Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 04:33 AM EDT

PDB ID	:	5WHQ
Title	:	Crystal structure of the catalase-peroxidase from Neurospora crassa at 2.9 A
Authors	:	Diaz-Vilchis, A.; Vega-Garcia, V.; Rudino-Pinera, E.; Hansberg, W.
Deposited on	:	2017-07-18
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

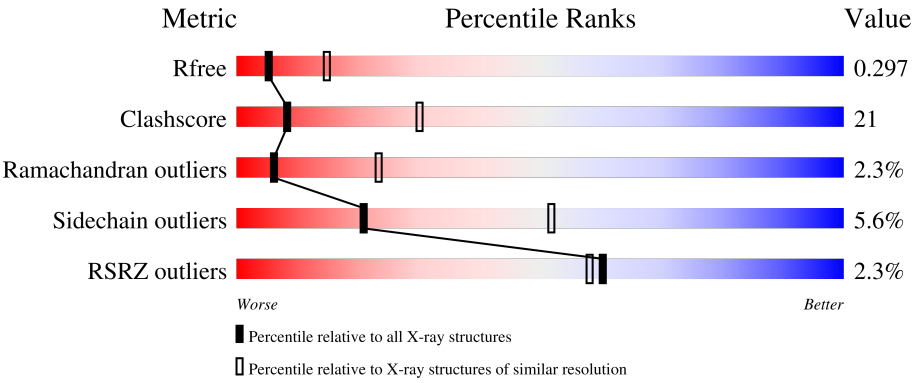
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	768	3% 58% 31% · 7%
1	B	768	% 69% 21% · 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11326 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5579	3545	975	1047	12			
1	B	711	Total	C	N	O	S	0	0	0
			5579	3545	975	1047	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP Q8X182
A	-13	ARG	-	expression tag	UNP Q8X182
A	-12	GLY	-	expression tag	UNP Q8X182
A	-11	SER	-	expression tag	UNP Q8X182
A	-10	HIS	-	expression tag	UNP Q8X182
A	-9	HIS	-	expression tag	UNP Q8X182
A	-8	HIS	-	expression tag	UNP Q8X182
A	-7	HIS	-	expression tag	UNP Q8X182
A	-6	HIS	-	expression tag	UNP Q8X182
A	-5	HIS	-	expression tag	UNP Q8X182
A	-4	GLY	-	expression tag	UNP Q8X182
A	-3	SER	-	expression tag	UNP Q8X182
A	-2	ALA	-	expression tag	UNP Q8X182
A	-1	CYS	-	expression tag	UNP Q8X182
A	0	GLU	-	expression tag	UNP Q8X182
A	1	LEU	-	expression tag	UNP Q8X182
B	-14	MET	-	initiating methionine	UNP Q8X182
B	-13	ARG	-	expression tag	UNP Q8X182
B	-12	GLY	-	expression tag	UNP Q8X182
B	-11	SER	-	expression tag	UNP Q8X182
B	-10	HIS	-	expression tag	UNP Q8X182
B	-9	HIS	-	expression tag	UNP Q8X182
B	-8	HIS	-	expression tag	UNP Q8X182
B	-7	HIS	-	expression tag	UNP Q8X182
B	-6	HIS	-	expression tag	UNP Q8X182

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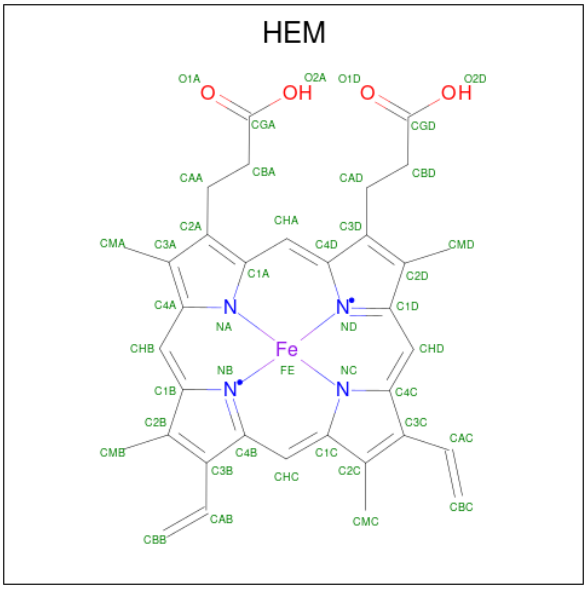
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8X182
B	-4	GLY	-	expression tag	UNP Q8X182
B	-3	SER	-	expression tag	UNP Q8X182
B	-2	ALA	-	expression tag	UNP Q8X182
B	-1	CYS	-	expression tag	UNP Q8X182
B	0	GLU	-	expression tag	UNP Q8X182
B	1	LEU	-	expression tag	UNP Q8X182

- 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		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	K		0	0
			1	1			
3	B	1	Total	K		0	0
			1	1			

- Molecule 4 is water.

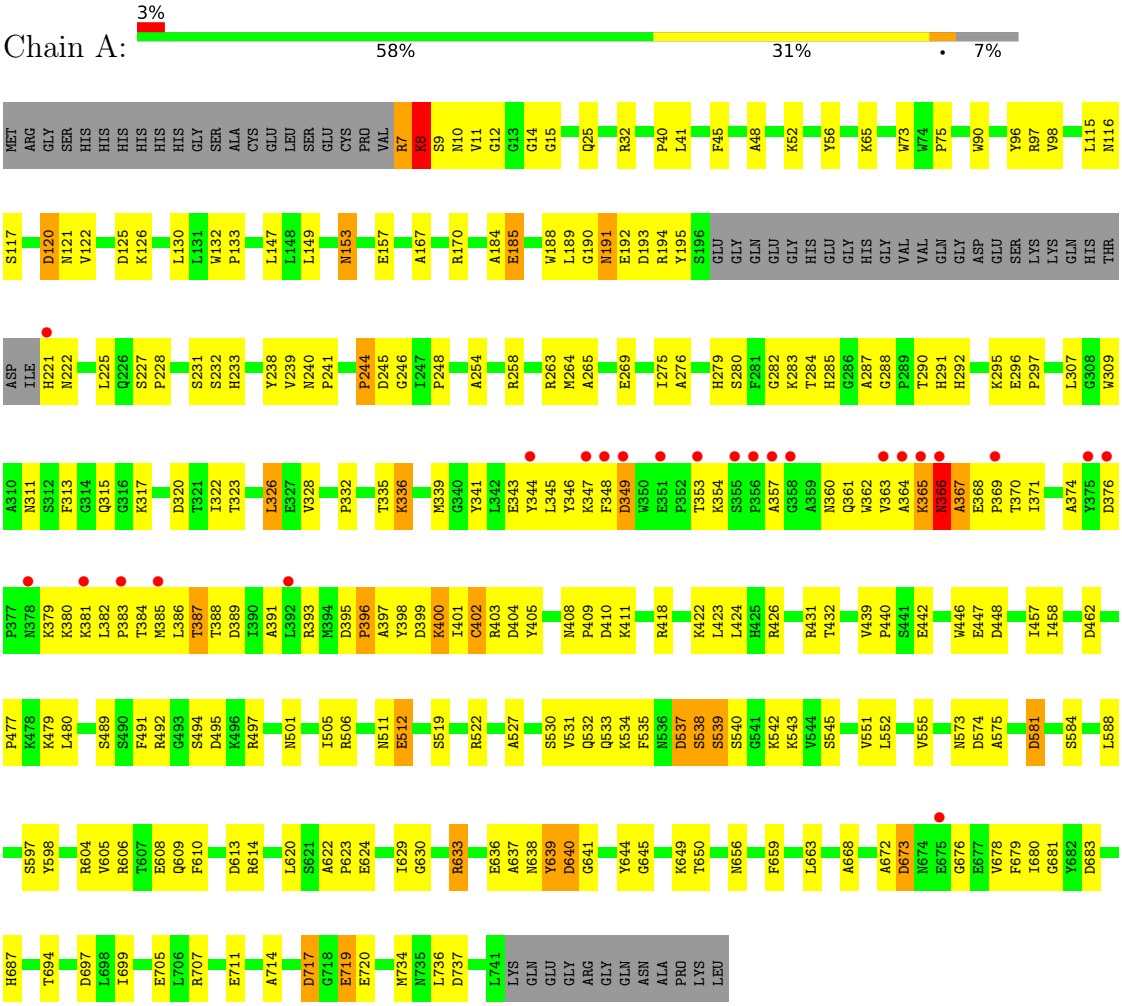
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	48	Total O 48 48	0	0

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.

