Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:21 am BST

PDB ID	:	6HQW
Title	:	Cytochrome P450-153 from Novosphingobium aromaticivorans
Authors	:	Fiorentini, F.; Mattevi, A.
Deposited on	:	2018-09-25
Resolution	:	2.90 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

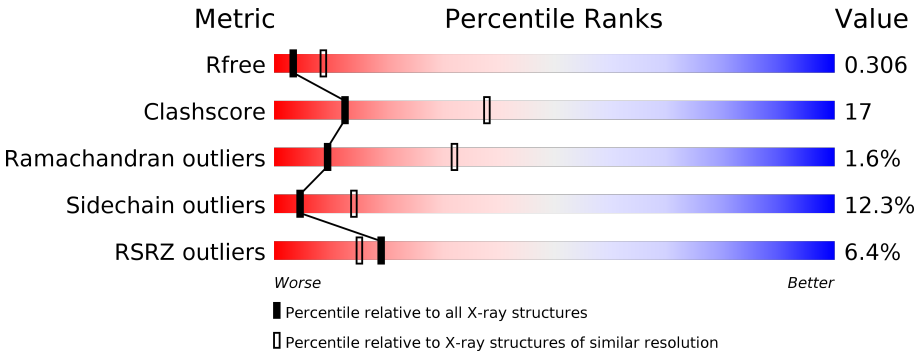
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

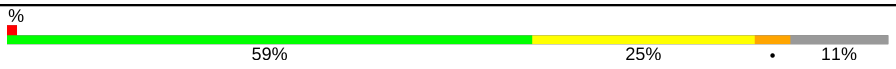
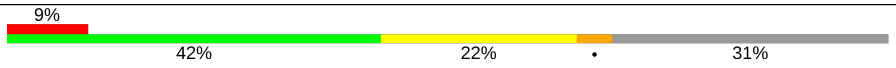
The reported resolution of this entry is 2.90 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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% 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	445	
1	B	445	

2 Entry composition

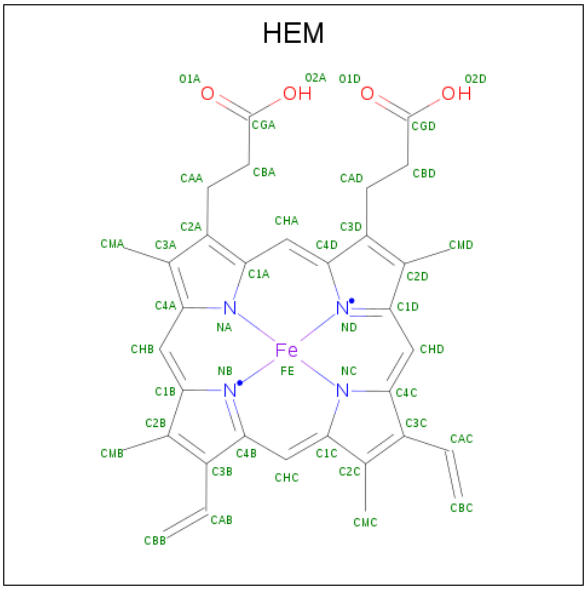
There are 2 unique types of molecules in this entry. The entry contains 5668 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3146	1990	567	568	21			
1	B	307	Total	C	N	O	S	0	0	0
			2436	1535	447	440	14			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

