



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:58 PM UTC

PDB ID : 1FAH / pdb_00001fah
Title : STRUCTURE OF CYTOCHROME P450
Authors : Li, H.Y.; Poulos, T.L.
Deposited on : 1996-08-01
Resolution : 2.30 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

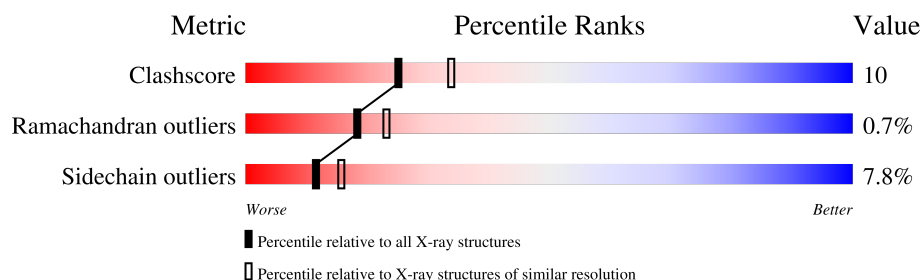
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	 73% 21% . .
1	B	471	 64% 28% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7819 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 BM-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3668	2344	623	684	17			
1	B	455	Total	C	N	O	S	0	0	0
			3668	2344	623	684	17			

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 (CCD ID: 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	216	Total	O	0	0
			216	216		
3	B	181	Total	O	0	0
			181	181		

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.

