Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 10:32 AM EST

PDB ID	:	5WHS
Title	:	Crystal structure of the catalase-peroxidase from Neurospora crassa at 2.6 A
Authors	:	Diaz-Vilchis, A.; Vega-Garcia, V.; Rudino-Pinera, E.; Hansberg, W.
Deposited on	:	2017-07-18
Resolution	:	2.60 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

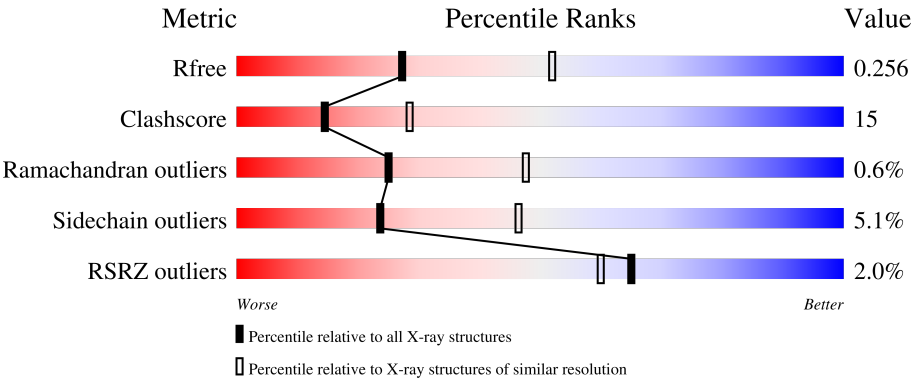
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	2% 67% 23% 7%
1	B	768	% 66% 23% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11962 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	713	Total 5597	C 3555	N 977	O 1053	S 12	0	0	0
1	B	713	Total 5597	C 3555	N 977	O 1053	S 12	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	expression tag	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
A	2	SER	-	expression tag	UNP Q8X182
A	3	GLU	-	expression tag	UNP Q8X182
A	4	CYS	-	expression tag	UNP Q8X182
A	5	PRO	-	expression tag	UNP Q8X182
A	6	VAL	-	expression tag	UNP Q8X182
A	742	LYS	-	expression tag	UNP Q8X182
A	743	GLN	-	expression tag	UNP Q8X182
A	744	GLU	-	expression tag	UNP Q8X182
A	745	GLY	-	expression tag	UNP Q8X182

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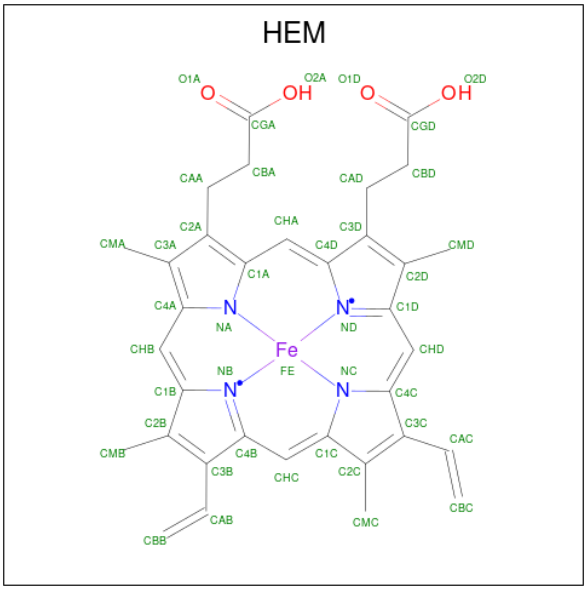
Chain	Residue	Modelled	Actual	Comment	Reference
A	746	ARG	-	expression tag	UNP Q8X182
A	747	GLY	-	expression tag	UNP Q8X182
A	748	GLN	-	expression tag	UNP Q8X182
A	749	ASN	-	expression tag	UNP Q8X182
A	750	ALA	-	expression tag	UNP Q8X182
A	751	PRO	-	expression tag	UNP Q8X182
A	752	LYS	-	expression tag	UNP Q8X182
A	753	LEU	-	expression tag	UNP Q8X182
B	-14	MET	-	expression tag	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
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
B	2	SER	-	expression tag	UNP Q8X182
B	3	GLU	-	expression tag	UNP Q8X182
B	4	CYS	-	expression tag	UNP Q8X182
B	5	PRO	-	expression tag	UNP Q8X182
B	6	VAL	-	expression tag	UNP Q8X182
B	742	LYS	-	expression tag	UNP Q8X182
B	743	GLN	-	expression tag	UNP Q8X182
B	744	GLU	-	expression tag	UNP Q8X182
B	745	GLY	-	expression tag	UNP Q8X182
B	746	ARG	-	expression tag	UNP Q8X182
B	747	GLY	-	expression tag	UNP Q8X182
B	748	GLN	-	expression tag	UNP Q8X182
B	749	ASN	-	expression tag	UNP Q8X182
B	750	ALA	-	expression tag	UNP Q8X182
B	751	PRO	-	expression tag	UNP Q8X182
B	752	LYS	-	expression tag	UNP Q8X182
B	753	LEU	-	expression tag	UNP Q8X182

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).



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 water.

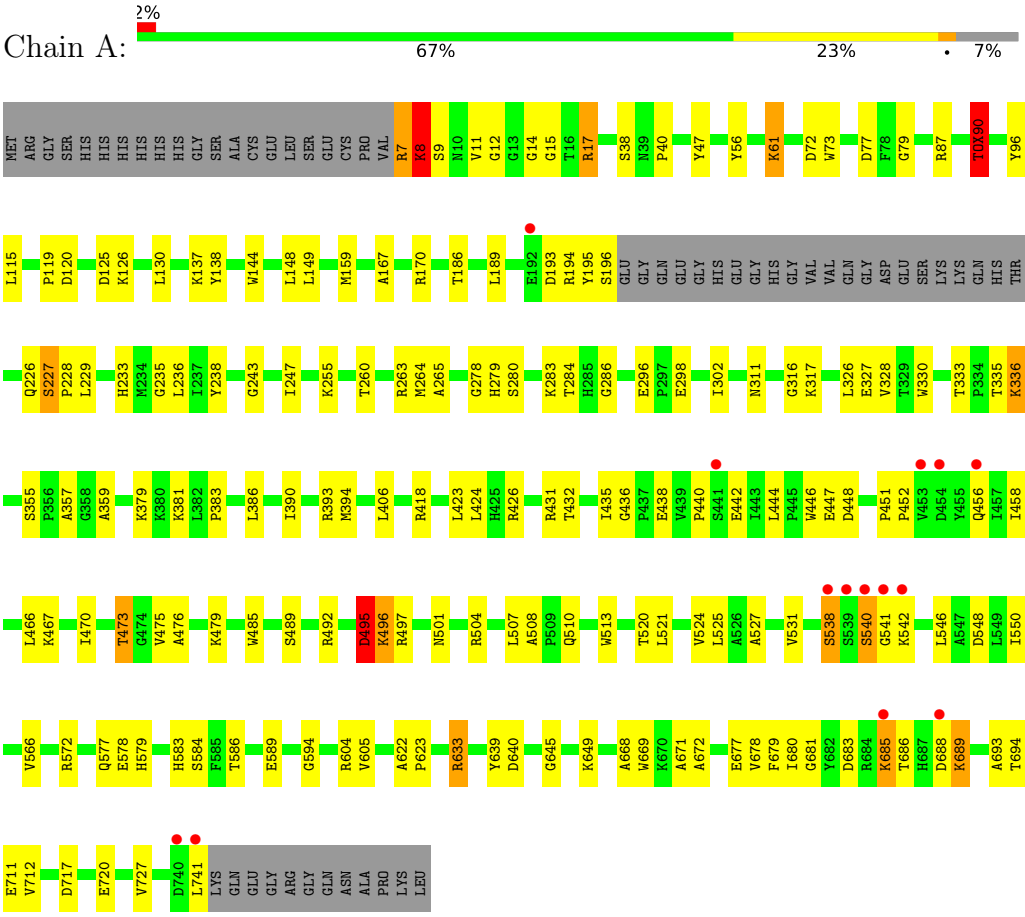
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	314	Total	O	0	0
			314	314		
3	B	368	Total	O	0	0
			368	368		

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.