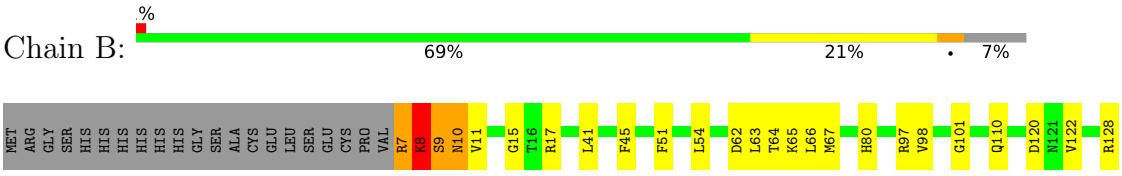
• Molecule 1: Catalase-peroxidase

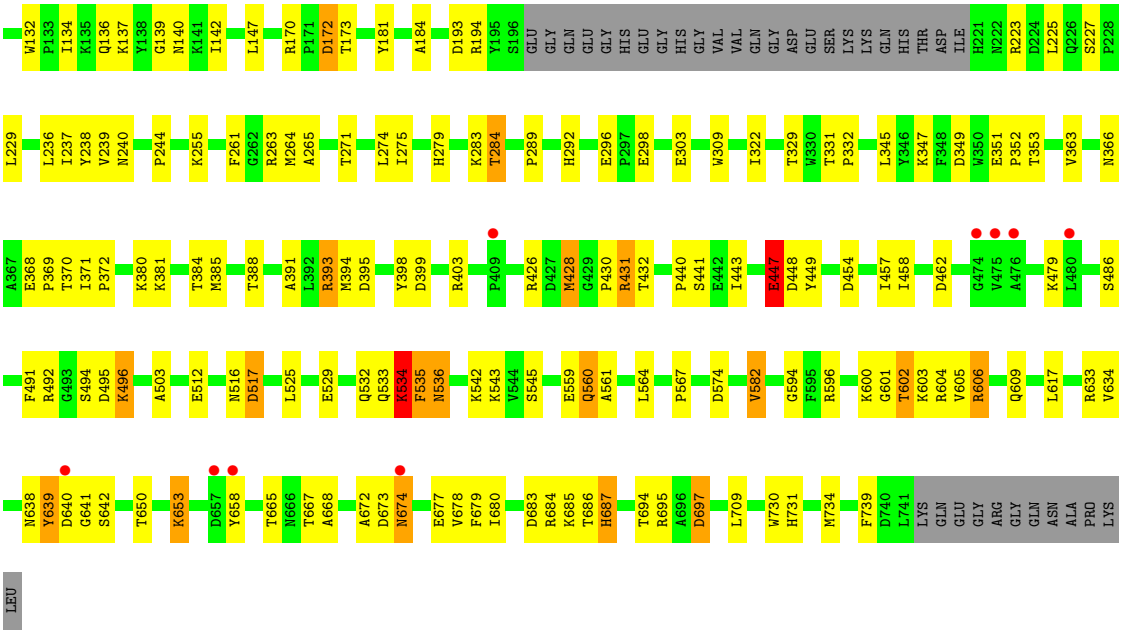
Chain A:



• Molecule 1: Catalase-peroxidase

Chain B:




W132 P133 I134 K135 Q136 K137 Y138 G139 N140 K141 I142 L147 R170 P171 D172 T173 Y181 A184 D193 R194 Y195 S196 H221 N222 R223 D224 L225 Q226 S227 P228
L229 L236 I237 Y238 V239 N240 P244 K255 F261 G262 R263 M264 A265 T271 L274 I275 H279 K283 T284 P289 H292 E296 P297 E298 E303 W309 I322 T329 W330 T331 P332 L345 Y346 K347 F348 D349 W350 E351 P352 T353 V363 N366
A367 E368 P369 T370 I371 P372 K380 K381 T384 M385 T388 A391 L392 R393 M394 D395 Y398 D399 R403 P409 R426 D427 M428 G429 P430 R431 T432 P440 S441 E442 I443 E447 D448 Y449 D454 I457 I458 D462 G474 V475 A476 K479 L480 S486
F491 R492 G493 S494 D495 K496 A503 E512 N516 D517 L525 E529 Q532 Q533 K534 F535 N536 K542 K543 V544 S545 E559 Q560 A561 L564 P567 D574 V582 G594 F596 R596 K600 G601 T602 K603 R604 V605 R606 Q609 L617 R633 V634
N638 Y639 D640 G641 S642 T650 K653 D657 Y658 T665 N666 T667 A668 A672 D673 N674 E677 V678 F679 I680 D683 R684 K685 T686 H687 T694 R695 A696 D697 L709 W730 H731 M734 F739 D740 L741 LYS GLN GLU GLY ARG GLY GLN ASN ALA PRO LYS
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.31Å 115.65Å 123.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.27 – 2.90 48.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (84.27-2.90) 96.3 (48.02-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.224 , 0.297 0.226 , 0.297	Depositor DCC
R_{free} test set	1652 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11326	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0111e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 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	0.84	1/5735 (0.0%)	0.79	5/7795 (0.1%)
1	B	0.86	1/5735 (0.0%)	0.81	1/7795 (0.0%)
All	All	0.85	2/11470 (0.0%)	0.80	6/15590 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	447	GLU	CD-OE2	-5.29	1.19	1.25
1	A	56	TYR	CE1-CZ	-5.26	1.31	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	349	ASP	N-CA-C	-6.62	93.13	111.00
1	A	282	GLY	N-CA-C	6.34	128.94	113.10
1	A	120	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	606	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	A	495	ASP	CB-CA-C	5.11	120.61	110.40
1	A	650	THR	C-N-CD	5.07	139.04	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5579	0	5397	298	1
1	B	5579	0	5397	170	1
2	A	43	0	30	15	0
2	B	43	0	30	13	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	0	1	0
4	B	48	0	0	5	0
All	All	11326	0	10854	465	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 21.