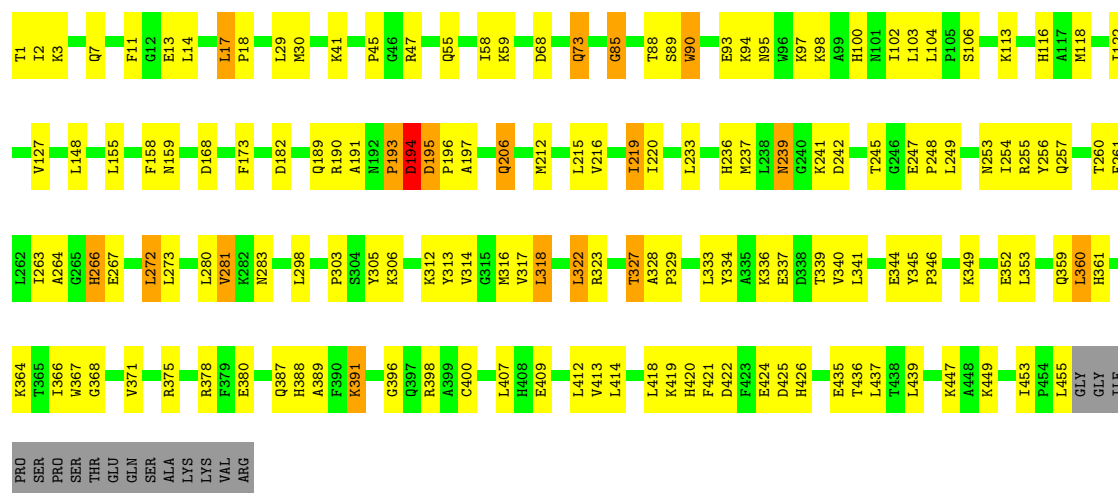
• Molecule 1: CYTOCHROME P450 BM-3

Chain A:  73% 21%



• Molecule 1: CYTOCHROME P450 BM-3

Chain B:  64% 28%



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, α , β , γ	59.50 Å 154.00 Å 62.40 Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	75.6 (10.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7819	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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	0.48	0/3753	0.96	13/5074 (0.3%)
1	B	0.46	0/3753	0.97	18/5074 (0.4%)
All	All	0.47	0/7506	0.97	31/10148 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	HIS	N-CA-C	8.35	120.01	111.07
1	B	168	ASP	N-CA-C	-8.13	100.50	111.96
1	A	437	LEU	N-CA-C	-7.66	102.93	111.82
1	B	266	HIS	N-CA-C	7.63	119.23	111.07
1	B	422	ASP	N-CA-C	-7.17	98.04	109.59
1	B	328	ALA	CA-C-N	6.78	126.47	119.56
1	B	328	ALA	C-N-CA	6.78	126.47	119.56
1	A	422	ASP	N-CA-C	-6.13	99.19	109.07
1	B	329	PRO	N-CA-C	6.10	121.77	113.84
1	B	283	ASN	CA-C-N	6.03	127.38	119.84
1	B	283	ASN	C-N-CA	6.03	127.38	119.84
1	B	328	ALA	N-CA-C	-5.99	95.71	108.66
1	A	329	PRO	N-CA-C	5.89	121.27	114.03
1	B	426	HIS	N-CA-C	5.87	120.06	113.01
1	B	396	GLY	N-CA-C	5.76	121.70	111.73
1	A	431	LEU	N-CA-C	5.72	118.88	110.30
1	B	437	LEU	N-CA-C	-5.70	105.58	112.54
1	B	421	PHE	N-CA-C	5.65	117.77	109.24
1	A	436	THR	N-CA-C	-5.64	98.78	110.80
1	A	86	LEU	N-CA-C	5.55	118.05	111.33
1	A	395	ASN	N-CA-C	5.53	118.24	109.50
1	B	85	GLY	N-CA-C	-5.46	105.55	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ALA	CA-C-N	5.32	125.40	119.87
1	A	328	ALA	C-N-CA	5.32	125.40	119.87
1	A	302	VAL	CA-C-N	5.24	125.16	119.76
1	A	302	VAL	C-N-CA	5.24	125.16	119.76
1	B	327	THR	N-CA-C	5.18	118.38	111.75
1	A	64	GLU	N-CA-C	5.09	118.60	112.38
1	B	436	THR	N-CA-C	-5.09	99.96	110.80
1	B	90	TRP	N-CA-C	-5.05	102.04	110.17
1	B	55	GLN	N-CA-C	-5.00	105.83	111.28

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	3668	0	3643	62	0
1	B	3668	0	3643	81	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	216	0	0	3	0
3	B	181	0	0	5	0
All	All	7819	0	7346	143	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 10.

