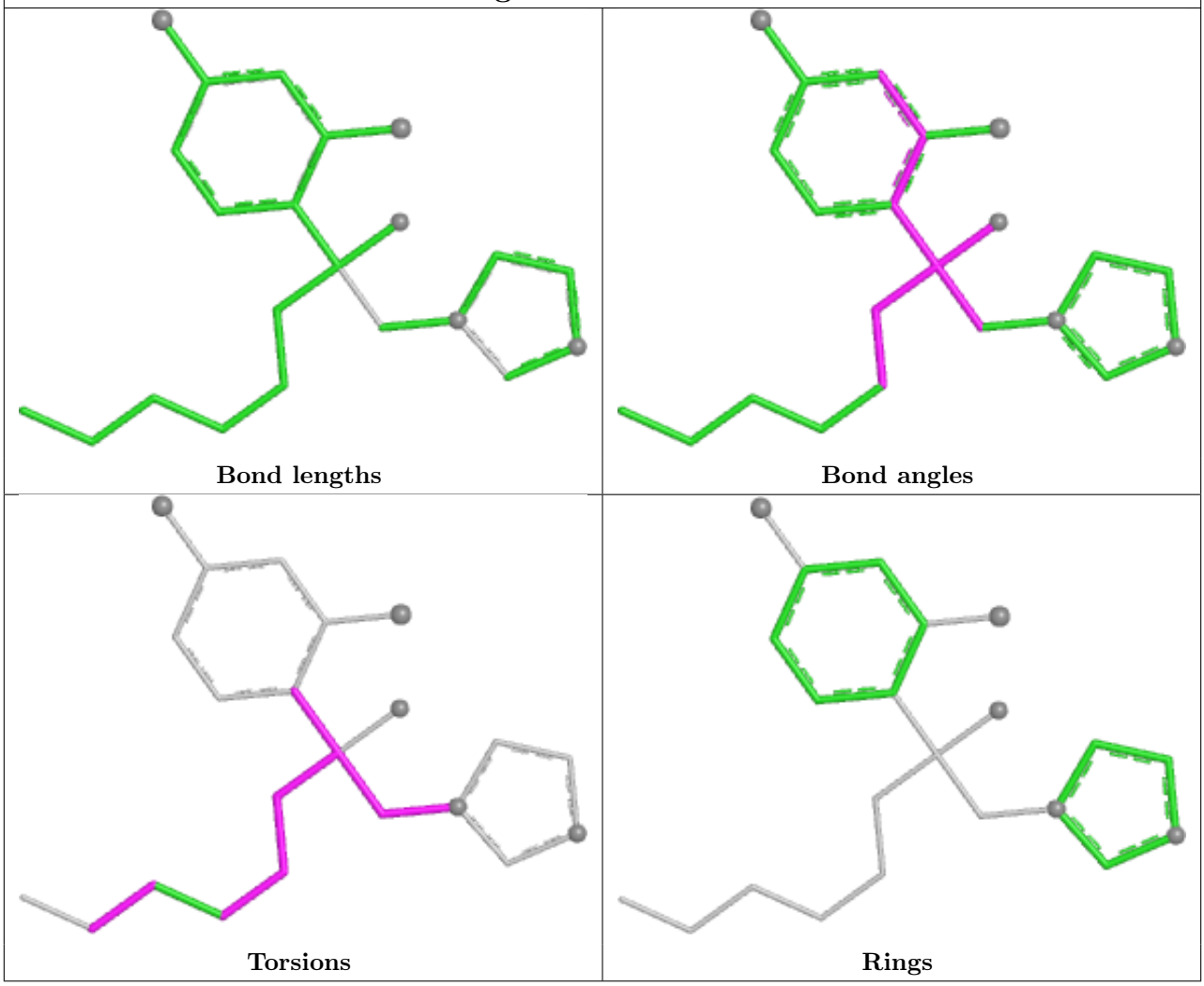
2 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	422	PFZ	27	0
2	A	417	HEM	7	0