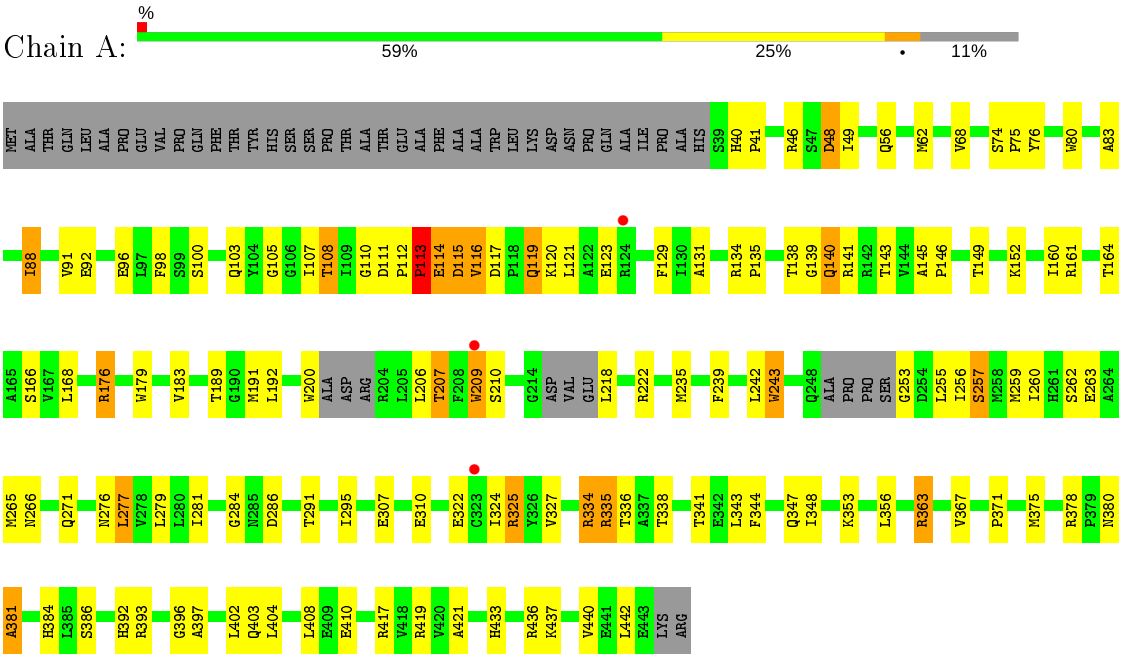


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

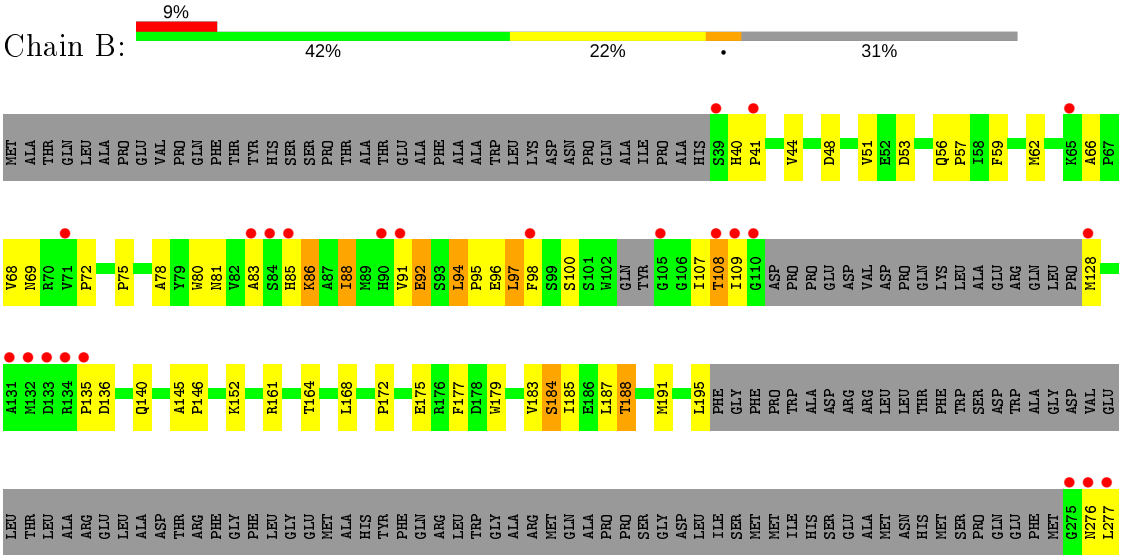
3 Residue-property plots (i)

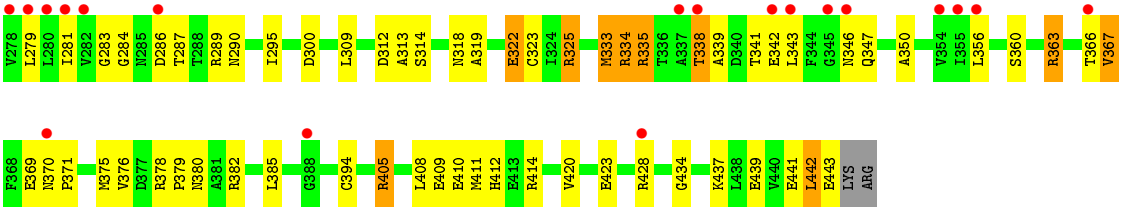
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Cytochrome P450



- Molecule 1: Cytochrome P450




V278 L279 L280 I281 V282 G283 G284 N285 D286 T287 T288 R289 N290 I295 D300 L309 D312 A313 S314 N318 A319 E322 C323 I324 R325 M333 R334 R335 T336 A337 T338 A339 D340 T341 E342 L343 F344 G345 N346 Q347 A350 V354 I355 L356 S360 R363 T366 V367
F368 E369 N370 P371 M375 V376 D377 R378 P379 N380 A381 R382 L385 G388 C394 R405 L408 E409 E410 M411 H412 E413 R414 V420 E423 R428 G434 K437 L438 E439 V440 E441 L442 E443 LYS ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	113.13Å 113.13Å 72.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.98 – 2.90 97.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (97.98-2.90) 98.6 (97.98-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.248 , 0.299 0.255 , 0.306	Depositor DCC
R_{free} test set	1142 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.030 for h,-h-k,-l 0.014 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5668	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	0/3221	0.74	0/4365
1	B	0.44	0/2488	0.64	0/3371
All	All	0.48	0/5709	0.70	0/7736

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	9
1	B	0	4
All	All	0	13

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	PRO	Peptide
1	A	113	PRO	Peptide
1	A	141	ARG	Sidechain
1	A	176	ARG	Sidechain
1	A	325	ARG	Sidechain
1	A	363	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	417	ARG	Sidechain
1	A	436	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	333	MET	Peptide
1	B	363	ARG	Sidechain
1	B	382	ARG	Sidechain
1	B	405	ARG	Sidechain

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	3146	0	3057	85	2
1	B	2436	0	2396	100	0
2	A	43	0	30	4	0
2	B	43	0	30	7	0
All	All	5668	0	5513	187	2

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 17.