All (143) 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:190:ARG:HD2	1:A:196:PRO:HD2	1.57	0.85
1:B:127:VAL:HG11	1:B:455:LEU:HD21	1.58	0.84
1:A:16:ASN:HB3	1:A:19:LEU:HD12	1.63	0.80
1:A:223:ARG:HH22	1:A:230:SER:HB2	1.54	0.73
1:A:190:ARG:NE	1:A:197:ALA:HB2	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.71	0.72
1:B:216:VAL:O	1:B:219:ILE:HG22	1.91	0.71
1:B:256:TYR:O	1:B:260:THR:HG23	1.92	0.69
1:A:190:ARG:HE	1:A:197:ALA:HB2	1.57	0.69
1:B:361:HIS:HE1	1:B:391:LYS:H	1.39	0.69
1:A:313:TYR:HA	1:A:316:MET:HE3	1.74	0.69
1:B:339:THR:HG22	1:B:340:VAL:H	1.58	0.69
1:B:281:VAL:CG1	1:B:425:ASP:HB2	2.26	0.65
1:A:8:PRO:HB2	1:A:19:LEU:CD1	2.29	0.62
1:A:236:HIS:HB3	3:A:590:HOH:O	1.99	0.62
1:B:420:HIS:CE1	1:B:455:LEU:HD23	2.35	0.61
1:A:361:HIS:HE1	1:A:391:LYS:H	1.47	0.61
1:B:253:ASN:O	1:B:257:GLN:HG2	2.00	0.61
1:A:223:ARG:HH11	1:A:223:ARG:HG2	1.66	0.61
1:B:233:LEU:HD13	1:B:261:PHE:CE2	2.37	0.60
1:A:100:HIS:HD2	3:A:556:HOH:O	1.86	0.59
1:B:85:GLY:HA3	1:B:260:THR:HG21	1.84	0.58
1:A:171:HIS:HD2	1:A:173:PHE:H	1.50	0.58
1:B:314:VAL:HG13	1:B:414:LEU:HD23	1.85	0.58
1:A:116:HIS:HE1	1:A:303:PRO:O	1.87	0.58
1:B:191:ALA:HB3	1:B:195:ASP:O	2.03	0.58
1:A:135:ALA:O	1:A:136:ASP:HB3	2.05	0.56
1:B:193:PRO:O	1:B:194:ASP:HB2	2.05	0.55
1:B:127:VAL:CG1	1:B:455:LEU:HD21	2.32	0.55
1:B:17:LEU:HD12	1:B:45:PRO:HD2	1.88	0.55
1:B:90:TRP:HB2	1:B:93:GLU:HG3	1.87	0.55
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.89	0.55
1:A:194:ASP:HA	1:A:197:ALA:O	2.06	0.55
1:A:447:LYS:HD2	1:A:449:LYS:HZ1	1.71	0.55
1:A:220:ILE:O	1:A:224:LYS:HG2	2.07	0.55
1:B:2:ILE:HA	1:B:344:GLU:O	2.06	0.55
1:B:7:GLN:HG3	1:B:41:LYS:O	2.07	0.54
1:B:267:GLU:HG2	3:B:652:HOH:O	2.07	0.54
1:B:30:MET:HG2	1:B:359:GLN:HG2	1.90	0.54
1:A:128:GLN:O	1:A:132:ARG:HG3	2.07	0.53
1:B:298:LEU:HD22	1:B:303:PRO:HB3	1.90	0.53
1:A:89:SER:O	1:A:398:ARG:NH2	2.38	0.53
1:A:74:ALA:O	1:A:78:VAL:HG23	2.09	0.53
1:A:160:TYR:OH	1:A:171:HIS:HE1	1.91	0.53
1:A:17:LEU:HB3	1:A:18:PRO:HD3	1.91	0.53
1:A:8:PRO:HB2	1:A:19:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HA	1:A:59:LYS:HE2	1.92	0.52
1:A:167:ARG:HG3	1:A:169:GLN:O	2.09	0.52
1:B:424:GLU:HB2	1:B:449:LYS:HE2	1.91	0.52