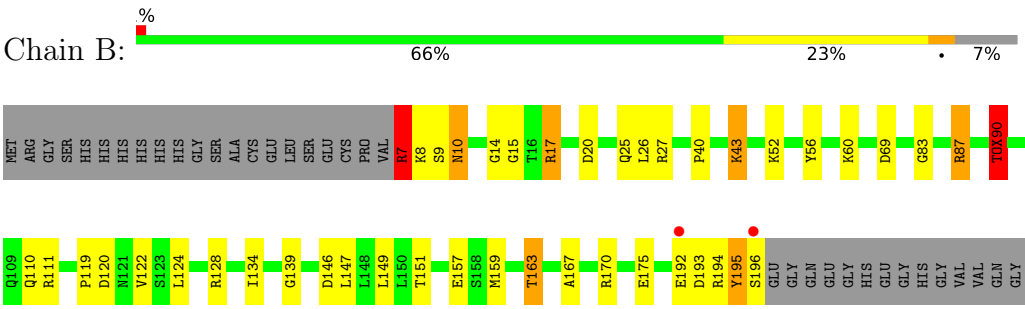
• Molecule 1: Catalase-peroxidase

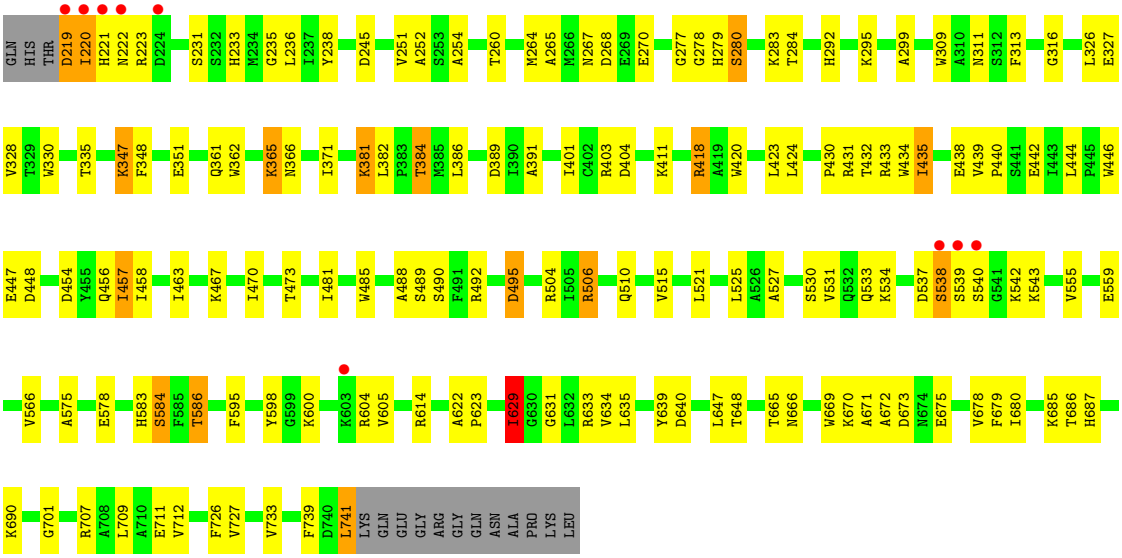
Chain A:



• Molecule 1: Catalase-peroxidase

Chain B:




GLN HIS THR D219 I220 H221 N222 R223 D224 S231 S232 H233 M234 G235 L236 I237 Y238 D245 V251 A252 S253 A254 T260 M264 A265 M266 N267 D268 E269 E270 G277 G278 H279 S280 K283 T284 H292 K295 A299 W309 A310 N311 S312 F313 G316 L326 E327
V328 T329 W330 T335 K347 F348 E351 Q361 W362 K365 N366 I371 K381 L382 P383 T384 M385 L386 D389 I390 A391 I401 C402 R403 D404 K411 R418 A419 W420 L423 L424 P430 R431 T432 R433 W434 I435 E438 V439 P440 S441 E442 I443 L444 P445 W446
E447 D448 D454 Y455 Q456 I457 I458 I463 K467 I470 T473 I481 W485 A488 S489 S490 F491 R492 D495 R504 I505 R506 Q510 V515 L521 L525 A526 A527 S530 V531 Q532 Q533 K534 D537 S538 S539 S540 G541 K542 K543 V555 E559
V566 A575 E578 H583 S584 F585 T586 F595 Y598 G599 K600 K603 R604 V605 R614 A622 P623 I629 G630 G631 L632 R633 V634 L635 Y639 D640 L647 T648 T665 N666 W669 K670 A671 A672 D673 N674 E675 V678 F679 I680 K685 T686 H687
K690 G701 R707 A708 L709 A710 E711 V712 F726 V727 V733 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	71.81Å 142.35Å 183.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.38 – 2.60 56.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (112.38-2.60) 99.9 (56.50-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.209 , 0.254 0.212 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11962	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, TOX

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	1.13	2/5734 (0.0%)	0.86	2/7791 (0.0%)
1	B	1.37	6/5734 (0.1%)	0.98	10/7791 (0.1%)
All	All	1.26	8/11468 (0.1%)	0.92	12/15582 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	GLU	CD-OE1	-6.08	1.19	1.25
1	B	195	TYR	CE1-CZ	-5.49	1.31	1.38
1	B	584	SER	CB-OG	-5.37	1.35	1.42
1	B	96	TYR	CE1-CZ	-5.17	1.31	1.38
1	A	47	TYR	CE1-CZ	-5.13	1.31	1.38
1	A	495	ASP	CB-CG	-5.12	1.41	1.51
1	B	446	TRP	CE3-CZ3	-5.07	1.29	1.38
1	B	420	TRP	CG-CD1	-5.05	1.29	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	ASP	CB-CG-OD1	6.49	124.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	629	ILE	CG1-CB-CG2	-6.19	97.78	111.40
1	B	418	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	69	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	27	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	B	673	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	673	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	10	ASN	N-CA-C	5.24	125.16	111.00
1	B	435	ILE	CG1-CB-CG2	-5.20	99.97	111.40
1	B	87	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	7	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	566	VAL	C-N-CD	5.08	139.08	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	TOX	Mainchain
1	B	90	TOX	Mainchain

