Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 03:07 pm GMT

PDB ID	:	4BIM
Title	:	CATALASE 3 FROM NEUROSPORA CRASSA IN TETRAGONAL FORM EXPOSES A MODIFIED TETRAMERIC ORGANIZATION
Authors	:	Zarate-Romero, A.; Rudino-Pinera, E.
Deposited on	:	2013-04-11
Resolution	:	2.95 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 (i)) were used in the production of this report:

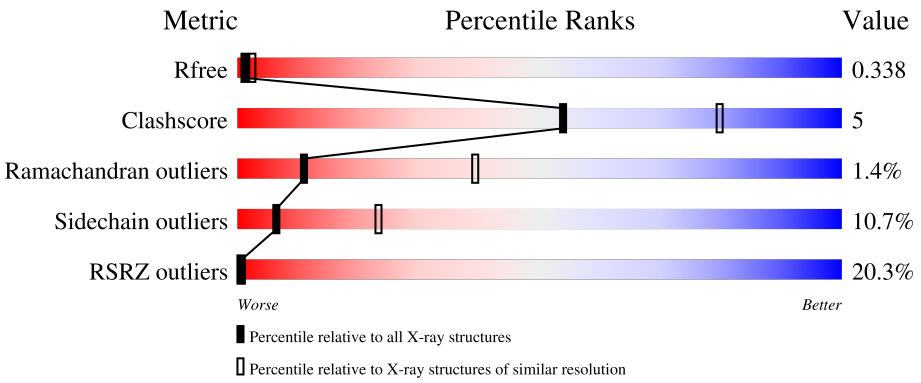
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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% 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	746	2%, 80%, 11%, • , 9%
1	B	746	6%, 78%, 12%, • , 9%
1	C	746	23%, 68%, 20%, • , 9%
1	D	746	42%, 65%, 22%, • • , 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21809 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 CATALASE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	681	5340	3381	941	1012	6	0	0	0
			Total	C	N	O	S			
1	B	679	5324	3371	939	1008	6	0	0	0
			Total	C	N	O	S			
1	C	681	5340	3381	941	1012	6	0	0	0
			Total	C	N	O	S			
1	D	680	5331	3376	940	1009	6	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	expression tag	UNP Q9C169
A	-25	ASN	-	expression tag	UNP Q9C169
A	-24	HIS	-	expression tag	UNP Q9C169
A	-23	LYS	-	expression tag	UNP Q9C169
A	-22	VAL	-	expression tag	UNP Q9C169
A	-21	HIS	-	expression tag	UNP Q9C169
A	-20	HIS	-	expression tag	UNP Q9C169
A	-19	HIS	-	expression tag	UNP Q9C169
A	-18	HIS	-	expression tag	UNP Q9C169
A	-17	HIS	-	expression tag	UNP Q9C169
A	-16	HIS	-	expression tag	UNP Q9C169
A	-15	ILE	-	expression tag	UNP Q9C169
A	-14	GLU	-	expression tag	UNP Q9C169
A	-13	GLY	-	expression tag	UNP Q9C169
A	-12	ARG	-	expression tag	UNP Q9C169
A	-11	HIS	-	expression tag	UNP Q9C169
A	-10	MET	-	expression tag	UNP Q9C169
A	-9	GLU	-	expression tag	UNP Q9C169
A	-8	LEU	-	expression tag	UNP Q9C169
A	-7	GLY	-	expression tag	UNP Q9C169
A	-6	THR	-	expression tag	UNP Q9C169

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP Q9C169
A	-4	GLU	-	expression tag	UNP Q9C169
A	-3	GLY	-	expression tag	UNP Q9C169
A	-2	SER	-	expression tag	UNP Q9C169
A	-1	GLU	-	expression tag	UNP Q9C169
A	0	PHE	-	expression tag	UNP Q9C169
B	-26	MET	-	expression tag	UNP Q9C169
B	-25	ASN	-	expression tag	UNP Q9C169
B	-24	HIS	-	expression tag	UNP Q9C169
B	-23	LYS	-	expression tag	UNP Q9C169
B	-22	VAL	-	expression tag	UNP Q9C169
B	-21	HIS	-	expression tag	UNP Q9C169
B	-20	HIS	-	expression tag	UNP Q9C169
B	-19	HIS	-	expression tag	UNP Q9C169
B	-18	HIS	-	expression tag	UNP Q9C169
B	-17	HIS	-	expression tag	UNP Q9C169
B	-16	HIS	-	expression tag	UNP Q9C169
B	-15	ILE	-	expression tag	UNP Q9C169
B	-14	GLU	-	expression tag	UNP Q9C169
B	-13	GLY	-	expression tag	UNP Q9C169
B	-12	ARG	-	expression tag	UNP Q9C169
B	-11	HIS	-	expression tag	UNP Q9C169
B	-10	MET	-	expression tag	UNP Q9C169
B	-9	GLU	-	expression tag	UNP Q9C169
B	-8	LEU	-	expression tag	UNP Q9C169
B	-7	GLY	-	expression tag	UNP Q9C169
B	-6	THR	-	expression tag	UNP Q9C169
B	-5	LEU	-	expression tag	UNP Q9C169
B	-4	GLU	-	expression tag	UNP Q9C169
B	-3	GLY	-	expression tag	UNP Q9C169
B	-2	SER	-	expression tag	UNP Q9C169
B	-1	GLU	-	expression tag	UNP Q9C169
B	0	PHE	-	expression tag	UNP Q9C169
C	-26	MET	-	expression tag	UNP Q9C169
C	-25	ASN	-	expression tag	UNP Q9C169
C	-24	HIS	-	expression tag	UNP Q9C169
C	-23	LYS	-	expression tag	UNP Q9C169
C	-22	VAL	-	expression tag	UNP Q9C169
C	-21	HIS	-	expression tag	UNP Q9C169
C	-20	HIS	-	expression tag	UNP Q9C169
C	-19	HIS	-	expression tag	UNP Q9C169
C	-18	HIS	-	expression tag	UNP Q9C169

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	HIS	-	expression tag	UNP Q9C169
C	-16	HIS	-	expression tag	UNP Q9C169
C	-15	ILE	-	expression tag	UNP Q9C169
C	-14	GLU	-	expression tag	UNP Q9C169
C	-13	GLY	-	expression tag	UNP Q9C169
C	-12	ARG	-	expression tag	UNP Q9C169
C	-11	HIS	-	expression tag	UNP Q9C169
C	-10	MET	-	expression tag	UNP Q9C169
C	-9	GLU	-	expression tag	UNP Q9C169
C	-8	LEU	-	expression tag	UNP Q9C169
C	-7	GLY	-	expression tag	UNP Q9C169
C	-6	THR	-	expression tag	UNP Q9C169
C	-5	LEU	-	expression tag	UNP Q9C169
C	-4	GLU	-	expression tag	UNP Q9C169
C	-3	GLY	-	expression tag	UNP Q9C169
C	-2	SER	-	expression tag	UNP Q9C169
C	-1	GLU	-	expression tag	UNP Q9C169
C	0	PHE	-	expression tag	UNP Q9C169
D	-26	MET	-	expression tag	UNP Q9C169
D	-25	ASN	-	expression tag	UNP Q9C169
D	-24	HIS	-	expression tag	UNP Q9C169
D	-23	LYS	-	expression tag	UNP Q9C169
D	-22	VAL	-	expression tag	UNP Q9C169
D	-21	HIS	-	expression tag	UNP Q9C169
D	-20	HIS	-	expression tag	UNP Q9C169
D	-19	HIS	-	expression tag	UNP Q9C169
D	-18	HIS	-	expression tag	UNP Q9C169
D	-17	HIS	-	expression tag	UNP Q9C169
D	-16	HIS	-	expression tag	UNP Q9C169
D	-15	ILE	-	expression tag	UNP Q9C169
D	-14	GLU	-	expression tag	UNP Q9C169
D	-13	GLY	-	expression tag	UNP Q9C169
D	-12	ARG	-	expression tag	UNP Q9C169
D	-11	HIS	-	expression tag	UNP Q9C169
D	-10	MET	-	expression tag	UNP Q9C169
D	-9	GLU	-	expression tag	UNP Q9C169
D	-8	LEU	-	expression tag	UNP Q9C169
D	-7	GLY	-	expression tag	UNP Q9C169
D	-6	THR	-	expression tag	UNP Q9C169
D	-5	LEU	-	expression tag	UNP Q9C169
D	-4	GLU	-	expression tag	UNP Q9C169
D	-3	GLY	-	expression tag	UNP Q9C169

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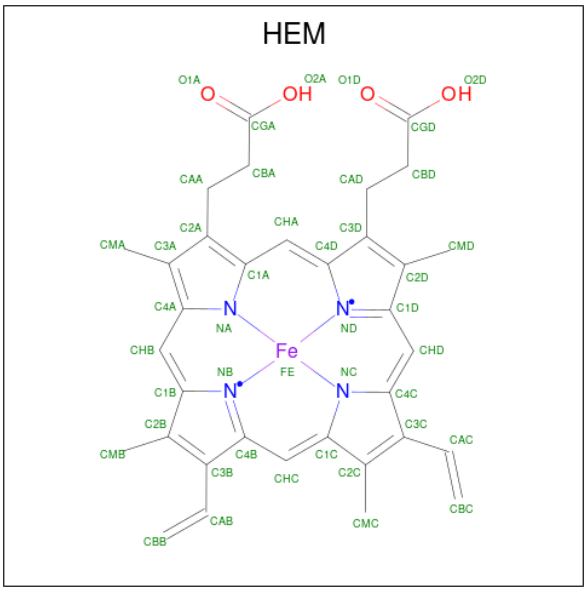
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q9C169
D	-1	GLU	-	expression tag	UNP Q9C169
D	0	PHE	-	expression tag	UNP Q9C169

- 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		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	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	90	Total	O	0	0
			90	90		
3	B	61	Total	O	0	0
			61	61		
3	C	54	Total	O	0	0
			54	54		

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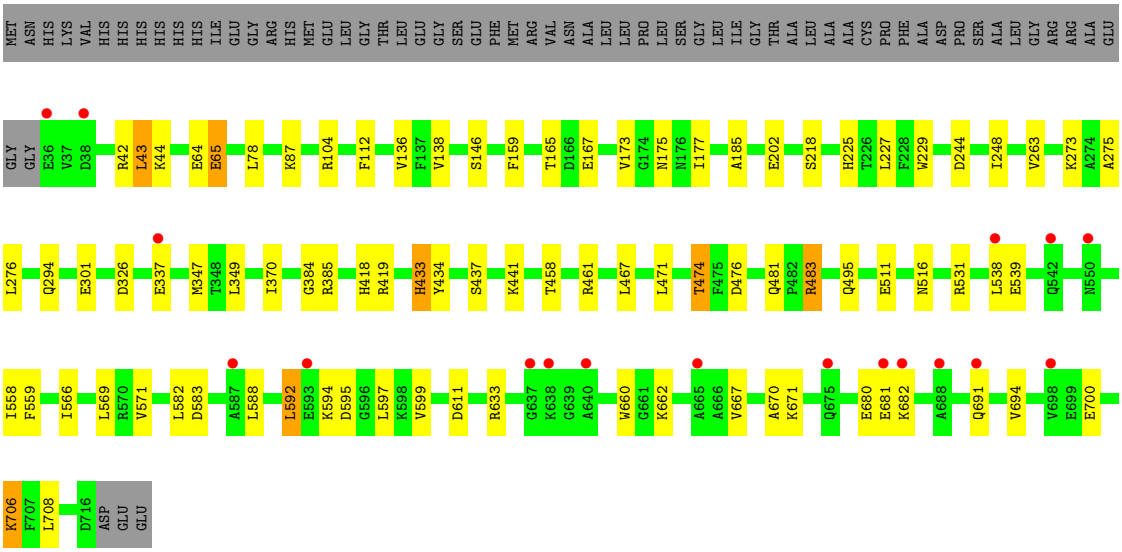
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	D	97	97	97	0	0

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 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.