All (465) 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:284:THR:HG22	2:B:801:HEM:CAA	1.54	1.38
1:A:511:ASN:OD1	1:A:512:GLU:HG2	1.35	1.24
1:A:288:GLY:O	1:A:357:ALA:HB2	1.31	1.24
1:A:221:HIS:ND1	1:A:222:ASN:N	1.91	1.19
1:A:717:ASP:OD2	1:B:139:GLY:HA3	1.39	1.18
1:B:284:THR:CG2	2:B:801:HEM:HAA1	1.76	1.16
1:A:362:TRP:O	1:A:384:THR:OG1	1.64	1.14
1:B:668:ALA:HB2	1:B:684:ARG:HH21	1.02	1.14
1:B:639:TYR:O	1:B:640:ASP:CG	1.91	1.09
1:A:345:LEU:O	1:A:393:ARG:NH1	1.86	1.09
1:B:331:THR:OG1	1:B:332:PRO:HD2	1.51	1.08
1:A:288:GLY:O	1:A:357:ALA:CB	2.04	1.06
1:B:673:ASP:OD1	1:B:674:ASN:OD1	1.73	1.05
1:A:506:ARG:NH2	1:A:575:ALA:O	1.91	1.03
1:A:457:ILE:O	1:A:542:LYS:NZ	1.94	1.00
1:A:96:TYR:O	1:A:264:MET:HG2	1.62	0.98
1:A:194:ARG:NH2	1:A:231:SER:O	1.95	0.98
1:B:8:LYS:HA	1:B:15:GLY:H	1.27	0.98
1:A:7:ARG:O	1:A:9:SER:N	1.97	0.98
1:A:604:ARG:O	1:B:9:SER:HB3	1.64	0.97
1:A:191:ASN:HB3	1:A:233:HIS:HD2	1.28	0.95
1:A:639:TYR:O	1:A:641:GLY:N	2.00	0.95
1:B:668:ALA:HB2	1:B:684:ARG:NH2	1.80	0.95
1:B:532:GLN:O	1:B:536:ASN:HB2	1.67	0.94
1:B:368:GLU:O	1:B:370:THR:HG23	1.67	0.94
1:B:193:ASP:OD1	1:B:604:ARG:NH2	1.99	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:ALA:CB	1:B:684:ARG:HH21	1.81	0.93
1:A:384:THR:O	1:A:385:MET:HG2	1.68	0.92
1:A:335:THR:O	1:A:336:LYS:HD3	1.70	0.91
1:A:239:VAL:HG22	1:A:240:ASN:H	1.37	0.89
1:A:385:MET:CE	1:A:389:ASP:HB3	2.05	0.87
1:A:537:ASP:O	1:A:539:SER:N	2.07	0.87
1:B:639:TYR:O	1:B:640:ASP:OD1	1.93	0.85
1:A:369:PRO:HB3	1:A:380:LYS:C	1.97	0.85
1:A:349:ASP:CB	1:A:365:LYS:HE2	2.07	0.84
1:B:673:ASP:HB2	1:B:678:VAL:HG22	1.60	0.84
1:B:264:MET:O	1:B:426:ARG:NH1	2.11	0.84
1:B:331:THR:OG1	1:B:332:PRO:CD	2.27	0.82
1:A:349:ASP:HB3	1:A:365:LYS:HE2	1.61	0.81
1:A:511:ASN:OD1	1:A:512:GLU:CG	2.26	0.81
1:A:115:LEU:O	1:A:121:ASN:ND2	2.12	0.81
1:A:353:THR:CG2	1:A:363:VAL:CG2	2.58	0.81
1:A:385:MET:HE1	1:A:389:ASP:HB3	1.62	0.80
1:B:533:GLN:O	1:B:534:LYS:O	1.98	0.80
1:B:677:GLU:OE2	4:B:901:HOH:O	2.00	0.80
1:B:284:THR:HG22	2:B:801:HEM:HAA1	0.81	0.80
1:A:311:ASN:HD21	1:A:322:ILE:HD12	1.46	0.80
1:A:385:MET:HE3	1:A:389:ASP:CB	2.12	0.79
1:A:343:GLU:O	1:A:347:LYS:HG2	1.82	0.79
1:A:349:ASP:HB3	1:A:365:LYS:CE	2.12	0.79
1:A:194:ARG:HH21	1:A:231:SER:C	1.86	0.79
1:A:492:ARG:NH1	1:A:588:LEU:HD12	1.98	0.78
1:A:349:ASP:CB	1:A:365:LYS:CE	2.61	0.78
1:B:284:THR:CG2	2:B:801:HEM:CAA	2.49	0.78
1:A:239:VAL:HG22	1:A:240:ASN:N	1.99	0.78
1:A:385:MET:CE	1:A:389:ASP:CB	2.61	0.77
2:A:801:HEM:HBC2	2:A:801:HEM:HMC2	1.67	0.77
1:B:633:ARG:NH1	1:B:697:ASP:OD1	2.18	0.77
1:A:283:LYS:NZ	1:A:374:ALA:HB2	1.99	0.77
1:A:343:GLU:O	1:A:347:LYS:CG	2.33	0.77
1:A:296:GLU:N	1:A:296:GLU:OE1	2.18	0.77
1:A:353:THR:HG21	1:A:363:VAL:CG2	2.15	0.77
1:B:7:ARG:O	1:B:9:SER:OG	2.03	0.76
1:A:639:TYR:C	1:A:641:GLY:H	1.88	0.76
1:A:283:LYS:NZ	1:A:374:ALA:CB	2.49	0.75
1:A:673:ASP:OD2	1:A:678:VAL:HG22	1.87	0.75
1:A:284:THR:HG22	2:A:801:HEM:HAA1	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLN:O	1:A:537:ASP:HB2	1.87	0.74
1:A:184:ALA:C	1:A:185:GLU:O	2.20	0.74
1:A:311:ASN:HD21	1:A:322:ILE:CD1	2.01	0.74
2:A:801:HEM:HBB2	2:A:801:HEM:HMB2	1.71	0.73
1:A:311:ASN:HD21	1:A:322:ILE:CG1	2.02	0.72
1:B:147:LEU:HD12	1:B:147:LEU:O	1.90	0.71
1:A:418:ARG:NH2	1:A:442:GLU:OE2	2.23	0.71
1:A:717:ASP:CG	1:B:139:GLY:HA3	2.09	0.71
1:A:311:ASN:ND2	1:A:322:ILE:HB	2.05	0.71
1:A:366:ASN:O	1:A:367:ALA:HB2	1.90	0.71
1:A:384:THR:C	1:A:385:MET:HG2	2.11	0.70
1:A:153:ASN:O	1:A:157:GLU:HG3	1.92	0.70
1:A:275:ILE:HD13	2:A:801:HEM:HHC	1.74	0.69
1:A:311:ASN:ND2	1:A:322:ILE:HD12	2.06	0.69
1:A:386:LEU:O	1:A:389:ASP:N	2.25	0.69
1:A:9:SER:HB2	1:B:605:VAL:HG22	1.75	0.69
1:B:542:LYS:C	1:B:543:LYS:HG3	2.12	0.69
1:B:8:LYS:HA	1:B:15:GLY:N	2.06	0.69
1:B:683:ASP:HB3	1:B:687:HIS:H	1.56	0.69
1:A:492:ARG:NH1	1:A:588:LEU:CD1	2.55	0.68
1:A:283:LYS:CE	1:A:374:ALA:HB2	2.23	0.68
1:A:369:PRO:HB3	1:A:381:LYS:N	2.08	0.68
1:A:604:ARG:O	1:B:9:SER:CB	2.40	0.68
1:A:194:ARG:NH2	1:A:231:SER:C	2.47	0.68
1:A:349:ASP:HB2	1:A:365:LYS:CE	2.24	0.68
1:B:172:ASP:OD1	4:B:902:HOH:O	2.11	0.67
1:B:677:GLU:O	1:B:679:PHE:CE1	2.46	0.67
1:A:191:ASN:HB3	1:A:233:HIS:CD2	2.20	0.67
1:B:640:ASP:OD1	1:B:641:GLY:N	2.28	0.67
1:A:633:ARG:HH12	1:A:697:ASP:CG	1.98	0.67
2:B:801:HEM:HMC1	2:B:801:HEM:HBC2	1.77	0.66
1:B:184:ALA:HB3	1:B:193:ASP:OD2	1.96	0.66
1:A:385:MET:HE3	1:A:389:ASP:HB2	1.76	0.66
1:A:353:THR:CG2	1:A:363:VAL:HG23	2.25	0.66
1:A:7:ARG:CB	1:A:7:ARG:HH21	2.08	0.66
1:A:239:VAL:HG12	2:A:801:HEM:HBB2	1.76	0.66
1:A:431:ARG:NH2	1:A:440:PRO:O	2.29	0.66
1:A:248:PRO:HG3	1:A:360:ASN:HB3	1.77	0.65
2:B:801:HEM:HMB1	2:B:801:HEM:HBB2	1.77	0.65
1:A:221:HIS:CG	1:A:222:ASN:H	2.10	0.65
1:A:184:ALA:O	1:A:185:GLU:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ARG:NH1	1:A:697:ASP:OD1	2.30	0.65
1:A:656:ASN:OD1	1:A:719:GLU:HG2	1.97	0.65
1:A:376:ASP:HB3	1:A:379:LYS:HB3	1.79	0.65
1:A:477:PRO:HA	1:A:480:LEU:HD12	1.79	0.65
1:B:7:ARG:CG	1:B:7:ARG:HH21	2.09	0.65
1:B:516:ASN:O	1:B:517:ASP:O	2.15	0.65
1:B:683:ASP:HB3	1:B:687:HIS:N	2.12	0.65
1:A:244:PRO:O	1:A:246:GLY:N	2.30	0.64
1:A:489:SER:OG	1:A:614:ARG:NH2	2.29	0.64
1:B:431:ARG:NH2	1:B:440:PRO:O	2.30	0.64
1:B:534:LYS:O	1:B:535:PHE:C	2.36	0.64
1:A:32:ARG:NH1	1:A:705:GLU:OE2	2.30	0.64
1:A:349:ASP:HB2	1:A:365:LYS:HE3	1.80	0.64
1:B:239:VAL:HG12	1:B:240:ASN:N	2.13	0.64
1:A:353:THR:HG22	1:A:363:VAL:HG23	1.80	0.64
1:B:395:ASP:O	1:B:399:ASP:HB2	1.98	0.63
1:A:348:PHE:CE1	1:A:366:ASN:O	2.52	0.63
1:A:598:TYR:HD1	1:A:639:TYR:CE2	2.16	0.63
1:B:329:THR:HB	1:B:371:ILE:HD12	1.81	0.63
1:B:447:GLU:OE2	1:B:449:TYR:HB2	1.98	0.63
1:A:194:ARG:HD2	1:A:232:SER:O	1.98	0.63
1:B:399:ASP:OD2	1:B:403:ARG:NH1	2.32	0.63
1:A:239:VAL:CG2	1:A:240:ASN:H	2.12	0.62
1:B:683:ASP:OD2	1:B:686:THR:HB	1.99	0.62
1:A:193:ASP:OD2	1:A:604:ARG:NH2	2.32	0.61
1:B:371:ILE:HD11	1:B:381:LYS:HG3	1.80	0.61
1:B:137:LYS:O	1:B:137:LYS:HG2	2.00	0.61
1:B:284:THR:HG22	2:B:801:HEM:HAA2	1.70	0.61
1:A:423:LEU:HD12	1:A:426:ARG:CZ	2.31	0.61
1:A:606:ARG:CZ	1:A:609:GLN:OE1	2.49	0.61
1:B:533:GLN:O	1:B:534:LYS:C	2.38	0.61
1:A:339:MET:CE	1:A:409:PRO:HB3	2.30	0.61
1:B:7:ARG:O	1:B:9:SER:N	2.33	0.61
1:A:188:TRP:O	1:A:189:LEU:HB2	2.01	0.61
1:A:365:LYS:C	1:A:366:ASN:OD1	2.39	0.61
1:B:694:THR:HG22	1:B:695:ARG:N	2.16	0.61
1:A:9:SER:O	1:A:11:VAL:N	2.33	0.60
1:B:237:ILE:HG22	1:B:238:TYR:CD2	2.37	0.60
1:A:239:VAL:HG12	2:A:801:HEM:CBB	2.30	0.60
1:A:386:LEU:O	1:A:387:THR:C	2.40	0.60
1:B:353:THR:HG21	1:B:363:VAL:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:801:HEM:HBC2	2:A:801:HEM:CMC	2.32	0.60
1:A:353:THR:HG23	1:A:354:LYS:N	2.17	0.59
1:B:559:GLU:HG2	1:B:564:LEU:O	2.01	0.59
1:A:7:ARG:HG3	1:A:8:LYS:N	2.17	0.59
1:A:364:ALA:O	1:A:366:ASN:N	2.35	0.59
