Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 07:10 PM EST

PDB ID	:	3VLM
Title	:	Crystal Structure Analysis of the Met244Ala Variant of KatG from Haloarcula marismortui
Authors	:	Sato, T.; Ten-i, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.
Deposited on	:	2011-12-01
Resolution	:	2.33 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:

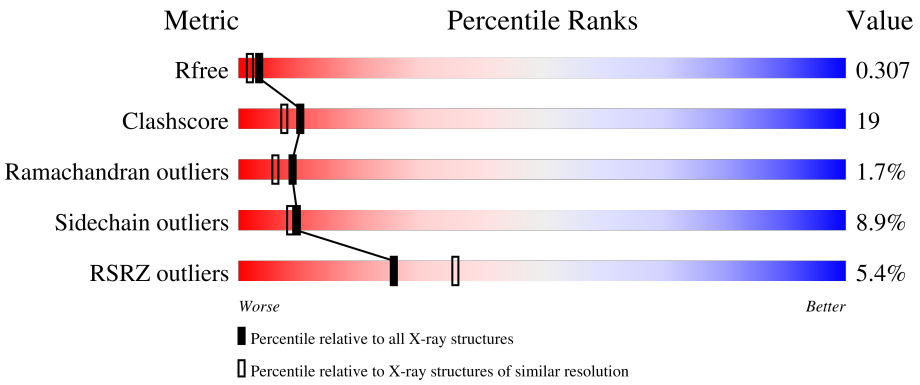
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	737	4% 54% 31% • 10%
1	B	737	5% 58% 29% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10623 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.

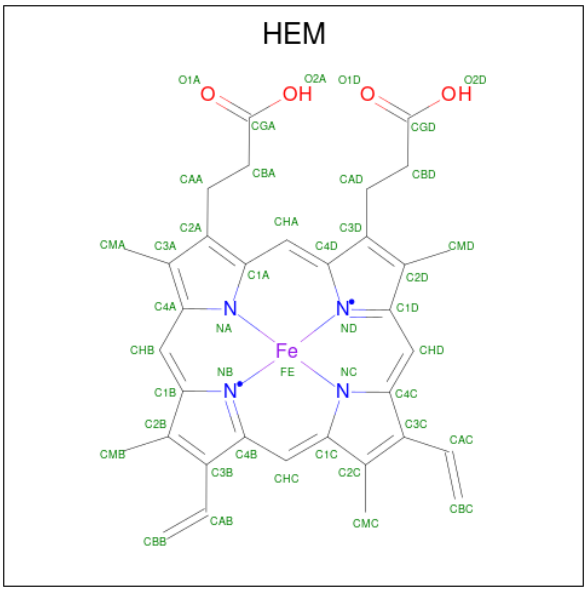
- Molecule 1 is a protein called Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	663	5201	3257	872	1054	18	0	0	0
1	B	660	5185	3247	872	1049	17	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ALA	MET	engineered mutation	UNP O59651
A	732	HIS	-	expression tag	UNP O59651
A	733	HIS	-	expression tag	UNP O59651
A	734	HIS	-	expression tag	UNP O59651
A	735	HIS	-	expression tag	UNP O59651
A	736	HIS	-	expression tag	UNP O59651
A	737	HIS	-	expression tag	UNP O59651
B	244	ALA	MET	engineered mutation	UNP O59651
B	732	HIS	-	expression tag	UNP O59651
B	733	HIS	-	expression tag	UNP O59651
B	734	HIS	-	expression tag	UNP O59651
B	735	HIS	-	expression tag	UNP O59651
B	736	HIS	-	expression tag	UNP O59651
B	737	HIS	-	expression tag	UNP O59651

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



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

- Molecule 3 is water.

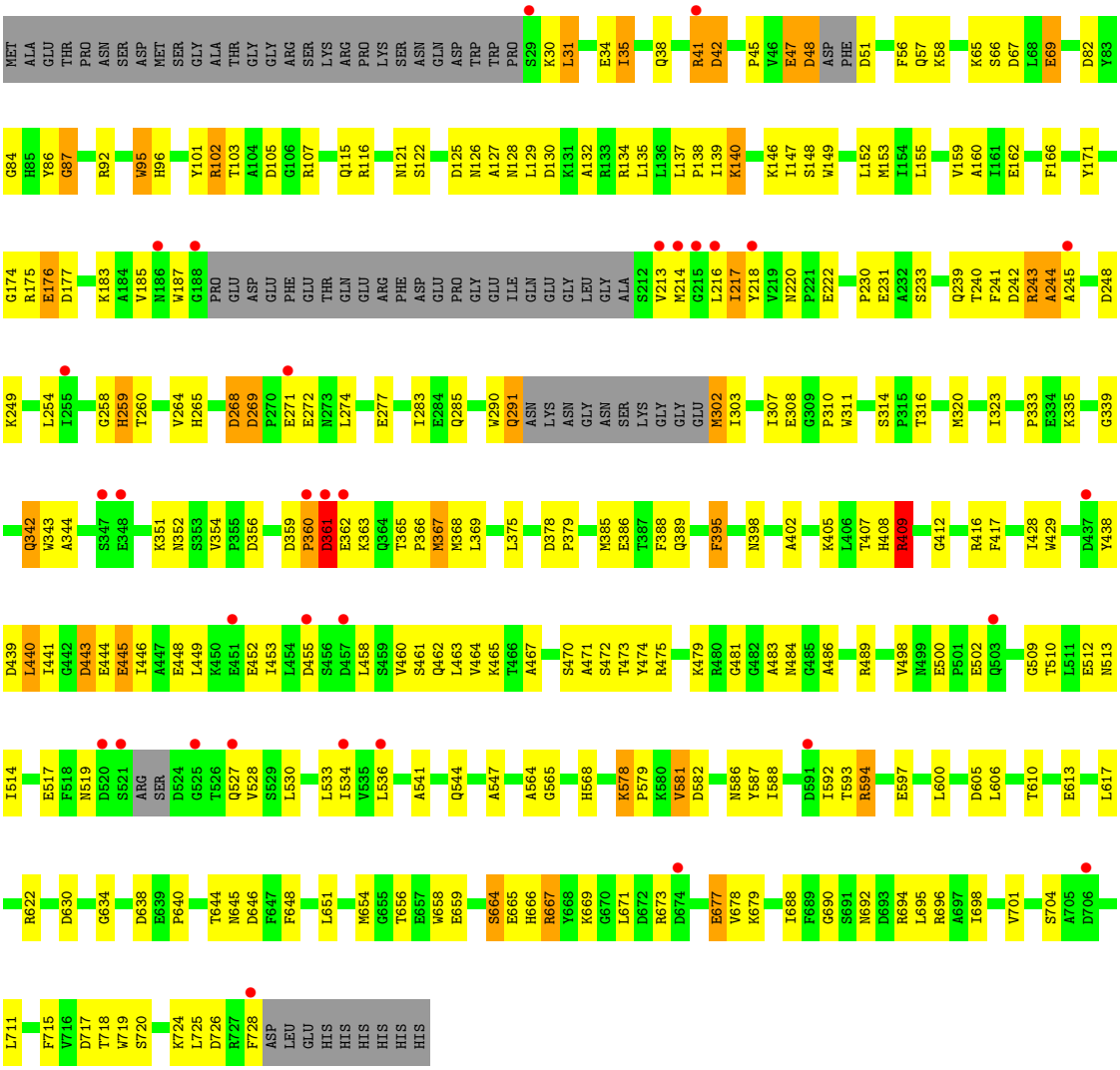
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	100	100	100	0	0
			Total	O		
3	B	51	51	51	0	0

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.