All (187) 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:108:THR:CA	1:B:334:ARG:HD3	1.61	1.31
1:A:410:GLU:OE2	1:B:410:GLU:OE1	1.72	1.06
1:B:108:THR:HA	1:B:334:ARG:CD	1.89	1.02
1:A:410:GLU:CD	1:B:410:GLU:OE1	1.95	1.01
1:B:108:THR:CA	1:B:334:ARG:CD	2.40	0.98
1:B:108:THR:HA	1:B:334:ARG:HD3	0.98	0.97
1:B:128:MET:HA	1:B:276:ASN:OD1	1.73	0.89
1:B:334:ARG:HB3	1:B:334:ARG:CZ	2.08	0.82
1:B:184:SER:O	1:B:188:THR:OG1	2.02	0.76
1:A:160:ILE:HG12	1:A:191:MET:CE	2.16	0.76
1:A:325:ARG:NH2	1:A:371:PRO:O	2.19	0.75
1:B:98:PHE:HB3	1:B:335:ARG:HG2	1.67	0.75
1:B:88:ILE:HD11	1:B:356:LEU:HB3	1.69	0.74
1:A:108:THR:HG23	1:A:110:GLY:H	1.52	0.74
1:B:108:THR:C	1:B:334:ARG:NE	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:HD11	1:B:356:LEU:CB	2.20	0.72
1:B:92:GLU:OE2	2:B:500:HEM:O1A	2.08	0.71
1:B:88:ILE:CG2	1:B:385:LEU:HD13	2.20	0.71
1:B:108:THR:N	1:B:334:ARG:HD3	2.06	0.71
1:B:88:ILE:CD1	1:B:356:LEU:HD22	2.23	0.69
1:B:107:ILE:HA	1:B:334:ARG:HB2	1.73	0.69
1:B:40:HIS:N	1:B:41:PRO:HD2	2.08	0.69
1:B:108:THR:N	1:B:334:ARG:HE	1.91	0.69
1:A:209:TRP:CD2	1:A:235:MET:HB3	2.28	0.68
1:A:92:GLU:OE2	2:A:500:HEM:O1A	2.11	0.67
1:A:334:ARG:HG3	1:A:335:ARG:N	2.10	0.66
1:B:86:LYS:NZ	1:B:366:THR:HG21	2.11	0.66
1:A:209:TRP:CE3	1:A:235:MET:HB3	2.31	0.66
1:A:140:GLN:HE21	1:A:276:ASN:HD21	1.44	0.66
1:A:189:THR:HG21	1:A:207:THR:HB	1.77	0.65
1:A:363:ARG:HG3	1:A:363:ARG:HH11	1.61	0.65
1:B:108:THR:N	1:B:334:ARG:CD	2.59	0.65
1:A:129:PHE:HB3	1:A:140:GLN:HG2	1.78	0.65
1:B:410:GLU:HB3	1:B:414:ARG:HH12	1.61	0.65
1:A:343:LEU:O	1:A:344:PHE:CD1	2.52	0.63
1:B:339:ALA:HA	1:B:350:ALA:HB2	1.80	0.63
1:A:105:GLY:HA3	1:A:334:ARG:HH22	1.64	0.62
1:B:108:THR:N	1:B:334:ARG:NE	2.47	0.62
1:B:97:LEU:O	1:B:338:THR:HB	1.99	0.62
1:B:333:MET:O	1:B:356:LEU:HB2	2.00	0.61
1:A:100:SER:O	1:A:131:ALA:HA	2.00	0.61
1:B:98:PHE:HB3	1:B:335:ARG:CG	2.30	0.61
1:A:143:THR:HG21	1:A:262:SER:OG	2.01	0.61
1:A:334:ARG:NH1	1:A:336:THR:OG1	2.34	0.61
1:B:68:VAL:HA	1:B:81:ASN:O	2.01	0.60
1:A:62:MET:CE	1:A:83:ALA:HB2	2.32	0.60
1:A:160:ILE:HG12	1:A:191:MET:HE1	1.83	0.59
1:B:107:ILE:HD12	1:B:107:ILE:O	2.02	0.59
1:B:107:ILE:O	1:B:334:ARG:HG3	2.01	0.59
1:B:318:ASN:ND2	1:B:376:VAL:O	2.34	0.59
1:A:343:LEU:HD13	1:A:344:PHE:HD1	1.67	0.59
1:B:108:THR:C	1:B:334:ARG:CD	2.70	0.59
1:B:423:GLU:HG2	1:B:439:GLU:OE2	2.03	0.58
1:A:134:ARG:HG2	1:A:138:THR:HG23	1.86	0.58
1:A:88:ILE:HD13	1:A:356:LEU:HB3	1.86	0.58
1:B:62:MET:CE	1:B:83:ALA:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HD3	1:A:49:ILE:HG23	1.86	0.57
1:B:334:ARG:O	1:B:335:ARG:NE	2.38	0.57
1:A:111:ASP:OD2	1:A:353:LYS:NZ	2.34	0.57
1:B:108:THR:CA	1:B:334:ARG:NE	2.67	0.57
1:B:107:ILE:C	1:B:334:ARG:HG3	2.26	0.56
1:B:405:ARG:NH1	1:B:409:GLU:OE2	2.38	0.56
1:B:363:ARG:HG3	1:B:363:ARG:HH11	1.70	0.56
1:B:88:ILE:HG21	1:B:385:LEU:HD13	1.88	0.55
1:A:139:GLY:O	1:A:143:THR:HG23	2.06	0.55
1:A:324:ILE:HG22	1:A:384:HIS:CD2	2.42	0.55
1:B:185:ILE:HG12	1:B:289:ARG:HD2	1.88	0.55
1:A:295:ILE:CD1	1:A:404:LEU:HD22	2.37	0.55
1:A:263:GLU:HA	1:A:266:ASN:ND2	2.21	0.54
2:B:500:HEM:HBB2	2:B:500:HEM:HMB2	1.88	0.54
1:A:140:GLN:NE2	1:A:276:ASN:HD21	2.05	0.54
1:B:86:LYS:HZ3	1:B:366:THR:HG21	1.73	0.54
1:B:85:HIS:O	1:B:88:ILE:HG22	2.07	0.54
1:B:88:ILE:HD11	1:B:356:LEU:CA	2.38	0.53
1:A:192:LEU:HD21	1:A:281:ILE:HA	1.90	0.53
1:A:48:ASP:N	1:A:48:ASP:OD1	2.39	0.53
1:A:40:HIS:N	1:A:41:PRO:HD2	2.23	0.53
1:A:80:TRP:CE2	1:A:348:ILE:HD13	2.43	0.53
1:B:66:ALA:O	1:B:69:ASN:ND2	2.40	0.53
1:A:327:VAL:O	1:A:433:HIS:CD2	2.61	0.53
1:B:313:ALA:HB2	1:B:412:HIS:CE1	2.44	0.53
1:B:325:ARG:NH2	1:B:371:PRO:O	2.42	0.53
1:A:74:SER:C	1:A:76:TYR:H	2.12	0.52
1:A:113:PRO:O	1:A:114:GLU:HG2	2.10	0.52
1:A:164:THR:O	1:A:168:LEU:HB2	2.10	0.52
1:A:239:PHE:HB3	1:A:277:LEU:HD21	1.92	0.51
1:B:80:TRP:HZ3	1:B:346:ASN:HD22	1.59	0.51
2:B:500:HEM:HBC2	2:B:500:HEM:HMC2	1.91	0.51
1:A:363:ARG:CG	1:A:363:ARG:HH11	2.25	0.50
1:B:168:LEU:HD21	1:B:411:MET:HG3	1.93	0.50
1:A:105:GLY:HA3	1:A:334:ARG:NH2	2.27	0.50
1:A:123:GLU:HA	1:A:271:GLN:HE21	1.75	0.50
1:B:319:ALA:HB2	1:B:376:VAL:HG13	1.93	0.50