1:B:672:ALA:HB2	1:B:680:ILE:HG13	1.84	0.59
1:A:290:THR:O	1:A:292:HIS:N	2.36	0.59
1:A:313:PHE:CB	1:A:322:ILE:HD11	2.33	0.59
1:A:366:ASN:OD1	1:A:366:ASN:N	2.35	0.59
2:B:801:HEM:HBC2	2:B:801:HEM:CMC	2.33	0.59
1:A:7:ARG:HH21	1:A:7:ARG:HB3	1.67	0.59
1:A:264:MET:HB3	1:A:426:ARG:HH12	1.66	0.59
1:A:275:ILE:CD1	2:A:801:HEM:HAB	2.33	0.59
1:A:279:HIS:CE1	2:A:801:HEM:C4B	2.90	0.59
1:A:633:ARG:HG3	1:A:645:GLY:O	2.03	0.58
1:B:371:ILE:CD1	1:B:381:LYS:HG3	2.33	0.58
1:A:116:ASN:OD1	1:A:117:SER:N	2.36	0.58
1:B:674:ASN:OD1	1:B:674:ASN:N	2.32	0.58
1:B:525:LEU:O	1:B:529:GLU:HG3	2.03	0.58
1:A:343:GLU:O	1:A:347:LYS:HG3	2.03	0.58
1:B:7:ARG:HH21	1:B:7:ARG:HG3	1.67	0.58
1:A:404:ASP:OD2	1:A:411:LYS:HE2	2.04	0.58
1:A:125:ASP:N	1:A:125:ASP:OD1	2.37	0.58
1:B:559:GLU:O	1:B:560:GLN:C	2.42	0.58
1:B:9:SER:O	1:B:11:VAL:N	2.36	0.57
1:A:636:GLU:O	1:A:638:ASN:N	2.36	0.57
1:B:495:ASP:C	1:B:496:LYS:HG2	2.23	0.57
1:B:516:ASN:O	1:B:517:ASP:C	2.42	0.57
1:A:339:MET:HE1	1:A:409:PRO:CB	2.35	0.57
1:B:142:ILE:HG23	1:B:142:ILE:O	2.04	0.57
1:A:227:SER:OG	1:A:228:PRO:HA	2.05	0.57
1:A:672:ALA:HB2	1:A:680:ILE:HG13	1.87	0.57
1:A:673:ASP:OD1	1:A:676:GLY:N	2.35	0.56
1:A:422:LYS:HD2	1:A:446:TRP:CD1	2.40	0.56
1:B:264:MET:HB3	1:B:426:ARG:HH12	1.68	0.56
1:B:686:THR:O	1:B:687:HIS:HB2	2.04	0.56
1:A:283:LYS:HZ3	1:A:374:ALA:CB	2.17	0.56
1:A:40:PRO:HG3	1:B:709:LEU:HD22	1.87	0.56
1:A:344:TYR:OH	1:A:370:THR:HG21	2.05	0.56
1:B:606:ARG:H	1:B:609:GLN:NE2	2.04	0.56
1:B:353:THR:CG2	1:B:363:VAL:HG23	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:HD2	1:A:232:SER:C	2.27	0.56
1:A:313:PHE:HB3	1:A:322:ILE:HD11	1.88	0.56
1:B:458:ILE:HB	1:B:462:ASP:HB2	1.88	0.56
1:A:362:TRP:N	1:A:362:TRP:CD1	2.73	0.56
1:A:545:SER:HB2	1:A:574:ASP:OD1	2.06	0.56
1:B:371:ILE:CG1	1:B:381:LYS:HG3	2.36	0.55
2:B:801:HEM:HBB2	2:B:801:HEM:CMB	2.36	0.55
1:A:283:LYS:HZ1	1:A:374:ALA:CB	2.17	0.55
1:A:167:ALA:O	1:A:170:ARG:NH2	2.39	0.55
1:B:371:ILE:HG13	1:B:381:LYS:HG3	1.88	0.55
1:A:194:ARG:HD3	1:A:231:SER:O	2.04	0.55
1:A:537:ASP:C	1:A:539:SER:H	2.06	0.54
1:A:269:GLU:OE2	4:A:901:HOH:O	2.18	0.54
1:A:458:ILE:HA	1:A:542:LYS:HZ1	1.72	0.54
1:B:62:ASP:OD1	1:B:65:LYS:NZ	2.37	0.54
1:B:602:THR:HG22	1:B:604:ARG:H	1.72	0.54
1:A:283:LYS:NZ	1:A:374:ALA:HB3	2.22	0.54
1:A:349:ASP:CB	1:A:365:LYS:HE3	2.35	0.54
1:B:45:PHE:CE1	1:B:140:ASN:ND2	2.76	0.54
1:A:73:TRP:CH2	1:A:130:LEU:CD1	2.91	0.54
1:A:279:HIS:HE1	2:A:801:HEM:C4B	2.25	0.54
1:B:457:ILE:HG22	1:B:458:ILE:N	2.22	0.54
1:B:181:TYR:CE2	1:B:229:LEU:HD21	2.43	0.54
1:B:535:PHE:O	1:B:536:ASN:O	2.24	0.54
1:A:9:SER:HB3	1:B:604:ARG:O	2.07	0.54
1:B:640:ASP:OD1	1:B:642:SER:N	2.38	0.54
1:A:283:LYS:HZ3	1:A:374:ALA:HB2	1.69	0.53
1:A:326:LEU:HD23	1:A:361:GLN:HB3	1.89	0.53
1:B:542:LYS:HB3	1:B:542:LYS:HZ2	1.73	0.53
1:A:364:ALA:C	1:A:366:ASN:H	2.11	0.53
1:B:239:VAL:CG1	1:B:240:ASN:N	2.71	0.53
1:B:486:SER:OG	1:B:596:ARG:NH1	2.41	0.53
1:B:602:THR:CG2	1:B:603:LYS:N	2.71	0.53
1:A:188:TRP:C	1:A:190:GLY:H	2.10	0.53
2:A:801:HEM:HBB2	2:A:801:HEM:CMB	2.37	0.53
1:A:7:ARG:HG3	1:A:8:LYS:H	1.73	0.53
1:A:349:ASP:HB2	1:A:365:LYS:HE2	1.87	0.53
1:A:605:VAL:HG22	1:B:9:SER:HB2	1.91	0.53
1:A:672:ALA:HB3	1:A:678:VAL:HG23	1.91	0.53
1:B:494:SER:OG	1:B:617:LEU:CD2	2.56	0.53
1:A:7:ARG:HH21	1:A:7:ARG:CG	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PRO:O	1:A:399:ASP:HB3	2.09	0.53
1:A:462:ASP:OD2	1:A:542:LYS:HE2	2.09	0.53
1:B:170:ARG:NH1	1:B:428:MET:SD	2.82	0.53
1:A:573:ASN:OD1	1:A:574:ASP:N	2.42	0.53
1:A:530:SER:O	1:A:534:LYS:HG3	2.09	0.52
1:B:399:ASP:OD1	1:B:403:ARG:NH1	2.42	0.52
1:A:491:PHE:CD2	1:A:736:LEU:HD13	2.44	0.52
1:A:264:MET:HB3	1:A:426:ARG:NH1	2.24	0.52
1:A:411:LYS:O	1:A:411:LYS:HG2	2.08	0.52
1:B:7:ARG:NH2	1:B:7:ARG:HB2	2.23	0.52
1:B:542:LYS:O	1:B:543:LYS:HG3	2.09	0.52
1:B:399:ASP:CG	1:B:403:ARG:NH1	2.63	0.52
1:A:98:VAL:CG2	1:A:265:ALA:HB2	2.40	0.52
1:A:348:PHE:CE1	1:A:367:ALA:HB2	2.45	0.52
1:A:630:GLY:HA3	1:A:659:PHE:CZ	2.45	0.52
1:B:7:ARG:NH2	1:B:7:ARG:CB	2.73	0.52
1:A:335:THR:O	1:A:336:LYS:CD	2.53	0.52
1:A:339:MET:HE1	1:A:409:PRO:HB3	1.89	0.52
1:B:639:TYR:O	1:B:641:GLY:N	2.43	0.52
1:A:73:TRP:CH2	1:A:130:LEU:HD12	2.44	0.52
1:B:602:THR:HG22	1:B:604:ARG:N	2.24	0.52
1:A:193:ASP:C	1:A:195:TYR:H	2.14	0.51
1:A:366:ASN:O	1:A:367:ALA:CB	2.57	0.51
1:A:369:PRO:HB3	1:A:381:LYS:CA	2.40	0.51
1:A:492:ARG:O	1:A:492:ARG:HG2	2.10	0.51
1:B:432:THR:OG1	1:B:739:PHE:HB2	2.10	0.51
1:A:328:VAL:HG13	1:A:384:THR:HG23	1.91	0.51
1:A:633:ARG:HD2	1:A:644:TYR:O	2.11	0.51
1:B:261:PHE:CD2	1:B:271:THR:HG23	2.45	0.51
1:A:448:ASP:OD2	1:A:497:ARG:NH1	2.43	0.51
1:A:408:ASN:C	1:A:410:ASP:H	2.14	0.51
1:B:559:GLU:O	1:B:561:ALA:N	2.43	0.51
1:A:7:ARG:CG	1:A:7:ARG:NH2	2.73	0.50
1:A:276:ALA:HA	1:A:341:TYR:CE1	2.46	0.50
1:A:315:GLN:HB2	1:A:320:ASP:OD2	2.11	0.50
1:A:371:ILE:HD13	1:A:383:PRO:HA	1.93	0.50
1:B:694:THR:CG2	4:B:901:HOH:O	2.58	0.50
1:A:193:ASP:CG	1:A:604:ARG:HH22	2.14	0.50
1:A:313:PHE:HB3	1:A:322:ILE:CD1	2.41	0.50
1:B:66:LEU:HD22	1:B:134:ILE:HD12	1.94	0.50
1:A:311:ASN:ND2	1:A:322:ILE:CB	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:THR:O	1:B:650:THR:OG1	2.29	0.50
1:A:8:LYS:HA	1:A:15:GLY:H	1.77	0.50
1:A:258:ARG:NH2	1:A:398:TYR:CE1	2.79	0.50
1:A:458:ILE:HA	1:A:542:LYS:NZ	2.25	0.50
1:B:730:TRP:O	1:B:734:MET:HG2	2.11	0.50
1:A:25:GLN:NE2	1:B:298:GLU:OE1	2.41	0.50
1:B:388:THR:O	1:B:391:ALA:HB3	2.12	0.50
1:A:225:LEU:HD11	1:A:231:SER:O	2.12	0.50
1:A:225:LEU:O	1:A:263:ARG:NH2	2.44	0.50
1:A:398:TYR:O	1:A:399:ASP:C	2.50	0.50
1:A:542:LYS:O	1:A:543:LYS:HG2	2.11	0.50
1:A:386:LEU:O	1:A:388:THR:N	2.45	0.49
1:A:363:VAL:HG12	1:A:364:ALA:N	2.27	0.49
1:B:120:ASP:HB2	1:B:236:LEU:HA	1.95	0.49
1:A:194:ARG:O	1:A:225:LEU:HA	2.13	0.49
1:A:457:ILE:C	1:A:542:LYS:HZ2	2.15	0.49
1:B:371:ILE:O	1:B:380:LYS:HD3	2.13	0.49
1:B:447:GLU:O	1:B:448:ASP:HB2	2.13	0.49
1:B:45:PHE:CZ	1:B:140:ASN:ND2	2.81	0.48
1:B:431:ARG:NH1	1:B:447:GLU:OE1	2.45	0.48
1:B:535:PHE:O	1:B:536:ASN:C	2.46	0.48
1:A:339:MET:O	1:A:339:MET:HG3	2.13	0.48
1:B:98:VAL:CG2	1:B:265:ALA:HB2	2.44	0.48
1:A:73:TRP:HB3	1:B:684:ARG:HD3	1.95	0.48
1:A:552:LEU:HD12	1:A:555:VAL:CG2	2.43	0.48
1:B:51:PHE:CE1	1:B:54:LEU:HD22	2.47	0.48
1:B:430:PRO:O	1:B:431:ARG:C	2.51	0.48
1:B:542:LYS:O	1:B:543:LYS:CG	2.62	0.48
1:A:285:HIS:O	1:A:323:THR:N	2.33	0.48
1:A:244:PRO:C	1:A:246:GLY:H	2.16	0.48
1:A:353:THR:HG21	1:A:363:VAL:HG21	1.96	0.47
1:A:644:TYR:N	1:A:644:TYR:CD1	2.79	0.47
1:B:132:TRP:CZ2	1:B:136:GLN:HG3	2.49	0.47
1:A:290:THR:C	1:A:292:HIS:N	2.67	0.47
1:A:239:VAL:CG2	1:A:240:ASN:N	2.70	0.47
1:B:67:MET:HB3	1:B:80:HIS:CE1	2.50	0.47
1:A:683:ASP:O	1:A:687:HIS:HA	2.14	0.47
1:B:110:GLN:HG2	1:B:128:ARG:NH1	2.29	0.47
1:B:694:THR:CG2	1:B:695:ARG:N	2.78	0.47