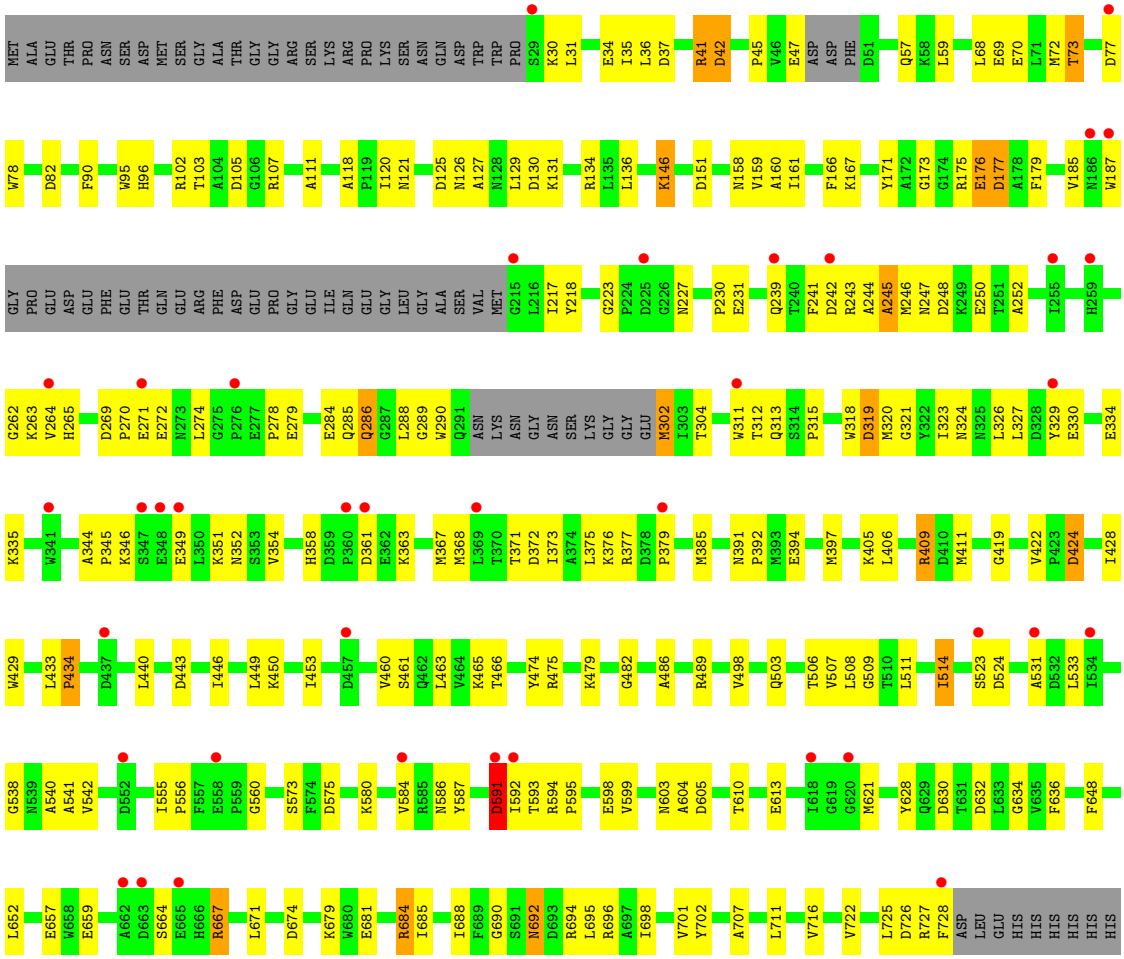
- Molecule 1: Catalase-peroxidase 2

Chain A: 4% 54% 31% • 10%



- Molecule 1: Catalase-peroxidase 2

Chain B: 5% 58% 29% • 10%


MET ALA GLU THR PRO ASN SER ASP MET SER GLY ALA THR GLY GLY ARG SER LYS ARG PRO LYS SER ASN GLN ASP TRP TRP PRO S29 K30 L31 E34 I35 L36 D37 R41 D42 P45 V46 E47 ASP ASP PHE D51 Q57 K58 L59 L68 E69 E70 L71 M72 T73 D77
W78 D82 F90 W95 H96 R102 T103 A104 D105 G106 R107 A111 A118 P119 I120 N121 D125 N126 A127 N128 L129 D130 K131 R134 L135 L136 K146 D151 N158 V159 A160 I161 F166 K167 Y171 A172 G173 G174 R175 E176 D177 A178 F179 V185 N186 W187
GLY PRO GLU ASP GLU PHE GLU THR GLN GLU ARG PHE ASP GLU PRO GLY GLU ILE GLN GLU GLY LEU GLY ALA SER VAL MET G215 L216 I217 Y218 G223 P224 D225 G226 N227 P230 E231 Q239 T240 F241 D242 R243 A244 A245 M246 N247 D248 K249 E250 T251 A252 I255 H259
G262 K263 V264 H265 D269 P270 E271 E272 N273 L274 G275 P276 E277 P278 E279 E284 Q285 Q286 G287 L288 G289 W290 Q291 ASN LYS ASN GLY ASN SER LYS GLY GLY GLU M302 I303 T304 W311 T312 Q313 S314 P315 W318 D319 M320 G321 Y322 I323 N324 N325 L326 L327 D328 Y329 E330 E334
K335 W341 A344 P345 K346 S347 E348 E349 L350 K351 N352 S353 V354 H358 D359 P360 D361 E362 K363 M367 M368 L369 T370 T371 D372 I373 A374 L375 K376 R377 D378 P379 M385 N391 P392 M393 E394 M397 K405 L406 R409 D410 M411 G419 V422 P423 D424 I428
W429 L433 P434 D437 L440 D443 I446 L449 K450 I453 D457 V460 S461 Q462 L463 V464 K465 T466 Y474 R475 K479 G482 A486 R489 V498 Q503 T506 V507 L508 G509 T510 L511 I514 S523 D524 A531 D532 L533 I534
G538 N539 A540 A541 V542 D552 I555 P556 F557 E558 P559 G560 S573 F574 D575 K580 V584 R585 N586 Y587 D591 I592 T593 R594 P595 E598 V599 N603 A604 D605 T610 E613 I618 G619 G620 M621 Y628 Q629 D630 T631 D632 L633 G634 V635 F636 F648
L652 E657 W658 E659 A662 D663 S664 E665 H666 R667 L671 D674 K679 W680 E681 R684 I685 I688 F689 G690 S691 N692 D693 R694 L695 R696 A697 I698 V701 Y702 A707 L711 V716 V722 L725 D726 R727 F728 ASP LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	315.83Å 81.05Å 74.84Å 90.00° 100.04° 90.00°	Depositor
Resolution (Å)	24.94 – 2.33 24.94 – 2.01	Depositor EDS
% Data completeness (in resolution range)	94.8 (24.94-2.33) 93.7 (24.94-2.01)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.01Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0109	Depositor
R, R_{free}	0.283 , 0.325 0.268 , 0.307	Depositor DCC
R_{free} test set	5841 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10623	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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	0.96	2/5322 (0.0%)	0.92	4/7230 (0.1%)
1	B	0.84	1/5307 (0.0%)	0.87	3/7211 (0.0%)
All	All	0.91	3/10629 (0.0%)	0.89	7/14441 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	GLU	CB-CG	5.51	1.62	1.52
1	B	176	GLU	CB-CG	5.43	1.62	1.52
1	A	140	LYS	CE-NZ	5.01	1.61	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	151	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	632	ASP	CB-CG-OD1	5.80	123.53	118.30
1	A	533	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	409	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	B	684	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	696	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	717	ASP	CB-CG-OD1	5.09	122.88	118.30

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	5201	0	4891	223	0
1	B	5185	0	4880	165	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
3	A	100	0	0	12	0
3	B	51	0	0	4	0
All	All	10623	0	9831	384	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 19.