1:B:40:HIS:N	1:B:41:PRO:CD	2.75	0.50
1:A:145:ALA:N	1:A:146:PRO:CD	2.75	0.49
1:A:179:TRP:CZ2	1:A:183:VAL:HG11	2.47	0.49
1:A:135:PRO:O	1:A:138:THR:OG1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLY:N	1:A:257:SER:HG	2.10	0.49
1:A:140:GLN:HE21	1:A:276:ASN:ND2	2.10	0.49
1:A:375:MET:O	1:A:378:ARG:N	2.39	0.49
1:B:62:MET:HE2	1:B:83:ALA:HB2	1.93	0.49
1:A:100:SER:HB2	1:A:107:ILE:HG22	1.95	0.48
1:B:145:ALA:N	1:B:146:PRO:CD	2.77	0.48
1:B:410:GLU:O	1:B:414:ARG:NH1	2.46	0.48
1:A:189:THR:HG21	1:A:207:THR:CG2	2.44	0.48
1:B:107:ILE:C	1:B:334:ARG:CD	2.82	0.48
1:B:94:LEU:HD22	1:B:97:LEU:HD23	1.96	0.48
1:B:161:ARG:NH2	1:B:409:GLU:OE2	2.47	0.48
1:A:239:PHE:CE2	1:A:281:ILE:HD11	2.49	0.48
1:A:91:VAL:HG11	1:A:356:LEU:HD21	1.96	0.47
1:B:164:THR:O	1:B:168:LEU:HB2	2.15	0.47
1:A:327:VAL:O	1:A:433:HIS:HD2	1.98	0.47
1:A:410:GLU:OE2	1:B:410:GLU:CD	2.44	0.47
1:B:410:GLU:HB3	1:B:414:ARG:NH1	2.29	0.47
1:A:143:THR:OG1	1:A:265:MET:CE	2.63	0.47
1:B:405:ARG:HH11	1:B:409:GLU:CD	2.19	0.46
1:A:143:THR:OG1	1:A:265:MET:HE2	2.16	0.46
1:B:88:ILE:HD11	1:B:356:LEU:HA	1.96	0.46
1:B:51:VAL:CG2	1:B:428:ARG:HA	2.46	0.46
1:A:189:THR:HG21	1:A:207:THR:CB	2.44	0.46
2:A:500:HEM:HMB2	2:A:500:HEM:HBB2	1.98	0.46
1:B:107:ILE:C	1:B:334:ARG:CG	2.84	0.46
1:B:284:GLY:HA2	2:B:500:HEM:C2C	2.51	0.46
1:B:312:ASP:O	1:B:312:ASP:OD1	2.35	0.45
1:A:121:LEU:HD23	1:A:121:LEU:O	2.16	0.45
1:A:396:GLY:O	1:A:397:ALA:C	2.55	0.45
1:B:375:MET:O	1:B:378:ARG:N	2.44	0.45
1:B:88:ILE:HD12	1:B:356:LEU:HD22	1.97	0.45
1:A:392:HIS:O	2:A:500:HEM:HBA2	2.17	0.45
1:B:80:TRP:HZ3	1:B:346:ASN:ND2	2.15	0.45
1:A:114:GLU:HG3	1:A:115:ASP:N	2.31	0.45
1:A:74:SER:C	1:A:76:TYR:N	2.70	0.45
1:B:91:VAL:HG11	1:B:356:LEU:HD21	1.99	0.45
1:B:179:TRP:CZ2	1:B:183:VAL:HG11	2.52	0.45
1:A:255:LEU:O	1:A:259:MET:HG3	2.17	0.44
1:A:88:ILE:O	1:A:92:GLU:HB2	2.17	0.44
1:A:98:PHE:O	1:A:335:ARG:HG2	2.17	0.44
1:A:191:MET:HG2	1:A:403:GLN:CD	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:SER:O	1:A:76:TYR:N	2.50	0.44
1:B:300:ASP:OD2	1:B:420:VAL:HG23	2.17	0.44
1:A:68:VAL:HG21	1:A:343:LEU:HD12	1.99	0.44
1:A:384:HIS:CD2	1:A:386:SER:H	2.35	0.44
1:B:283:GLY:O	2:B:500:HEM:C1C	2.71	0.44
1:A:123:GLU:HA	1:A:271:GLN:NE2	2.33	0.44
1:B:177:PHE:O	1:B:439:GLU:HA	2.18	0.44
1:B:86:LYS:HZ1	1:B:366:THR:HG21	1.83	0.44
1:A:192:LEU:HD13	1:A:284:GLY:O	2.17	0.43
1:B:107:ILE:O	1:B:107:ILE:CD1	2.66	0.43
1:A:123:GLU:CA	1:A:271:GLN:HE21	2.32	0.43
1:B:187:LEU:O	1:B:191:MET:N	2.46	0.43
1:B:295:ILE:HG12	1:B:323:CYS:SG	2.58	0.43
2:A:500:HEM:HBC2	2:A:500:HEM:HMC1	2.01	0.43
1:B:72:PRO:O	1:B:78:ALA:HB2	2.18	0.43
1:B:109:ILE:N	1:B:334:ARG:CD	2.82	0.43
1:B:94:LEU:N	1:B:95:PRO:CD	2.82	0.43
1:A:176:ARG:HA	1:A:440:VAL:O	2.18	0.43
1:A:322:GLU:OE2	1:A:378:ARG:HD2	2.19	0.43
1:B:394:CYS:SG	2:B:500:HEM:C4B	3.10	0.42
1:B:56:GLN:HB2	1:B:57:PRO:HD3	2.01	0.42
1:B:423:GLU:CG	1:B:439:GLU:OE2	2.66	0.42
1:A:307:GLU:HA	1:A:310:GLU:HB2	2.01	0.42
1:B:322:GLU:HG3	1:B:375:MET:C	2.39	0.42
1:B:88:ILE:HG21	1:B:385:LEU:CD1	2.49	0.42
1:B:88:ILE:HD12	1:B:88:ILE:HA	1.85	0.42
1:A:380:ASN:O	1:A:381:ALA:C	2.57	0.42
1:B:322:GLU:HG3	1:B:375:MET:O	2.19	0.42
1:B:59:PHE:CD1	1:B:360:SER:HB2	2.55	0.42
1:A:149:THR:HG23	1:A:152:LYS:H	1.85	0.42
1:A:176:ARG:HD3	1:A:421:ALA:HB1	2.00	0.42
1:B:290:ASN:CG	1:B:434:GLY:HA3	2.40	0.42
2:B:500:HEM:HBB2	2:B:500:HEM:CMB	2.50	0.41
1:B:441:GLU:C	1:B:442:LEU:HD13	2.41	0.41
1:B:97:LEU:HD12	1:B:97:LEU:C	2.39	0.41
1:A:160:ILE:CG1	1:A:191:MET:HE1	2.50	0.41
1:A:140:GLN:NE2	1:A:276:ASN:ND2	2.67	0.41
1:B:378:ARG:HA	1:B:379:PRO:HD3	1.97	0.41
1:B:312:ASP:OD1	1:B:312:ASP:C	2.58	0.41
1:B:369:GLU:C	1:B:370:ASN:HD22	2.24	0.41
1:B:367:VAL:HG23	1:B:380:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HA	1:A:277:LEU:HD12	1.89	0.41
1:A:243:TRP:CD2	1:A:260:ILE:HD11	2.56	0.41
1:A:291:THR:HG21	1:A:404:LEU:HD11	2.02	0.41
1:A:256:ILE:O	1:A:257:SER:C	2.59	0.40
1:B:107:ILE:C	1:B:334:ARG:HD3	2.39	0.40
1:A:114:GLU:HG3	1:A:115:ASP:H	1.85	0.40
1:B:309:LEU:HD13	1:B:376:VAL:HG11	2.04	0.40
1:B:366:THR:HG22	1:B:366:THR:O	2.20	0.40