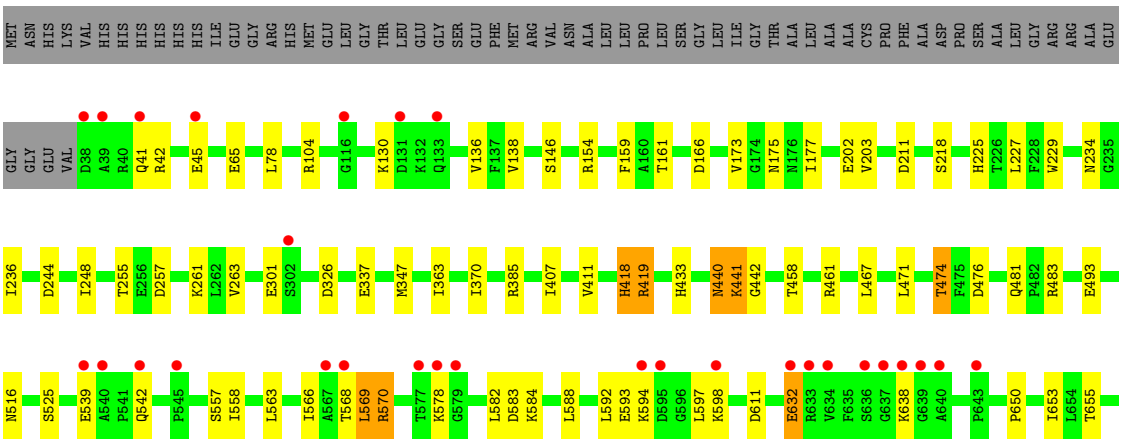
- Molecule 1: CATALASE 3

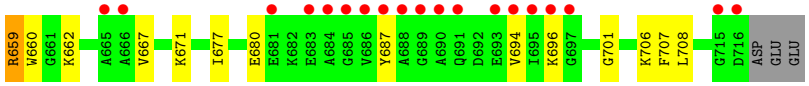
Chain A:



- Molecule 1: CATALASE 3

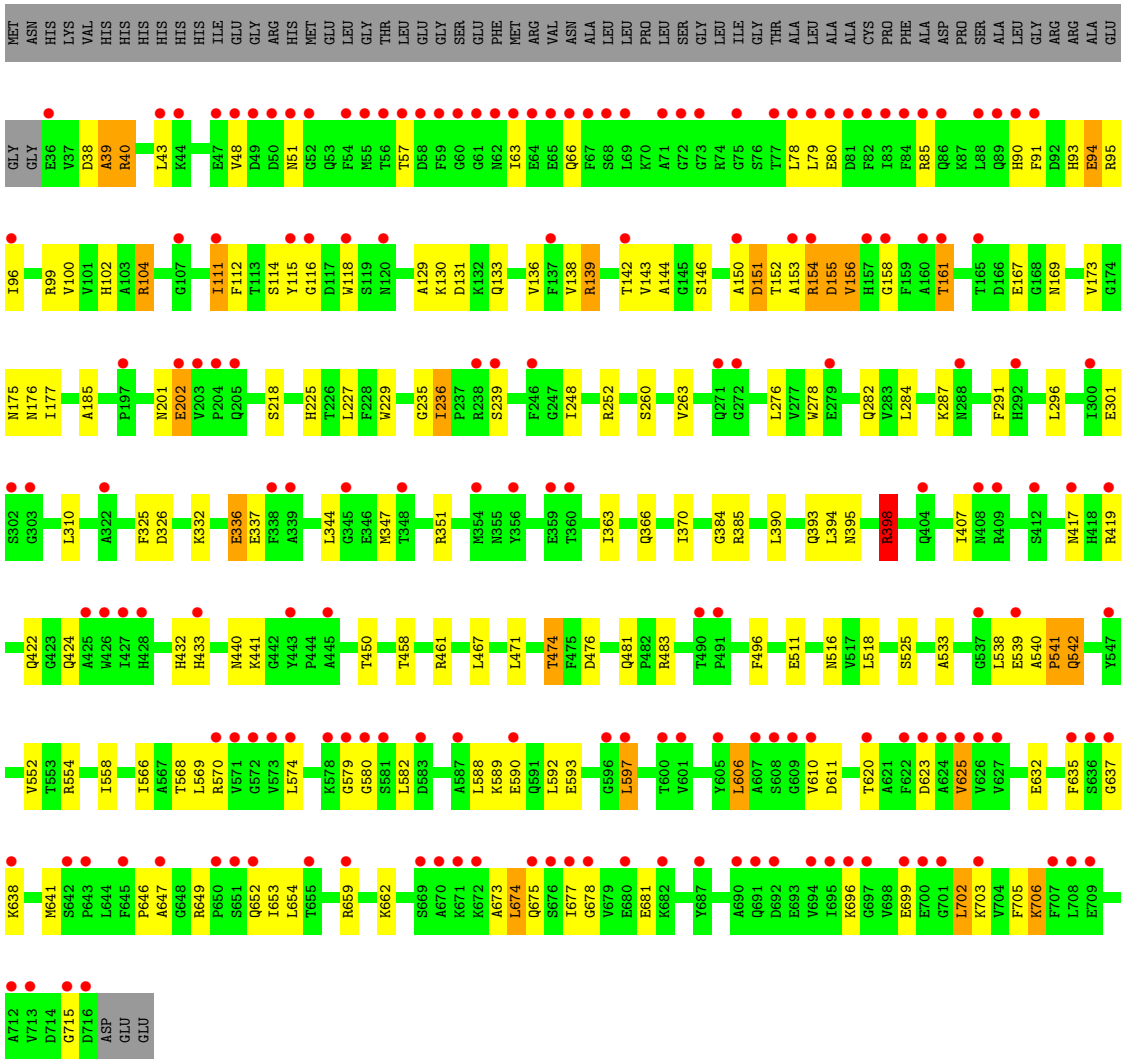
Chain B:





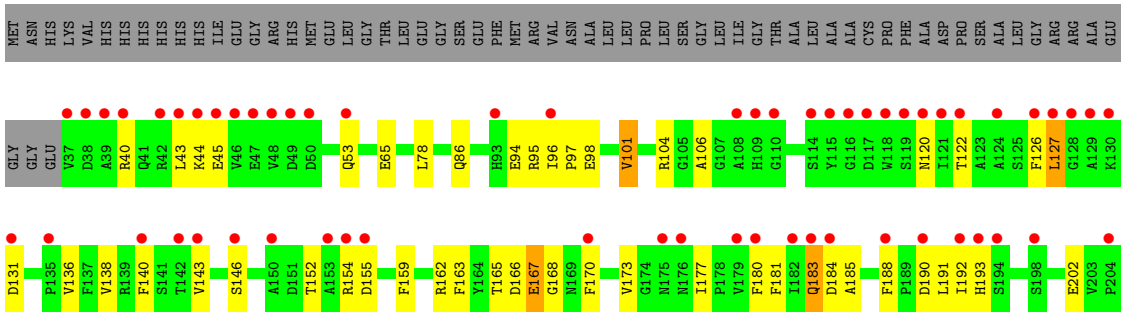
- Molecule 1: CATALASE 3

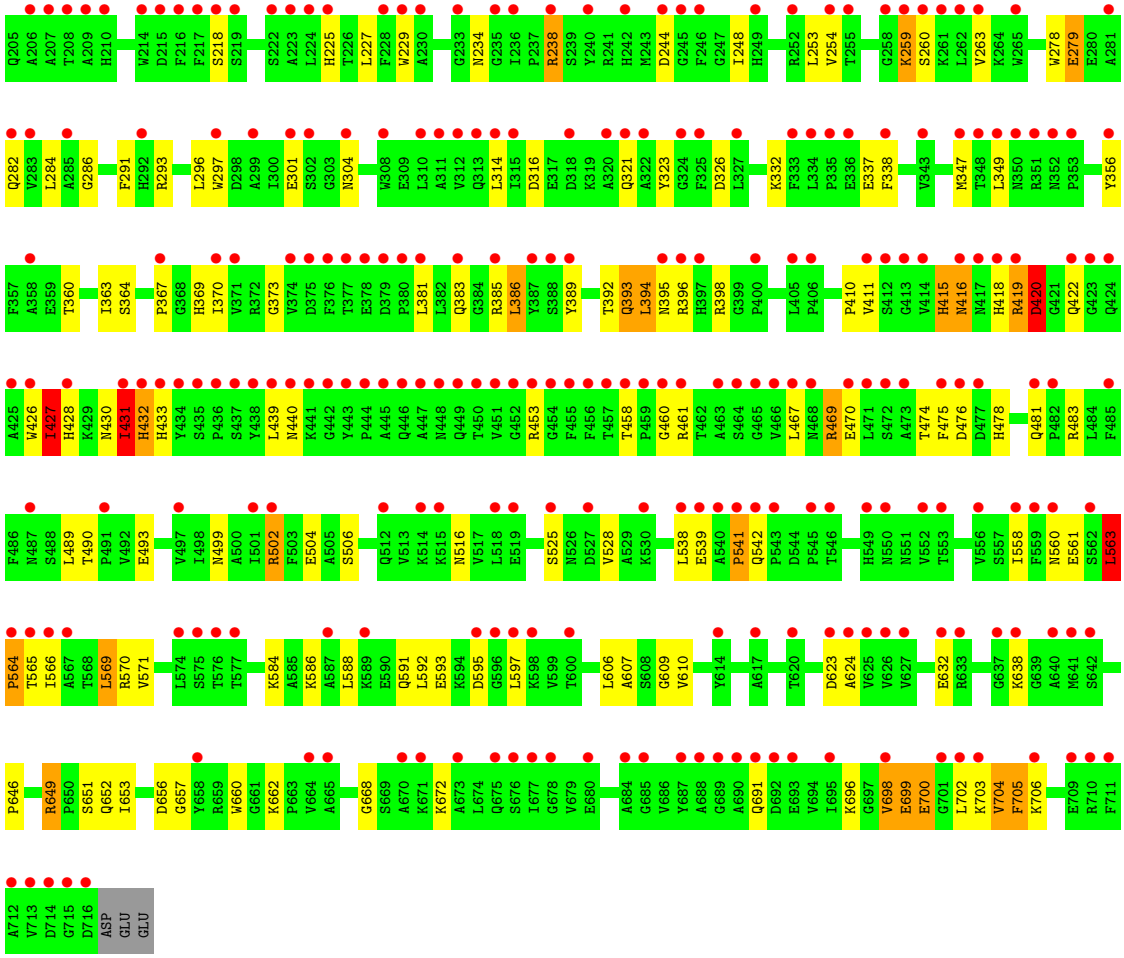
Chain C:



- Molecule 1: CATALASE 3

Chain D:




Q205 A206 A207 T208 A209 H210 W214 D215 F216 F217 S218 S219 S222 A223 L224 H225 T226 L227 F228 W229 A230 G233 N234 G235 I236 P237 R238 S239 Y240 R241 H242 M243 D244 G245 F246 G247 I248 H249 R252 L253 V254 T255 G258 K259 S260 K261 L262 V263 K264 W265 W278 E279 E280 A281
Q282 V283 L284 A285 G286 F291 H292 R293 L296 W297 D298 A299 I300 E301 S302 S303 N304 W308 E309 L310 A311 V312 Q313 L314 I315 D316 E317 D318 K319 A320 Q321 A322 Y323 G324 F325 D326 L327 K332 F333 L334 P335 E336 E337 F338 V343 M347 T348 L349 N350 R351 N352 P353 Y356
F357 A358 E359 T360 I363 S364 P367 G368 H369 I370 V371 R372 G373 V374 D375 F376 T377 E378 D379 P380 L381 L382 Q383 G384 R385 L386 Y387 S388 Y389 T392 Q393 L394 N395 R396 H397 R398 G399 P400 L405 P406 P410 V411 S412 G413 V414 H415 N416 M417 H418 R419 D420 G421 Q422 G423 Q424
A425 W426 I427 H428 K429 N430 I431 H432 H433 Y434 S435 P436 S437 Y438 L439 N440 K441 G442 Y443 P444 A445 Q446 A447 N448 Q449 T450 V451 G452 R453 G454 F455 F456 T457 T458 P459 G460 R461 T462 A463 S464 G465 V466 L467 N468 R469 E470 L471 S472 A473 T474 F475 D476 D477 H478 Q481 P482 R483 L484 F485
F486 N487 S488 L489 T490 P491 V492 E493 V497 I498 N499 A500 I501 R502 F503 E504 A505 S506 Q512 V513 K514 K515 N516 V517 L518 E519 S525 N526 D527 V528 A529 K530 L538 E539 A540 P541 Q542 P543 D544 P545 T546 H549 N550 N551 V552 T553 V556 S557 I558 F559 N560 E561 S562 L563
P564 T565 I566 A567 T568 L569 R570 V571 L574 S575 T576 T577 K584 A585 K586 A587 L588 K589 E590 Q591 L592 E593 K594 D595 G596 L597 K598 V599 T600 L606 A607 S608 G609 V610 Y614 A617 T620 D623 A624 V625 V626 V627 E632 R633 G637 K638 G639 A640 M641 S642
P646 R649 P650 S651 Q652 I653 D656 G657 Y658 R659 W660 G661 K662 P663 V664 A665 G668 S669 A670 K671 K672 A673 L674 Q675 S676 I677 G678 V679 E680 A684 G685 V686 Y687 A688 G689 A690 Q691 D692 E693 V694 I695 K696 G697 V698 E699 E700 G701 L702 K703 V704 F705 K706 E709 R710 F711
A712 V713 D714 G715 D716 ASP GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	207.51Å 207.51Å 137.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.30 – 2.95 29.30 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.30-2.95) 98.9 (29.30-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.255 , 0.304 0.285 , 0.338	Depositor DCC
R_{free} test set	3166 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 68.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	21809	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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 (i)

5.1 Standard geometry (i)

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	0.45	0/5473	0.64	0/7424
1	B	0.45	0/5457	0.65	2/7402 (0.0%)
1	C	0.47	0/5473	0.70	4/7424 (0.1%)
1	D	0.48	0/5464	0.73	2/7412 (0.0%)
All	All	0.46	0/21867	0.68	8/29662 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	541	PRO	C-N-CA	7.57	140.63	121.70
1	B	632	GLU	C-N-CA	6.37	137.63	121.70
1	C	702	LEU	C-N-CA	5.85	136.31	121.70
1	C	39	ALA	C-N-CA	5.37	135.13	121.70
1	C	150	ALA	C-N-CA	5.32	134.99	121.70
1	D	698	VAL	C-N-CA	5.24	134.79	121.70
1	D	609	GLY	C-N-CA	5.13	134.53	121.70
1	B	566	ILE	C-N-CA	5.09	134.43	121.70

There are no chirality outliers.