All (384) 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:95:TRP:CH2	1:B:218:TYR:HE1	1.12	1.62
1:B:95:TRP:HH2	1:B:218:TYR:CE1	1.19	1.59
1:B:95:TRP:CH2	1:B:218:TYR:CE1	1.94	1.52
1:B:95:TRP:CZ2	1:B:218:TYR:HE1	1.58	1.22
1:B:95:TRP:HH2	1:B:218:TYR:CZ	1.69	1.08
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.38	1.03
1:A:105:ASP:OD2	1:A:107:ARG:HD2	1.63	0.98
1:B:95:TRP:CZ2	1:B:218:TYR:CE1	2.43	0.94
1:A:474:TYR:CD1	1:A:725:LEU:HB3	2.08	0.89
1:A:474:TYR:CE1	1:A:725:LEU:HB3	2.10	0.87
1:B:555:ILE:HD12	1:B:716:VAL:HG13	1.57	0.86
1:A:245:ALA:HB3	1:A:409:ARG:NH1	1.94	0.82
1:A:41:ARG:HD2	1:B:41:ARG:HD2	1.62	0.81
1:A:101:TYR:CD2	1:A:409:ARG:HD3	2.19	0.78
1:A:101:TYR:CE2	1:A:409:ARG:HD3	2.20	0.77
1:A:470:SER:OG	1:A:483:ALA:HB1	1.82	0.77
1:B:486:ALA:HB2	1:B:531:ALA:HB2	1.68	0.75
1:A:581:VAL:HG12	1:A:581:VAL:O	1.85	0.75
1:A:320:MET:HE3	1:A:323:ILE:HB	1.69	0.74
1:A:405:LYS:HE3	1:A:429:TRP:CD1	2.22	0.74
1:A:245:ALA:HB3	1:A:409:ARG:HH12	1.52	0.74
1:B:692:ASN:ND2	1:B:695:LEU:H	1.85	0.74
1:A:34:GLU:OE2	1:A:183:LYS:HE2	1.88	0.73
1:A:95:TRP:HH2	1:A:218:TYR:CD1	2.07	0.72
1:B:449:LEU:O	1:B:453:ILE:HG13	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:TRP:O	1:B:319:ASP:HB3	1.88	0.72
1:A:677:GLU:O	1:A:677:GLU:HG2	1.89	0.72
1:A:308:GLU:H	1:A:342:GLN:HE22	1.34	0.72
1:A:479:LYS:HD2	1:A:728:PHE:CZ	2.24	0.71
1:A:565:GLY:H	1:A:568:HIS:HD2	1.38	0.71
1:A:412:GLY:HA3	1:A:479:LYS:HB2	1.73	0.71
1:B:34:GLU:HB2	3:B:753:HOH:O	1.90	0.70
1:B:95:TRP:HE3	1:B:406:LEU:HD21	1.56	0.69
1:A:486:ALA:HB3	1:A:489:ARG:NH1	2.09	0.68
1:A:597:GLU:O	1:A:600:LEU:HB3	1.93	0.68
1:A:239:GLN:NE2	1:A:243:ARG:HH21	1.92	0.68
1:A:613:GLU:HA	3:A:760:HOH:O	1.94	0.67
1:B:610:THR:OG1	1:B:613:GLU:HG3	1.94	0.67
1:B:440:LEU:HD21	1:B:560:GLY:HA2	1.77	0.67
1:B:131:LYS:NZ	1:B:289:GLY:O	2.28	0.66
1:B:376:LYS:HG2	1:B:376:LYS:O	1.96	0.66
1:B:90:PHE:CE1	1:B:136:LEU:HD21	2.31	0.66
1:B:368:MET:HG3	1:B:372:ASP:HB2	1.78	0.66
1:A:645:ASN:HA	1:A:711:LEU:HD23	1.78	0.65
1:B:95:TRP:CH2	1:B:218:TYR:CZ	2.58	0.65
1:B:685:ILE:O	1:B:688:ILE:HG22	1.97	0.65
1:A:30:LYS:HG2	3:A:802:HOH:O	1.95	0.65
1:A:95:TRP:HH2	1:A:218:TYR:HD1	1.43	0.64
1:B:319:ASP:OD1	1:B:319:ASP:C	2.35	0.64
1:A:471:ALA:N	1:A:483:ALA:HB2	2.13	0.64
1:B:391:ASN:OD1	1:B:394:GLU:HB2	1.97	0.64
1:B:701:VAL:O	1:B:707:ALA:HB2	1.97	0.64
1:A:122:SER:HB3	1:A:277:GLU:HG3	1.79	0.64
1:A:310:PRO:HG3	1:A:354:VAL:HG11	1.80	0.64
1:A:308:GLU:H	1:A:342:GLN:NE2	1.96	0.64
1:A:38:GLN:NE2	1:A:183:LYS:HD2	2.13	0.63
1:A:474:TYR:CD2	1:A:475:ARG:N	2.66	0.63
1:A:388:PHE:CG	1:A:395:PHE:HB2	2.33	0.63
1:A:264:VAL:HG23	1:A:307:ILE:O	1.99	0.63
1:A:259:HIS:HB3	1:A:311:TRP:CD2	2.34	0.63
1:A:470:SER:OG	1:A:483:ALA:CB	2.47	0.63
1:B:591:ASP:OD2	1:B:591:ASP:N	2.31	0.63
1:A:259:HIS:HB3	1:A:311:TRP:CE2	2.33	0.62
1:B:584:VAL:HG13	1:B:621:MET:CG	2.23	0.62
1:B:371:THR:HG21	2:B:800:HEM:HMB3	1.80	0.62
1:B:465:LYS:HD3	3:B:749:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TRP:CH2	1:B:218:TYR:OH	2.52	0.62
1:A:333:PRO:HD3	1:A:343:TRP:CZ3	2.35	0.62
2:B:800:HEM:HMB1	2:B:800:HEM:HBB2	1.82	0.62
1:A:486:ALA:HB3	1:A:489:ARG:HH11	1.63	0.61
1:A:87:GLY:HA2	1:A:160:ALA:HB1	1.82	0.61
1:A:386:GLU:HG3	3:A:761:HOH:O	2.00	0.61
1:A:128:ASN:HA	1:A:130:ASP:OD2	2.00	0.60
1:A:242:ASP:O	1:A:244:ALA:N	2.32	0.60
1:A:409:ARG:HH21	1:A:409:ARG:HG3	1.66	0.60
1:B:450:LYS:HG3	1:B:540:ALA:HB2	1.82	0.60
1:A:65:LYS:HE3	1:A:159:VAL:HG22	1.83	0.60
1:A:594:ARG:H	1:A:594:ARG:HE	1.50	0.60
1:A:474:TYR:HD1	1:A:725:LEU:CB	2.14	0.60
1:A:140:LYS:HG2	1:A:149:TRP:CE2	2.37	0.59
1:A:460:VAL:HG23	3:A:741:HOH:O	2.01	0.59
1:B:120:ILE:HD11	1:B:187:TRP:CZ2	2.37	0.59
1:B:244:ALA:O	1:B:245:ALA:HB3	2.02	0.59
1:A:162:GLU:HA	1:A:166:PHE:O	2.02	0.59
1:A:474:TYR:HD1	1:A:725:LEU:HB3	1.62	0.59
1:B:223:GLY:HA3	1:B:227:ASN:O	2.01	0.59
1:B:274:LEU:HD22	1:B:290:TRP:HB3	1.85	0.59
1:B:368:MET:HG3	1:B:372:ASP:CB	2.33	0.59
1:B:35:ILE:HG13	1:B:36:LEU:N	2.17	0.59
1:A:35:ILE:HD11	1:A:605:ASP:HB2	1.83	0.59
1:A:102:ARG:HH21	1:A:105:ASP:CG	2.06	0.59
1:B:134:ARG:CZ	1:B:288:LEU:HD21	2.33	0.59
1:B:479:LYS:HB3	1:B:728:PHE:CZ	2.38	0.58
1:A:245:ALA:CB	1:A:409:ARG:HH12	2.15	0.58
1:A:361:ASP:O	1:A:362:GLU:HB2	2.03	0.58
1:B:711:LEU:O	1:B:711:LEU:HG	2.03	0.58
1:A:470:SER:C	1:A:483:ALA:HB2	2.24	0.58
1:B:68:LEU:HB3	1:B:159:VAL:HG11	1.86	0.58
1:A:359:ASP:OD1	1:A:360:PRO:HD2	2.03	0.58
1:A:474:TYR:CD1	1:A:725:LEU:CB	2.84	0.58
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.86	0.58
1:A:41:ARG:H	1:A:41:ARG:HD3	1.69	0.58
1:A:335:LYS:HE2	1:A:339:GLY:O	2.04	0.58
1:A:344:ALA:HB2	3:A:778:HOH:O	2.04	0.58
1:A:692:ASN:ND2	1:A:694:ARG:H	2.03	0.57
1:A:320:MET:HE2	1:A:389:GLN:HA	1.84	0.57
1:A:320:MET:CE	1:A:323:ILE:HB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ALA:HA	1:A:534:ILE:HG22	1.86	0.57
1:B:367:MET:HE1	1:B:368:MET:O	2.04	0.57
1:A:115:GLN:O	1:A:121:ASN:HB3	2.05	0.57
1:B:270:PRO:HB3	1:B:274:LEU:HD12	1.84	0.57
1:A:354:VAL:HG23	1:A:366:PRO:HD3	1.86	0.57
1:A:474:TYR:HE1	1:A:725:LEU:HB3	1.67	0.56
1:A:354:VAL:O	1:A:363:LYS:HA	2.05	0.56
1:A:648:PHE:HE1	1:A:711:LEU:CD2	2.18	0.56
1:B:330:GLU:HB3	1:B:346:LYS:HE3	1.87	0.56
2:B:800:HEM:HBB2	2:B:800:HEM:CMB	2.36	0.56
1:B:244:ALA:O	1:B:245:ALA:CB	2.53	0.56
1:B:449:LEU:HD22	1:B:533:LEU:HD21	1.87	0.56
1:A:452:GLU:HG2	1:A:514:ILE:HG23	1.87	0.56
1:B:166:PHE:HD1	1:B:318:TRP:CD2	2.24	0.55
1:A:412:GLY:CA	1:A:479:LYS:HB2	2.35	0.55
1:B:134:ARG:CZ	1:B:288:LEU:CD2	2.84	0.55
1:A:245:ALA:HB3	1:A:409:ARG:CZ	2.36	0.55
1:A:405:LYS:HA	1:A:429:TRP:CZ2	2.41	0.55
1:B:344:ALA:HB1	1:B:345:PRO:HD2	1.89	0.55
1:A:498:VAL:HG23	1:A:587:TYR:CG	2.43	0.54