All (2) 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:119:GLN:OE1	1:A:134:ARG:NH2[2_544]	2.16	0.04
1:A:103:GLN:OE1	1:A:343:LEU:O[2_544]	2.18	0.02

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	387/445 (87%)	345 (89%)	34 (9%)	8 (2%)	7 26
1	B	299/445 (67%)	262 (88%)	34 (11%)	3 (1%)	15 45
All	All	686/890 (77%)	607 (88%)	68 (10%)	11 (2%)	9 32

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PRO
1	A	114	GLU
1	A	116	VAL
1	A	119	GLN

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Mol	Chain	Res	Type
1	B	75	PRO
1	A	56	GLN
1	A	381	ALA
1	A	402	LEU
1	B	53	ASP
1	B	172	PRO
1	A	75	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	329/378 (87%)	295 (90%)	34 (10%)	7 22
1	B	257/378 (68%)	219 (85%)	38 (15%)	3 9
All	All	586/756 (78%)	514 (88%)	72 (12%)	4 14

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	88	ILE
1	A	96	GLU
1	A	108	THR
1	A	115	ASP
1	A	116	VAL
1	A	117	ASP
1	A	120	LYS
1	A	140	GLN
1	A	161	ARG
1	A	166	SER
1	A	200	TRP
1	A	206	LEU
1	A	207	THR
1	A	209	TRP
1	A	210	SER

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Mol	Chain	Res	Type
1	A	218	LEU
1	A	222	ARG
1	A	242	LEU
1	A	243	TRP
1	A	257	SER
1	A	277	LEU
1	A	279	LEU
1	A	286	ASP
1	A	334	ARG
1	A	335	ARG
1	A	338	THR
1	A	341	THR
1	A	347	GLN
1	A	367	VAL
1	A	408	LEU
1	A	419	ARG
1	A	437	LYS
1	A	442	LEU
1	B	44	VAL
1	B	48	ASP
1	B	86	LYS
1	B	88	ILE
1	B	92	GLU
1	B	94	LEU
1	B	96	GLU
1	B	97	LEU
1	B	100	SER
1	B	108	THR
1	B	135	PRO
1	B	136	ASP
1	B	140	GLN
1	B	152	LYS
1	B	175	GLU
1	B	184	SER
1	B	188	THR
1	B	195	LEU
1	B	277	LEU
1	B	279	LEU
1	B	281	ILE
1	B	286	ASP
1	B	287	THR
1	B	314	SER

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Mol	Chain	Res	Type
1	B	322	GLU
1	B	325	ARG
1	B	334	ARG
1	B	335	ARG
1	B	338	THR
1	B	341	THR
1	B	342	GLU
1	B	343	LEU
1	B	347	GLN
1	B	367	VAL
1	B	408	LEU
1	B	437	LYS
1	B	442	LEU
1	B	443	GLU