1:A:75:PRO:HD3	1:A:317:LYS:HD2	1.96	0.47
1:A:184:ALA:O	1:A:185:GLU:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:THR:CG2	2:A:801:HEM:HAA1	2.43	0.47
1:A:369:PRO:HB3	1:A:380:LYS:O	2.13	0.47
1:A:369:PRO:HB2	1:A:380:LYS:HB2	1.97	0.47
1:A:639:TYR:C	1:A:641:GLY:N	2.53	0.47
1:B:454:ASP:OD1	1:B:454:ASP:N	2.41	0.47
1:B:457:ILE:CG2	1:B:458:ILE:N	2.77	0.47
1:A:122:VAL:HG22	1:A:309:TRP:CE2	2.50	0.47
1:A:633:ARG:HG3	1:A:645:GLY:C	2.35	0.47
1:B:98:VAL:HG21	1:B:265:ALA:HB2	1.97	0.47
1:B:225:LEU:O	1:B:263:ARG:NH2	2.47	0.47
1:B:639:TYR:C	1:B:640:ASP:CG	2.71	0.47
1:A:126:LYS:O	1:A:130:LEU:HD13	2.15	0.46
1:B:345:LEU:HD13	1:B:385:MET:HE2	1.97	0.46
1:A:283:LYS:HZ1	1:A:374:ALA:HB3	1.80	0.46
1:A:633:ARG:NH1	1:A:697:ASP:OD2	2.48	0.46
1:A:633:ARG:CG	1:A:645:GLY:O	2.64	0.46
1:B:63:LEU:HD23	1:B:134:ILE:HD13	1.97	0.46
1:A:232:SER:O	1:A:233:HIS:CD2	2.68	0.46
1:A:636:GLU:C	1:A:638:ASN:H	2.18	0.46
1:A:348:PHE:HE1	1:A:366:ASN:O	1.98	0.46
1:A:346:TYR:C	1:A:347:LYS:HG2	2.36	0.46
1:B:7:ARG:CG	1:B:7:ARG:NH2	2.72	0.46
1:B:393:ARG:HG2	1:B:394:MET:CE	2.46	0.46
1:A:90:TRP:HZ3	1:A:238:TYR:HH	1.58	0.45
1:A:264:MET:O	1:A:265:ALA:HB3	2.16	0.45
1:A:361:GLN:C	1:A:362:TRP:HD1	2.19	0.45
1:B:443:ILE:HG23	1:B:447:GLU:OE2	2.16	0.45
1:A:296:GLU:HB2	1:A:297:PRO:HD2	1.97	0.45
1:A:408:ASN:O	1:A:410:ASP:N	2.42	0.45
1:A:551:VAL:HG13	1:A:734:MET:SD	2.56	0.45
1:A:639:TYR:CD1	1:A:640:ASP:N	2.85	0.45
1:A:194:ARG:HH22	1:A:231:SER:CB	2.29	0.45
1:A:581:ASP:HB3	1:A:584:SER:HB2	1.98	0.45
1:A:346:TYR:O	1:A:347:LYS:HG2	2.15	0.45
1:A:290:THR:C	1:A:292:HIS:H	2.20	0.45
1:A:707:ARG:O	1:A:711:GLU:HG3	2.16	0.45
1:A:606:ARG:NH2	1:A:606:ARG:HG3	2.31	0.45
1:B:685:LYS:HD2	1:B:685:LYS:HA	1.63	0.45
1:A:447:GLU:O	1:A:448:ASP:HB2	2.17	0.45
1:B:283:LYS:HG3	1:B:284:THR:O	2.17	0.45
1:B:639:TYR:C	1:B:641:GLY:H	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:HD13	1:B:385:MET:CE	2.47	0.45
1:B:686:THR:O	1:B:687:HIS:CB	2.65	0.45
1:A:41:LEU:HD13	1:A:45:PHE:CE2	2.52	0.44
1:A:284:THR:OG1	1:A:326:LEU:O	2.19	0.44
1:B:683:ASP:O	1:B:687:HIS:N	2.46	0.44
1:A:132:TRP:HB3	1:A:133:PRO:HD3	1.98	0.44
1:B:353:THR:HG22	1:B:363:VAL:HG23	2.00	0.44
1:A:371:ILE:HG12	1:A:381:LYS:O	2.18	0.44
1:A:339:MET:HE3	1:A:409:PRO:HB3	1.99	0.44
1:A:633:ARG:HA	1:A:633:ARG:HD3	1.64	0.44
1:B:279:HIS:CE1	2:B:801:HEM:C4B	3.06	0.44
1:A:147:LEU:O	1:A:147:LEU:HG	2.17	0.44
1:A:353:THR:HG21	1:A:363:VAL:HG22	1.97	0.44
1:A:395:ASP:O	1:A:399:ASP:HB2	2.17	0.44
1:B:494:SER:OG	1:B:617:LEU:HD22	2.17	0.44
1:B:542:LYS:C	1:B:543:LYS:CG	2.84	0.44
1:A:98:VAL:HG21	1:A:265:ALA:HB2	1.98	0.44
1:A:363:VAL:HG12	1:A:364:ALA:H	1.82	0.44
1:A:644:TYR:N	1:A:644:TYR:HD1	2.16	0.44
1:A:361:GLN:C	1:A:362:TRP:CD1	2.91	0.43
1:B:602:THR:HG22	1:B:603:LYS:N	2.33	0.43
1:B:667:THR:O	1:B:684:ARG:NH2	2.51	0.43
1:B:672:ALA:HB2	1:B:680:ILE:CG1	2.46	0.43
1:B:10:ASN:OD1	1:B:10:ASN:N	2.51	0.43
1:A:279:HIS:CE1	2:A:801:HEM:CHC	3.01	0.43
1:A:608:GLU:CB	1:A:699:ILE:HD13	2.49	0.43
1:A:48:ALA:O	1:A:52:LYS:HE3	2.17	0.43
1:A:254:ALA:HB1	1:A:395:ASP:OD1	2.18	0.43
1:A:400:LYS:O	1:A:403:ARG:N	2.49	0.43
1:A:364:ALA:C	1:A:366:ASN:N	2.71	0.43
1:B:274:LEU:C	2:B:801:HEM:HMC3	2.39	0.43
1:A:311:ASN:HD21	1:A:322:ILE:HG13	1.81	0.43
1:A:519:SER:O	1:A:522:ARG:HG2	2.18	0.43
1:B:351:GLU:HG2	1:B:352:PRO:HD2	2.00	0.43
2:B:801:HEM:HMB1	2:B:801:HEM:CBB	2.47	0.43
1:A:362:TRP:N	1:A:362:TRP:HD1	2.16	0.43
1:A:396:PRO:O	1:A:399:ASP:CB	2.66	0.43
1:B:122:VAL:HG22	1:B:309:TRP:CE2	2.54	0.43
1:B:639:TYR:CE1	1:B:640:ASP:OD2	2.72	0.43
1:A:439:VAL:HA	1:A:440:PRO:HD2	1.87	0.43
1:A:11:VAL:HG13	1:A:12:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:MET:CE	1:A:389:ASP:HB2	2.38	0.43
1:A:386:LEU:HB2	1:A:389:ASP:OD2	2.19	0.43
1:A:638:ASN:O	1:A:639:TYR:C	2.54	0.43
1:A:191:ASN:O	1:A:193:ASP:N	2.50	0.42
1:A:283:LYS:HE2	1:A:374:ALA:HB2	2.01	0.42
1:A:287:ALA:O	1:A:313:PHE:CE2	2.72	0.42
1:A:620:LEU:HA	1:A:624:GLU:OE2	2.19	0.42
1:A:7:ARG:CG	1:A:8:LYS:N	2.82	0.42
1:A:188:TRP:C	1:A:190:GLY:N	2.73	0.42
1:A:388:THR:O	1:A:391:ALA:HB3	2.19	0.42
1:A:511:ASN:OD1	1:A:512:GLU:N	2.52	0.42
1:B:41:LEU:HD13	1:B:45:PHE:CD2	2.54	0.42
1:A:479:LYS:O	1:A:480:LEU:C	2.57	0.42
1:A:244:PRO:C	1:A:246:GLY:N	2.70	0.42
1:B:594:GLY:O	1:B:633:ARG:NH2	2.48	0.42
1:A:149:LEU:HD23	1:A:424:LEU:HB3	2.00	0.42
1:A:248:PRO:HG3	1:A:360:ASN:CB	2.46	0.42
1:A:527:ALA:O	1:A:531:VAL:HG23	2.19	0.42
1:A:264:MET:O	1:A:426:ARG:NH1	2.53	0.42
1:B:223:ARG:H	1:B:223:ARG:HG2	1.70	0.42
1:B:503:ALA:HA	4:B:905:HOH:O	2.18	0.42
1:A:679:PHE:CE2	1:B:303:GLU:HG3	2.55	0.42
1:A:401:ILE:CG2	1:A:405:TYR:CE2	3.02	0.42
1:B:638:ASN:OD1	4:B:903:HOH:O	2.21	0.42
1:A:606:ARG:HG3	1:A:606:ARG:HH21	1.85	0.42
1:A:663:LEU:HD12	1:A:714:ALA:CB	2.50	0.42
1:B:430:PRO:O	1:B:432:THR:N	2.53	0.42
1:B:431:ARG:O	1:B:432:THR:C	2.55	0.42
1:A:275:ILE:CD1	2:A:801:HEM:HHC	2.48	0.42
1:A:535:PHE:CD1	1:A:535:PHE:O	2.73	0.42
1:A:501:ASN:HB2	1:A:737:ASP:OD2	2.21	0.41
1:A:240:ASN:OD1	1:A:241:PRO:CD	2.68	0.41
1:A:597:SER:CB	1:A:638:ASN:ND2	2.82	0.41
2:A:801:HEM:HMC2	2:A:801:HEM:CBC	2.45	0.41
1:B:331:THR:OG1	1:B:332:PRO:N	2.53	0.41
1:A:694:THR:O	1:A:697:ASP:HB2	2.19	0.41
1:B:697:ASP:OD1	1:B:697:ASP:N	2.51	0.41
1:B:322:ILE:HD13	1:B:322:ILE:HG21	1.84	0.41
1:B:395:ASP:O	1:B:399:ASP:CB	2.67	0.41
1:A:431:ARG:NH1	1:A:447:GLU:OE1	2.49	0.41
1:A:126:LYS:HG3	1:A:307:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:HH22	1:A:231:SER:HB2	1.86	0.41
1:A:365:LYS:O	1:A:366:ASN:CB	2.67	0.41
1:A:537:ASP:C	1:A:539:SER:N	2.68	0.41
1:A:610:PHE:O	1:A:613:ASP:HB3	2.20	0.41
1:A:672:ALA:O	1:A:673:ASP:HB3	2.20	0.41
1:B:275:ILE:CD1	2:B:801:HEM:HHC	2.51	0.41
1:A:40:PRO:HG3	1:B:709:LEU:CD2	2.49	0.41
1:A:353:THR:HG22	1:A:363:VAL:CG2	2.39	0.41
1:A:622:ALA:HB3	1:A:623:PRO:HD3	2.03	0.41
1:B:289:PRO:HD2	1:B:292:HIS:CD2	2.56	0.41
1:B:567:PRO:HB2	1:B:731:HIS:CE1	2.56	0.41
1:B:658:TYR:OH	1:B:697:ASP:HB3	2.21	0.41
1:B:667:THR:HG22	1:B:668:ALA:N	2.36	0.41
1:A:365:LYS:O	1:A:366:ASN:HB3	2.20	0.41
1:A:367:ALA:O	1:A:382:LEU:HG	2.20	0.41
1:A:598:TYR:CD1	1:A:639:TYR:CE2	3.05	0.41
1:A:246:GLY:O	1:A:360:ASN:ND2	2.54	0.40
1:A:423:LEU:O	1:A:426:ARG:HG2	2.21	0.40
1:A:14:GLY:O	1:B:181:TYR:HD1	2.05	0.40
1:A:535:PHE:CD1	1:A:535:PHE:C	2.95	0.40
1:A:668:ALA:O	1:A:681:GLY:HA2	2.21	0.40
1:B:491:PHE:CG	1:B:492:ARG:N	2.90	0.40
1:B:634:VAL:HG12	1:B:653:LYS:O	2.21	0.40
1:B:395:ASP:HB3	1:B:398:TYR:HB2	2.03	0.40
1:A:367:ALA:O	1:A:368:GLU:C	2.59	0.40
1:A:391:ALA:O	1:A:395:ASP:HB2	2.21	0.40
1:A:397:ALA:O	1:A:398:TYR:C	2.57	0.40
1:A:399:ASP:O	1:A:402:CYS:HB2	2.22	0.40
1:B:101:GLY:C	1:B:494:SER:HB3	2.42	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)
1:A:687:HIS:ND1	1:B:582:VAL:CG1[2_465]	2.06	0.14