1:A:587:TYR:O	1:A:588:ILE:HG13	2.06	0.54
1:B:262:GLY:HA3	2:B:800:HEM:O2D	2.07	0.54
1:A:320:MET:CE	1:A:389:GLN:HA	2.38	0.54
1:B:95:TRP:CE3	1:B:406:LEU:HD21	2.42	0.54
1:B:511:LEU:HA	1:B:514:ILE:HG13	1.89	0.54
1:A:463:LEU:HB2	1:A:541:ALA:HB2	1.90	0.54
1:B:443:ASP:HA	1:B:446:ILE:HD12	1.88	0.54
1:A:86:TYR:O	1:A:87:GLY:C	2.47	0.54
1:B:323:ILE:HG23	1:B:327:LEU:HD12	1.89	0.54
1:A:87:GLY:CA	1:A:160:ALA:HB1	2.38	0.53
1:A:125:ASP:HB2	1:A:216:LEU:HD23	1.91	0.53
1:B:118:ALA:HB2	1:B:279:GLU:HG3	1.91	0.53
1:B:482:GLY:HA3	1:B:726:ASP:OD2	2.09	0.53
1:A:95:TRP:NE1	1:A:96:HIS:HD2	2.06	0.53
1:A:405:LYS:HA	1:A:429:TRP:CH2	2.43	0.53
1:B:161:ILE:HG22	1:B:166:PHE:HB3	1.90	0.53
1:B:692:ASN:HD22	1:B:695:LEU:H	1.54	0.53
1:A:95:TRP:NE1	1:A:96:HIS:CD2	2.76	0.53
1:A:95:TRP:CH2	1:A:218:TYR:CD1	2.94	0.53
1:A:87:GLY:HA2	1:A:160:ALA:CB	2.39	0.53
1:A:416:ARG:HD3	1:A:479:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:TYR:CD1	1:A:527:GLN:HB2	2.44	0.52
1:A:458:LEU:HA	1:A:462:GLN:OE1	2.09	0.52
2:A:800:HEM:HBC2	2:A:800:HEM:CMC	2.39	0.52
1:B:440:LEU:CD2	1:B:560:GLY:HA2	2.40	0.52
1:B:95:TRP:CD1	1:B:96:HIS:HD2	2.27	0.52
1:B:177:ASP:HB2	3:B:755:HOH:O	2.08	0.52
1:A:241:PHE:O	1:A:244:ALA:HB3	2.09	0.52
1:A:720:SER:OG	1:A:724:LYS:NZ	2.42	0.52
1:A:66:SER:O	1:A:69:GLU:HB2	2.10	0.52
1:A:645:ASN:HA	1:A:711:LEU:CD2	2.38	0.52
1:B:466:THR:OG1	1:B:507:VAL:HG11	2.10	0.51
1:B:587:TYR:HD1	1:B:628:TYR:CD1	2.28	0.51
1:B:555:ILE:HD12	1:B:716:VAL:CG1	2.35	0.51
1:A:249:LYS:HG2	1:A:398:ASN:OD1	2.11	0.51
1:A:35:ILE:CD1	1:A:605:ASP:HB2	2.40	0.51
1:A:610:THR:OG1	1:A:613:GLU:HG3	2.10	0.51
1:B:326:LEU:O	1:B:376:LYS:NZ	2.36	0.51
1:A:95:TRP:CD1	1:A:96:HIS:HD2	2.29	0.51
1:A:149:TRP:O	1:A:153:MET:HG3	2.11	0.51
1:A:486:ALA:O	1:A:489:ARG:HG2	2.10	0.51
1:A:82:ASP:OD1	1:A:265:HIS:NE2	2.43	0.50
1:A:213:VAL:HB	1:A:216:LEU:HD12	1.93	0.50
1:B:722:VAL:HA	1:B:725:LEU:HG	1.92	0.50
1:A:692:ASN:HD22	1:A:695:LEU:H	1.58	0.50
1:A:45:PRO:HG3	1:B:698:ILE:HG23	1.92	0.50
1:A:648:PHE:HE1	1:A:711:LEU:HD21	1.77	0.50
1:B:173:GLY:O	1:B:411:MET:HE1	2.11	0.50
1:A:582:ASP:C	1:A:582:ASP:OD1	2.50	0.50
1:B:159:VAL:O	1:B:160:ALA:C	2.49	0.50
1:B:185:VAL:HG11	1:B:187:TRP:CZ3	2.47	0.50
1:B:270:PRO:CB	1:B:274:LEU:HD12	2.41	0.50
1:A:171:TYR:HD2	3:A:757:HOH:O	1.94	0.50
1:A:174:GLY:O	3:A:746:HOH:O	2.20	0.50
1:B:95:TRP:CD1	1:B:96:HIS:CD2	3.00	0.50
1:B:270:PRO:C	1:B:272:GLU:H	2.15	0.49
1:A:314:SER:O	1:A:316:THR:N	2.44	0.49
1:B:405:LYS:HE3	1:B:429:TRP:CD1	2.46	0.49
1:B:474:TYR:CD2	1:B:726:ASP:HB3	2.47	0.49
1:B:460:VAL:O	1:B:461:SER:C	2.49	0.49
1:B:684:ARG:HG3	3:B:757:HOH:O	2.13	0.49
1:A:593:THR:H	1:A:594:ARG:HH21	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:TRP:NE1	1:B:372:ASP:OD2	2.39	0.49
1:A:666:HIS:H	1:A:667:ARG:HD3	1.77	0.49
1:A:701:VAL:O	1:A:704:SER:HB2	2.12	0.49
1:B:538:GLY:O	1:B:542:VAL:HG23	2.12	0.49
1:B:125:ASP:OD1	1:B:217:ILE:HG12	2.13	0.49
1:B:486:ALA:HB2	1:B:531:ALA:CB	2.41	0.49
1:A:82:ASP:C	1:A:84:GLY:N	2.67	0.49
1:A:125:ASP:OD2	1:A:125:ASP:O	2.30	0.49
1:A:264:VAL:HG23	1:A:264:VAL:O	2.12	0.49
1:A:644:THR:OG1	1:A:646:ASP:HB2	2.13	0.49
1:A:665:GLU:HB3	1:A:666:HIS:CE1	2.48	0.49
1:A:82:ASP:C	1:A:84:GLY:H	2.16	0.48
1:A:254:LEU:HG	1:A:402:ALA:HB1	1.95	0.48
1:B:158:ASN:ND2	1:B:171:TYR:HB2	2.28	0.48
1:A:694:ARG:O	1:A:698:ILE:HG13	2.14	0.48
1:B:265:HIS:HD2	1:B:302:MET:HG2	1.77	0.48
1:B:409:ARG:NH2	1:B:409:ARG:HG3	2.28	0.48
1:A:470:SER:HG	1:A:483:ALA:HB1	1.77	0.48
1:A:473:THR:O	1:A:481:GLY:HA3	2.13	0.48
1:B:68:LEU:O	1:B:72:MET:HG2	2.13	0.48
1:B:694:ARG:O	1:B:698:ILE:HG13	2.13	0.48
1:A:519:ASN:HD21	1:A:528:VAL:H	1.62	0.48
1:B:648:PHE:O	1:B:652:LEU:HG	2.13	0.48
1:A:140:LYS:HD3	1:A:149:TRP:CD2	2.49	0.48
1:A:474:TYR:HD2	1:A:475:ARG:H	1.62	0.48
1:A:484:ASN:HB3	1:A:726:ASP:OD2	2.14	0.48
1:A:259:HIS:CE1	2:A:800:HEM:NB	2.80	0.48
1:A:449:LEU:O	1:A:453:ILE:HG13	2.13	0.48
1:B:241:PHE:O	1:B:244:ALA:HB3	2.14	0.48
1:B:329:TYR:O	1:B:376:LYS:NZ	2.46	0.48
1:B:252:ALA:HB1	1:B:385:MET:SD	2.54	0.47
1:A:386:GLU:CD	3:A:761:HOH:O	2.53	0.47
1:B:373:ILE:O	1:B:376:LYS:N	2.47	0.47
1:A:352:ASN:HB3	1:A:363:LYS:HB2	1.96	0.47
1:B:424:ASP:N	1:B:424:ASP:OD1	2.47	0.47
1:B:474:TYR:CD1	1:B:474:TYR:C	2.88	0.47
1:A:48:ASP:OD2	1:A:48:ASP:N	2.47	0.47
1:A:409:ARG:HG3	1:A:409:ARG:NH2	2.30	0.47
1:B:320:MET:HB2	1:B:324:ASN:ND2	2.30	0.47
1:A:218:TYR:HD2	1:A:218:TYR:HA	1.53	0.47
1:A:486:ALA:CB	1:A:489:ARG:HH11	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ARG:HD3	1:B:78:TRP:HB3	1.97	0.47
1:B:524:ASP:OD2	1:B:524:ASP:C	2.53	0.47
1:A:444:GLU:HG3	1:A:445:GLU:H	1.79	0.46
1:B:486:ALA:CB	1:B:531:ALA:HB2	2.44	0.46
1:A:175:ARG:NH2	1:A:407:THR:O	2.41	0.46
1:B:111:ALA:O	1:B:175:ARG:HB3	2.14	0.46
1:B:134:ARG:NH1	1:B:288:LEU:HD21	2.29	0.46
1:B:664:SER:OG	1:B:667:ARG:HB2	2.15	0.46
1:B:634:GLY:HA2	1:B:636:PHE:CE2	2.51	0.46
1:B:727:ARG:HD2	1:B:727:ARG:HA	1.61	0.46
1:A:140:LYS:HG2	1:A:149:TRP:CZ2	2.51	0.46
1:A:361:ASP:O	1:A:362:GLU:CB	2.62	0.46
1:A:664:SER:OG	1:A:667:ARG:HB2	2.15	0.46
1:B:95:TRP:CZ3	1:B:218:TYR:OH	2.67	0.46
1:B:127:ALA:HB3	1:B:304:THR:HG23	1.96	0.46
1:A:137:LEU:HB3	1:A:138:PRO:HD3	1.97	0.46
1:A:395:PHE:O	1:A:395:PHE:CD1	2.68	0.46
1:B:242:ASP:C	1:B:244:ALA:H	2.19	0.46
1:A:42:ASP:OD1	1:A:42:ASP:N	2.49	0.46
1:A:386:GLU:CG	3:A:761:HOH:O	2.61	0.46
1:A:544:GLN:O	1:A:547:ALA:N	2.49	0.46
1:A:502:GLU:CD	1:A:502:GLU:H	2.18	0.46
1:B:474:TYR:HD2	1:B:726:ASP:HB3	1.81	0.46
1:A:443:ASP:OD1	1:A:443:ASP:N	2.41	0.45
1:B:692:ASN:ND2	1:B:692:ASN:C	2.69	0.45
1:A:56:PHE:C	1:A:58:LYS:H	2.19	0.45
1:A:471:ALA:CA	1:A:483:ALA:HB2	2.47	0.45
1:A:509:GLY:O	1:A:513:ASN:OD1	2.34	0.45