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

Mol	Chain	Res	Type
1	A	85	HIS
1	A	140	GLN
1	A	384	HIS
1	A	403	GLN
1	A	433	HIS
1	B	85	HIS
1	B	140	GLN
1	B	370	ASN
1	B	433	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 carbohydrates 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	500	1	27,50,50	0.82	0	17,82,82	1.70	5 (29%)
2	HEM	A	500	1	27,50,50	0.99	1 (3%)	17,82,82	2.19	8 (47%)

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	500	1	-	2/6/54/54	-
2	HEM	A	500	1	-	0/6/54/54	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C4D-C3D	2.29	1.47	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	CBD-CAD-C3D	-5.40	102.53	112.48
2	B	500	HEM	CAA-CBA-CGA	3.70	118.88	112.67
2	B	500	HEM	C4A-C3A-C2A	3.16	109.19	107.00
2	A	500	HEM	CBA-CAA-C2A	-2.63	107.63	112.49
2	A	500	HEM	CMD-C2D-C1D	-2.40	124.77	128.46
2	A	500	HEM	C4C-C3C-C2C	-2.37	105.24	106.90
2	A	500	HEM	CMB-C2B-C3B	2.28	128.95	124.68
2	B	500	HEM	CBD-CAD-C3D	-2.26	108.31	112.48
2	A	500	HEM	CMA-C3A-C4A	-2.22	125.05	128.46
2	A	500	HEM	CMA-C3A-C2A	2.19	129.06	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	CMD-C2D-C3D	2.19	129.06	124.94
2	B	500	HEM	CMA-C3A-C4A	-2.02	125.35	128.46
2	B	500	HEM	CAD-CBD-CGD	-2.00	109.31	112.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HEM	C1A-C2A-CAA-CBA
2	B	500	HEM	C3A-C2A-CAA-CBA

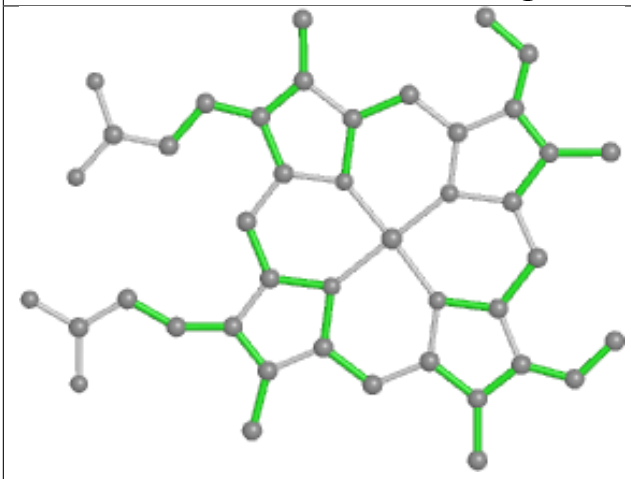
There are no ring outliers.

2 monomers are involved in 11 short contacts:

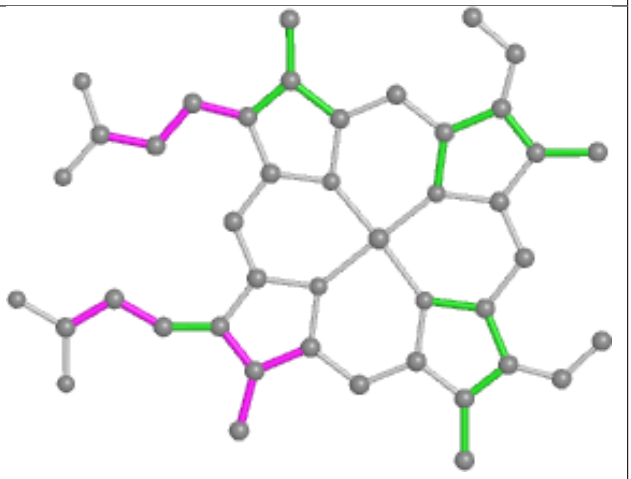
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	7	0
2	A	500	HEM	4	0

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.