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	707/768 (92%)	637 (90%)	52 (7%)	18 (2%)	5	21
1	B	707/768 (92%)	655 (93%)	38 (5%)	14 (2%)	7	27
All	All	1414/1536 (92%)	1292 (91%)	90 (6%)	32 (2%)	6	23

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	10	ASN
1	A	245	ASP
1	A	365	LYS
1	A	538	SER
1	B	8	LYS
1	B	10	ASN
1	B	534	LYS
1	B	536	ASN
1	A	185	GLU
1	A	192	GLU
1	A	291	HIS
1	A	366	ASN
1	A	637	ALA
1	A	640	ASP
1	B	560	GLN
1	A	367	ALA
1	A	387	THR
1	B	369	PRO
1	B	431	ARG
1	B	601	GLY
1	A	191	ASN
1	A	494	SER
1	A	581	ASP
1	B	244	PRO

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Mol	Chain	Res	Type
1	B	296	GLU
1	B	366	ASN
1	B	535	PHE
1	B	517	ASP
1	A	396	PRO
1	A	244	PRO
1	B	372	PRO

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	576/622 (93%)	546 (95%)	30 (5%)	23	55
1	B	576/622 (93%)	542 (94%)	34 (6%)	19	49
All	All	1152/1244 (93%)	1088 (94%)	64 (6%)	21	52

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	LYS
1	A	65	LYS
1	A	97	ARG
1	A	120	ASP
1	A	153	ASN
1	A	280	SER
1	A	295	LYS
1	A	326	LEU
1	A	332	PRO
1	A	336	LYS
1	A	366	ASN
1	A	400	LYS
1	A	402	CYS
1	A	432	THR
1	A	505	ILE

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Mol	Chain	Res	Type
1	A	512	GLU
1	A	532	GLN
1	A	537	ASP
1	A	538	SER
1	A	539	SER
1	A	540	SER
1	A	629	ILE
1	A	633	ARG
1	A	639	TYR
1	A	649	LYS
1	A	673	ASP
1	A	717	ASP
1	A	719	GLU
1	A	720	GLU
1	B	7	ARG
1	B	8	LYS
1	B	9	SER
1	B	17	ARG
1	B	64	THR
1	B	97	ARG
1	B	172	ASP
1	B	173	THR
1	B	194	ARG
1	B	227	SER
1	B	255	LYS
1	B	284	THR
1	B	347	LYS
1	B	349	ASP
1	B	384	THR
1	B	393	ARG
1	B	428	MET
1	B	441	SER
1	B	447	GLU
1	B	479	LYS
1	B	496	LYS
1	B	512	GLU
1	B	534	LYS
1	B	545	SER
1	B	574	ASP
1	B	582	VAL
1	B	600	LYS
1	B	602	THR