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	5597	0	5411	189	0
1	B	5597	0	5411	162	0
2	A	43	0	30	5	0
2	B	43	0	30	7	0
3	A	314	0	0	12	2
3	B	368	0	0	10	2
All	All	11962	0	10882	342	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:THR:OG1	1:A:326:LEU:O	1.62	1.17
1:B:431:ARG:NH2	1:B:440:PRO:O	1.85	1.08
1:A:219:ASP:O	1:A:220:ILE:HG13	1.55	1.06
1:B:267:ASN:OD1	1:B:270:GLU:HG3	1.56	1.04
1:A:8:LYS:HA	1:A:15:GLY:H	1.21	1.01
1:B:56:TYR:OH	1:B:438:GLU:OE1	1.77	1.00
1:B:7:ARG:HH21	1:B:7:ARG:HG3	1.24	0.99
1:A:467:LYS:NZ	1:A:559:GLU:OE1	1.99	0.95
1:A:633:ARG:HG2	1:A:645:GLY:O	1.67	0.93
1:B:159:MET:HE1	1:B:335:THR:HA	1.48	0.93
1:A:555:VAL:O	1:A:559:GLU:HG3	1.70	0.91
1:B:14:GLY:O	1:B:17:ARG:NH1	2.03	0.91
1:B:284:THR:OG1	1:B:326:LEU:O	1.91	0.89
1:B:220:ILE:HG12	1:B:221:HIS:N	1.88	0.88
1:A:456:GLN:NE2	1:A:542:LYS:CE	2.38	0.87
1:A:479:LYS:HD3	1:A:520:THR:HG23	1.58	0.86
1:A:195:TYR:O	1:A:196:SER:OG	1.94	0.85
1:A:96:TYR:O	1:A:264:MET:HE2	1.78	0.84
1:A:473:THR:CG2	1:A:475:VAL:HG23	2.08	0.83
1:A:431:ARG:HD2	1:A:447:GLU:OE2	1.77	0.81
1:A:219:ASP:O	1:A:220:ILE:CG1	2.28	0.81
1:B:220:ILE:HG23	1:B:222:ASN:H	1.45	0.81
1:B:533:GLN:O	1:B:537:ASP:HB2	1.80	0.81
1:A:456:GLN:NE2	1:A:542:LYS:HE3	1.96	0.81
1:A:7:ARG:NH2	3:A:902:HOH:O	2.13	0.80
1:A:7:ARG:O	1:A:9:SER:N	2.13	0.80
1:B:159:MET:CE	1:B:335:THR:HA	2.11	0.80
1:A:72:ASP:O	1:A:317:LYS:HE3	1.81	0.80
1:A:96:TYR:O	1:A:264:MET:CE	2.31	0.79
1:A:9:SER:HB3	1:B:605:VAL:HG22	1.65	0.78
1:A:709:LEU:CD2	1:B:40:PRO:HG3	2.14	0.78
1:A:605:VAL:HG22	1:B:9:SER:HB2	1.66	0.77
1:A:473:THR:HG22	1:A:475:VAL:HG23	1.65	0.77
1:B:98:VAL:HG11	1:B:265:ALA:HB2	1.66	0.76
1:A:8:LYS:HA	1:A:15:GLY:N	2.00	0.76
1:A:672:ALA:HB3	1:A:678:VAL:HG23	1.66	0.76
1:A:14:GLY:O	1:A:17:ARG:NH1	2.17	0.76
1:B:431:ARG:HD2	1:B:447:GLU:OE2	1.86	0.75
1:B:467:LYS:NZ	1:B:559:GLU:OE1	2.19	0.74
1:A:685:LYS:HG3	1:A:686:THR:HG23	1.69	0.73
1:A:513:TRP:CE2	1:A:589:GLU:HG3	2.24	0.72
1:A:345:LEU:O	1:A:393:ARG:NH1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ILE:O	1:B:473:THR:OG1	2.05	0.72
1:B:506:ARG:NH2	1:B:575:ALA:O	2.18	0.72
1:A:467:LYS:HG2	1:A:556:ALA:HB2	1.72	0.72
1:B:220:ILE:HG23	1:B:221:HIS:H	1.55	0.72
1:A:418:ARG:NH2	1:A:442:GLU:OE2	2.23	0.71
1:B:8:LYS:HA	1:B:15:GLY:H	1.54	0.71
1:A:456:GLN:HB3	1:A:542:LYS:HG2	1.72	0.71
1:B:17:ARG:O	1:B:20:ASP:HB2	1.91	0.70
1:B:220:ILE:HG12	1:B:221:HIS:H	1.53	0.70
1:A:435:ILE:HG22	1:A:436:GLY:N	2.05	0.70
1:B:7:ARG:HG3	1:B:7:ARG:NH2	1.98	0.70
1:A:38:SER:OG	3:A:901:HOH:O	2.09	0.69
1:B:220:ILE:CG1	1:B:221:HIS:H	2.05	0.69
1:A:604:ARG:O	1:B:9:SER:HB3	1.93	0.69
1:B:98:VAL:CG1	1:B:265:ALA:HB2	2.22	0.69
1:A:504:ARG:NH1	1:A:579:HIS:O	2.27	0.68
1:B:7:ARG:HH21	1:B:7:ARG:CG	2.03	0.68
1:B:149:LEU:HD22	1:B:424:LEU:HD22	1.76	0.68
1:B:741:LEU:O	3:B:901:HOH:O	2.12	0.68
1:A:393:ARG:O	1:A:393:ARG:HG2	1.92	0.67
1:A:167:ALA:O	1:A:170:ARG:NH2	2.27	0.67
1:A:40:PRO:HG3	1:B:709:LEU:CD2	2.25	0.67
1:A:456:GLN:NE2	1:A:542:LYS:HE2	2.09	0.67
1:A:685:LYS:HG3	1:A:686:THR:CG2	2.24	0.67
2:B:800:HEM:HBC2	2:B:800:HEM:CMC	2.24	0.67
1:B:220:ILE:HG23	1:B:221:HIS:N	2.09	0.67
1:B:542:LYS:O	1:B:543:LYS:HG2	1.95	0.67
1:A:219:ASP:O	1:A:220:ILE:CB	2.42	0.66
1:A:220:ILE:HG22	1:A:221:HIS:N	2.09	0.66
1:A:467:LYS:CE	1:A:559:GLU:OE1	2.42	0.66
1:A:447:GLU:O	1:A:448:ASP:HB2	1.94	0.66
1:A:283:LYS:HE3	1:A:284:THR:O	1.95	0.65
1:A:459:ASP:O	1:A:461:ASN:N	2.30	0.65
1:B:194:ARG:NH1	1:B:231:SER:O	2.29	0.65
2:B:800:HEM:HBC2	2:B:800:HEM:HMC1	1.78	0.65
2:A:800:HEM:HBC2	2:A:800:HEM:CMC	2.27	0.65
1:B:167:ALA:O	1:B:170:ARG:NH2	2.30	0.64
1:A:520:THR:O	1:A:524:VAL:HG23	1.97	0.64
1:A:685:LYS:CG	1:A:686:THR:HG23	2.27	0.64
1:A:538:SER:C	1:A:540:SER:H	2.01	0.64
1:A:456:GLN:HE22	1:A:542:LYS:CE	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ALA:HB3	1:A:479:LYS:HG3	1.78	0.64
1:A:7:ARG:CB	1:A:7:ARG:HH21	2.10	0.64
1:A:456:GLN:HE22	1:A:542:LYS:HE3	1.60	0.63
1:A:495:ASP:O	1:A:496:LYS:HB2	1.96	0.63
1:A:485:TRP:O	1:A:489:SER:HB2	1.98	0.63
2:A:800:HEM:HBC2	2:A:800:HEM:HMC1	1.81	0.63
1:B:504:ARG:NH1	3:B:909:HOH:O	2.31	0.63
1:B:686:THR:O	1:B:687:HIS:HB2	1.97	0.63
1:A:604:ARG:O	1:B:9:SER:CB	2.46	0.62
1:B:690:LYS:HE2	3:B:1221:HOH:O	1.99	0.62
1:A:279:HIS:HB3	1:A:330:TRP:CE2	2.34	0.62
1:A:243:GLY:HA3	1:A:247:ILE:O	1.99	0.62
1:B:279:HIS:HB3	1:B:330:TRP:CE2	2.35	0.62
1:B:672:ALA:HB3	1:B:678:VAL:HG23	1.80	0.62
1:A:504:ARG:HG2	1:A:507:LEU:HD12	1.82	0.62
1:A:456:GLN:CD	1:A:542:LYS:HE3	2.20	0.61
1:B:555:VAL:O	1:B:559:GLU:HG3	2.01	0.61
1:A:546:LEU:O	1:A:550:ILE:HG13	2.00	0.60
1:A:495:ASP:HB3	1:A:497:ARG:HG3	1.84	0.60
1:A:709:LEU:HD22	1:B:40:PRO:HG3	1.82	0.60
1:A:462:ASP:O	1:A:466:LEU:HG	2.02	0.60
1:B:157:GLU:OE2	1:B:163:THR:OG1	2.19	0.60
1:A:223:ARG:NH1	3:A:909:HOH:O	2.34	0.60
1:A:594:GLY:O	1:A:633:ARG:NH2	2.28	0.59
1:A:189:LEU:O	1:A:233:HIS:ND1	2.30	0.59
1:B:481:ILE:HD13	1:B:635:LEU:HD13	1.84	0.59
1:B:600:LYS:HE3	1:B:675:GLU:OE2	2.03	0.59
1:A:220:ILE:HG22	1:A:222:ASN:H	1.68	0.59
1:A:448:ASP:OD2	1:A:497:ARG:NH1	2.36	0.58