1:B:316:MET:HE1	1:B:380:GLU:HG2	1.92	0.52
1:A:391:LYS:NZ	1:A:395:ASN:HD22	2.08	0.51
1:B:281:VAL:HG11	1:B:425:ASP:HB2	1.93	0.51
1:A:434:LYS:HB2	1:A:442:GLU:HB2	1.91	0.51
1:A:223:ARG:HD3	1:A:234:LEU:HD23	1.91	0.51
1:A:116:HIS:HD2	1:A:408:HIS:NE2	2.07	0.51
1:B:14:LEU:HD23	1:B:18:PRO:CG	2.40	0.51
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.92	0.51
1:B:419:LYS:HE2	1:B:453:ILE:HG21	1.93	0.50
1:B:47:ARG:HH12	1:B:73:GLN:HB2	1.75	0.50
1:A:69:LYS:HD3	1:A:398:ARG:CZ	2.42	0.50
1:B:387:GLN:HG2	1:B:388:HIS:CD2	2.47	0.50
1:A:127:VAL:CG1	1:A:455:LEU:HD11	2.42	0.49
1:B:206:GLN:HE21	1:B:206:GLN:HA	1.77	0.49
1:A:51:TYR:CE2	1:A:354:MET:HG2	2.48	0.49
1:B:59:LYS:HG3	1:B:388:HIS:CD2	2.48	0.48
1:A:92:HIS:H	1:A:92:HIS:CD2	2.31	0.48
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.94	0.48
1:B:103:LEU:O	1:B:106:SER:HB2	2.14	0.48
1:B:263:ILE:HG13	1:B:264:ALA:N	2.28	0.48
1:B:190:ARG:HG3	1:B:196:PRO:HD2	1.95	0.47
1:A:141:VAL:HB	1:A:142:PRO:HD3	1.97	0.47
1:B:216:VAL:O	1:B:220:ILE:HG13	2.15	0.47
1:B:249:LEU:HD22	1:B:253:ASN:OD1	2.15	0.47
1:B:239:ASN:HD22	1:B:239:ASN:N	2.11	0.47
1:B:113:LYS:HE2	1:B:305:TYR:CE2	2.50	0.47
1:A:8:PRO:HB2	1:A:19:LEU:HD13	1.97	0.47
1:B:313:TYR:O	1:B:317:VAL:HG23	2.15	0.47
1:B:435:GLU:HG2	1:B:439:LEU:CD2	2.46	0.46
1:B:14:LEU:HB3	1:B:18:PRO:HD3	1.97	0.46
1:B:89:SER:O	1:B:398:ARG:NH2	2.44	0.46
1:B:336:LYS:O	1:B:349:LYS:HG3	2.15	0.46
1:B:14:LEU:HD23	1:B:18:PRO:HG2	1.97	0.46
1:B:237:MET:CE	1:B:254:ILE:HA	2.45	0.46
1:B:122:ILE:HG22	1:B:148:LEU:HD12	1.97	0.45
1:A:377:GLU:O	1:A:380:GLU:HB2	2.16	0.45
1:B:272:LEU:HG	1:B:322:LEU:HD13	1.99	0.45
1:B:58:ILE:HD13	1:B:360:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HG11	1:A:455:LEU:HD11	1.98	0.45
1:A:158:PHE:CD1	1:A:158:PHE:N	2.85	0.45
1:B:1:THR:HG23	1:B:1:THR:O	2.16	0.45
1:B:94:LYS:HE3	3:B:646:HOH:O	2.17	0.45
1:A:2:ILE:HG13	1:A:2:ILE:O	2.17	0.44
1:B:118:MET:HE2	1:B:155:LEU:HG	1.99	0.44
1:B:219:ILE:HD13	1:B:219:ILE:O	2.17	0.44
1:B:345:TYR:HA	1:B:346:PRO:HD3	1.83	0.44
1:B:400:CYS:HB2	2:B:472:HEM:C4A	2.52	0.44
1:B:420:HIS:CD2	1:B:453:ILE:HB	2.53	0.44
1:A:5:MET:SD	1:A:50:ARG:HG2	2.58	0.44
1:A:38:GLU:OE2	1:A:56:ARG:NH1	2.51	0.44
1:A:302:VAL:HA	1:A:303:PRO:HD3	1.85	0.44