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Mol	Chain	Res	Type
1	B	639	TYR
1	B	653	LYS
1	B	665	THR
1	B	674	ASN
1	B	687	HIS
1	B	697	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	191	ASN
1	A	226	GLN
1	A	233	HIS
1	A	305	GLN
1	A	378	ASN
1	A	638	ASN
1	B	33	GLN
1	B	226	GLN
1	B	292	HIS
1	B	532	GLN
1	B	609	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	801	1	41,50,50	1.35	6 (14%)	45,82,82	1.74	8 (17%)
2	HEM	B	801	1	41,50,50	1.37	6 (14%)	45,82,82	1.72	9 (20%)

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	801	1	-	2/12/54/54	-
2	HEM	B	801	1	-	2/12/54/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C1B-NB	-3.79	1.33	1.40
2	B	801	HEM	C1B-NB	-3.73	1.33	1.40
2	B	801	HEM	C4D-ND	-3.49	1.34	1.40
2	A	801	HEM	C4D-ND	-3.20	1.34	1.40
2	A	801	HEM	C4B-NB	-2.96	1.32	1.38
2	B	801	HEM	C4B-NB	-2.37	1.33	1.38
2	A	801	HEM	CHB-C1B	2.36	1.41	1.35
2	A	801	HEM	FE-NB	2.30	2.08	1.96
2	A	801	HEM	O2A-CGA	-2.20	1.23	1.30
2	B	801	HEM	CHB-C1B	2.18	1.40	1.35
2	B	801	HEM	C3B-C4B	2.16	1.49	1.44
2	B	801	HEM	FE-NB	2.12	2.07	1.96

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HEM	C1B-NB-C4B	6.25	111.52	105.07
2	B	801	HEM	C1B-NB-C4B	5.54	110.79	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	HEM	CHC-C4B-NB	4.55	129.37	124.43
2	A	801	HEM	CHC-C4B-NB	4.47	129.29	124.43
2	A	801	HEM	CHD-C1D-ND	3.72	128.47	124.43
2	B	801	HEM	CHD-C1D-ND	3.64	128.39	124.43
2	A	801	HEM	CHA-C4D-ND	2.86	127.92	124.38
2	A	801	HEM	CHB-C1B-NB	2.66	127.67	124.38
2	B	801	HEM	CHA-C4D-ND	2.66	127.67	124.38
2	B	801	HEM	CHD-C1D-C2D	-2.45	121.15	124.98
2	B	801	HEM	CHA-C4D-C3D	-2.44	120.74	125.33
2	B	801	HEM	CHB-C1B-NB	2.37	127.31	124.38
2	A	801	HEM	CHD-C1D-C2D	-2.34	121.33	124.98
2	A	801	HEM	CHA-C4D-C3D	-2.24	121.13	125.33
2	B	801	HEM	CAD-C3D-C4D	2.19	128.48	124.66
2	A	801	HEM	O2D-CGD-O1D	-2.11	118.03	123.30
2	B	801	HEM	O2D-CGD-CBD	2.08	120.70	114.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

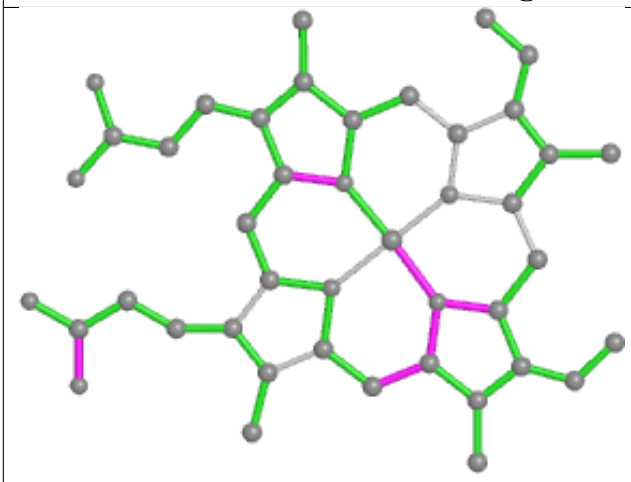
2 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	15	0
2	B	801	HEM	13	0

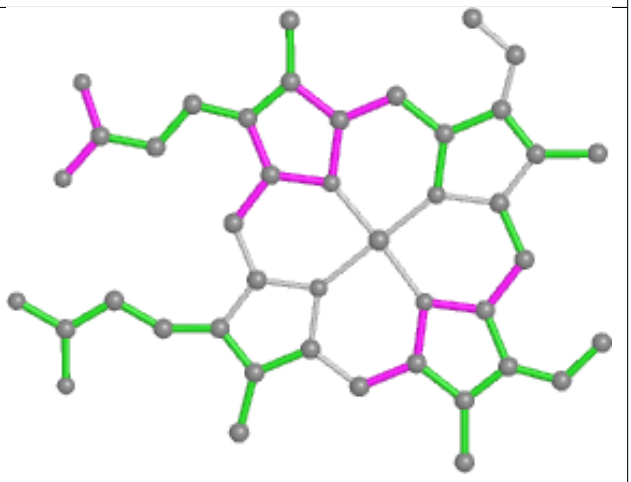
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