1:B:34:GLU:OE1	1:B:34:GLU:N	2.50	0.45
1:A:269:ASP:OD1	1:A:271:GLU:HB2	2.17	0.45
1:A:440:LEU:HD23	1:A:440:LEU:HA	1.81	0.45
1:B:312:THR:OG1	1:B:315:PRO:HA	2.16	0.45
1:A:258:GLY:O	1:A:260:THR:N	2.50	0.45
1:A:379:PRO:HD2	3:A:832:HOH:O	2.17	0.45
1:B:42:ASP:OD1	1:B:42:ASP:N	2.50	0.45
1:B:105:ASP:OD2	1:B:107:ARG:HD2	2.15	0.45
1:A:148:SER:HB2	1:A:177:ASP:CG	2.38	0.45
1:B:166:PHE:HE1	1:B:318:TRP:CZ2	2.35	0.45
1:B:264:VAL:HG12	2:B:800:HEM:HAA1	1.98	0.45
1:B:118:ALA:HB2	1:B:279:GLU:CG	2.46	0.44
1:A:248:ASP:HA	3:A:739:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:HB3	1:A:139:ILE:HD13	2.00	0.44
1:A:213:VAL:HG12	1:A:214:MET:N	2.33	0.44
1:A:264:VAL:HG23	1:A:307:ILE:C	2.38	0.44
1:B:82:ASP:OD2	1:B:358:HIS:CE1	2.70	0.44
1:B:555:ILE:CG2	1:B:556:PRO:HD2	2.48	0.44
1:A:67:ASP:HB3	1:A:139:ILE:CD1	2.47	0.44
1:A:47:GLU:H	1:A:47:GLU:HG2	1.55	0.44
1:A:147:ILE:HG23	1:A:147:ILE:O	2.18	0.44
1:B:603:ASN:C	1:B:605:ASP:N	2.71	0.44
1:A:230:PRO:HG2	1:A:231:GLU:OE2	2.18	0.44
1:A:283:ILE:HD11	1:B:688:ILE:N	2.33	0.44
1:B:134:ARG:NH2	1:B:288:LEU:HD23	2.33	0.44
1:B:659:GLU:OE1	1:B:671:LEU:HD11	2.18	0.44
1:A:408:HIS:HB3	1:A:417:PHE:CE1	2.52	0.44
1:B:405:LYS:O	1:B:409:ARG:HB2	2.17	0.44
1:A:134:ARG:CZ	1:B:696:ARG:NH2	2.81	0.44
1:B:45:PRO:HD2	1:B:179:PHE:CZ	2.52	0.43
1:B:166:PHE:CD1	1:B:318:TRP:CD2	3.05	0.43
1:A:58:LYS:HB3	1:A:146:LYS:HZ2	1.83	0.43
1:A:578:LYS:HA	1:A:579:PRO:HD3	1.88	0.43
1:A:658:TRP:CD1	1:A:658:TRP:N	2.85	0.43
1:B:508:LEU:O	1:B:509:GLY:C	2.55	0.43
1:A:412:GLY:HA3	1:A:479:LYS:CB	2.46	0.43
1:A:656:THR:HA	1:A:671:LEU:O	2.18	0.43
1:B:166:PHE:HD2	1:B:167:LYS:H	1.59	0.43
1:B:603:ASN:O	1:B:604:ALA:C	2.57	0.43
1:A:92:ARG:HA	1:A:95:TRP:HD1	1.84	0.43
1:A:351:LYS:HA	1:A:365:THR:OG1	2.19	0.43
1:B:59:LEU:HB2	1:B:146:LYS:HB3	1.99	0.43
1:A:489:ARG:NH2	1:A:564:ALA:O	2.49	0.43
1:A:715:PHE:C	1:A:715:PHE:CD2	2.91	0.43
1:B:103:THR:O	1:B:475:ARG:NH1	2.51	0.43
1:B:285:GLN:O	1:B:286:GLN:C	2.56	0.43
1:A:56:PHE:C	1:A:58:LYS:N	2.72	0.43
1:A:264:VAL:O	1:A:308:GLU:HA	2.19	0.43
1:A:479:LYS:HD2	1:A:728:PHE:CE2	2.53	0.43
1:A:30:LYS:O	1:A:31:LEU:C	2.56	0.43
1:A:285:GLN:NE2	1:A:291:GLN:HE22	2.17	0.43
1:B:103:THR:O	1:B:475:ARG:NH2	2.51	0.43
1:A:41:ARG:HD2	1:B:41:ARG:CD	2.43	0.43
1:A:265:HIS:ND1	1:A:265:HIS:N	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:MET:N	3:A:811:HOH:O	2.51	0.42
1:A:443:ASP:HA	1:A:446:ILE:HD12	2.01	0.42
2:A:800:HEM:HBC2	2:A:800:HEM:HMC1	2.01	0.42
1:B:166:PHE:CD2	1:B:167:LYS:N	2.77	0.42
1:B:329:TYR:CD1	1:B:329:TYR:N	2.87	0.42
1:B:373:ILE:HG22	1:B:377:ARG:HG3	2.00	0.42
1:B:419:GLY:O	1:B:422:VAL:HG23	2.19	0.42
1:B:595:PRO:O	1:B:598:GLU:HB2	2.19	0.42
1:A:405:LYS:HB2	1:A:429:TRP:CZ2	2.55	0.42
1:B:70:GLU:O	1:B:72:MET:N	2.51	0.42
1:B:246:MET:HA	1:B:250:GLU:OE1	2.20	0.42
1:A:259:HIS:CG	1:A:311:TRP:CZ2	3.07	0.42
1:A:688:ILE:C	1:A:690:GLY:H	2.23	0.42
1:A:581:VAL:O	1:A:581:VAL:CG1	2.54	0.42
1:A:665:GLU:HB3	1:A:666:HIS:ND1	2.34	0.42
1:B:230:PRO:O	1:B:231:GLU:C	2.58	0.42
1:B:503:GLN:O	1:B:506:THR:HB	2.20	0.42
1:B:702:TYR:O	1:B:707:ALA:HB3	2.19	0.42
1:A:367:MET:HE2	1:A:367:MET:HB2	1.81	0.42
1:A:126:ASN:HA	1:A:129:LEU:HD12	2.01	0.42
1:A:65:LYS:HD2	1:A:155:LEU:HD11	2.02	0.42
1:A:185:VAL:HG11	1:A:187:TRP:CE2	2.54	0.42
1:A:354:VAL:CG2	1:A:366:PRO:HD3	2.50	0.42
1:B:95:TRP:HZ3	1:B:406:LEU:HD11	1.84	0.42
1:B:463:LEU:HB2	1:B:541:ALA:HB2	2.01	0.42
1:B:688:ILE:C	1:B:690:GLY:H	2.23	0.42
1:A:471:ALA:O	1:A:472:SER:C	2.59	0.42
1:A:283:ILE:HD11	1:B:688:ILE:HA	2.02	0.41
1:A:127:ALA:HA	1:A:290:TRP:CH2	2.54	0.41
1:B:313:GLN:C	1:B:315:PRO:HD3	2.40	0.41
1:A:107:ARG:CZ	1:A:606:LEU:HD21	2.51	0.41
1:B:73:THR:O	1:B:73:THR:OG1	2.38	0.41
1:A:220:ASN:OD1	1:A:222:GLU:HB2	2.21	0.41
1:A:536:LEU:HD12	1:A:536:LEU:HA	1.88	0.41
1:B:376:LYS:O	1:B:376:LYS:CG	2.66	0.41
1:A:264:VAL:HG12	2:A:800:HEM:HAA1	2.01	0.41
1:A:405:LYS:HE3	1:A:429:TRP:CG	2.53	0.41
1:A:461:SER:O	1:A:465:LYS:HB3	2.21	0.41
1:A:622:ARG:HB3	1:A:634:GLY:O	2.20	0.41
1:A:718:THR:O	1:A:719:TRP:C	2.55	0.41
1:B:217:ILE:N	1:B:217:ILE:HD13	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:PRO:HB2	1:A:361:ASP:H	1.28	0.41
1:A:428:ILE:HD12	1:A:428:ILE:HA	1.80	0.41
1:A:464:VAL:HG23	1:A:541:ALA:HB1	2.02	0.41
1:A:617:LEU:HA	1:A:715:PHE:CD1	2.55	0.41
1:B:247:ASN:N	1:B:250:GLU:OE1	2.51	0.41
1:A:217:ILE:O	1:A:218:TYR:CD2	2.74	0.41
1:A:268:ASP:H	1:A:303:ILE:HG12	1.85	0.41
1:B:555:ILE:HG22	1:B:556:PRO:HD2	2.01	0.41
1:A:147:ILE:HD13	1:A:152:LEU:HD13	2.03	0.41
1:A:724:LYS:HZ3	1:A:724:LYS:HG3	1.64	0.41
1:B:95:TRP:HZ3	1:B:218:TYR:HH	1.58	0.41
1:B:126:ASN:O	1:B:129:LEU:HB2	2.21	0.41
1:B:352:ASN:HB3	1:B:363:LYS:HB3	2.03	0.41
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.90	0.41
1:B:433:LEU:HA	1:B:434:PRO:HD2	1.68	0.41
1:A:441:ILE:HA	1:A:445:GLU:OE1	2.21	0.41
1:A:512:GLU:HG3	1:A:530:LEU:HD22	2.02	0.41
1:B:34:GLU:HA	1:B:37:ASP:OD2	2.21	0.41
1:A:367:MET:HE1	1:A:369:LEU:HD23	2.03	0.40
1:A:95:TRP:CD1	1:A:96:HIS:CD2	3.09	0.40
1:A:510:THR:O	1:A:514:ILE:HG12	2.22	0.40
1:A:587:TYR:C	1:A:588:ILE:HG13	2.41	0.40
1:B:409:ARG:CG	1:B:409:ARG:HH21	2.34	0.40
1:B:31:LEU:HA	1:B:31:LEU:HD23	1.65	0.40
1:A:132:ALA:O	1:A:135:LEU:HB2	2.21	0.40
1:A:375:LEU:HD22	1:A:385:MET:HE1	2.04	0.40
1:A:654:MET:HE1	1:B:288:LEU:HD11	2.04	0.40
1:A:116:ARG:HD3	1:A:149:TRP:HB3	2.03	0.40
1:A:274:LEU:HD13	1:A:290:TRP:HB3	2.03	0.40
1:B:320:MET:SD	1:B:392:PRO:HB3	2.62	0.40
1:B:391:ASN:HA	1:B:392:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	653/737 (89%)	573 (88%)	68 (10%)	12 (2%)	8 5
1	B	652/737 (88%)	558 (86%)	84 (13%)	10 (2%)	10 7
All	All	1305/1474 (88%)	1131 (87%)	152 (12%)	22 (2%)	9 6