1:A:313:TYR:O	1:A:317:VAL:HG23	2.17	0.44
1:A:223:ARG:HH22	1:A:230:SER:CB	2.27	0.44
1:B:360:LEU:HD22	3:B:642:HOH:O	2.17	0.44
1:A:94:LYS:HE2	1:A:98:LYS:HD2	1.99	0.43
1:B:281:VAL:HG13	1:B:425:ASP:HB2	1.98	0.43
1:B:102:ILE:HD12	1:B:249:LEU:HG	2.00	0.43
1:B:14:LEU:O	1:B:17:LEU:HB2	2.18	0.43
1:A:192:ASN:ND2	1:A:195:ASP:HB3	2.34	0.43
1:B:116:HIS:HE1	1:B:303:PRO:O	2.02	0.43
1:B:158:PHE:CD1	1:B:158:PHE:N	2.87	0.43
1:A:171:HIS:CD2	1:A:172:PRO:HD2	2.54	0.42
1:A:366:ILE:HD12	1:A:386:PRO:HG2	2.00	0.42
1:A:320:GLU:OE1	1:A:379:PHE:HE2	2.02	0.42
1:B:236:HIS:HB3	3:B:558:HOH:O	2.18	0.42
1:B:14:LEU:HD23	1:B:18:PRO:HG3	2.01	0.42
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.91	0.42
1:B:247:GLU:HA	1:B:248:PRO:HD3	1.84	0.42
1:B:337:GLU:HG3	3:B:521:HOH:O	2.19	0.42
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.86	0.42
1:B:375:ARG:O	1:B:378:ARG:HG3	2.19	0.42
1:B:323:ARG:HA	1:B:361:HIS:CD2	2.54	0.42
1:B:352:GLU:HG2	1:B:353:LEU:N	2.34	0.42
1:B:414:LEU:O	1:B:418:LEU:HG	2.20	0.41
1:B:364:LYS:HA	1:B:368:GLY:O	2.20	0.41
1:A:95:ASN:HD22	1:A:95:ASN:HA	1.72	0.41
1:A:286:VAL:HG13	1:A:313:TYR:OH	2.20	0.41
1:A:317:VAL:HG13	1:A:374:PHE:HZ	1.86	0.41
1:B:306:LYS:HA	1:B:306:LYS:HD2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ILE:O	1:A:178:VAL:HG13	2.20	0.41
1:A:426:HIS:HE1	3:A:602:HOH:O	2.03	0.41
1:B:100:HIS:O	1:B:104:LEU:HB2	2.21	0.41
1:B:212:MET:HE2	1:B:212:MET:HB3	1.92	0.41
1:B:173:PHE:CD2	1:B:215:LEU:HD23	2.55	0.41
1:A:148:LEU:HD11	1:A:413:VAL:HG21	2.01	0.41
1:A:223:ARG:HG2	1:A:223:ARG:NH1	2.34	0.41
1:A:158:PHE:CD2	1:A:219:ILE:HD13	2.56	0.40
1:B:68:ASP:HB3	1:B:334:TYR:CE1	2.57	0.40
1:A:9:LYS:HD3	1:A:11:PHE:CZ	2.55	0.40
1:B:366:ILE:HG21	1:B:389:ALA:HB1	2.01	0.40
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.98	0.40
1:B:11:PHE:O	1:B:14:LEU:HB2	2.20	0.40
1:B:98:LYS:HG2	1:B:242:ASP:HB2	2.03	0.40
1:B:341:LEU:N	1:B:345:TYR:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/471 (96%)	424 (94%)	27 (6%)	2 (0%)	30	38
1	B	453/471 (96%)	432 (95%)	17 (4%)	4 (1%)	14	17
All	All	906/942 (96%)	856 (94%)	44 (5%)	6 (1%)	18	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	A	194	ASP
1	B	194	ASP