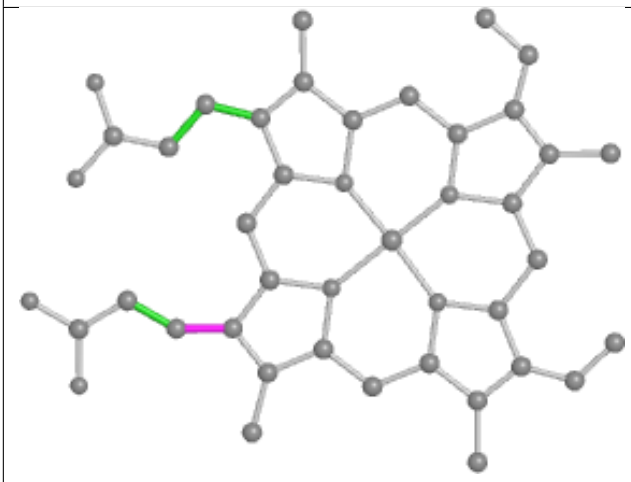
Ligand HEM B 500



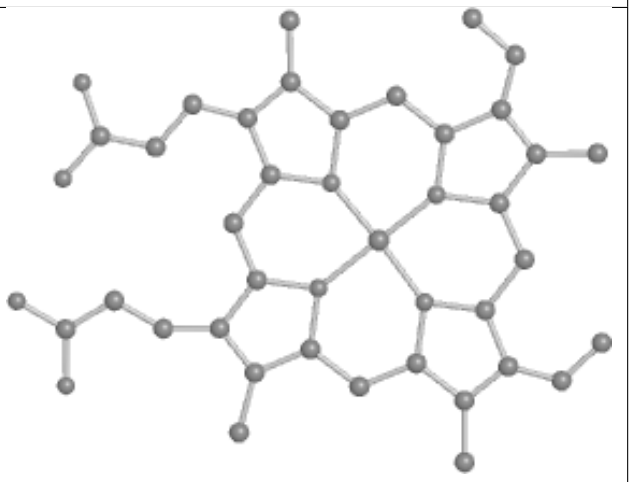
Bond lengths



Bond angles

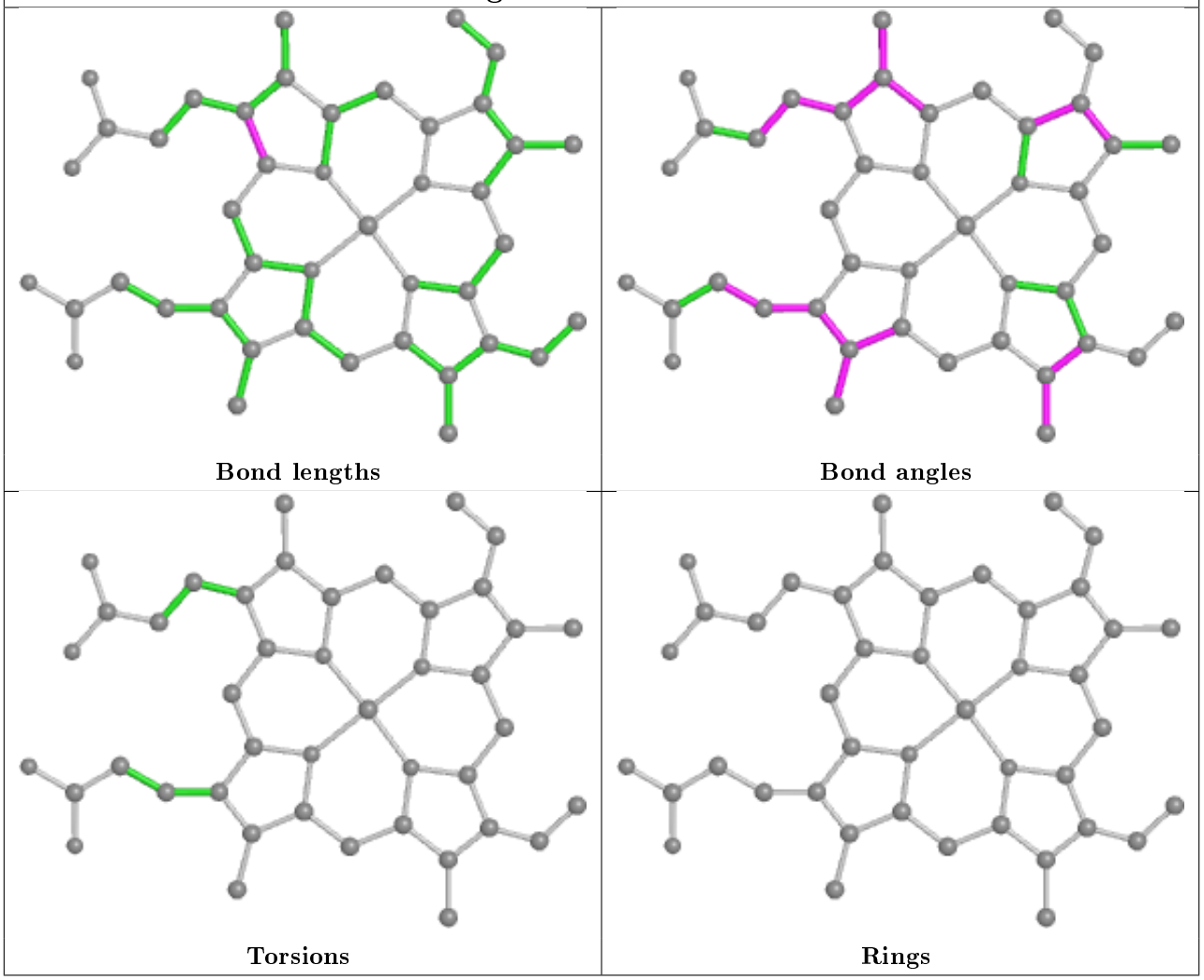


Torsions



Rings

Ligand HEM A 500



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^{th} 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^2)	Q<0.9
1	A	395/445 (88%)	0.28	3 (0%) 86 86	28, 55, 93, 134	0
1	B	307/445 (68%)	0.91	42 (13%) 3 2	43, 85, 132, 175	0
All	All	702/890 (78%)	0.56	45 (6%) 19 15	28, 69, 120, 175	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	GLY	9.1
1	B	276	ASN	7.7
1	B	343	LEU	7.6
1	B	342	GLU	6.3
1	B	90	HIS	6.3
1	B	278	VAL	5.4
1	B	109	ILE	5.4
1	B	39	SER	4.3
1	B	108	THR	4.3
1	B	110	GLY	4.3
1	B	279	LEU	4.2
1	B	338	THR	4.1
1	B	354	VAL	4.0
1	B	135	PRO	3.8
1	B	337	ALA	3.7
1	B	282	VAL	3.5
1	B	128	MET	3.5
1	B	105	GLY	3.4
1	B	134	ARG	3.4
1	B	91	VAL	3.1
1	B	370	ASN	3.0
1	B	281	ILE	3.0
1	B	83	ALA	2.8
1	B	71	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	277	LEU	2.7
1	B	85	HIS	2.7
1	B	132	MET	2.6
1	A	124	ARG	2.6
1	B	41	PRO	2.6
1	A	323	CYS	2.5
1	B	84	SER	2.4
1	B	366	THR	2.4
1	B	345	GLY	2.4
1	B	346	ASN	2.4
1	B	355	ILE	2.4
1	B	356	LEU	2.4
1	B	131	ALA	2.3
1	B	65	LYS	2.3
1	B	428	ARG	2.2
1	B	388	GLY	2.2
1	B	98	PHE	2.1
1	B	133	ASP	2.0
1	B	286	ASP	2.0
1	A	209	TRP	2.0
1	B	280	LEU	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