1:A:7:ARG:HH21	1:A:7:ARG:CG	2.16	0.58
1:A:548:ASP:OD1	1:A:572:ARG:HB2	2.03	0.58
1:B:537:ASP:C	1:B:539:SER:H	2.07	0.58
1:B:220:ILE:CG1	1:B:221:HIS:N	2.56	0.58
1:A:219:ASP:C	1:A:220:ILE:HG13	2.23	0.57
1:A:284:THR:HB	2:A:800:HEM:HAA2	1.86	0.57
1:B:159:MET:HG2	1:B:335:THR:O	2.04	0.57
1:A:709:LEU:HD23	1:B:40:PRO:HG3	1.87	0.57
1:B:371:ILE:O	1:B:381:LYS:N	2.35	0.57
1:B:284:THR:HB	2:B:800:HEM:HAA2	1.87	0.57
1:A:521:LEU:O	1:A:525:LEU:HG	2.06	0.56
1:B:539:SER:O	1:B:540:SER:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:ASP:OD1	1:B:139:GLY:HA3	2.06	0.56
1:A:458:ILE:HB	1:A:462:ASP:HB2	1.87	0.56
1:A:444:LEU:CD2	3:A:953:HOH:O	2.54	0.56
1:A:444:LEU:HD22	1:A:446:TRP:HE1	1.70	0.56
1:B:17:ARG:NH1	3:B:915:HOH:O	2.38	0.56
1:A:61:LYS:HE3	3:A:915:HOH:O	2.06	0.55
1:B:25:GLN:HG3	1:B:26:LEU:N	2.21	0.55
1:A:264:MET:O	1:A:426:ARG:NH1	2.39	0.55
1:A:435:ILE:HG22	1:A:436:GLY:H	1.71	0.55
1:B:260:THR:O	1:B:264:MET:HG3	2.07	0.55
1:B:485:TRP:CZ3	1:B:733:VAL:HG11	2.41	0.55
1:A:671:ALA:HA	1:A:679:PHE:CD1	2.42	0.55
1:A:220:ILE:CG2	1:A:221:HIS:N	2.69	0.55
1:A:355:SER:C	1:A:357:ALA:H	2.10	0.55
1:A:119:PRO:HD2	1:A:235:GLY:HA3	1.89	0.54
1:A:492:ARG:NH2	1:A:495:ASP:OD2	2.40	0.54
1:B:119:PRO:HD2	1:B:235:GLY:HA3	1.89	0.54
1:A:431:ARG:NH1	1:A:447:GLU:OE1	2.40	0.54
1:A:460:ASP:HA	1:A:463:ILE:HD12	1.89	0.54
1:A:40:PRO:HG3	1:B:709:LEU:HD22	1.89	0.54
1:B:220:ILE:CG2	1:B:221:HIS:H	2.14	0.54
1:A:219:ASP:O	1:A:220:ILE:HB	2.08	0.54
1:A:485:TRP:O	1:A:489:SER:CB	2.55	0.54
1:A:649:LYS:NZ	3:A:916:HOH:O	2.40	0.54
1:A:125:ASP:OD2	1:A:126:LYS:HE3	2.08	0.53
1:A:87:ARG:HD3	3:A:903:HOH:O	2.07	0.53
1:B:403:ARG:HD2	3:B:1156:HOH:O	2.07	0.53
1:B:559:GLU:HG2	1:B:566:VAL:HG23	1.90	0.53
1:A:431:ARG:HH11	1:A:447:GLU:CD	2.12	0.53
1:A:435:ILE:CG2	1:A:436:GLY:N	2.72	0.53
1:B:96:TYR:O	1:B:264:MET:CE	2.57	0.53
1:B:431:ARG:HD2	1:B:447:GLU:CD	2.29	0.53
1:A:90:TOX:H9	1:A:238:TYR:OH	2.09	0.53
1:B:279:HIS:HB3	1:B:330:TRP:CD2	2.44	0.53
1:A:279:HIS:HB3	1:A:330:TRP:CD2	2.44	0.52
1:A:193:ASP:OD2	1:A:604:ARG:NH2	2.41	0.52
1:A:260:THR:O	1:A:264:MET:HG3	2.09	0.52
1:A:296:GLU:OE1	1:A:296:GLU:N	2.33	0.52
1:A:346:TYR:CE1	1:A:393:ARG:HG3	2.45	0.52
1:B:159:MET:HE2	1:B:335:THR:HB	1.92	0.51
1:B:583:HIS:O	1:B:586:THR:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ASP:OD1	1:A:685:LYS:HG2	2.10	0.51
1:A:479:LYS:HD3	1:A:520:THR:CG2	2.37	0.51
1:B:90:TOX:H8	1:B:423:LEU:HD21	1.93	0.51
1:B:311:ASN:ND2	1:B:316:GLY:HA2	2.25	0.51
1:A:233:HIS:HB2	1:A:236:LEU:HD12	1.92	0.51
1:B:521:LEU:O	1:B:525:LEU:HG	2.10	0.51
1:B:146:ASP:OD1	1:B:170:ARG:HB2	2.11	0.51
1:A:326:LEU:HD23	1:A:359:ALA:HB3	1.93	0.50
1:A:633:ARG:HG2	1:A:645:GLY:C	2.30	0.50
1:B:195:TYR:O	1:B:196:SER:OG	2.21	0.50
1:B:431:ARG:CD	1:B:447:GLU:OE2	2.57	0.50
1:B:488:ALA:C	1:B:490:SER:H	2.13	0.50
1:A:311:ASN:ND2	1:A:316:GLY:HA2	2.27	0.50
1:A:677:GLU:O	1:A:694:THR:HA	2.12	0.50
1:B:90:TOX:H9	1:B:238:TYR:OH	2.12	0.50
1:B:454:ASP:OD1	1:B:454:ASP:N	2.43	0.50
1:A:459:ASP:O	1:A:462:ASP:N	2.41	0.50
1:B:527:ALA:O	1:B:531:VAL:HG23	2.11	0.49
1:A:40:PRO:HG2	1:B:712:VAL:HG21	1.94	0.49
1:B:510:GLN:NE2	3:B:917:HOH:O	2.45	0.49
1:B:542:LYS:C	1:B:543:LYS:HG2	2.32	0.49
1:B:634:VAL:HG12	1:B:648:THR:HB	1.94	0.49
1:A:7:ARG:NH2	1:A:7:ARG:CG	2.74	0.49
1:A:194:ARG:CZ	1:A:229:LEU:HD13	2.43	0.49
1:B:254:ALA:HB2	1:B:391:ALA:HB1	1.94	0.49
1:B:277:GLY:O	1:B:280:SER:HB2	2.12	0.49
1:A:98:VAL:CG1	1:A:265:ALA:HB2	2.43	0.49
1:A:444:LEU:HD22	3:A:953:HOH:O	2.12	0.49
1:B:110:GLN:HG2	1:B:128:ARG:NH1	2.28	0.49
1:B:278:GLY:C	1:B:280:SER:H	2.15	0.49
1:A:501:ASN:HA	1:A:572:ARG:HG2	1.95	0.49
1:A:513:TRP:CD2	1:A:589:GLU:HG3	2.48	0.48
1:B:403:ARG:CD	3:B:1156:HOH:O	2.61	0.48
1:A:527:ALA:O	1:A:531:VAL:HG23	2.12	0.48
1:A:328:VAL:HG21	1:A:386:LEU:HD23	1.96	0.48
1:B:492:ARG:NH2	1:B:495:ASP:OD2	2.31	0.48
1:A:431:ARG:CD	1:A:447:GLU:OE2	2.56	0.48
1:B:351:GLU:HB3	1:B:365:LYS:HE3	1.95	0.48
1:A:96:TYR:HB2	3:A:938:HOH:O	2.12	0.48
2:B:800:HEM:HMC1	2:B:800:HEM:CBC	2.42	0.48
1:A:221:HIS:CE1	1:A:255:LYS:HE3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLY:O	1:B:111:ARG:HG2	2.14	0.48
1:A:680:ILE:HG23	1:A:689:LYS:HE3	1.95	0.48
1:B:87:ARG:NH2	1:B:120:ASP:O	2.46	0.48
1:B:221:HIS:CE1	1:B:252:ALA:HB2	2.48	0.47
1:A:355:SER:C	1:A:357:ALA:N	2.68	0.47
1:A:90:TOX:H8	1:A:423:LEU:HD21	1.96	0.47
1:A:195:TYR:CD1	1:A:223:ARG:HB2	2.48	0.47
1:A:326:LEU:HD23	1:A:359:ALA:CB	2.44	0.47
2:A:800:HEM:HMC1	2:A:800:HEM:CBC	2.44	0.47
1:A:98:VAL:HG11	1:A:265:ALA:HB2	1.96	0.47
1:A:508:ALA:H	1:A:577:GLN:HE22	1.63	0.47
1:A:712:VAL:HG21	1:B:40:PRO:HG2	1.96	0.47
1:B:362:TRP:N	1:B:362:TRP:CD1	2.82	0.47
1:B:488:ALA:O	1:B:490:SER:N	2.48	0.47
1:A:221:HIS:HE1	1:A:255:LYS:HE3	1.79	0.47
1:A:456:GLN:OE1	1:A:542:LYS:HE3	2.15	0.47
1:B:671:ALA:HA	1:B:679:PHE:CD2	2.50	0.47
1:A:96:TYR:O	1:A:264:MET:HE3	2.13	0.46
1:A:286:GLY:O	1:A:327:GLU:HG2	2.14	0.46
1:B:122:VAL:HA	1:B:309:TRP:CZ3	2.50	0.46
1:B:647:LEU:N	1:B:647:LEU:HD23	2.30	0.46
1:B:330:TRP:HH2	2:B:800:HEM:CHA	2.27	0.46