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	PRO
1	A	361	ASP
1	B	321	GLY
1	B	592	ILE
1	A	87	GLY
1	A	409	ARG
1	A	630	ASP
1	B	245	ALA
1	B	271	GLU
1	A	243	ARG
1	A	244	ALA
1	B	434	PRO
1	A	259	HIS
1	A	581	VAL
1	A	592	ILE
1	B	243	ARG
1	B	319	ASP
1	B	674	ASP
1	A	217	ILE
1	B	286	GLN
1	B	591	ASP
1	A	678	VAL

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	545/607 (90%)	497 (91%)	48 (9%)	10 9
1	B	543/607 (90%)	494 (91%)	49 (9%)	9 8
All	All	1088/1214 (90%)	991 (91%)	97 (9%)	9 8

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	35	ILE
1	A	41	ARG
1	A	42	ASP
1	A	47	GLU
1	A	48	ASP
1	A	51	ASP
1	A	57	GLN
1	A	69	GLU
1	A	95	TRP
1	A	102	ARG
1	A	103	THR
1	A	176	GLU
1	A	233	SER
1	A	240	THR
1	A	268	ASP
1	A	269	ASP
1	A	272	GLU
1	A	291	GLN
1	A	302	MET
1	A	342	GLN
1	A	356	ASP
1	A	361	ASP
1	A	367	MET
1	A	368	MET
1	A	378	ASP
1	A	395	PHE
1	A	409	ARG
1	A	439	ASP
1	A	440	LEU
1	A	443	ASP
1	A	445	GLU
1	A	448	GLU
1	A	455	ASP
1	A	500	GLU

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Mol	Chain	Res	Type
1	A	517	GLU
1	A	578	LYS
1	A	586	ASN
1	A	594	ARG
1	A	638	ASP
1	A	640	PRO
1	A	651	LEU
1	A	659	GLU
1	A	664	SER
1	A	667	ARG
1	A	669	LYS
1	A	677	GLU
1	A	679	LYS
1	B	30	LYS
1	B	41	ARG
1	B	42	ASP
1	B	47	GLU
1	B	57	GLN
1	B	69	GLU
1	B	73	THR
1	B	77	ASP
1	B	102	ARG
1	B	121	ASN
1	B	130	ASP
1	B	146	LYS
1	B	176	GLU
1	B	177	ASP
1	B	239	GLN
1	B	248	ASP
1	B	263	LYS
1	B	269	ASP
1	B	278	PRO
1	B	284	GLU
1	B	302	MET
1	B	334	GLU
1	B	335	LYS
1	B	349	GLU
1	B	351	LYS
1	B	361	ASP
1	B	379	PRO
1	B	397	MET
1	B	409	ARG

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Mol	Chain	Res	Type
1	B	424	ASP
1	B	428	ILE
1	B	489	ARG
1	B	498	VAL
1	B	514	ILE
1	B	523	SER
1	B	573	SER
1	B	575	ASP
1	B	580	LYS
1	B	586	ASN
1	B	591	ASP
1	B	593	THR
1	B	594	ARG
1	B	599	VAL
1	B	630	ASP
1	B	657	GLU
1	B	667	ARG
1	B	679	LYS
1	B	681	GLU
1	B	692	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	39	ASN
1	A	186	ASN
1	A	239	GLN
1	A	285	GLN
1	A	286	GLN
1	A	291	GLN
1	A	342	GLN
1	A	503	GLN
1	A	515	GLN
1	A	519	ASN
1	A	568	HIS
1	A	586	ASN
1	A	666	HIS
1	A	692	ASN
1	B	32	ASN
1	B	38	GLN
1	B	96	HIS

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Mol	Chain	Res	Type
1	B	126	ASN
1	B	291	GLN
1	B	342	GLN
1	B	358	HIS
1	B	495	ASN
1	B	515	GLN
1	B	519	ASN
1	B	586	ASN
1	B	608	ASN
1	B	692	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)

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	800	1	41,50,50	1.93	7 (17%)	45,82,82	1.89	9 (20%)
2	HEM	A	800	1	41,50,50	1.96	7 (17%)	45,82,82	2.26	10 (22%)