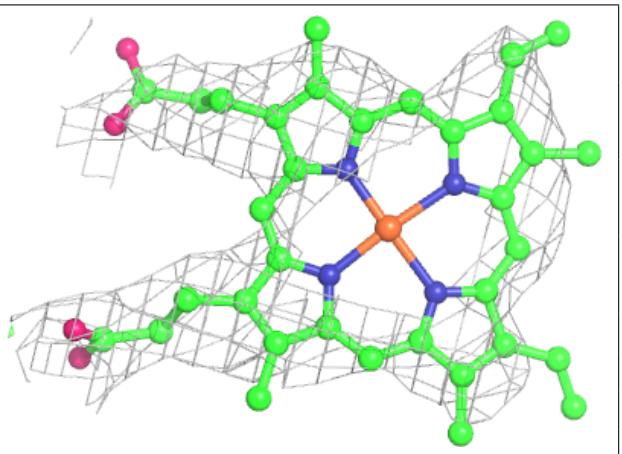
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

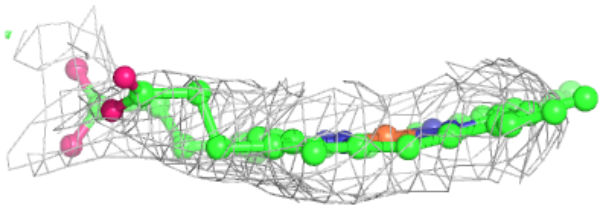
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	500	43/43	0.94	0.28	62,93,102,122	0
2	HEM	A	500	43/43	0.98	0.22	31,44,49,56	0

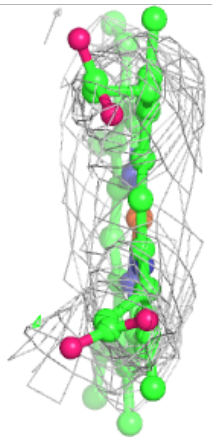
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM B 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

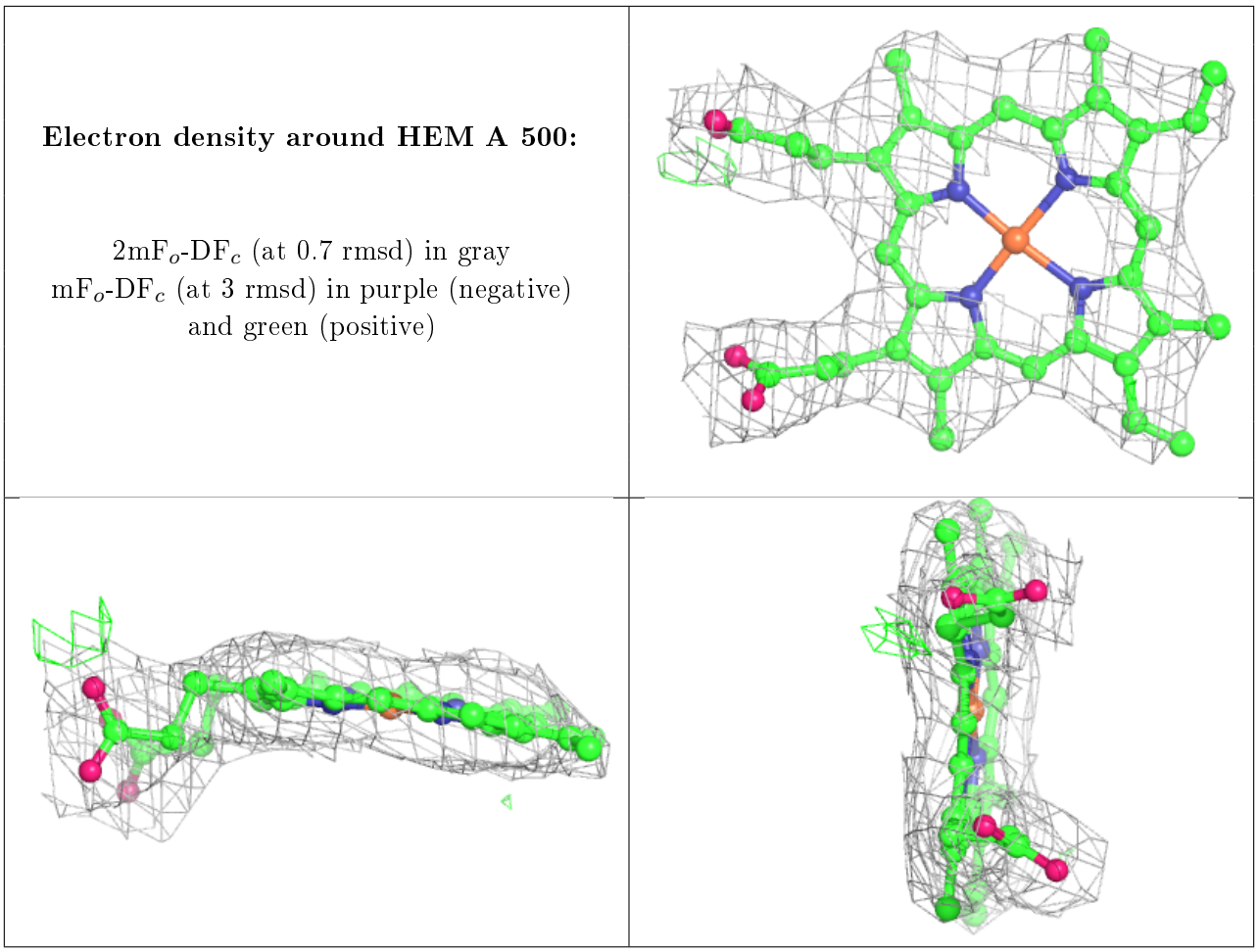






Electron density around HEM A 500:

$2mF_o$-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.