1:A:73:TRP:CZ2	1:A:130:LEU:HD23	2.50	0.46
1:A:195:TYR:C	1:A:196:SER:HG	2.04	0.46
1:A:278:GLY:C	1:A:280:SER:H	2.17	0.46
1:A:538:SER:C	1:A:540:SER:N	2.68	0.46
1:A:159:MET:HE1	1:A:335:THR:HA	1.98	0.46
1:B:219:ASP:O	1:B:220:ILE:HB	2.15	0.46
1:A:77:ASP:C	1:A:79:GLY:H	2.20	0.46
1:A:583:HIS:O	1:A:586:THR:HG22	2.16	0.46
1:B:640:ASP:OD1	1:B:640:ASP:N	2.49	0.46
1:A:456:GLN:CD	1:A:542:LYS:CE	2.83	0.46
1:B:530:SER:O	1:B:534:LYS:HG3	2.16	0.46
1:B:147:LEU:O	1:B:151:THR:OG1	2.27	0.45
1:B:223:ARG:NH1	1:B:245:ASP:OD1	2.30	0.45
1:B:233:HIS:HB2	1:B:236:LEU:HD12	1.97	0.45
1:B:122:VAL:HG22	1:B:309:TRP:CE2	2.51	0.45
1:B:669:TRP:HA	1:B:680:ILE:O	2.15	0.45
1:A:9:SER:OG	1:B:604:ARG:O	2.20	0.45
1:A:87:ARG:NH2	1:A:120:ASP:O	2.50	0.45
1:B:595:PHE:CD1	1:B:629:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:PRO:HG3	1:B:709:LEU:HD23	1.98	0.45
1:A:98:VAL:HG22	1:A:263:ARG:O	2.16	0.45
1:A:126:LYS:NZ	3:A:912:HOH:O	2.40	0.45
1:A:9:SER:HA	3:A:910:HOH:O	2.17	0.45
1:A:333:THR:HB	1:A:336:LYS:HB3	1.98	0.45
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.79	0.45
1:B:431:ARG:HG2	1:B:434:TRP:CZ3	2.52	0.45
1:B:457:ILE:H	1:B:457:ILE:HG12	1.61	0.45
1:A:390:ILE:O	1:A:394:MET:HG2	2.17	0.45
1:A:219:ASP:C	1:A:220:ILE:CG1	2.85	0.45
1:B:386:LEU:O	1:B:389:ASP:HB2	2.17	0.45
1:A:473:THR:HG22	1:A:475:VAL:H	1.82	0.44
1:B:404:ASP:OD2	1:B:411:LYS:HE2	2.18	0.44
1:B:622:ALA:HB3	1:B:623:PRO:HD3	1.99	0.44
1:A:577:GLN:HG3	1:A:577:GLN:O	2.17	0.44
1:A:298:GLU:OE1	1:B:25:GLN:NE2	2.43	0.44
1:B:418:ARG:NH2	1:B:442:GLU:OE2	2.49	0.44
1:B:515:VAL:HG23	1:B:598:TYR:CG	2.52	0.44
1:A:381:LYS:HE2	3:A:968:HOH:O	2.17	0.44
1:B:433:ARG:HD3	1:B:739:PHE:CE1	2.53	0.44
1:A:467:LYS:HG2	1:A:556:ALA:CB	2.46	0.44
1:B:295:LYS:HD2	1:B:299:ALA:HB3	1.99	0.44
1:B:43:LYS:HA	1:B:43:LYS:HD3	1.73	0.44
1:A:622:ALA:HB3	1:A:623:PRO:HD3	1.99	0.43
1:B:685:LYS:HG3	3:B:1050:HOH:O	2.18	0.43
1:A:11:VAL:HG13	1:A:12:GLY:O	2.18	0.43
1:A:125:ASP:OD1	1:A:125:ASP:N	2.51	0.43
1:A:193:ASP:CG	1:A:604:ARG:HH22	2.21	0.43
1:A:668:ALA:O	1:A:681:GLY:HA2	2.19	0.43
1:A:669:TRP:HA	1:A:680:ILE:O	2.18	0.43
1:A:220:ILE:CG2	1:A:221:HIS:H	2.32	0.43
1:B:170:ARG:NH1	1:B:424:LEU:O	2.52	0.43
1:B:328:VAL:HG22	1:B:384:THR:HB	2.00	0.43
1:A:56:TYR:OH	1:A:438:GLU:OE1	2.25	0.43
1:A:7:ARG:NH2	1:A:7:ARG:HG3	2.33	0.43
1:A:149:LEU:HG	1:A:424:LEU:HD22	2.01	0.43
2:A:800:HEM:CMC	2:A:800:HEM:CBC	2.97	0.43
1:B:538:SER:O	1:B:539:SER:OG	2.26	0.43
1:A:227:SER:HA	1:A:228:PRO:HA	1.71	0.43
1:A:264:MET:O	1:A:265:ALA:HB3	2.19	0.43
1:A:671:ALA:HA	1:A:679:PHE:HD1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:HE2	1:B:435:ILE:CG2	2.49	0.42
1:A:470:ILE:O	1:A:473:THR:HB	2.19	0.42
1:B:193:ASP:CG	1:B:604:ARG:HH22	2.22	0.42
1:A:137:LYS:HD3	1:A:138:TYR:CE1	2.54	0.42
1:A:540:SER:HB3	1:A:541:GLY:H	1.39	0.42
1:B:537:ASP:C	1:B:539:SER:N	2.73	0.42
1:B:707:ARG:O	1:B:711:GLU:HG3	2.19	0.42
1:A:431:ARG:NH2	1:A:440:PRO:O	2.52	0.42
1:A:707:ARG:O	1:A:711:GLU:HG3	2.19	0.42
1:B:159:MET:CE	1:B:335:THR:CA	2.92	0.42
1:B:595:PHE:HE2	1:B:614:ARG:HG2	1.85	0.42
1:A:355:SER:O	1:A:357:ALA:N	2.52	0.42
1:B:631:GLY:HA3	1:B:726:PHE:CE2	2.55	0.42
1:B:268:ASP:HB3	1:B:401:ILE:CD1	2.50	0.42
1:A:326:LEU:CD2	1:A:359:ALA:HB1	2.50	0.42
1:A:513:TRP:NE1	1:A:589:GLU:HG3	2.34	0.42
1:B:347:LYS:HE2	1:B:348:PHE:CZ	2.55	0.42
1:B:439:VAL:CG1	1:B:440:PRO:HD2	2.50	0.42
1:B:537:ASP:O	1:B:539:SER:N	2.52	0.42
1:B:96:TYR:O	1:B:264:MET:HE2	2.19	0.41
1:B:295:LYS:HA	1:B:295:LYS:HD3	1.86	0.41
1:B:670:LYS:HB3	3:B:924:HOH:O	2.20	0.41
1:B:292:HIS:CG	1:B:313:PHE:HB2	2.55	0.41
1:B:439:VAL:HG13	1:B:440:PRO:HD2	2.02	0.41
1:B:458:ILE:HD12	1:B:463:ILE:CG1	2.50	0.41
1:B:488:ALA:C	1:B:490:SER:N	2.73	0.41
1:B:685:LYS:HG3	1:B:685:LYS:H	1.51	0.41
1:A:144:TRP:O	1:A:148:LEU:HG	2.20	0.41
1:A:346:TYR:CZ	1:A:393:ARG:HG3	2.56	0.41
1:A:604:ARG:O	1:B:9:SER:HB2	2.20	0.41
1:B:595:PHE:CE1	1:B:629:ILE:HD12	2.55	0.41
1:B:701:GLY:O	1:B:707:ARG:NH1	2.48	0.41
1:B:83:GLY:O	2:B:800:HEM:HBD2	2.21	0.41
1:A:451:PRO:HA	1:A:452:PRO:HD3	1.96	0.41
1:B:458:ILE:HD12	1:B:463:ILE:HG12	2.02	0.41
1:B:578:GLU:CD	1:B:578:GLU:H	2.24	0.41
1:A:435:ILE:CG2	1:A:436:GLY:H	2.32	0.41
1:A:510:GLN:HG2	1:A:513:TRP:CZ3	2.56	0.41
1:A:678:VAL:HA	1:A:693:ALA:O	2.21	0.41
1:B:629:ILE:O	1:B:633:ARG:HG2	2.21	0.41
1:A:342:LEU:HB3	1:A:406:LEU:HG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:ASP:OD1	1:A:640:ASP:N	2.46	0.40
1:B:447:GLU:O	1:B:448:ASP:HB2	2.21	0.40
1:A:77:ASP:C	1:A:79:GLY:N	2.74	0.40
1:B:283:LYS:HG3	1:B:284:THR:O	2.22	0.40
1:B:284:THR:HG22	2:B:800:HEM:CAA	2.51	0.40
1:B:361:GLN:C	1:B:362:TRP:CD1	2.94	0.40
1:B:666:ASN:HB3	3:B:1050:HOH:O	2.20	0.40
1:A:467:LYS:HE3	1:A:559:GLU:OE1	2.20	0.40
1:B:430:PRO:C	1:B:432:THR:N	2.74	0.40
1:B:559:GLU:HG2	1:B:566:VAL:CG2	2.51	0.40
1:B:96:TYR:O	1:B:264:MET:HE3	2.22	0.40
1:B:295:LYS:HD2	1:B:299:ALA:CB	2.52	0.40
1:B:456:GLN:HB3	1:B:542:LYS:CG	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1179:HOH:O	3:B:949:HOH:O[3_555]	2.14	0.06
3:A:1200:HOH:O	3:B:1177:HOH:O[3_555]	2.15	0.05