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	800	1	-	6/12/54/54	-
2	HEM	A	800	1	-	5/12/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	C3D-C2D	7.73	1.53	1.36
2	B	800	HEM	C3D-C2D	7.20	1.52	1.36
2	B	800	HEM	C3C-C2C	-4.98	1.33	1.40
2	A	800	HEM	C3C-C2C	-4.71	1.33	1.40
2	A	800	HEM	C3C-CAC	3.96	1.55	1.47
2	B	800	HEM	C3C-CAC	3.07	1.54	1.47
2	A	800	HEM	CAB-C3B	2.50	1.54	1.47
2	A	800	HEM	CMB-C2B	2.50	1.56	1.50
2	B	800	HEM	CAB-C3B	2.31	1.53	1.47
2	B	800	HEM	CAA-C2A	2.26	1.55	1.52
2	A	800	HEM	C2A-C3A	-2.25	1.31	1.37
2	B	800	HEM	C1A-CHA	-2.23	1.34	1.41
2	B	800	HEM	CMA-C3A	2.07	1.56	1.51
2	A	800	HEM	C1D-ND	2.06	1.43	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	HEM	C4C-CHD-C1D	7.63	132.62	122.56
2	B	800	HEM	C4D-ND-C1D	5.12	110.36	105.07
2	A	800	HEM	CMC-C2C-C3C	5.00	134.03	124.68
2	B	800	HEM	CAA-CBA-CGA	-4.96	99.86	113.76
2	A	800	HEM	C4D-ND-C1D	4.95	110.19	105.07
2	A	800	HEM	CAD-CBD-CGD	-4.68	103.53	113.60
2	B	800	HEM	C4C-CHD-C1D	4.57	128.59	122.56
2	A	800	HEM	C4A-C3A-C2A	4.46	110.10	107.00
2	B	800	HEM	CBA-CAA-C2A	4.38	120.09	112.62
2	A	800	HEM	CMD-C2D-C1D	4.28	131.56	125.04
2	A	800	HEM	CAA-CBA-CGA	-3.43	104.14	113.76
2	B	800	HEM	CHB-C1B-NB	3.02	128.12	124.38
2	B	800	HEM	CAD-CBD-CGD	-2.78	107.61	113.60
2	B	800	HEM	CHA-C4D-ND	2.59	127.58	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	HEM	CHB-C1B-NB	2.52	127.50	124.38
2	A	800	HEM	C1D-C2D-C3D	-2.34	104.50	106.96
2	B	800	HEM	C3B-C2B-C1B	2.33	108.21	106.49
2	B	800	HEM	CMD-C2D-C1D	2.30	128.54	125.04
2	A	800	HEM	C3C-C4C-NC	-2.27	106.66	110.94

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	800	HEM	C3A-C2A-CAA-CBA
2	B	800	HEM	C1A-C2A-CAA-CBA
2	B	800	HEM	CAD-CBD-CGD-O1D
2	A	800	HEM	CAA-CBA-CGA-O2A
2	A	800	HEM	C4B-C3B-CAB-CBB
2	A	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	CAA-CBA-CGA-O2A
2	B	800	HEM	CAD-CBD-CGD-O2D
2	A	800	HEM	CAD-CBD-CGD-O2D
2	B	800	HEM	CAA-CBA-CGA-O1A
2	A	800	HEM	C2D-C3D-CAD-CBD

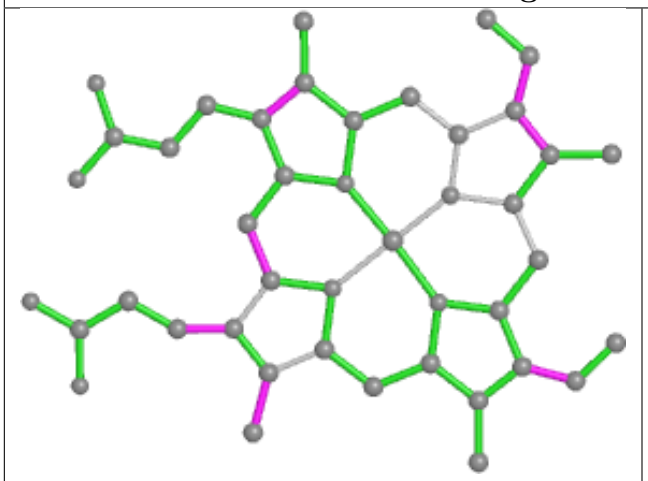
There are no ring outliers.

2 monomers are involved in 9 short contacts:

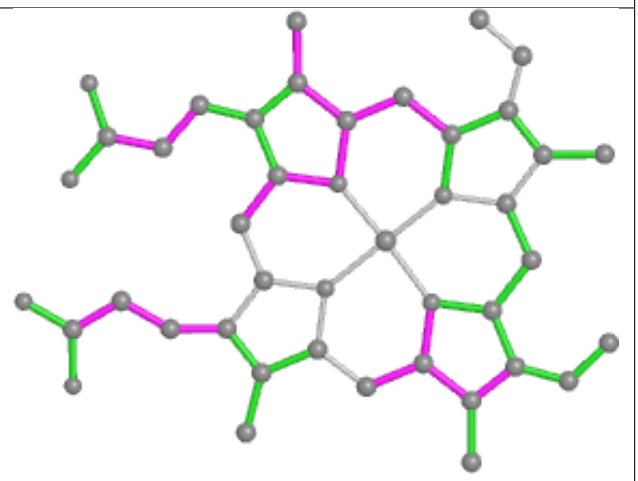
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	HEM	5	0
2	A	800	HEM	4	0

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.