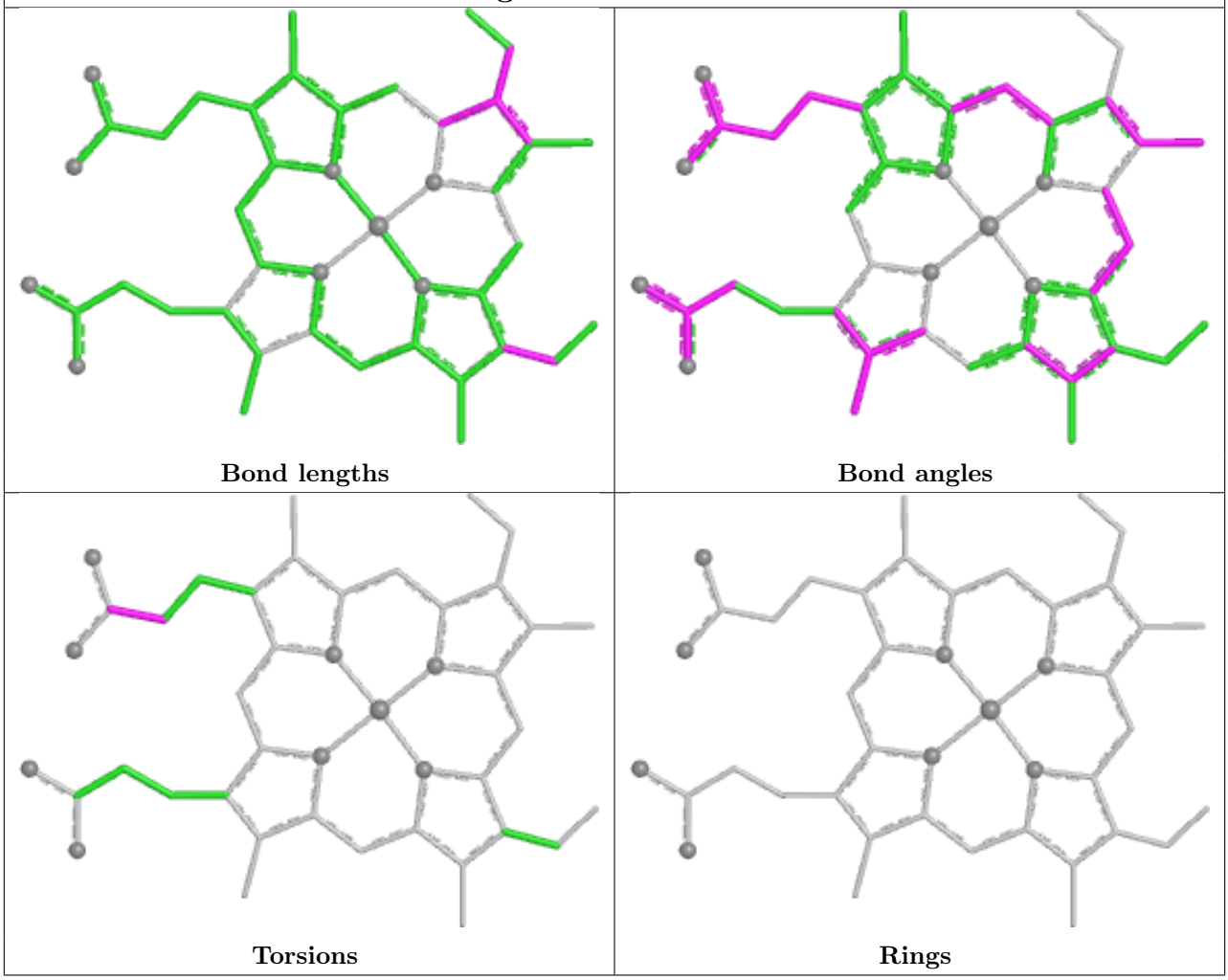
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand PFZ A 422



Ligand HEM A 417



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.