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	708/768 (92%)	672 (95%)	33 (5%)	3 (0%)	34	57
1	B	708/768 (92%)	682 (96%)	21 (3%)	5 (1%)	22	43
All	All	1416/1536 (92%)	1354 (96%)	54 (4%)	8 (1%)	25	47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	220	ILE
1	A	460	ASP
1	B	220	ILE
1	B	10	ASN
1	B	43	LYS
1	B	538	SER
1	B	489	SER

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	577/621 (93%)	546 (95%)	31 (5%)	22	44
1	B	577/621 (93%)	549 (95%)	28 (5%)	25	48
All	All	1154/1242 (93%)	1095 (95%)	59 (5%)	24	46

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	LYS
1	A	17	ARG
1	A	61	LYS
1	A	99	THR
1	A	115	LEU
1	A	186	THR
1	A	222	ASN
1	A	223	ARG
1	A	226	GLN
1	A	227	SER
1	A	302	ILE
1	A	336	LYS
1	A	379	LYS
1	A	383	PRO
1	A	432	THR

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Mol	Chain	Res	Type
1	A	473	THR
1	A	495	ASP
1	A	496	LYS
1	A	538	SER
1	A	540	SER
1	A	578	GLU
1	A	584	SER
1	A	633	ARG
1	A	639	TYR
1	A	685	LYS
1	A	688	ASP
1	A	689	LYS
1	A	720	GLU
1	A	727	VAL
1	A	741	LEU
1	B	7	ARG
1	B	17	ARG
1	B	60	LYS
1	B	97	ARG
1	B	134	ILE
1	B	163	THR
1	B	175	GLU
1	B	192	GLU
1	B	219	ASP
1	B	251	VAL
1	B	280	SER
1	B	347	LYS
1	B	365	LYS
1	B	366	ASN
1	B	381	LYS
1	B	382	LEU
1	B	384	THR
1	B	444	LEU
1	B	457	ILE
1	B	495	ASP
1	B	506	ARG
1	B	584	SER
1	B	586	THR
1	B	629	ILE
1	B	639	TYR
1	B	665	THR
1	B	727	VAL