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Mol	Chain	Res	Type
1	B	197	ALA
1	B	193	PRO
1	B	195	ASP

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	398/411 (97%)	370 (93%)	28 (7%)	14	19
1	B	398/411 (97%)	364 (92%)	34 (8%)	10	13
All	All	796/822 (97%)	734 (92%)	62 (8%)	11	16

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	13	GLU
1	A	31	LYS
1	A	45	PRO
1	A	92	HIS
1	A	97	LYS
1	A	103	LEU
1	A	104	LEU
1	A	132	ARG
1	A	133	LEU
1	A	158	PHE
1	A	190	ARG
1	A	194	ASP
1	A	204	GLN
1	A	223	ARG
1	A	249	LEU
1	A	250	ASP
1	A	255	ARG
1	A	267	GLU
1	A	272	LEU

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Mol	Chain	Res	Type
1	A	281	VAL
1	A	302	VAL
1	A	318	LEU
1	A	322	LEU
1	A	337	GLU
1	A	398	ARG
1	A	414	LEU
1	A	445	VAL
1	B	3	LYS
1	B	13	GLU
1	B	17	LEU
1	B	29	LEU
1	B	73	GLN
1	B	88	THR
1	B	95	ASN
1	B	97	LYS
1	B	159	ASN
1	B	182	ASP
1	B	189	GLN
1	B	194	ASP
1	B	206	GLN
1	B	219	ILE
1	B	239	ASN
1	B	241	LYS
1	B	245	THR
1	B	255	ARG
1	B	266	HIS
1	B	272	LEU
1	B	273	LEU
1	B	280	LEU
1	B	281	VAL
1	B	312	LYS
1	B	318	LEU
1	B	322	LEU
1	B	327	THR
1	B	333	LEU
1	B	360	LEU
1	B	391	LYS
1	B	407	LEU
1	B	409	GLU
1	B	412	LEU
1	B	447	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	70	ASN
1	A	73	GLN
1	A	92	HIS
1	A	95	ASN
1	A	100	HIS
1	A	116	HIS
1	A	128	GLN
1	A	159	ASN
1	A	171	HIS
1	A	201	ASN
1	A	206	GLN
1	A	229	GLN
1	A	239	ASN
1	A	266	HIS
1	A	285	HIS
1	A	319	ASN
1	A	361	HIS
1	A	388	HIS
1	A	395	ASN
1	A	403	GLN
1	B	21	ASN
1	B	27	GLN
1	B	70	ASN
1	B	95	ASN
1	B	116	HIS
1	B	163	ASN
1	B	201	ASN
1	B	206	GLN
1	B	213	ASN
1	B	229	GLN
1	B	239	ASN
1	B	361	HIS
1	B	387	GLN
1	B	388	HIS
1	B	395	ASN
1	B	420	HIS
1	B	428	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	A	472	3,1	50,50,50	1.25	4 (8%)	67,82,82	1.14	6 (8%)
2	HEM	B	472	3,1	50,50,50	1.12	4 (8%)	67,82,82	1.27	5 (7%)

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	472	3,1	-	6/14/54/54	-
2	HEM	B	472	3,1	-	3/14/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	472	HEM	CMB-C2B	2.78	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	472	HEM	CAB-C3B	-2.72	1.40	1.47
2	B	472	HEM	CAB-C3B	-2.69	1.40	1.47
2	A	472	HEM	FE-ND	2.62	2.03	1.94
2	A	472	HEM	CAC-C3C	-2.51	1.40	1.47
2	B	472	HEM	CAC-C3C	-2.42	1.40	1.47
2	B	472	HEM	FE-NB	2.26	2.01	1.94
2	B	472	HEM	FE-ND	2.20	2.01	1.94

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	472	HEM	C3B-C4B-NB	4.43	112.65	109.47
2	A	472	HEM	CMA-C3A-C4A	3.02	130.02	125.42
2	A	472	HEM	CMC-C2C-C1C	2.98	129.97	124.73
2	B	472	HEM	C1D-C2D-C3D	-2.65	104.20	106.98
2	B	472	HEM	CAD-C3D-C2D	-2.52	123.14	127.87
2	B	472	HEM	CMA-C3A-C4A	2.50	129.23	125.42
2	B	472	HEM	C2D-C1D-ND	2.20	112.44	109.90
2	A	472	HEM	C3B-C4B-NB	2.18	111.04	109.47
2	A	472	HEM	CMC-C2C-C3C	-2.18	123.16	128.43
2	A	472	HEM	CHD-C4C-C3C	-2.10	121.67	125.21
2	A	472	HEM	C2B-C1B-NB	2.03	112.17	109.84

There are no chirality outliers.

All (9) torsion outliers are listed below:

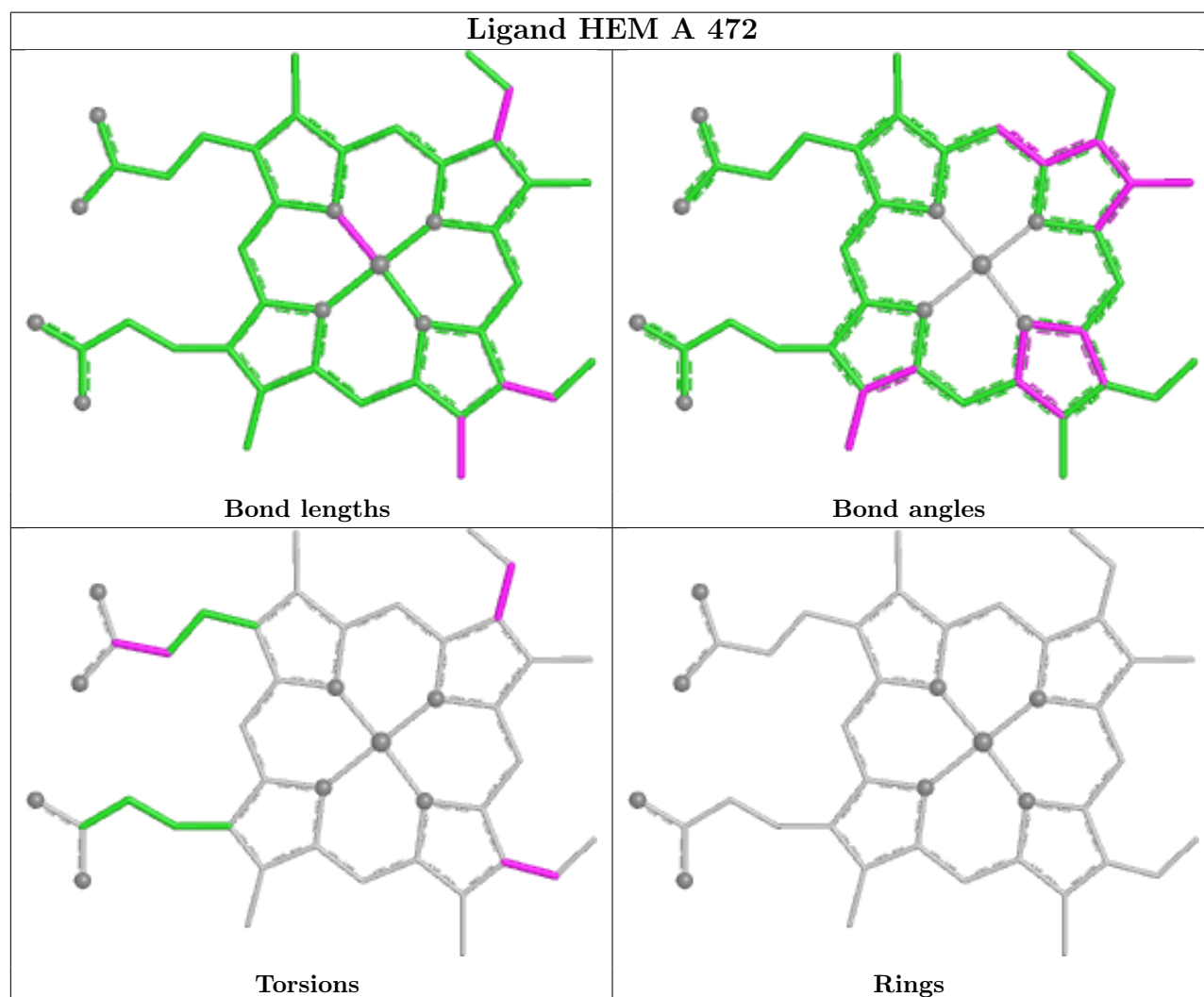
Mol	Chain	Res	Type	Atoms
2	A	472	HEM	C2C-C3C-CAC-CBC
2	B	472	HEM	C2B-C3B-CAB-CBB
2	A	472	HEM	C2B-C3B-CAB-CBB
2	A	472	HEM	C4C-C3C-CAC-CBC
2	A	472	HEM	C4B-C3B-CAB-CBB
2	B	472	HEM	C4B-C3B-CAB-CBB
2	A	472	HEM	CAD-CBD-CGD-O1D
2	A	472	HEM	CAD-CBD-CGD-O2D
2	B	472	HEM	C2C-C3C-CAC-CBC