There are no planarity outliers.

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	5340	0	5156	33	0
1	B	5324	0	5141	33	0
1	C	5340	0	5156	85	0
1	D	5331	0	5151	88	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	1	0
3	A	90	0	0	1	0
3	B	61	0	0	1	0
3	C	54	0	0	0	0
3	D	97	0	0	2	1
All	All	21809	0	20724	223	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (223) 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:D:704:VAL:HA	1:D:705:PHE:HB3	1.17	1.13
1:C:153:ALA:HB1	1:C:154:ARG:HA	1.22	1.10
1:D:415:HIS:HB2	1:D:416:ASN:HA	1.34	1.09
1:C:102:HIS:HA	1:C:142:THR:O	1.69	0.92
1:D:431:ILE:HD13	1:D:432:HIS:H	1.35	0.91
1:C:646:PRO:HB3	1:D:279:GLU:HG2	1.63	0.79
1:C:39:ALA:HB1	1:C:351:ARG:HG3	1.64	0.79
1:D:152:THR:HG21	1:D:284:LEU:HG	1.67	0.76
1:D:704:VAL:CA	1:D:705:PHE:HB3	2.09	0.75
1:C:153:ALA:HB1	1:C:154:ARG:CA	2.13	0.73
1:D:699:GLU:HG3	1:D:700:GLU:HG2	1.75	0.69
1:B:655:THR:O	1:B:659:ARG:HG2	1.93	0.68
1:C:654:LEU:HB3	1:C:674:LEU:HD13	1.74	0.68
1:D:426:TRP:HA	1:D:427:ILE:HB	1.75	0.68
1:C:287:LYS:HE2	1:D:282:GLN:HG3	1.76	0.68
1:B:593:GLU:HB3	1:C:580:GLY:HA3	1.77	0.67
1:C:104:ARG:HE	1:C:151:ASP:HB2	1.58	0.67
1:C:158:GLY:HA2	1:C:175:ASN:HA	1.77	0.67
1:C:91:PHE:O	1:C:94:GLU:HB2	1.95	0.67
1:C:332:LYS:HG2	1:C:481:GLN:HG3	1.76	0.66
1:D:180:PHE:HB2	1:D:248:ILE:HD13	1.78	0.65
1:C:646:PRO:HG3	1:C:649:ARG:HE	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:VAL:HG11	1:D:349:LEU:HD11	1.78	0.65
1:D:385:ARG:HG2	1:D:389:TYR:HE1	1.62	0.65
1:A:248:ILE:HD13	2:A:4000:HEM:HMB1	1.80	0.64
1:D:238:ARG:HH22	1:D:291:PHE:HZ	1.44	0.64
1:C:278:TRP:H	1:C:496:PHE:HE1	1.45	0.64
1:D:431:ILE:CD1	1:D:432:HIS:H	2.10	0.64
1:A:483:ARG:NH2	3:A:2070:HOH:O	2.30	0.63
1:D:260:SER:HB3	1:D:458:THR:HG21	1.80	0.63
1:D:563:LEU:HB3	1:D:564:PRO:HA	1.80	0.63
1:D:704:VAL:HA	1:D:705:PHE:CB	2.08	0.63
1:A:571:VAL:HG11	1:A:592:LEU:HD22	1.81	0.62
1:C:625:VAL:HB	1:C:654:LEU:HD12	1.81	0.62
1:C:606:LEU:HD21	1:D:506:SER:HB2	1.80	0.62
1:D:563:LEU:H	1:D:703:LYS:HG2	1.64	0.62
1:C:248:ILE:HD13	2:C:4000:HEM:HMB1	1.82	0.61
1:B:248:ILE:HD13	2:B:4000:HEM:HMB1	1.82	0.61
1:C:417:ASN:HB3	1:C:433:HIS:O	2.01	0.61
1:D:419:ARG:HE	1:D:420:ASP:HB3	1.66	0.60
1:C:40:ARG:HD2	1:C:43:LEU:HD12	1.82	0.60
1:C:540:ALA:HB1	1:C:541:PRO:CD	2.32	0.60
1:D:668:GLY:HA3	3:D:2064:HOH:O	2.02	0.59
1:C:153:ALA:CB	1:C:154:ARG:HA	2.12	0.58
1:C:93:HIS:ND1	1:D:395:ASN:HB2	2.18	0.58
1:B:569:LEU:HD13	1:B:598:LYS:H	1.68	0.58
1:D:154:ARG:HH12	1:D:504:GLU:HG3	1.69	0.58
1:C:702:LEU:HD12	1:C:705:PHE:HA	1.84	0.58
1:D:415:HIS:HB2	1:D:416:ASN:CA	2.23	0.57
1:C:57:THR:HG23	1:C:63:ILE:HG12	1.86	0.57
1:D:571:VAL:HG22	1:D:624:ALA:HB3	1.84	0.57
1:D:563:LEU:HB3	1:D:564:PRO:CA	2.34	0.57
1:D:183:GLN:HG2	1:D:475:PHE:HD2	1.69	0.57
1:C:284:LEU:HD13	1:C:620:THR:HB	1.87	0.57
1:C:177:ILE:HG12	1:C:229:TRP:HB3	1.87	0.56
1:D:415:HIS:CB	1:D:416:ASN:HA	2.22	0.56
1:D:646:PRO:HD2	1:D:649:ARG:HG3	1.87	0.56
1:D:489:LEU:HB3	1:D:493:GLU:HB3	1.88	0.55
1:A:177:ILE:HG12	1:A:229:TRP:HB3	1.89	0.54
1:D:431:ILE:HD13	1:D:432:HIS:N	2.14	0.54
1:D:385:ARG:HG2	1:D:389:TYR:CE1	2.43	0.54
1:C:483:ARG:HD2	1:C:525:SER:HB2	1.89	0.54
1:B:177:ILE:HG12	1:B:229:TRP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:ALA:HB1	1:C:539:GLU:HA	1.90	0.54
1:D:177:ILE:HG12	1:D:229:TRP:HB3	1.90	0.54
1:D:483:ARG:HD2	1:D:525:SER:HB2	1.90	0.54
1:A:136:VAL:HG21	1:A:347:MET:HG3	1.90	0.53
1:B:136:VAL:HG21	1:B:347:MET:HG3	1.90	0.53
1:C:138:VAL:HG22	1:C:161:THR:HG22	1.89	0.53
1:D:180:PHE:CD2	1:D:381:LEU:HD21	2.43	0.53
1:D:165:THR:OG1	1:D:168:GLY:O	2.25	0.53
1:A:275:ALA:HB3	1:A:558:ILE:HD13	1.90	0.53
1:A:467:LEU:HD22	1:B:78:LEU:HD11	1.90	0.53
1:C:632:GLU:HG3	1:C:673:ALA:HB2	1.91	0.52
1:D:136:VAL:HG21	1:D:347:MET:HG3	1.92	0.52
1:D:97:PRO:HD2	1:D:396:ARG:HA	1.91	0.52
1:C:100:VAL:HA	1:D:95:ARG:HG3	1.90	0.52
1:C:39:ALA:CB	1:C:351:ARG:HG3	2.38	0.52
1:C:282:GLN:O	1:D:286:GLY:HA3	2.10	0.52
1:B:483:ARG:HD2	1:B:525:SER:HB2	1.92	0.52
1:C:90:HIS:H	1:C:93:HIS:HD2	1.58	0.52
1:B:660:TRP:HE3	1:B:662:LYS:HE3	1.75	0.51
1:C:635:PHE:CE1	1:C:674:LEU:HD12	2.45	0.51
1:D:185:ALA:HA	2:D:4000:HEM:HBB1	1.92	0.51
1:A:419:ARG:HG3	1:A:433:HIS:HD2	1.76	0.51
1:A:458:THR:HB	1:A:461:ARG:HG3	1.92	0.51
1:A:276:LEU:HA	1:A:706:LYS:HE3	1.92	0.51
1:D:660:TRP:HE3	1:D:662:LYS:HE3	1.76	0.50
1:B:138:VAL:HG22	1:B:161:THR:HG23	1.94	0.50
1:C:156:VAL:HG23	1:C:177:ILE:HD12	1.94	0.50
1:C:102:HIS:CE1	1:C:143:VAL:HG22	2.46	0.50
1:C:574:LEU:HD21	1:C:653:ILE:HG23	1.92	0.50
1:C:589:LYS:O	1:C:593:GLU:HB2	2.10	0.50
1:D:323:TYR:HD1	1:D:338:PHE:CD2	2.29	0.50
1:A:660:TRP:HE3	1:A:662:LYS:HE3	1.76	0.49
1:A:273:LYS:HB3	1:A:558:ILE:HG22	1.93	0.49
1:D:696:LYS:HA	1:D:699:GLU:HG2	1.93	0.49
1:A:78:LEU:HD11	1:B:467:LEU:HD22	1.94	0.49
1:B:234:ASN:ND2	1:B:558:ILE:HD11	2.27	0.49
1:D:278:TRP:O	1:D:282:GLN:HG2	2.12	0.49
1:A:42:ARG:HG2	1:A:43:LEU:HD22	1.95	0.49
1:B:568:THR:OG1	1:B:569:LEU:HA	2.13	0.49
1:C:136:VAL:HG21	1:C:347:MET:HG3	1.94	0.49
1:B:458:THR:HB	1:B:461:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:PHE:HB2	1:C:332:LYS:HD3	1.94	0.48
1:D:418:HIS:CG	1:D:419:ARG:H	2.29	0.48
1:D:699:GLU:HA	1:D:700:GLU:HA	1.65	0.48
1:B:418:HIS:O	1:B:419:ARG:HD3	2.13	0.48
1:C:94:GLU:O	1:C:95:ARG:NH1	2.46	0.48
1:D:383:GLN:O	1:D:386:LEU:HG	2.13	0.48
1:C:366:GLN:HG2	1:C:390:LEU:HD22	1.95	0.48
1:C:566:ILE:HD13	1:C:699:GLU:HG2	1.95	0.48
1:C:458:THR:HB	1:C:461:ARG:HG3	1.94	0.48
1:B:667:VAL:HG22	1:B:694:VAL:HG21	1.95	0.48
1:C:39:ALA:HB3	1:C:40:ARG:HB3	1.95	0.48
1:D:234:ASN:ND2	1:D:558:ILE:HD11	2.29	0.48
1:C:276:LEU:HA	1:C:706:LYS:HE3	1.96	0.47
1:C:606:LEU:HA	1:C:610:VAL:HB	1.97	0.47
1:D:122:THR:HB	1:D:253:LEU:HB3	1.95	0.47
1:C:153:ALA:HB2	1:C:235:GLY:O	2.14	0.47
1:D:652:GLN:NE2	1:D:656:ASP:OD2	2.46	0.47
1:C:39:ALA:HB2	1:C:351:ARG:HH11	1.79	0.47
1:C:518:LEU:HB3	1:C:540:ALA:HB2	1.96	0.47
1:D:260:SER:HB3	1:D:458:THR:CG2	2.45	0.47
1:A:566:ILE:HA	1:A:569:LEU:HD12	1.96	0.47
1:A:495:GLN:OE1	1:A:531:ARG:NH2	2.37	0.47
1:B:708:LEU:HD22	1:B:708:LEU:H	1.79	0.47
1:C:144:ALA:HB3	1:C:155:ASP:OD2	2.15	0.46
1:C:202:GLU:HB2	1:D:356:TYR:CG	2.50	0.46
1:C:225:HIS:CE1	1:C:481:GLN:HB3	2.49	0.46
1:D:323:TYR:HD1	1:D:338:PHE:HD2	1.61	0.46
1:C:637:GLY:O	1:C:641:MET:HB2	2.16	0.46
1:D:254:VAL:N	1:D:373:GLY:O	2.47	0.46
1:B:154:ARG:HG3	1:B:236:ILE:HG23	1.97	0.46
1:B:175:ASN:HB2	1:B:248:ILE:HD11	1.97	0.46
1:C:111:ILE:HD11	1:C:133:GLN:HG2	1.97	0.46
1:C:284:LEU:HD11	1:C:291:PHE:CD1	2.51	0.46
1:C:569:LEU:HB2	1:C:597:LEU:HD23	1.96	0.46
1:C:310:LEU:HD23	1:C:344:LEU:HB2	1.98	0.46
1:C:432:HIS:HB2	1:C:440:ASN:HB3	1.96	0.46
1:D:360:THR:O	1:D:363:ILE:HG22	2.16	0.46
1:C:540:ALA:HB1	1:C:541:PRO:HD3	1.98	0.45
1:D:188:PHE:CZ	1:D:192:ILE:HD11	2.51	0.45
1:C:623:ASP:HB3	1:C:702:LEU:HD11	1.98	0.45
1:A:175:ASN:HB2	1:A:248:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:LEU:CB	1:D:564:PRO:HA	2.46	0.45
1:D:106:ALA:HB2	1:D:293:ARG:HG2	1.98	0.45
1:C:143:VAL:HG23	1:C:156:VAL:O	2.17	0.45
1:C:218:SER:HB2	1:C:516:ASN:HB3	1.99	0.45
1:D:623:ASP:O	1:D:662:LYS:HB3	2.16	0.45
1:B:261:LYS:HB2	3:B:2013:HOH:O	2.16	0.45
1:C:116:GLY:HA2	1:C:130:LYS:HG3	1.99	0.45
1:B:440:ASN:HD22	1:B:442:GLY:H	1.65	0.45
1:C:467:LEU:HD22	1:D:78:LEU:HD11	1.98	0.45
1:A:138:VAL:HG23	1:A:349:LEU:HD21	1.99	0.45
1:A:559:PHE:CD2	1:A:708:LEU:HD21	2.51	0.45
1:D:490:THR:OG1	1:D:493:GLU:HB2	2.17	0.45
1:B:569:LEU:HD22	1:B:597:LEU:HA	1.99	0.44
1:D:314:LEU:HD23	1:D:314:LEU:H	1.82	0.44
1:D:418:HIS:HB3	1:D:430:ASN:HD22	1.82	0.44
1:B:650:PRO:HA	1:B:653:ILE:HD12	1.99	0.44
1:D:564:PRO:HD2	3:D:2026:HOH:O	2.16	0.44
1:A:571:VAL:HG13	1:A:599:VAL:HG13	1.99	0.44
1:C:93:HIS:HE1	1:D:394:LEU:HG	1.83	0.44
1:C:173:VAL:HB	1:C:385:ARG:HH22	1.83	0.44
1:D:569:LEU:O	1:D:623:ASP:HB2	2.17	0.44
1:A:559:PHE:HB3	1:A:708:LEU:HD11	2.00	0.44
1:D:181:PHE:HB2	1:D:191:LEU:HD11	2.00	0.43
1:B:363:ILE:HD12	1:B:407:ILE:HG13	2.00	0.43
1:D:218:SER:HB2	1:D:516:ASN:HB3	2.00	0.43
1:C:336:GLU:H	1:C:336:GLU:HG2	1.59	0.43
1:C:652:GLN:NE2	1:D:652:GLN:OE1	2.52	0.43
1:C:153:ALA:CB	1:C:236:ILE:HG23	2.49	0.43
1:A:173:VAL:HB	1:A:385:ARG:HH22	1.83	0.43
1:C:394:LEU:O	1:C:398:ARG:HA	2.18	0.43
1:C:635:PHE:CE2	1:C:673:ALA:HB1	2.54	0.43
1:B:493:GLU:OE1	1:B:557:SER:OG	2.35	0.43
1:D:364:SER:HB3	1:D:393:GLN:CD	2.39	0.43
1:D:541:PRO:HB2	1:D:542:GLN:H	1.64	0.43
1:A:434:TYR:CE2	1:A:437:SER:HB2	2.54	0.42
1:C:326:ASP:HB2	1:C:474:THR:HB	2.00	0.42
1:B:594:LYS:HA	1:C:579:GLY:H	1.84	0.42
1:D:173:VAL:HB	1:D:367:PRO:HG3	2.01	0.42
1:A:65:GLU:HB2	1:A:87:LYS:HD2	2.01	0.42
1:C:112:PHE:HD1	1:C:347:MET:HB2	1.83	0.42
1:A:218:SER:HB2	1:A:516:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:VAL:HB	1:B:385:ARG:HH22	1.84	0.42
1:B:255:THR:OG1	1:B:257:ASP:OD1	2.33	0.42
1:B:326:ASP:HB2	1:B:474:THR:HB	2.01	0.42
1:D:101:VAL:HG11	1:D:192:ILE:HD12	2.00	0.42
1:D:225:HIS:CE1	1:D:481:GLN:HB3	2.55	0.42
1:C:115:TYR:HD2	1:C:118:TRP:HZ2	1.67	0.42
1:D:162:ARG:NH2	1:D:369:HIS:CE1	2.87	0.42
1:B:225:HIS:CE1	1:B:481:GLN:HB3	2.55	0.41
1:D:326:ASP:HB2	1:D:474:THR:HB	2.02	0.41
1:C:201:ASN:HB3	1:D:297:TRP:CE3	2.56	0.41
1:D:136:VAL:HG12	1:D:163:PHE:HA	2.02	0.41
1:A:326:ASP:HB2	1:A:474:THR:HB	2.01	0.41
1:A:566:ILE:HD12	1:A:597:LEU:HD11	2.01	0.41
1:C:646:PRO:N	1:C:647:ALA:HA	2.35	0.41
1:C:185:ALA:HB3	1:C:384:GLY:HA3	2.02	0.41
1:C:252:ARG:NH1	1:C:461:ARG:HD3	2.35	0.41
1:D:163:PHE:HB2	1:D:170:PHE:O	2.20	0.41
1:C:260:SER:HB3	1:C:458:THR:CG2	2.51	0.41
1:D:234:ASN:HD21	1:D:558:ILE:HD11	1.86	0.41
1:D:389:TYR:HA	1:D:392:THR:HG22	2.01	0.41
1:D:499:ASN:HA	1:D:502:ARG:HD2	2.03	0.41
1:A:294:GLN:OE1	1:B:203:VAL:HG11	2.21	0.41
1:B:218:SER:HB2	1:B:516:ASN:HB3	2.02	0.41
1:C:398:ARG:NH1	1:D:398:ARG:HG2	2.36	0.41
1:A:667:VAL:HG22	1:A:694:VAL:HG21	2.02	0.41
1:C:139:ARG:HD3	2:C:4000:HEM:O2A	2.21	0.41
1:D:98:GLU:HA	1:D:396:ARG:HH21	1.85	0.41
1:C:363:ILE:HD12	1:C:407:ILE:HG13	2.03	0.41
1:B:701:GLY:HA2	1:B:707:PHE:HZ	1.86	0.41
1:A:225:HIS:CE1	1:A:481:GLN:HB3	2.57	0.40
1:D:657:GLY:HA2	1:D:662:LYS:HD2	2.03	0.40
1:A:112:PHE:HD1	1:A:347:MET:HB2	1.86	0.40
1:A:185:ALA:HB3	1:A:384:GLY:HA3	2.03	0.40
2:C:4000:HEM:HMB1	2:C:4000:HEM:HBB2	2.02	0.40
1:D:140:PHE:HE1	1:D:159:PHE:CZ	2.39	0.40
1:D:653:ILE:O	1:D:656:ASP:O	2.39	0.40
1:A:165:THR:C	1:A:167:GLU:H	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2016:HOH:O	3:D:2016:HOH:O[8_554]	2.19	0.01