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Mol	Chain	Res	Type
1	B	741	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	226	GLN
1	A	305	GLN
1	A	360	ASN
1	A	456	GLN
1	A	577	GLN
1	A	638	ASN
1	B	221	HIS
1	B	226	GLN
1	B	378	ASN
1	B	510	GLN
1	B	533	GLN
1	B	638	ASN
1	B	666	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TOX	B	90	1	10,17,18	2.65	3 (30%)	10,23,25	1.35	1 (10%)
1	TOX	A	90	1	10,17,18	2.67	4 (40%)	10,23,25	1.51	3 (30%)

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
1	TOX	B	90	1	-	2/4/8/10	0/2/2/2
1	TOX	A	90	1	-	2/4/8/10	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	TOX	CD1-NE1	-5.18	1.34	1.39
1	B	90	TOX	O-C	5.10	1.40	1.19
1	A	90	TOX	O-C	5.09	1.40	1.19
1	B	90	TOX	CD1-NE1	-5.00	1.34	1.39
1	B	90	TOX	CE3-CD2	-2.83	1.36	1.42
1	A	90	TOX	CE3-CD2	-2.30	1.37	1.42
1	A	90	TOX	CH2-CZ2	2.02	1.41	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	90	TOX	CZ3-CH2-CZ2	-2.66	116.71	120.44
1	A	90	TOX	CZ3-CH2-CZ2	-2.54	116.88	120.44
1	A	90	TOX	CZ3-CE3-CD2	-2.40	117.56	120.89
1	A	90	TOX	CE3-CD2-CG	-2.01	130.72	134.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	90	TOX	N-CA-CB-CG
1	A	90	TOX	C-CA-CB-CG
1	B	90	TOX	N-CA-CB-CG
1	B	90	TOX	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	90	TOX	2	0
1	A	90	TOX	2	0

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	A	800	1	41,50,50	1.32	6 (14%)	45,82,82	1.72	8 (17%)
2	HEM	B	800	1	41,50,50	1.30	5 (12%)	45,82,82	1.73	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	800	1	-	4/12/54/54	-
2	HEM	B	800	1	-	4/12/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	C1B-NB	-3.85	1.33	1.40
2	A	800	HEM	C1B-NB	-3.61	1.34	1.40
2	A	800	HEM	C4D-ND	-3.43	1.34	1.40
2	B	800	HEM	C4D-ND	-3.31	1.34	1.40
2	B	800	HEM	CHB-C1B	2.71	1.41	1.35
2	A	800	HEM	CHB-C1B	2.69	1.41	1.35
2	B	800	HEM	C4B-NB	-2.35	1.34	1.38
2	A	800	HEM	C4B-NB	-2.30	1.34	1.38
2	A	800	HEM	C3B-C4B	2.14	1.49	1.44
2	A	800	HEM	O2D-CGD	-2.11	1.23	1.30
2	B	800	HEM	O2D-CGD	-2.01	1.24	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	800	HEM	C1B-NB-C4B	5.11	110.35	105.07
2	A	800	HEM	CHC-C4B-NB	5.07	129.94	124.43
2	A	800	HEM	C1B-NB-C4B	4.84	110.08	105.07
2	B	800	HEM	CHC-C4B-NB	4.73	129.57	124.43
2	B	800	HEM	CHB-C1B-NB	3.97	129.28	124.38
2	A	800	HEM	CHB-C1B-NB	3.56	128.78	124.38
2	A	800	HEM	CHD-C1D-ND	2.93	127.62	124.43
2	B	800	HEM	CHD-C1D-ND	2.86	127.54	124.43
2	B	800	HEM	C4D-ND-C1D	2.47	107.62	105.07
2	B	800	HEM	CHA-C4D-ND	2.33	127.26	124.38
2	A	800	HEM	C4D-ND-C1D	2.31	107.46	105.07
2	A	800	HEM	O2D-CGD-CBD	2.19	121.07	114.03
2	A	800	HEM	CAD-CBD-CGD	-2.07	109.16	113.60
2	A	800	HEM	O2A-CGA-CBA	2.02	120.53	114.03
2	B	800	HEM	O2D-CGD-CBD	2.02	120.52	114.03
2	B	800	HEM	CBA-CAA-C2A	-2.01	109.19	112.62
2	B	800	HEM	O2A-CGA-CBA	2.00	120.46	114.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	HEM	C4B-C3B-CAB-CBB
2	B	800	HEM	C4B-C3B-CAB-CBB
2	A	800	HEM	C2B-C3B-CAB-CBB
2	B	800	HEM	C2B-C3B-CAB-CBB
2	B	800	HEM	CAA-CBA-CGA-O1A
2	A	800	HEM	CAA-CBA-CGA-O1A
2	A	800	HEM	CAA-CBA-CGA-O2A
2	B	800	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

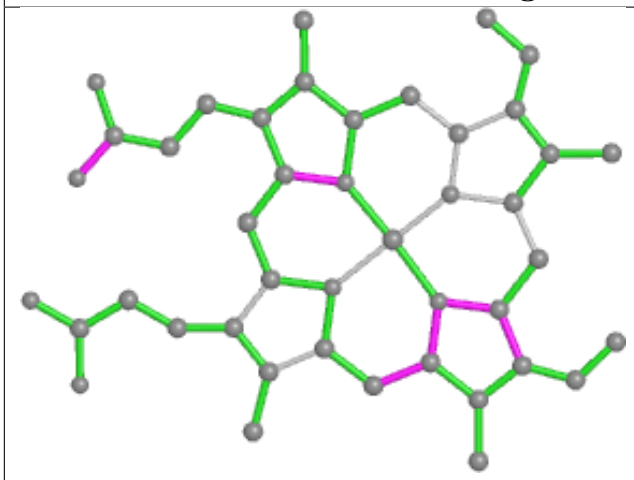
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	HEM	5	0
2	B	800	HEM	7	0

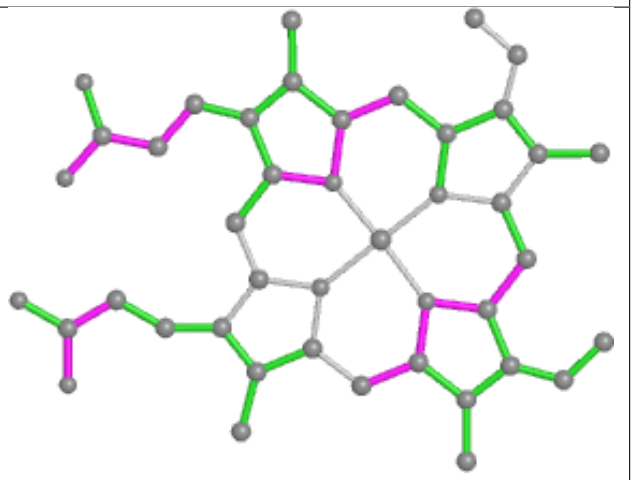
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