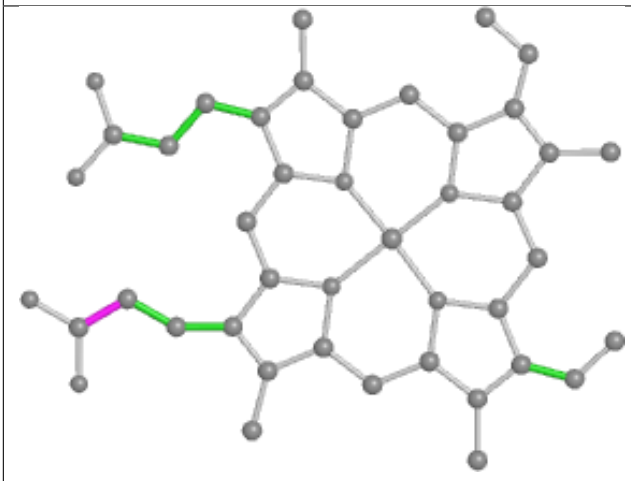
Ligand HEM A 801



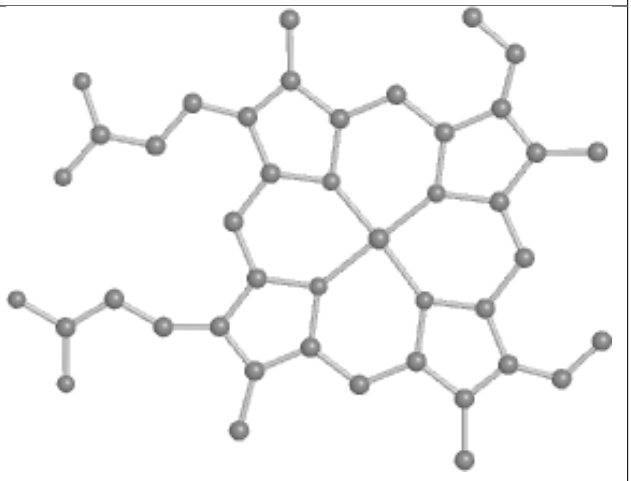
Bond lengths



Bond angles

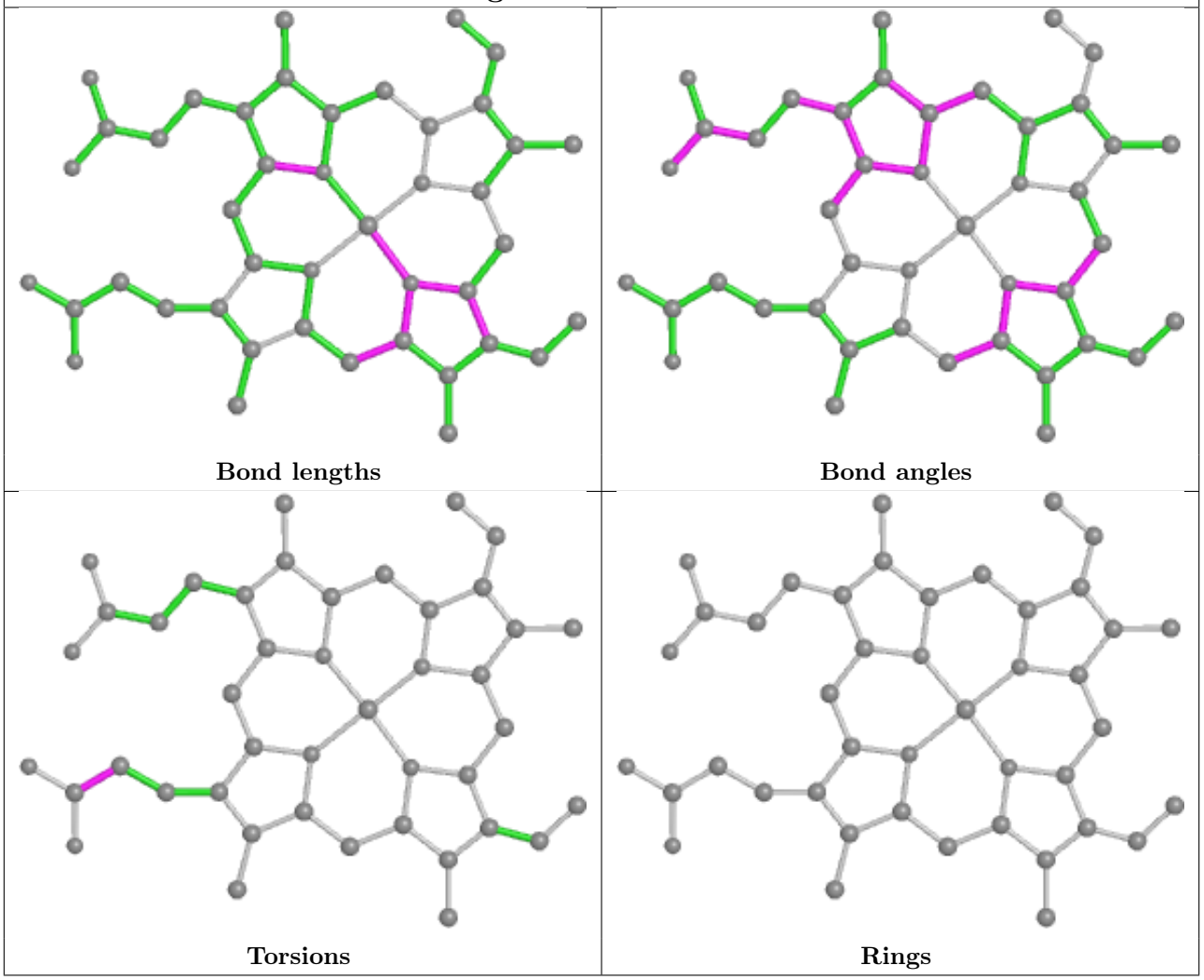


Torsions



Rings

Ligand HEM B 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	711/768 (92%)	0.18	24 (3%) 45 40	26, 45, 75, 101	0
1	B	711/768 (92%)	0.05	9 (1%) 77 77	24, 42, 63, 87	0
All	All	1422/1536 (92%)	0.12	33 (2%) 60 58	24, 43, 70, 101	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	VAL	5.5
1	A	369	PRO	3.7
1	A	356	PRO	3.5
1	A	348	PHE	3.2
1	A	375	TYR	3.0
1	A	357	ALA	3.0
1	B	474	GLY	2.9
1	A	349	ASP	2.8
1	A	381	LYS	2.7
1	A	355	SER	2.7
1	B	674	ASN	2.6
1	B	640	ASP	2.5
1	A	365	LYS	2.5
1	A	378	ASN	2.4
1	A	392	LEU	2.4
1	B	657	ASP	2.4
1	A	351	GLU	2.3
1	A	376	ASP	2.3
1	A	385	MET	2.3
1	A	383	PRO	2.3
1	A	344	TYR	2.2
1	A	675	GLU	2.2
1	A	366	ASN	2.2
1	A	353	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	409	PRO	2.1
1	A	364	ALA	2.1
1	A	358	GLY	2.1
1	B	480	LEU	2.1
1	B	476	ALA	2.1
1	A	221	HIS	2.1
1	B	475	VAL	2.0
1	B	658	TYR	2.0
1	A	347	LYS	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)

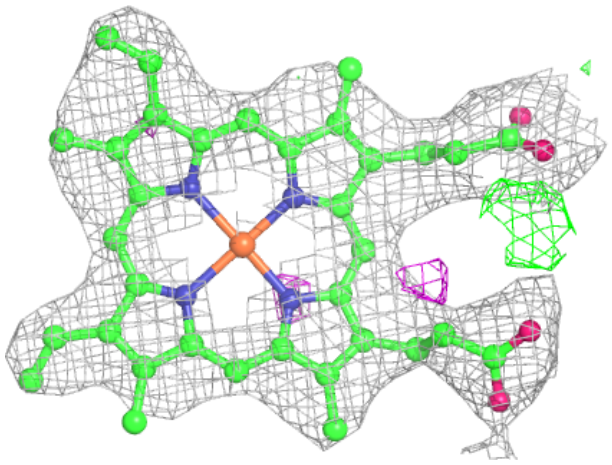
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

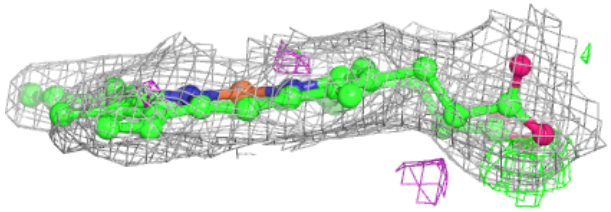
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	A	802	1/1	0.93	0.17	59,59,59,59	0
2	HEM	B	801	43/43	0.94	0.18	30,41,44,46	0
2	HEM	A	801	43/43	0.95	0.17	40,45,52,59	0
3	K	B	802	1/1	0.95	0.20	49,49,49,49	0

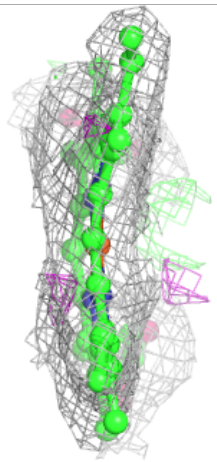
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM B 801:

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

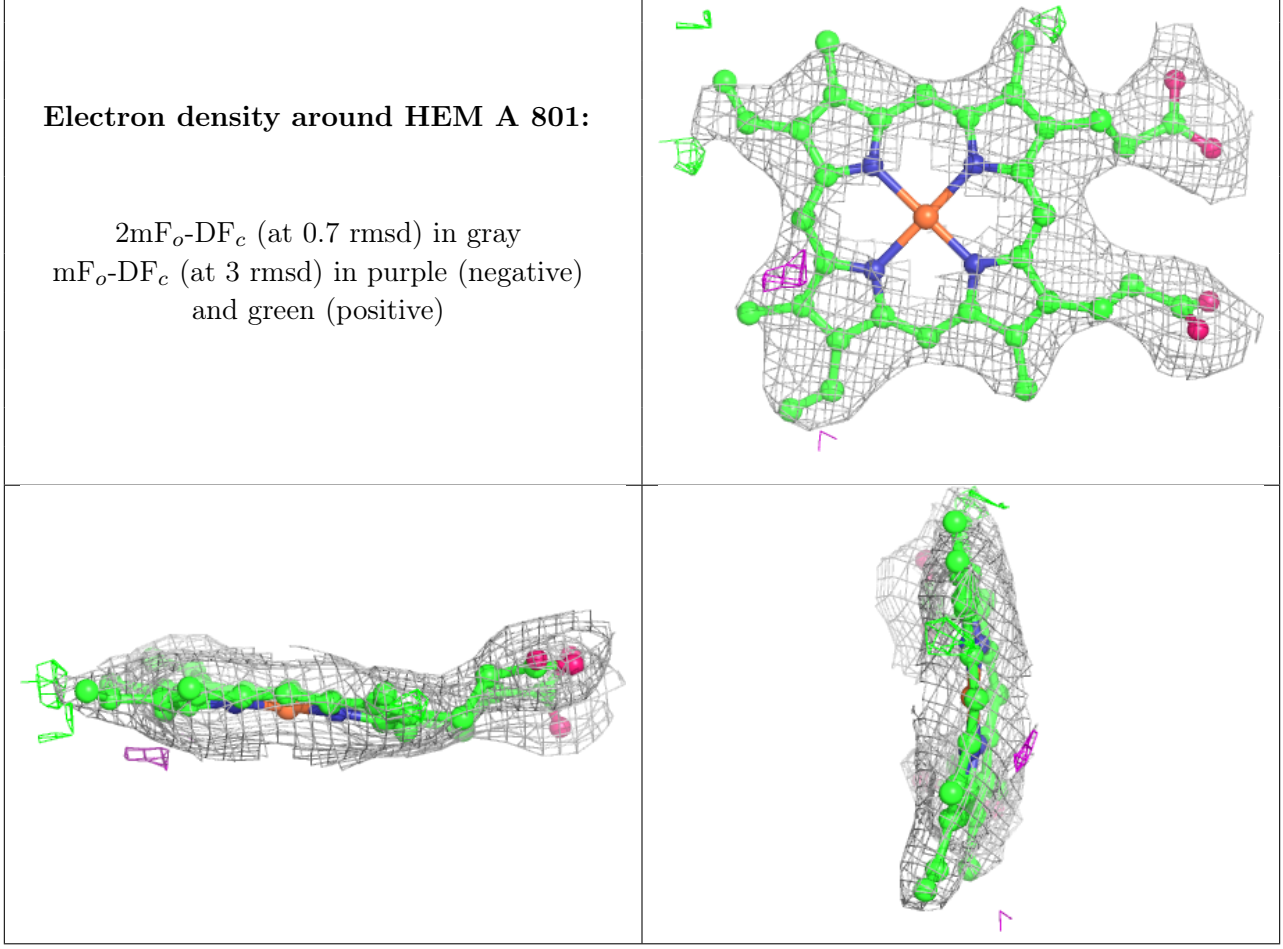






Electron density around HEM A 801:

$2mF_o$-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

There are no such residues in this entry.