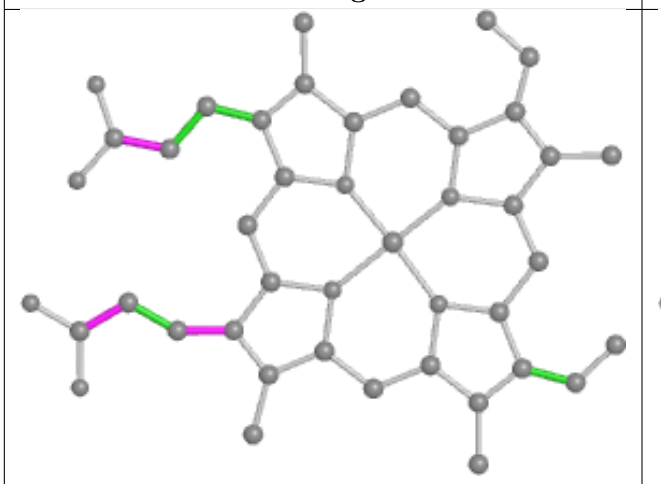
Ligand HEM B 800



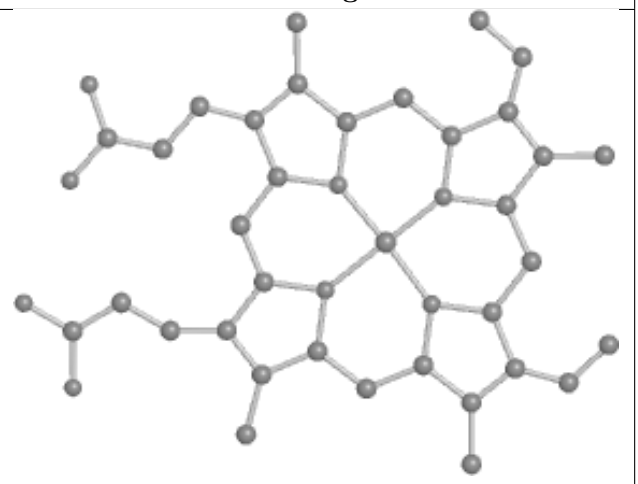
Bond lengths



Bond angles

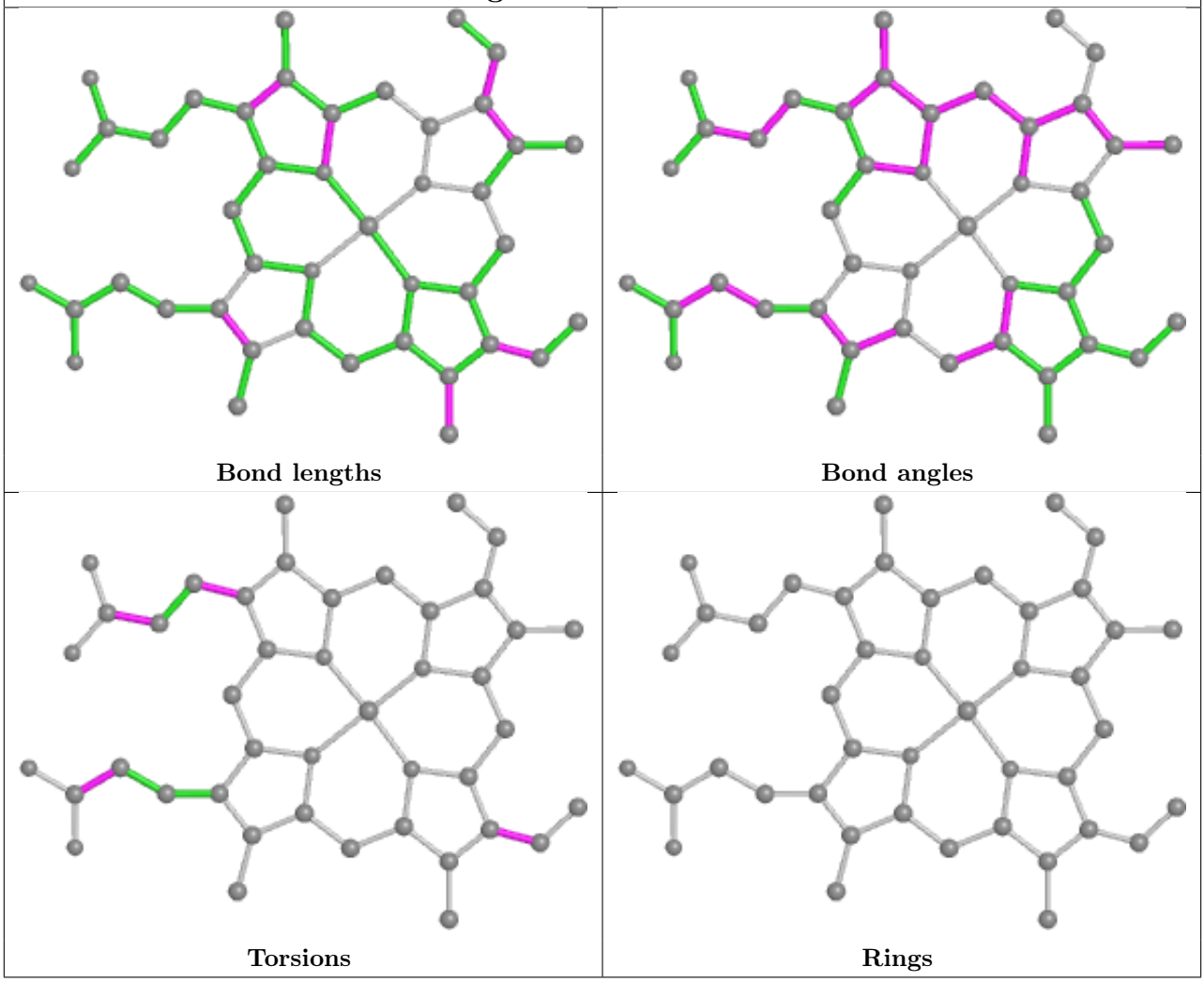


Torsions



Rings

Ligand HEM A 800



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	663/737 (89%)	0.19	32 (4%)	30	41	14, 35, 55, 68	0
1	B	660/737 (89%)	0.43	39 (5%)	22	31	24, 43, 60, 71	0
All	All	1323/1474 (89%)	0.31	71 (5%)	25	36	14, 39, 58, 71	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	MET	5.2
1	A	360	PRO	5.0
1	B	348	GLU	4.7
1	B	663	ASP	4.6
1	A	361	ASP	4.4
1	B	592	ILE	4.1
1	B	361	ASP	4.1
1	B	239	GLN	4.1
1	A	525	GLY	4.1
1	A	591	ASP	4.0
1	A	186	ASN	3.9
1	B	271	GLU	3.9
1	B	665	GLU	3.7
1	B	29	SER	3.6
1	B	591	ASP	3.6
1	B	662	ALA	3.5
1	A	188	GLY	3.3
1	A	437	ASP	3.2
1	A	29	SER	3.1
1	A	245	ALA	3.0
1	B	534	ILE	3.0
1	B	77	ASP	3.0
1	B	523	SER	3.0
1	B	311	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	520	ASP	2.9
1	B	347	SER	2.9
1	A	213	VAL	2.9
1	B	264	VAL	2.9
1	B	360	PRO	2.9
1	A	271	GLU	2.8
1	B	276	PRO	2.7
1	B	437	ASP	2.7
1	A	521	SER	2.7
1	B	242	ASP	2.7
1	A	215	GLY	2.7
1	A	706	ASP	2.6
1	B	618	ILE	2.6
1	A	216	LEU	2.6
1	A	362	GLU	2.6
1	B	558	GLU	2.6
1	B	215	GLY	2.6
1	B	187	TRP	2.5
1	A	218	TYR	2.5
1	A	457	ASP	2.5
1	B	620	GLY	2.5
1	B	369	LEU	2.5
1	B	259	HIS	2.4
1	A	455	ASP	2.4
1	A	348	GLU	2.4
1	B	584	VAL	2.4
1	B	728	PHE	2.4
1	B	341	TRP	2.3
1	A	255	ILE	2.3
1	B	379	PRO	2.3
1	A	728	PHE	2.3
1	A	503	GLN	2.3
1	A	347	SER	2.2
1	B	255	ILE	2.2
1	A	674	ASP	2.2
1	B	457	ASP	2.2
1	A	534	ILE	2.2
1	B	186	ASN	2.2
1	B	349	GLU	2.2
1	A	527	GLN	2.1
1	B	552	ASP	2.1
1	B	531	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	536	LEU	2.1
1	B	329	TYR	2.1
1	A	41	ARG	2.0
1	B	225	ASP	2.0
1	A	451	GLU	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)

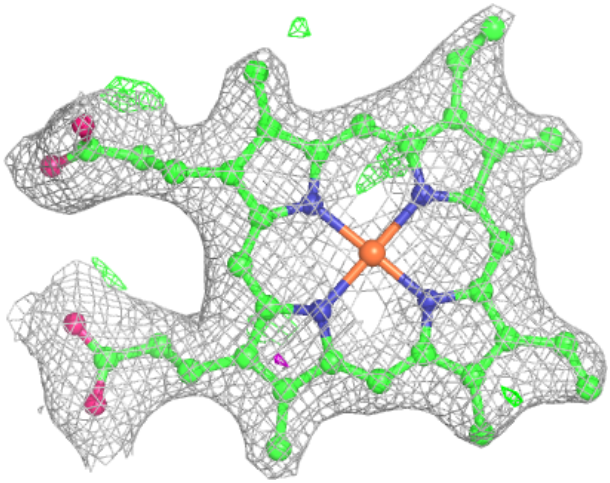
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

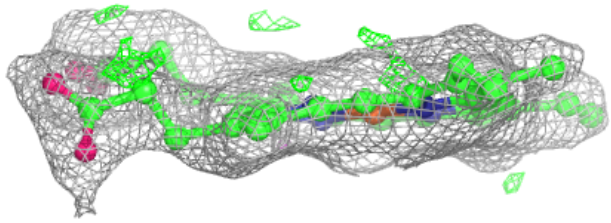
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	800	43/43	0.93	0.23	39,42,46,48	0
2	HEM	A	800	43/43	0.94	0.18	17,22,25,29	0

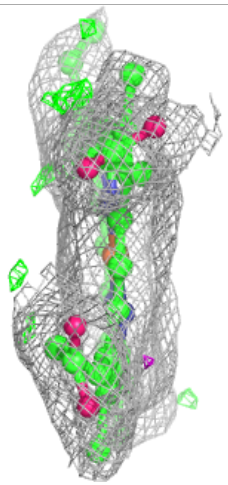
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM B 800:

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

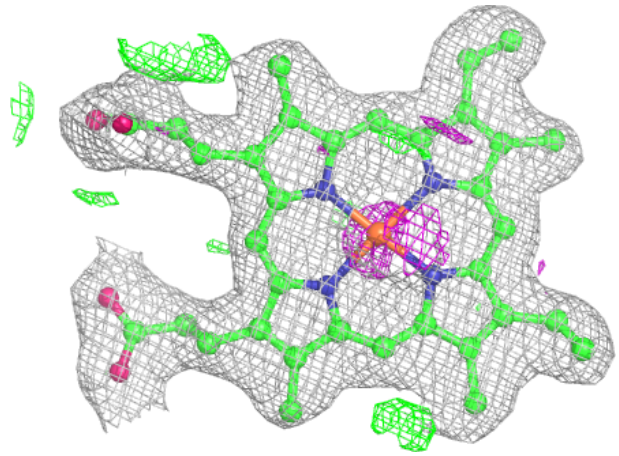


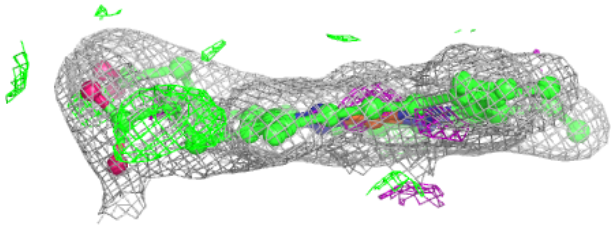


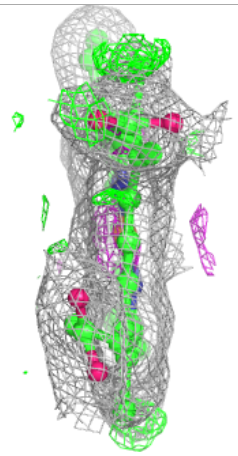


Electron density around HEM A 800:

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.