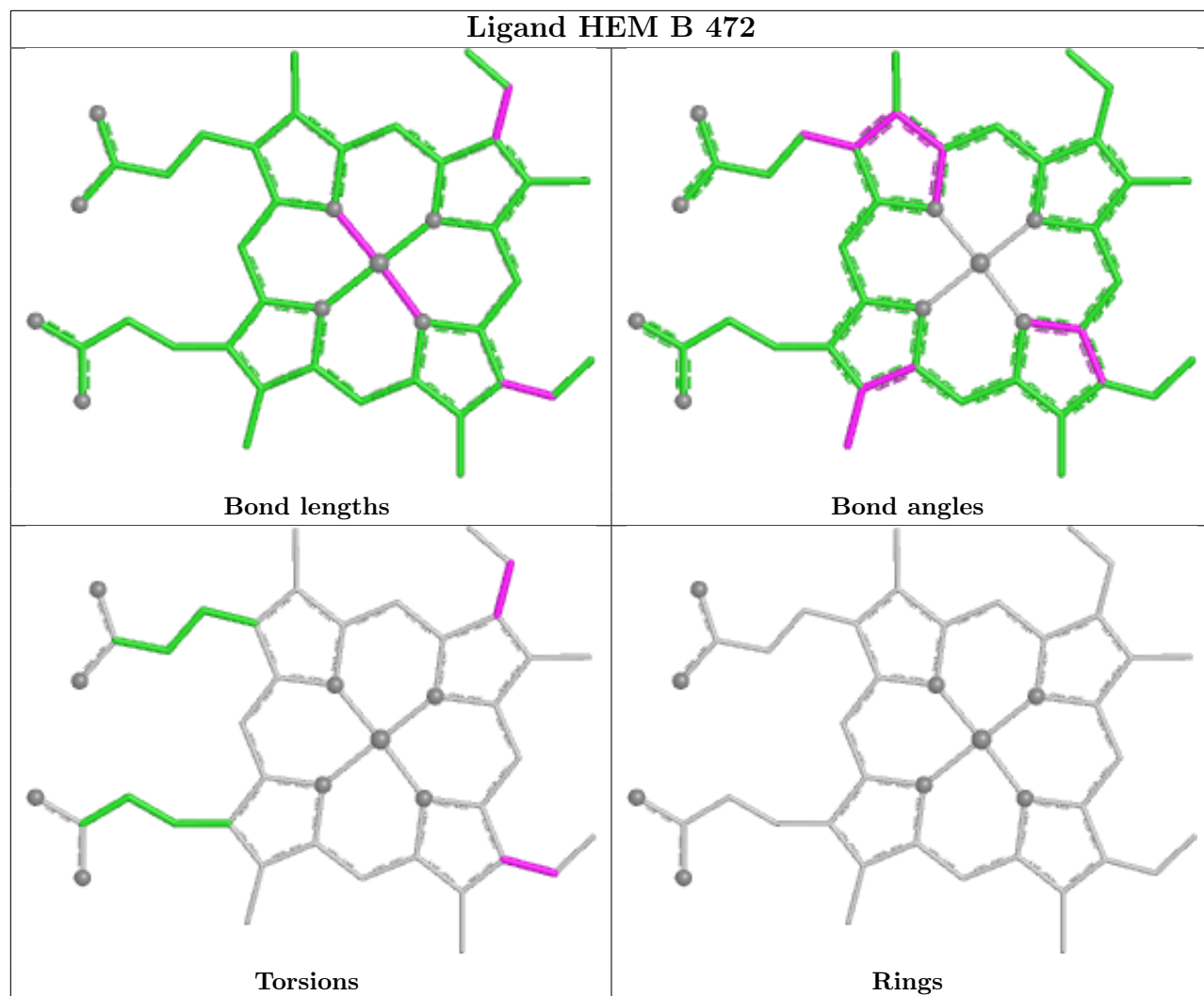
There are no ring outliers.

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

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.