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	679/746 (91%)	640 (94%)	38 (6%)	1 (0%)	51 83
1	B	677/746 (91%)	628 (93%)	46 (7%)	3 (0%)	34 69
1	C	679/746 (91%)	619 (91%)	49 (7%)	11 (2%)	9 36
1	D	678/746 (91%)	585 (86%)	70 (10%)	23 (3%)	3 17
All	All	2713/2984 (91%)	2472 (91%)	203 (8%)	38 (1%)	11 39

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	THR
1	C	568	THR
1	D	427	ILE
1	D	563	LEU
1	D	564	PRO
1	D	705	PHE
1	B	632	GLU
1	C	152	THR
1	C	398	ARG
1	C	678	GLY
1	D	94	GLU
1	D	259	LYS
1	D	411	VAL
1	D	415	HIS
1	D	428	HIS
1	D	541	PRO
1	B	570	ARG

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Mol	Chain	Res	Type
1	C	40	ARG
1	C	169	ASN
1	D	143	VAL
1	D	410	PRO
1	D	469	ARG
1	D	699	GLU
1	D	704	VAL
1	A	670	ALA
1	B	441	LYS
1	D	127	LEU
1	D	607	ALA
1	D	610	VAL
1	C	38	ASP
1	C	129	ALA
1	C	542	GLN
1	D	167	GLU
1	C	715	GLY
1	D	419	ARG
1	D	420	ASP
1	D	431	ILE
1	D	460	GLY

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	559/609 (92%)	520 (93%)	39 (7%)	15 43
1	B	557/609 (92%)	511 (92%)	46 (8%)	11 35
1	C	559/609 (92%)	491 (88%)	68 (12%)	5 19
1	D	558/609 (92%)	472 (85%)	86 (15%)	2 11
All	All	2233/2436 (92%)	1994 (89%)	239 (11%)	6 23

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	44	LYS
1	A	64	GLU
1	A	65	GLU
1	A	104	ARG
1	A	146	SER
1	A	159	PHE
1	A	202	GLU
1	A	227	LEU
1	A	244	ASP
1	A	263	VAL
1	A	301	GLU
1	A	337	GLU
1	A	370	ILE
1	A	418	HIS
1	A	433	HIS
1	A	441	LYS
1	A	471	LEU
1	A	474	THR
1	A	476	ASP
1	A	483	ARG
1	A	511	GLU
1	A	538	LEU
1	A	539	GLU
1	A	582	LEU
1	A	583	ASP
1	A	588	LEU
1	A	592	LEU
1	A	594	LYS
1	A	595	ASP
1	A	611	ASP
1	A	633	ARG
1	A	671	LYS
1	A	680	GLU
1	A	681	GLU
1	A	682	LYS
1	A	691	GLN
1	A	700	GLU
1	A	706	LYS
1	B	41	GLN
1	B	42	ARG
1	B	45	GLU
1	B	65	GLU

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Mol	Chain	Res	Type
1	B	104	ARG
1	B	130	LYS
1	B	146	SER
1	B	159	PHE
1	B	166	ASP
1	B	202	GLU
1	B	211	ASP
1	B	227	LEU
1	B	244	ASP
1	B	263	VAL
1	B	301	GLU
1	B	337	GLU
1	B	370	ILE
1	B	411	VAL
1	B	418	HIS
1	B	419	ARG
1	B	433	HIS
1	B	440	ASN
1	B	441	LYS
1	B	471	LEU
1	B	474	THR
1	B	476	ASP
1	B	539	GLU
1	B	542	GLN
1	B	563	LEU
1	B	569	LEU
1	B	570	ARG
1	B	578	LYS
1	B	582	LEU
1	B	583	ASP
1	B	584	LYS
1	B	588	LEU
1	B	592	LEU
1	B	611	ASP
1	B	638	LYS
1	B	659	ARG
1	B	671	LYS
1	B	677	ILE
1	B	680	GLU
1	B	687	TYR
1	B	696	LYS
1	B	706	LYS

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Mol	Chain	Res	Type
1	C	48	VAL
1	C	51	ASN
1	C	66	GLN
1	C	78	LEU
1	C	79	LEU
1	C	80	GLU
1	C	85	ARG
1	C	94	GLU
1	C	96	ILE
1	C	99	ARG
1	C	104	ARG
1	C	111	ILE
1	C	114	SER
1	C	131	ASP
1	C	139	ARG
1	C	146	SER
1	C	151	ASP
1	C	154	ARG
1	C	155	ASP
1	C	156	VAL
1	C	167	GLU
1	C	176	ASN
1	C	202	GLU
1	C	227	LEU
1	C	236	ILE
1	C	239	SER
1	C	263	VAL
1	C	296	LEU
1	C	301	GLU
1	C	336	GLU
1	C	337	GLU
1	C	370	ILE
1	C	393	GLN
1	C	395	ASN
1	C	398	ARG
1	C	419	ARG
1	C	422	GLN
1	C	424	GLN
1	C	441	LYS
1	C	450	THR
1	C	471	LEU
1	C	474	THR

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Mol	Chain	Res	Type
1	C	476	ASP
1	C	511	GLU
1	C	538	LEU
1	C	542	GLN
1	C	552	VAL
1	C	554	ARG
1	C	558	ILE
1	C	570	ARG
1	C	582	LEU
1	C	588	LEU
1	C	590	GLU
1	C	592	LEU
1	C	597	LEU
1	C	606	LEU
1	C	611	ASP
1	C	625	VAL
1	C	638	LYS
1	C	659	ARG
1	C	662	LYS
1	C	674	LEU
1	C	675	GLN
1	C	677	ILE
1	C	681	GLU
1	C	696	LYS
1	C	703	LYS
1	C	706	LYS
1	D	40	ARG
1	D	43	LEU
1	D	44	LYS
1	D	45	GLU
1	D	53	GLN
1	D	65	GLU
1	D	86	GLN
1	D	96	ILE
1	D	101	VAL
1	D	104	ARG
1	D	120	ASN
1	D	126	PHE
1	D	127	LEU
1	D	131	ASP
1	D	146	SER
1	D	155	ASP

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Mol	Chain	Res	Type
1	D	166	ASP
1	D	167	GLU
1	D	183	GLN
1	D	184	ASP
1	D	190	ASP
1	D	193	HIS
1	D	202	GLU
1	D	227	LEU
1	D	238	ARG
1	D	244	ASP
1	D	259	LYS
1	D	263	VAL
1	D	279	GLU
1	D	296	LEU
1	D	301	GLU
1	D	304	ASN
1	D	316	ASP
1	D	321	GLN
1	D	332	LYS
1	D	337	GLU
1	D	370	ILE
1	D	386	LEU
1	D	393	GLN
1	D	394	LEU
1	D	416	ASN
1	D	420	ASP
1	D	422	GLN
1	D	427	ILE
1	D	431	ILE
1	D	432	HIS
1	D	433	HIS
1	D	439	LEU
1	D	440	ASN
1	D	453	ARG
1	D	461	ARG
1	D	467	LEU
1	D	469	ARG
1	D	470	GLU
1	D	476	ASP
1	D	478	HIS
1	D	502	ARG
1	D	528	VAL

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Mol	Chain	Res	Type
1	D	538	LEU
1	D	539	GLU
1	D	560	ASN
1	D	561	GLU
1	D	563	LEU
1	D	565	THR
1	D	566	ILE
1	D	569	LEU
1	D	570	ARG
1	D	584	LYS
1	D	586	LYS
1	D	588	LEU
1	D	591	GLN
1	D	592	LEU
1	D	593	GLU
1	D	595	ASP
1	D	597	LEU
1	D	606	LEU
1	D	632	GLU
1	D	638	LYS
1	D	649	ARG
1	D	651	SER
1	D	672	LYS
1	D	691	GLN
1	D	698	VAL
1	D	700	GLU
1	D	702	LEU
1	D	706	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	ASN
1	A	468	ASN
1	A	516	ASN
1	A	591	GLN
1	A	652	GLN
1	B	234	ASN
1	B	440	ASN
1	B	516	ASN
1	B	522	ASN
1	B	526	ASN

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Mol	Chain	Res	Type
1	B	652	GLN
1	C	176	ASN
1	C	516	ASN
1	C	652	GLN
1	C	691	GLN
1	D	86	GLN
1	D	234	ASN
1	D	304	ASN
1	D	417	ASN
1	D	432	HIS
1	D	468	ASN
1	D	516	ASN

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)

4 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	4000	1	41,50,50	1.49	7 (17%)	45,82,82	1.73	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	C	4000	1	41,50,50	1.57	7 (17%)	45,82,82	1.72	13 (28%)
2	HEM	D	4000	-	41,50,50	1.68	10 (24%)	45,82,82	1.90	14 (31%)
2	HEM	B	4000	1	41,50,50	1.56	8 (19%)	45,82,82	1.70	11 (24%)

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	4000	1	-	2/12/54/54	-
2	HEM	C	4000	1	-	2/12/54/54	-
2	HEM	D	4000	-	-	4/12/54/54	-
2	HEM	B	4000	1	-	2/12/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4000	HEM	C4D-ND	-4.36	1.32	1.40
2	D	4000	HEM	O1D-CGD	4.29	1.36	1.22
2	C	4000	HEM	C4D-ND	-4.11	1.33	1.40
2	B	4000	HEM	C4D-ND	-3.93	1.33	1.40
2	C	4000	HEM	C1B-NB	-3.73	1.33	1.40
2	B	4000	HEM	C1B-NB	-3.49	1.34	1.40
2	A	4000	HEM	C1B-NB	-3.36	1.34	1.40
2	D	4000	HEM	C1B-NB	-3.21	1.34	1.40
2	D	4000	HEM	C4D-C3D	3.17	1.50	1.45
2	C	4000	HEM	CAA-C2A	-3.17	1.47	1.52
2	B	4000	HEM	C3D-C2D	-2.98	1.30	1.36
2	A	4000	HEM	C3D-C2D	-2.96	1.30	1.36
2	D	4000	HEM	C1D-C2D	2.78	1.49	1.44
2	B	4000	HEM	C4B-NB	-2.75	1.33	1.38
2	D	4000	HEM	O2D-CGD	-2.75	1.21	1.30
2	D	4000	HEM	C3B-C4B	2.66	1.50	1.44
2	D	4000	HEM	C3B-C2B	-2.57	1.32	1.37
2	A	4000	HEM	C3C-CAC	2.50	1.52	1.47
2	B	4000	HEM	C1D-C2D	2.49	1.49	1.44
2	B	4000	HEM	C4D-C3D	2.47	1.49	1.45
2	A	4000	HEM	C3B-C4B	2.45	1.49	1.44
2	D	4000	HEM	C1A-CHA	-2.37	1.34	1.41
2	C	4000	HEM	C4B-NB	-2.35	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4000	HEM	C1D-ND	-2.35	1.34	1.38
2	A	4000	HEM	C4B-NB	-2.34	1.34	1.38
2	C	4000	HEM	C3D-C2D	-2.32	1.31	1.36
2	B	4000	HEM	C4A-CHB	-2.31	1.34	1.41
2	D	4000	HEM	C4D-ND	-2.28	1.36	1.40
2	B	4000	HEM	C1D-ND	-2.26	1.34	1.38
2	A	4000	HEM	C1D-ND	-2.20	1.34	1.38
2	D	4000	HEM	C4B-NB	-2.12	1.34	1.38
2	C	4000	HEM	C3B-C4B	2.11	1.49	1.44

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4000	HEM	CAD-CBD-CGD	-5.67	101.39	113.60
2	A	4000	HEM	C4B-C3B-C2B	-4.55	103.50	107.11
2	B	4000	HEM	C4B-C3B-C2B	-4.18	103.80	107.11
2	D	4000	HEM	CMB-C2B-C1B	4.01	131.14	125.04
2	D	4000	HEM	CMA-C3A-C4A	-3.80	122.62	128.46
2	C	4000	HEM	C2C-C3C-C4C	-3.75	104.28	106.90
2	C	4000	HEM	C4B-C3B-C2B	-3.64	104.22	107.11
2	A	4000	HEM	CMA-C3A-C4A	-3.32	123.36	128.46
2	D	4000	HEM	CMA-C3A-C2A	3.22	131.02	124.94
2	A	4000	HEM	CMA-C3A-C2A	3.21	131.00	124.94
2	D	4000	HEM	C2D-C1D-ND	3.20	113.71	109.88
2	C	4000	HEM	CMA-C3A-C2A	3.15	130.89	124.94
2	B	4000	HEM	CMA-C3A-C2A	3.08	130.74	124.94
2	B	4000	HEM	CHD-C1D-C2D	-3.07	120.18	124.98
2	B	4000	HEM	CMA-C3A-C4A	-2.98	123.88	128.46
2	D	4000	HEM	CHD-C1D-C2D	-2.92	120.42	124.98
2	C	4000	HEM	CHD-C1D-C2D	-2.89	120.46	124.98
2	C	4000	HEM	CMA-C3A-C4A	-2.88	124.03	128.46
2	A	4000	HEM	C2C-C3C-C4C	-2.85	104.91	106.90
2	C	4000	HEM	C4A-C3A-C2A	-2.83	105.02	107.00
2	B	4000	HEM	CBD-CAD-C3D	-2.74	105.02	112.63
2	D	4000	HEM	C2B-C1B-NB	2.71	113.05	109.84
2	C	4000	HEM	CBD-CAD-C3D	-2.61	105.37	112.63
2	A	4000	HEM	CHC-C4B-NB	2.59	127.25	124.43
2	C	4000	HEM	C1D-C2D-C3D	-2.59	104.23	106.96
2	B	4000	HEM	C2C-C3C-C4C	-2.57	105.10	106.90
2	C	4000	HEM	C2B-C1B-NB	2.53	112.84	109.84
2	C	4000	HEM	CHD-C1D-ND	2.53	127.18	124.43
2	B	4000	HEM	CHD-C1D-ND	2.53	127.18	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4000	HEM	CBD-CAD-C3D	-2.49	105.70	112.63
2	A	4000	HEM	CHD-C1D-C2D	-2.49	121.09	124.98
2	A	4000	HEM	C2B-C1B-NB	2.47	112.77	109.84
2	B	4000	HEM	O2D-CGD-CBD	2.42	121.81	114.03
2	D	4000	HEM	C4D-ND-C1D	-2.36	102.63	105.07
2	B	4000	HEM	C1D-C2D-C3D	-2.34	104.49	106.96
2	B	4000	HEM	C4A-C3A-C2A	-2.34	105.37	107.00
2	B	4000	HEM	C2D-C1D-ND	2.30	112.64	109.88
2	D	4000	HEM	C3D-C4D-ND	2.27	112.70	110.17
2	D	4000	HEM	CMB-C2B-C3B	-2.23	122.83	128.30
2	A	4000	HEM	CHC-C4B-C3B	-2.21	121.18	124.57
2	A	4000	HEM	C2D-C1D-ND	2.19	112.50	109.88
2	C	4000	HEM	CHC-C4B-NB	2.18	126.80	124.43
2	A	4000	HEM	C1D-C2D-C3D	-2.16	104.69	106.96
2	A	4000	HEM	CMC-C2C-C3C	2.16	128.71	124.68
2	C	4000	HEM	O2D-CGD-CBD	2.13	120.87	114.03
2	A	4000	HEM	O2D-CGD-CBD	2.13	120.87	114.03
2	D	4000	HEM	C1D-C2D-C3D	-2.11	104.74	106.96
2	D	4000	HEM	C4B-C3B-C2B	-2.10	105.45	107.11
2	D	4000	HEM	CHC-C4B-NB	2.07	126.68	124.43
2	C	4000	HEM	C2D-C1D-ND	2.05	112.34	109.88
2	D	4000	HEM	CHA-C4D-C3D	-2.04	121.51	125.33
2	A	4000	HEM	C4A-C3A-C2A	-2.01	105.60	107.00

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4000	HEM	C2B-C3B-CAB-CBB
2	D	4000	HEM	C4B-C3B-CAB-CBB
2	A	4000	HEM	CAA-CBA-CGA-O2A
2	B	4000	HEM	CAA-CBA-CGA-O2A
2	C	4000	HEM	CAA-CBA-CGA-O2A
2	B	4000	HEM	CAA-CBA-CGA-O1A
2	A	4000	HEM	CAA-CBA-CGA-O1A
2	C	4000	HEM	CAA-CBA-CGA-O1A
2	D	4000	HEM	CAD-CBD-CGD-O1D
2	D	4000	HEM	CAD-CBD-CGD-O2D

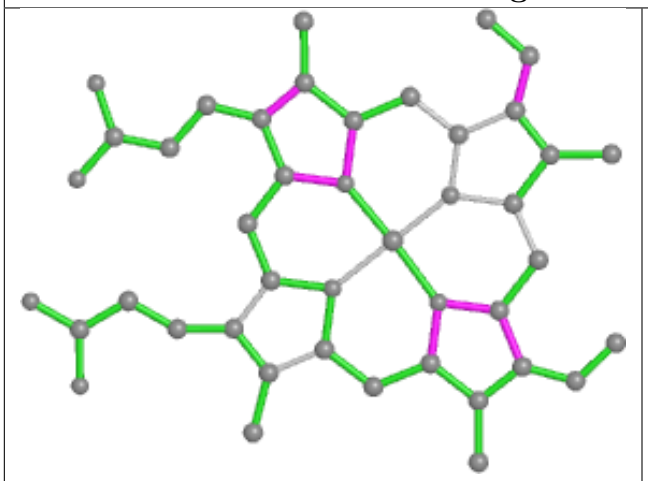
There are no ring outliers.

4 monomers are involved in 6 short contacts:

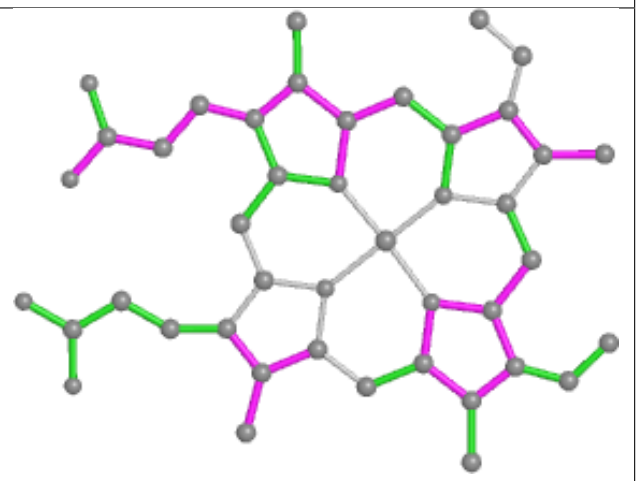
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4000	HEM	1	0
2	C	4000	HEM	3	0
2	D	4000	HEM	1	0
2	B	4000	HEM	1	0

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 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.

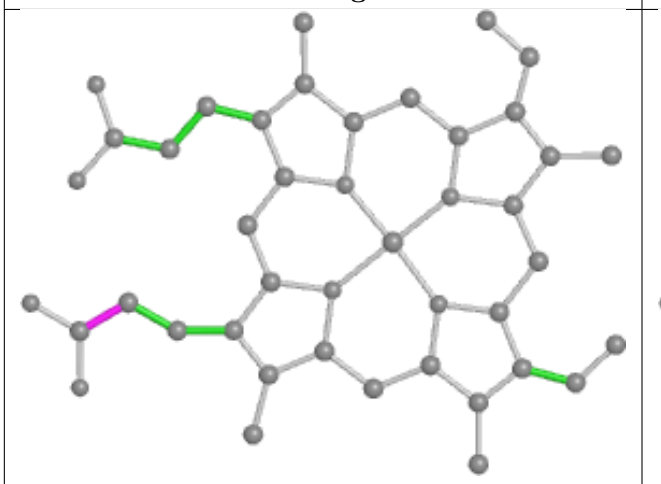
Ligand HEM A 4000



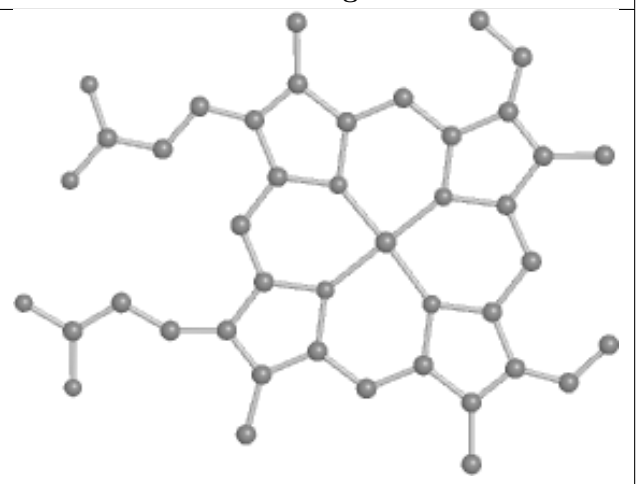
Bond lengths



Bond angles

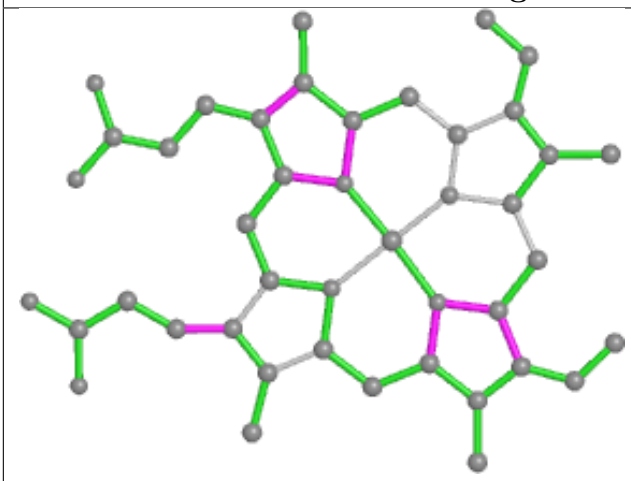


Torsions

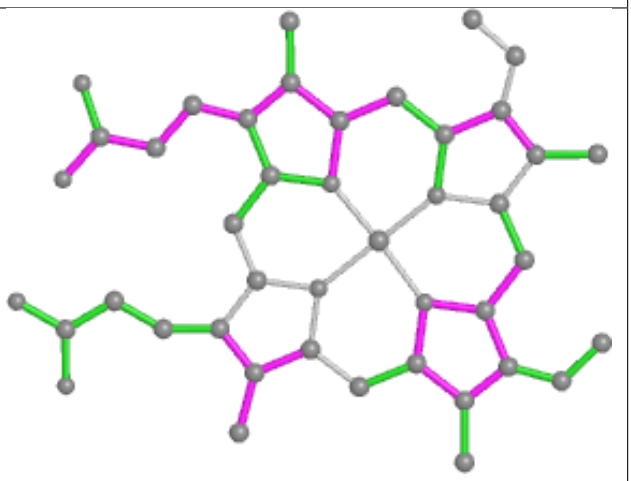


Rings

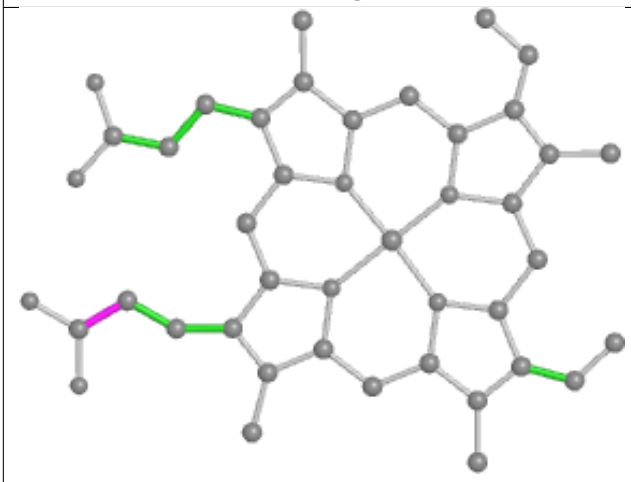
Ligand HEM C 4000



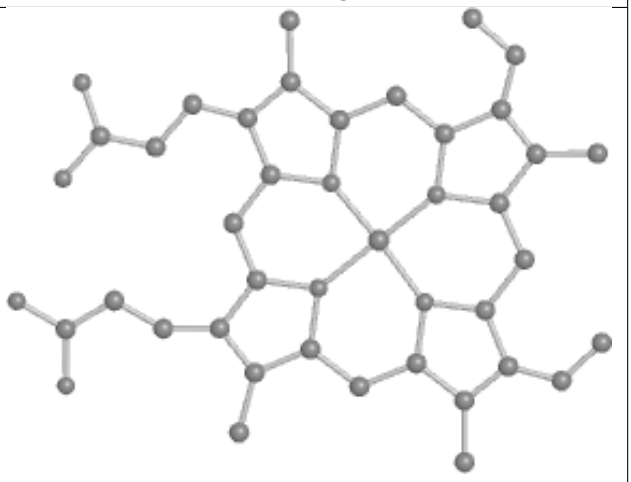
Bond lengths



Bond angles



Torsions



Rings

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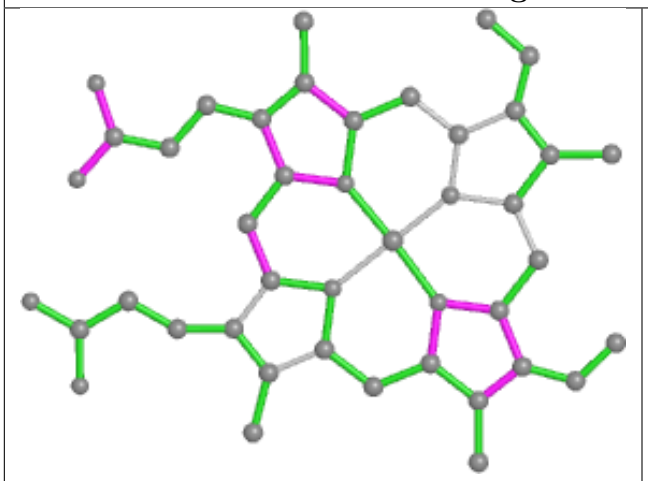
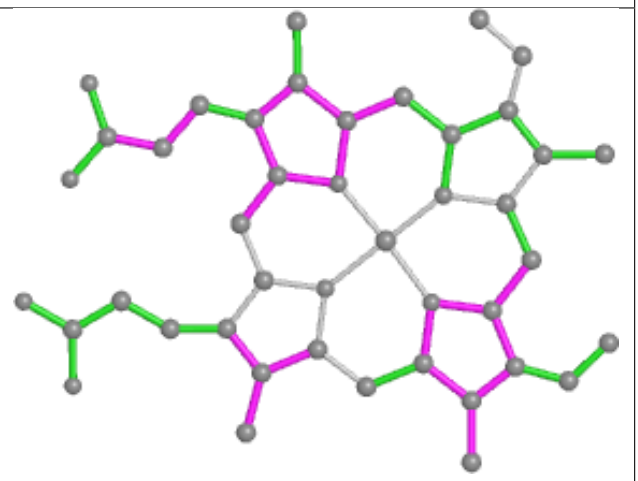
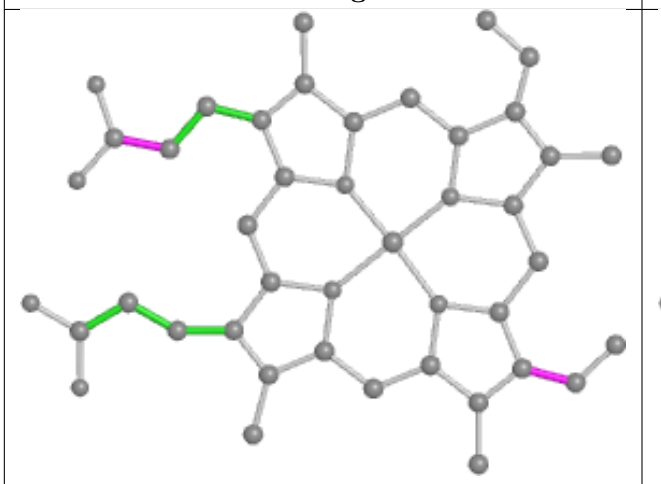


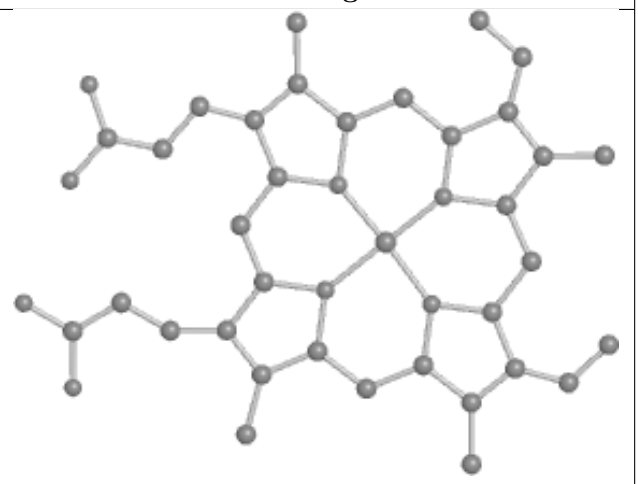
Bond lengths



Bond angles

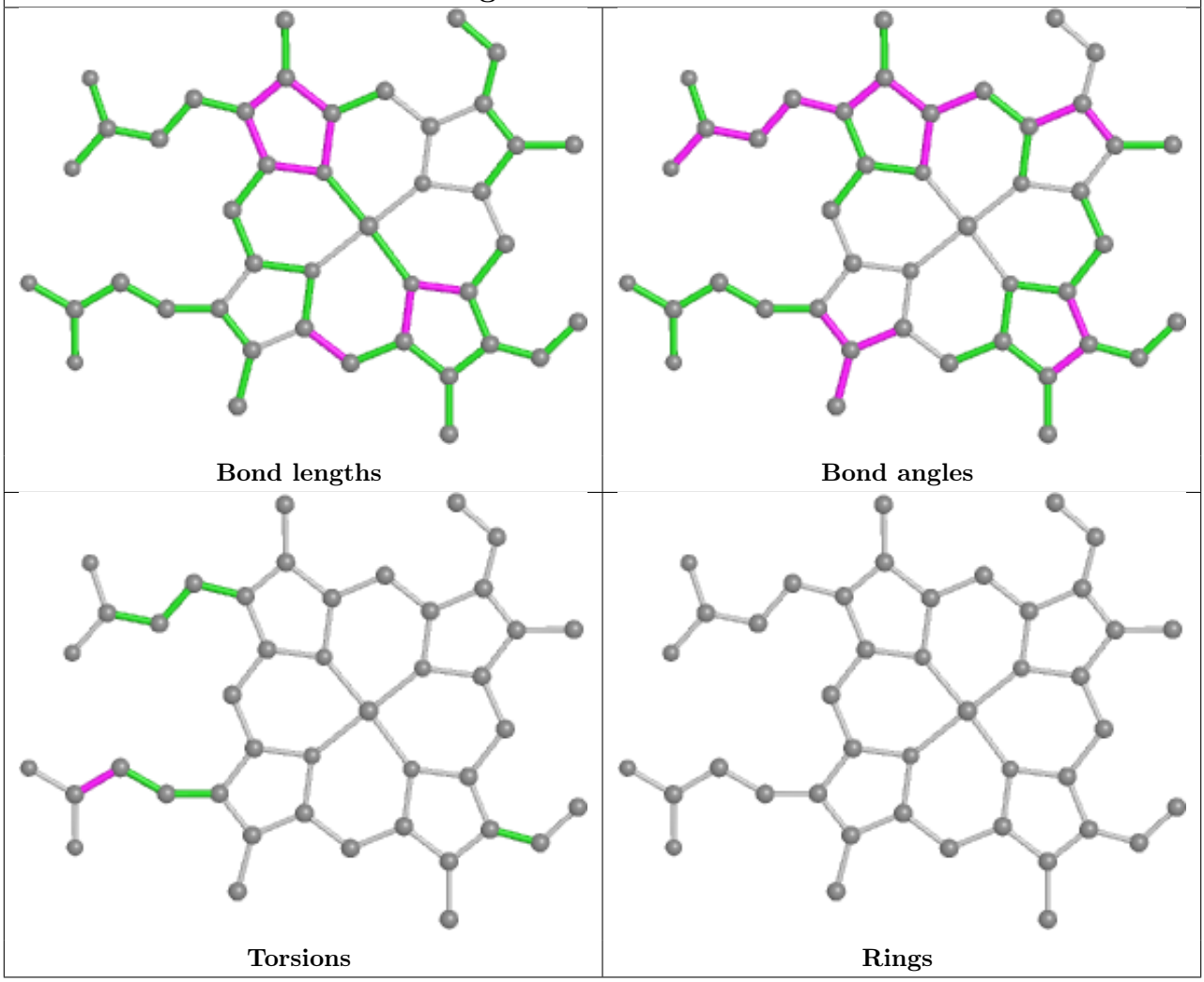


Torsions



Rings

Ligand HEM B 4000



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)

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, 95th 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	681/746 (91%)	-0.03	18 (2%)	56	39	15, 51, 103, 141	0
1	B	679/746 (91%)	0.27	48 (7%)	16	9	19, 63, 154, 227	0
1	C	681/746 (91%)	1.34	173 (25%)	0	0	32, 79, 138, 169	0
1	D	680/746 (91%)	2.17	313 (46%)	0	0	32, 94, 149, 188	0
All	All	2721/2984 (91%)	0.94	552 (20%)	1	0	15, 75, 140, 227	0

All (552) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	579	GLY	10.5
1	D	443	TYR	9.9
1	D	446	GLN	9.5
1	D	444	PRO	9.5
1	C	708	LEU	9.0
1	D	445	ALA	8.7
1	C	605	TYR	8.2
1	D	466	VAL	8.1
1	D	127	LEU	8.0
1	C	60	GLY	7.6
1	B	687	TYR	7.2
1	D	455	PHE	7.1
1	D	322	ALA	7.1
1	D	321	GLN	7.0
1	C	651	SER	7.0
1	D	315	ILE	6.9
1	D	215	ASP	6.8
1	C	428	HIS	6.7
1	D	126	PHE	6.7
1	B	633	ARG	6.7
1	C	66	GLN	6.7

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Mol	Chain	Res	Type	RSRZ
1	D	128	GLY	6.7
1	D	314	LEU	6.6
1	D	447	ALA	6.6
1	D	120	ASN	6.6
1	D	388	SER	6.5
1	D	468	ASN	6.4
1	D	473	ALA	6.4
1	D	678	GLY	6.2
1	D	715	GLY	6.1
1	D	311	ALA	6.1
1	B	568	THR	6.1
1	D	442	GLY	5.8
1	B	688	ALA	5.8
1	D	559	PHE	5.8
1	D	416	ASN	5.7
1	D	690	ALA	5.6
1	D	37	VAL	5.6
1	C	84	PHE	5.6
1	D	417	ASN	5.4
1	D	434	TYR	5.3
1	D	552	VAL	5.3
1	B	691	GLN	5.3
1	D	687	TYR	5.2
1	D	491	PRO	5.2
1	C	609	GLY	5.2
1	D	121	ILE	5.2
1	C	345	GLY	5.1
1	D	441	LYS	5.1
1	D	418	HIS	5.1
1	D	450	THR	5.1
1	C	83	ILE	5.0
1	C	75	GLY	5.0
1	D	433	HIS	5.0
1	D	38	ASP	5.0
1	C	637	GLY	5.0
1	D	412	SER	5.0
1	C	635	PHE	4.9
1	C	623	ASP	4.9
1	D	688	ALA	4.9
1	D	150	ALA	4.8
1	C	659	ARG	4.8
1	D	566	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	645	PHE	4.8
1	C	691	GLN	4.8
1	D	400	PRO	4.8
1	D	456	PHE	4.8
1	C	56	THR	4.8
1	D	641	MET	4.7
1	C	687	TYR	4.7
1	C	573	VAL	4.7
1	C	59	PHE	4.7
1	D	219	SER	4.7
1	D	464	SER	4.7
1	D	684	ALA	4.6
1	D	677	ILE	4.6
1	D	675	GLN	4.6
1	B	686	VAL	4.6
1	C	625	VAL	4.6
1	C	572	GLY	4.6
1	C	607	ALA	4.6
1	C	360	THR	4.6
1	D	545	PRO	4.6
1	B	545	PRO	4.6
1	B	685	GLY	4.5
1	C	676	SER	4.5
1	D	414	VAL	4.5
1	C	624	ALA	4.4
1	D	53	GLN	4.4
1	D	377	THR	4.4
1	C	49	ASP	4.3
1	C	643	PRO	4.3
1	D	223	ALA	4.3
1	C	73	GLY	4.3
1	D	115	TYR	4.3
1	D	449	GLN	4.3
1	D	324	GLY	4.3
1	D	153	ALA	4.3
1	D	370	ILE	4.3
1	C	608	SER	4.3
1	D	285	ALA	4.2
1	D	116	GLY	4.2
1	C	427	ILE	4.2
1	C	69	LEU	4.2
1	C	636	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	207	ALA	4.2
1	D	689	GLY	4.1
1	C	642	SER	4.1
1	C	412	SER	4.1
1	D	190	ASP	4.1
1	D	482	PRO	4.1
1	D	454	GLY	4.1
1	C	63	ILE	4.1
1	D	623	ASP	4.1
1	D	353	PRO	4.0
1	C	580	GLY	4.0
1	D	110	GLY	4.0
1	D	304	ASN	4.0
1	C	47	GLU	4.0
1	D	665	ALA	4.0
1	D	352	ASN	4.0
1	C	672	LYS	4.0
1	D	155	ASP	4.0
1	D	238	ARG	4.0
1	D	435	SER	4.0
1	D	432	HIS	4.0
1	C	88	LEU	4.0
1	B	637	GLY	4.0
1	D	472	SER	4.0
1	C	116	GLY	3.9
1	D	283	VAL	3.9
1	C	610	VAL	3.9
1	D	565	THR	3.9
1	C	50	ASP	3.9
1	D	214	TRP	3.9
1	B	638	LYS	3.9
1	C	90	HIS	3.9
1	C	67	PHE	3.9
1	C	627	VAL	3.8
1	C	62	ASN	3.8
1	D	465	GLY	3.8
1	D	575	SER	3.8
1	D	206	ALA	3.8
1	D	595	ASP	3.8
1	D	122	THR	3.8
1	C	696	LYS	3.7
1	D	242	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	539	GLU	3.7
1	D	325	PHE	3.7
1	D	439	LEU	3.7
1	B	695	ILE	3.7
1	D	436	PRO	3.7
1	D	183	GLN	3.7
1	C	68	SER	3.7
1	D	378	GLU	3.7
1	C	79	LEU	3.7
1	D	225	HIS	3.6
1	D	338	PHE	3.6
1	D	519	GLU	3.6
1	D	541	PRO	3.6
1	D	664	VAL	3.6
1	A	682	LYS	3.6
1	D	431	ILE	3.6
1	D	49	ASP	3.6
1	C	699	GLU	3.6
1	B	639	GLY	3.6
1	B	715	GLY	3.6
1	D	193	HIS	3.6
1	D	380	PRO	3.6
1	D	633	ARG	3.6
1	D	525	SER	3.6
1	C	96	ILE	3.6
1	D	676	SER	3.6
1	C	65	GLU	3.5
1	D	374	VAL	3.5
1	B	696	LYS	3.5
1	D	313	GLN	3.5
1	D	131	ASP	3.5
1	C	443	TYR	3.5
1	C	712	ALA	3.5
1	C	638	LYS	3.5
1	C	52	GLY	3.5
1	D	413	GLY	3.5
1	D	538	LEU	3.5
1	D	260	SER	3.5
1	D	297	TRP	3.5
1	D	587	ALA	3.5
1	B	578	LYS	3.5
1	D	476	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	335	PRO	3.5
1	B	38	ASP	3.5
1	C	490	THR	3.4
1	D	389	TYR	3.4
1	D	438	TYR	3.4
1	C	239	SER	3.4
1	A	637	GLY	3.4
1	D	176	ASN	3.4
1	C	338	PHE	3.4
1	D	246	PHE	3.4
1	B	39	ALA	3.4
1	C	288	ASN	3.4
1	D	453	ARG	3.4
1	B	579	GLY	3.4
1	D	119	SER	3.4
1	A	36	GLU	3.4
1	C	713	VAL	3.4
1	D	550	ASN	3.4
1	A	538	LEU	3.4
1	D	281	ALA	3.4
1	C	81	ASP	3.4
1	C	655	THR	3.4
1	D	39	ALA	3.4
1	C	707	PHE	3.4
1	C	61	GLY	3.3
1	D	625	VAL	3.3
1	D	713	VAL	3.3
1	D	458	THR	3.3
1	C	80	GLU	3.3
1	D	109	HIS	3.3
1	C	596	GLY	3.3
1	C	118	TRP	3.3
1	B	689	GLY	3.3
1	D	451	VAL	3.3
1	C	581	SER	3.3
1	D	376	PHE	3.2
1	D	358	ALA	3.2
1	D	259	LYS	3.2
1	D	512	GLN	3.2
1	D	129	ALA	3.2
1	D	701	GLY	3.2
1	D	282	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	709	GLU	3.2
1	D	224	LEU	3.2
1	D	691	GLN	3.2
1	D	597	LEU	3.2
1	D	333	PHE	3.2
1	D	426	TRP	3.2
1	D	463	ALA	3.1
1	D	47	GLU	3.1
1	C	58	ASP	3.1
1	C	539	GLU	3.1
1	A	681	GLU	3.1
1	C	590	GLU	3.1
1	C	491	PRO	3.1
1	D	437	SER	3.1
1	D	600	THR	3.1
1	D	459	PRO	3.1
1	C	71	ALA	3.1
1	C	570	ARG	3.1
1	D	208	THR	3.1
1	D	560	ASN	3.1
1	D	198	SER	3.1
1	C	158	GLY	3.1
1	C	72	GLY	3.1
1	D	210	HIS	3.1
1	C	682	LYS	3.1
1	D	194	SER	3.1
1	D	236	ILE	3.1
1	D	406	PRO	3.1
1	B	643	PRO	3.1
1	B	636	SER	3.0
1	D	422	GLN	3.1
1	C	51	ASN	3.0
1	D	343	VAL	3.0
1	D	118	TRP	3.0
1	D	440	ASN	3.0
1	C	425	ALA	3.0
1	D	50	ASP	3.0
1	B	567	ALA	3.0
1	C	160	ALA	3.0
1	D	423	GLY	3.0
1	C	354	MET	3.0
1	D	680	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	518	LEU	3.0
1	C	675	GLN	3.0
1	C	695	ILE	3.0
1	C	703	LYS	3.0
1	D	249	HIS	3.0
1	D	460	GLY	3.0
1	D	230	ALA	3.0
1	C	669	SER	2.9
1	D	562	SER	2.9
1	C	694	VAL	2.9
1	C	86	GLN	2.9
1	C	426	TRP	2.9
1	D	114	SER	2.9
1	A	638	LYS	2.9
1	B	684	ALA	2.9
1	D	596	GLY	2.9
1	D	45	GLU	2.9
1	C	115	TYR	2.9
1	C	626	VAL	2.9
1	B	665	ALA	2.9
1	D	514	LYS	2.9
1	D	702	LEU	2.9
1	C	157	HIS	2.8
1	D	577	THR	2.8
1	A	691	GLN	2.8
1	D	461	ARG	2.8
1	A	688	ALA	2.8
1	C	107	GLY	2.8
1	C	700	GLU	2.8
1	D	117	ASP	2.8
1	D	240	TYR	2.8
1	B	577	THR	2.8
1	C	583	ASP	2.8
1	C	716	ASP	2.8
1	D	244	ASP	2.8
1	D	471	LEU	2.8
1	B	690	ALA	2.8
1	D	233	GLY	2.8
1	C	650	PRO	2.8
1	D	558	ILE	2.8
1	C	680	GLU	2.8
1	D	130	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	381	LEU	2.7
1	D	542	GLN	2.7
1	D	299	ALA	2.7
1	C	419	ARG	2.7
1	D	228	PHE	2.7
1	B	302	SER	2.7
1	C	48	VAL	2.7
1	D	310	LEU	2.7
1	D	348	THR	2.7
1	D	312	VAL	2.7
1	D	564	PRO	2.7
1	B	693	GLU	2.7
1	D	638	LYS	2.7
1	B	716	ASP	2.7
1	C	78	LEU	2.7
1	D	477	ASP	2.7
1	C	120	ASN	2.7
1	D	334	LEU	2.7
1	D	292	HIS	2.7
1	D	397	HIS	2.7
1	D	396	ARG	2.7
1	B	595	ASP	2.7
1	A	698	VAL	2.7
1	B	131	ASP	2.6
1	D	549	HIS	2.6
1	D	182	ILE	2.6
1	A	550	ASN	2.6
1	C	578	LYS	2.6
1	D	658	TYR	2.6
1	C	701	GLY	2.6
1	D	714	ASP	2.6
1	C	161	THR	2.6
1	D	501	ILE	2.6
1	D	351	ARG	2.6
1	D	385	ARG	2.6
1	D	502	ARG	2.6
1	D	485	PHE	2.6
1	D	627	VAL	2.6
1	C	571	VAL	2.6
1	D	448	ASN	2.6
1	D	712	ALA	2.6
1	A	675	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	715	GLY	2.6
1	D	48	VAL	2.6
1	D	302	SER	2.6
1	D	371	VAL	2.6
1	A	640	ALA	2.6
1	B	683	GLU	2.6
1	C	709	GLU	2.6
1	D	93	HIS	2.6
1	C	622	PHE	2.6
1	D	457	THR	2.5
1	B	634	VAL	2.5
1	D	670	ALA	2.5
1	D	204	PRO	2.5
1	D	695	ILE	2.5
1	D	671	LYS	2.5
1	D	698	VAL	2.5
1	D	142	THR	2.5
1	D	411	VAL	2.5
1	D	209	ALA	2.5
1	D	387	TYR	2.5
1	D	673	ALA	2.5
1	B	542	GLN	2.5
1	D	556	VAL	2.5
1	C	82	PHE	2.5
1	C	36	GLU	2.5
1	C	204	PRO	2.5
1	D	543	PRO	2.5
1	D	350	ASN	2.5
1	D	527	ASP	2.5
1	C	647	ALA	2.5
1	D	567	ALA	2.5
1	D	716	ASP	2.5
1	C	57	THR	2.5
1	C	409	ARG	2.5
1	D	624	ALA	2.5
1	C	404	GLN	2.5
1	C	44	LYS	2.5
1	D	43	LEU	2.5
1	D	428	HIS	2.5
1	B	539	GLU	2.4
1	C	671	LYS	2.4
1	C	292	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	540	ALA	2.4
1	D	135	PRO	2.4
1	D	146	SER	2.4
1	A	542	GLN	2.4
1	C	271	GLN	2.4
1	C	652	GLN	2.4
1	D	424	GLN	2.4
1	C	64	GLU	2.4
1	D	261	LYS	2.4
1	D	140	PHE	2.4
1	B	640	ALA	2.4
1	D	217	PHE	2.4
1	D	318	ASP	2.4
1	B	41	GLN	2.4
1	D	154	ARG	2.4
1	D	262	LEU	2.4
1	D	375	ASP	2.4
1	D	692	ASP	2.4
1	D	710	ARG	2.4
1	D	467	LEU	2.4
1	D	452	GLY	2.4
1	B	632	GLU	2.4
1	B	681	GLU	2.4
1	D	179	VAL	2.4
1	D	367	PRO	2.4
1	C	620	THR	2.4
1	C	670	ALA	2.4
1	C	537	GLY	2.4
1	C	348	THR	2.4
1	D	252	ARG	2.4
1	D	263	VAL	2.3
1	C	302	SER	2.3
1	D	40	ARG	2.3
1	D	336	GLU	2.3
1	D	470	GLU	2.3
1	C	85	ARG	2.3
1	C	322	ALA	2.3
1	D	265	TRP	2.3
1	D	614	TYR	2.3
1	C	77	THR	2.3
1	D	349	LEU	2.3
1	D	383	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	678	GLY	2.3
1	D	245	GLY	2.3
1	C	597	LEU	2.3
1	D	108	ALA	2.3
1	D	530	LYS	2.3
1	D	42	ARG	2.3
1	D	180	PHE	2.3
1	D	222	SER	2.3
1	D	395	ASN	2.3
1	D	553	THR	2.3
1	B	694	VAL	2.3
1	A	593	GLU	2.3
1	B	598	LYS	2.3
1	D	184	ASP	2.3
1	C	300	ILE	2.3
1	C	574	LEU	2.3
1	C	587	ALA	2.3
1	D	711	PHE	2.3
1	D	46	VAL	2.3
1	C	433	HIS	2.3
1	C	153	ALA	2.3
1	D	419	ARG	2.3
1	C	272	GLY	2.3
1	D	216	PHE	2.3
1	C	692	ASP	2.3
1	C	356	TYR	2.3
1	D	188	PHE	2.3
1	A	337	GLU	2.3
1	C	43	LEU	2.2
1	D	576	THR	2.2
1	C	111	ILE	2.2
1	D	546	THR	2.2
1	D	475	PHE	2.2
1	D	693	GLU	2.2
1	C	205	GLN	2.2
1	C	547	TYR	2.2
1	D	515	LYS	2.2
1	D	598	LYS	2.2
1	D	487	ASN	2.2
1	C	339	ALA	2.2
1	C	445	ALA	2.2
1	D	143	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	202	GLU	2.2
1	C	408	ASN	2.2
1	D	379	ASP	2.2
1	D	574	LEU	2.2
1	B	540	ALA	2.2
1	B	666	ALA	2.2
1	B	45	GLU	2.2
1	D	175	ASN	2.2
1	C	197	PRO	2.2
1	D	192	ILE	2.2
1	C	154	ARG	2.2
1	D	327	LEU	2.2
1	C	91	PHE	2.2
1	D	356	TYR	2.2
1	D	308	TRP	2.2
1	D	124	ALA	2.2
1	D	320	ALA	2.2
1	A	38	ASP	2.1
1	D	617	ALA	2.1
1	C	238	ARG	2.1
1	B	697	GLY	2.1
1	C	203	VAL	2.1
1	D	497	VAL	2.1
1	A	665	ALA	2.1
1	D	96	ILE	2.1
1	C	55	MET	2.1
1	C	601	VAL	2.1
1	C	359	GLU	2.1
1	D	425	ALA	2.1
1	D	254	VAL	2.1
1	C	142	THR	2.1
1	C	54	PHE	2.1
1	D	170	PHE	2.1
1	A	587	ALA	2.1
1	D	626	VAL	2.1
1	D	685	GLY	2.1
1	D	255	THR	2.1
1	D	235	GLY	2.1
1	D	218	SER	2.1
1	D	642	SER	2.1
1	D	632	GLU	2.1
1	D	703	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	637	GLY	2.1
1	D	229	TRP	2.1
1	D	301	GLU	2.1
1	D	405	LEU	2.1
1	B	594	LYS	2.1
1	C	150	ALA	2.1
1	C	697	GLY	2.1
1	D	258	GLY	2.1
1	C	417	ASN	2.1
1	D	589	LYS	2.1
1	D	481	GLN	2.0
1	C	677	ILE	2.0
1	C	303	GLY	2.0
1	C	279	GLU	2.0
1	D	347	MET	2.0
1	C	690	ALA	2.0
1	C	165	THR	2.0
1	D	706	LYS	2.0
1	D	44	LYS	2.0
1	B	116	GLY	2.0
1	C	246	PHE	2.0
1	C	89	GLN	2.0
1	D	640	ALA	2.0
1	C	600	THR	2.0
1	D	620	THR	2.0
1	C	137	PHE	2.0
1	B	133	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

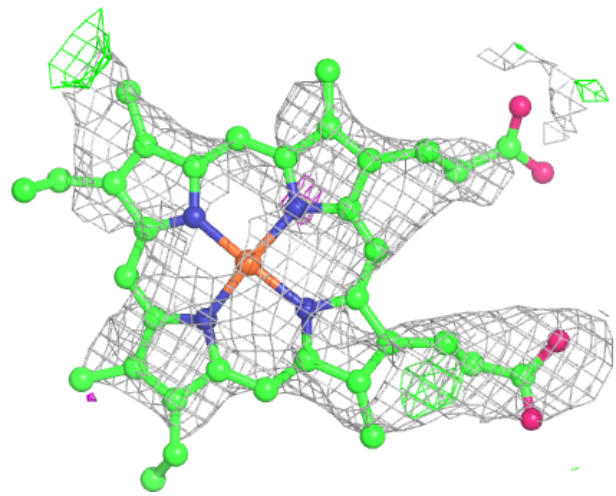
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

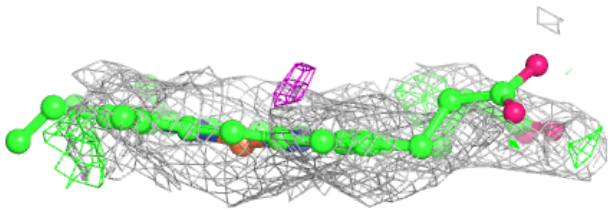
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	D	4000	43/43	0.78	0.36	92,93,97,101	0
2	HEM	C	4000	43/43	0.93	0.19	60,62,68,73	0
2	HEM	B	4000	43/43	0.94	0.16	43,46,50,59	0
2	HEM	A	4000	43/43	0.96	0.15	31,34,38,40	0

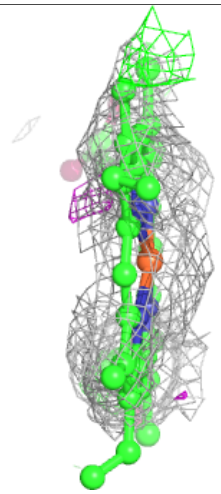
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM D 4000:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

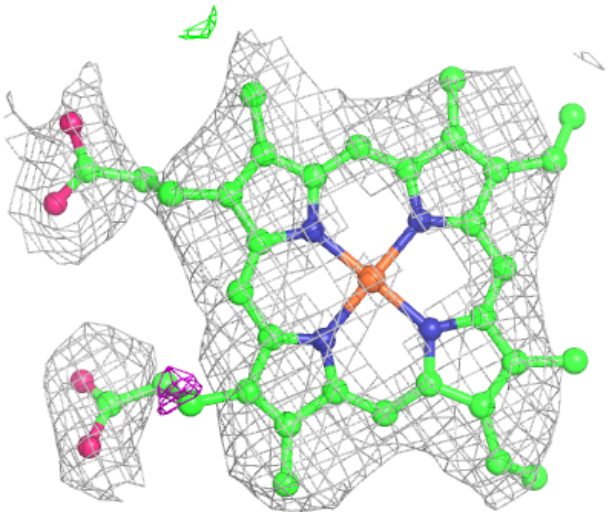


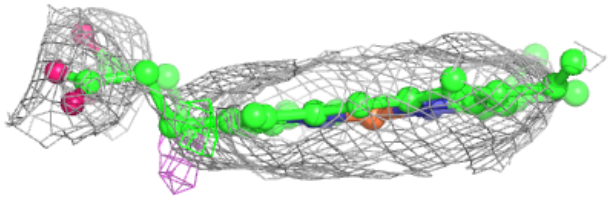


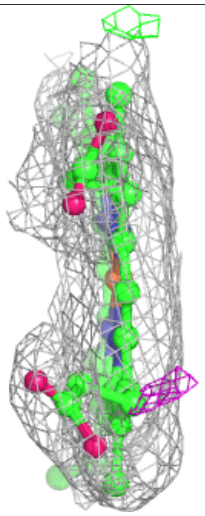


Electron density around HEM C 4000:

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

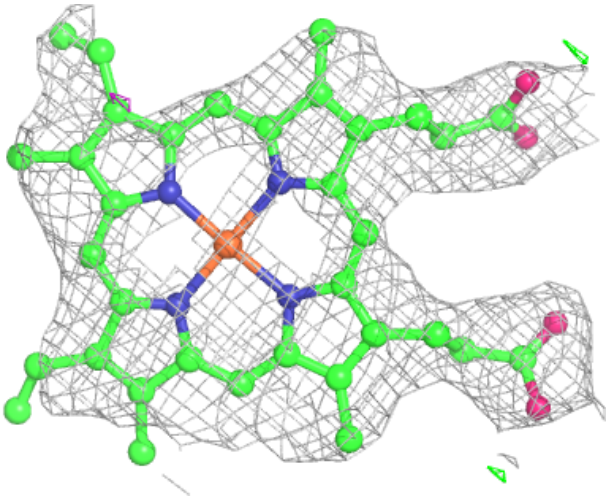


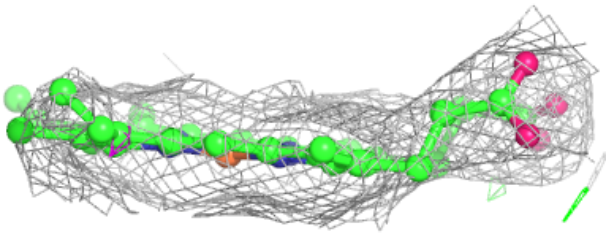


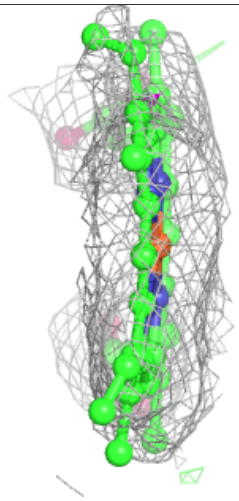


Electron density around HEM B 4000:

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

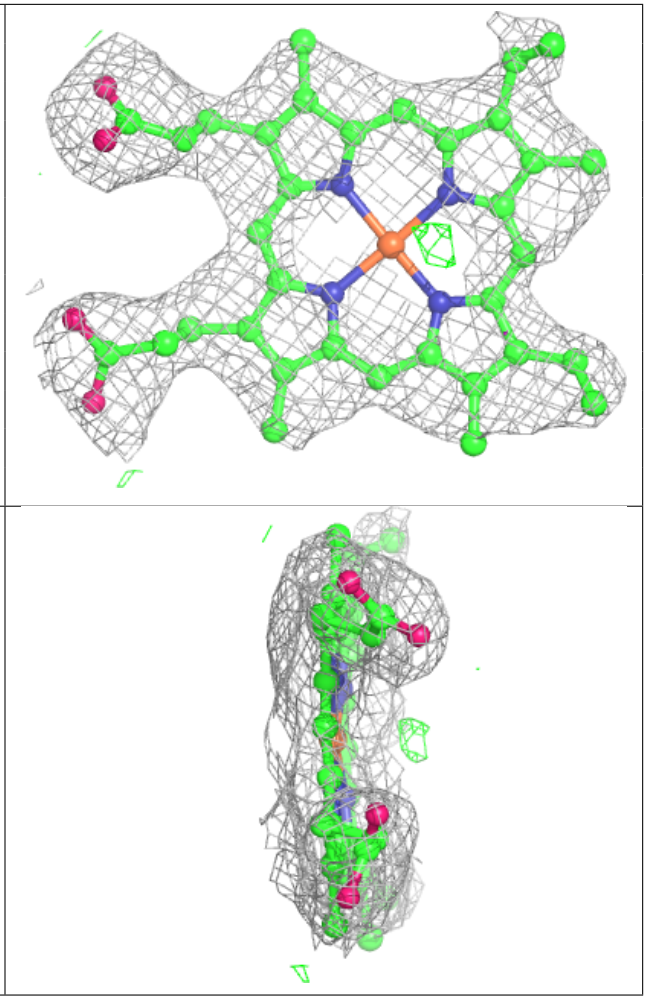






Electron density around HEM A 4000:

$2mF_o$-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.