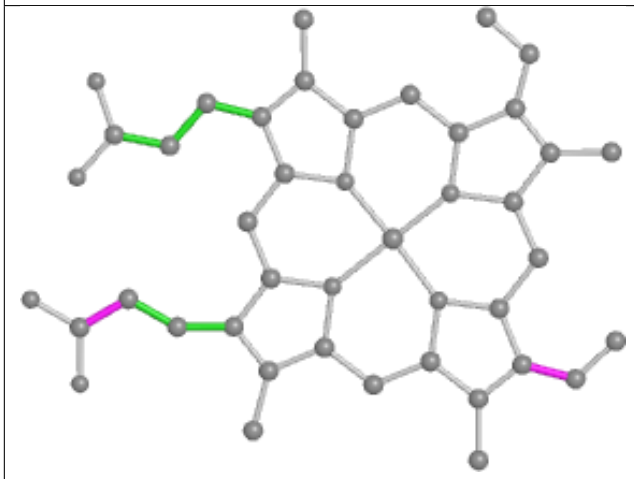
Ligand HEM A 800



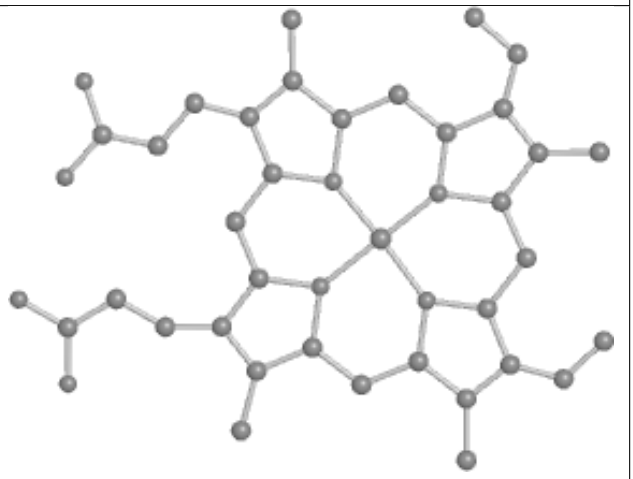
Bond lengths



Bond angles

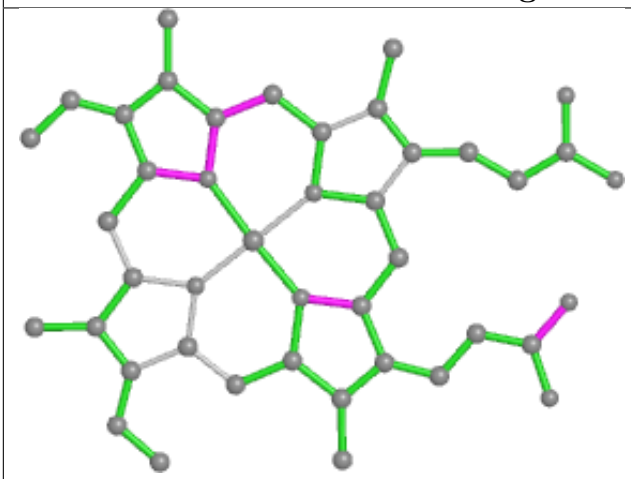


Torsions

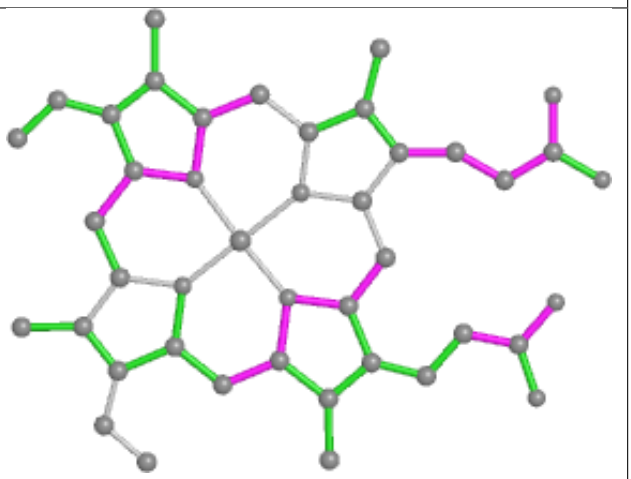


Rings

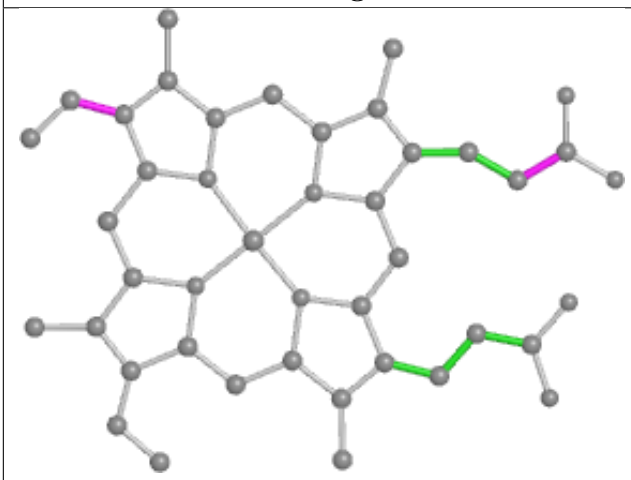
Ligand HEM B 800



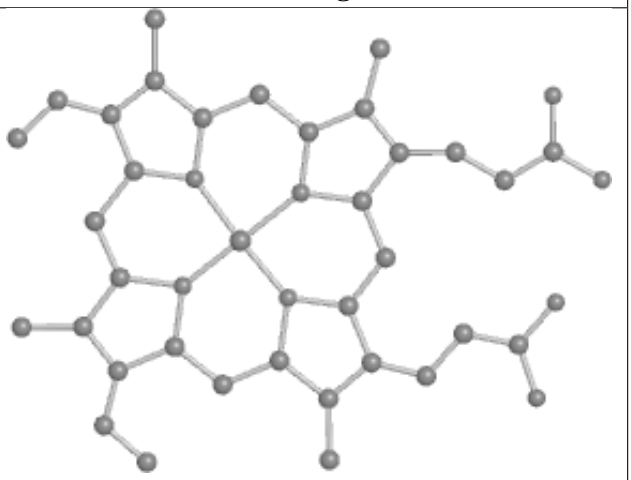
Bond lengths



Bond angles



Torsions



Rings

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	712/768 (92%)	-0.17	18 (2%)	57	51	14, 29, 49, 91	0
1	B	712/768 (92%)	-0.26	11 (1%)	73	70	13, 24, 47, 106	0
All	All	1424/1536 (92%)	-0.21	29 (2%)	65	60	13, 27, 48, 106	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	538	SER	5.9
1	B	221	HIS	4.8
1	B	219	ASP	4.6
1	B	222	ASN	4.6
1	A	219	ASP	3.9
1	A	222	ASN	3.9
1	A	221	HIS	3.8
1	B	196	SER	3.7
1	A	539	SER	3.6
1	B	539	SER	3.6
1	A	538	SER	3.6
1	A	541	GLY	3.4
1	A	540	SER	3.0
1	B	224	ASP	3.0
1	B	540	SER	3.0
1	A	220	ILE	2.8
1	A	542	LYS	2.8
1	A	456	GLN	2.5
1	A	192	GLU	2.5
1	B	192	GLU	2.5
1	B	603	LYS	2.3
1	A	441	SER	2.2
1	A	741	LEU	2.1
1	A	453	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	454	ASP	2.1
1	B	220	ILE	2.1
1	A	688	ASP	2.1
1	A	685	LYS	2.1
1	A	740	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TOX	A	90	16/17	0.95	0.16	21,23,28,33	0
1	TOX	B	90	16/17	0.96	0.14	12,14,19,23	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

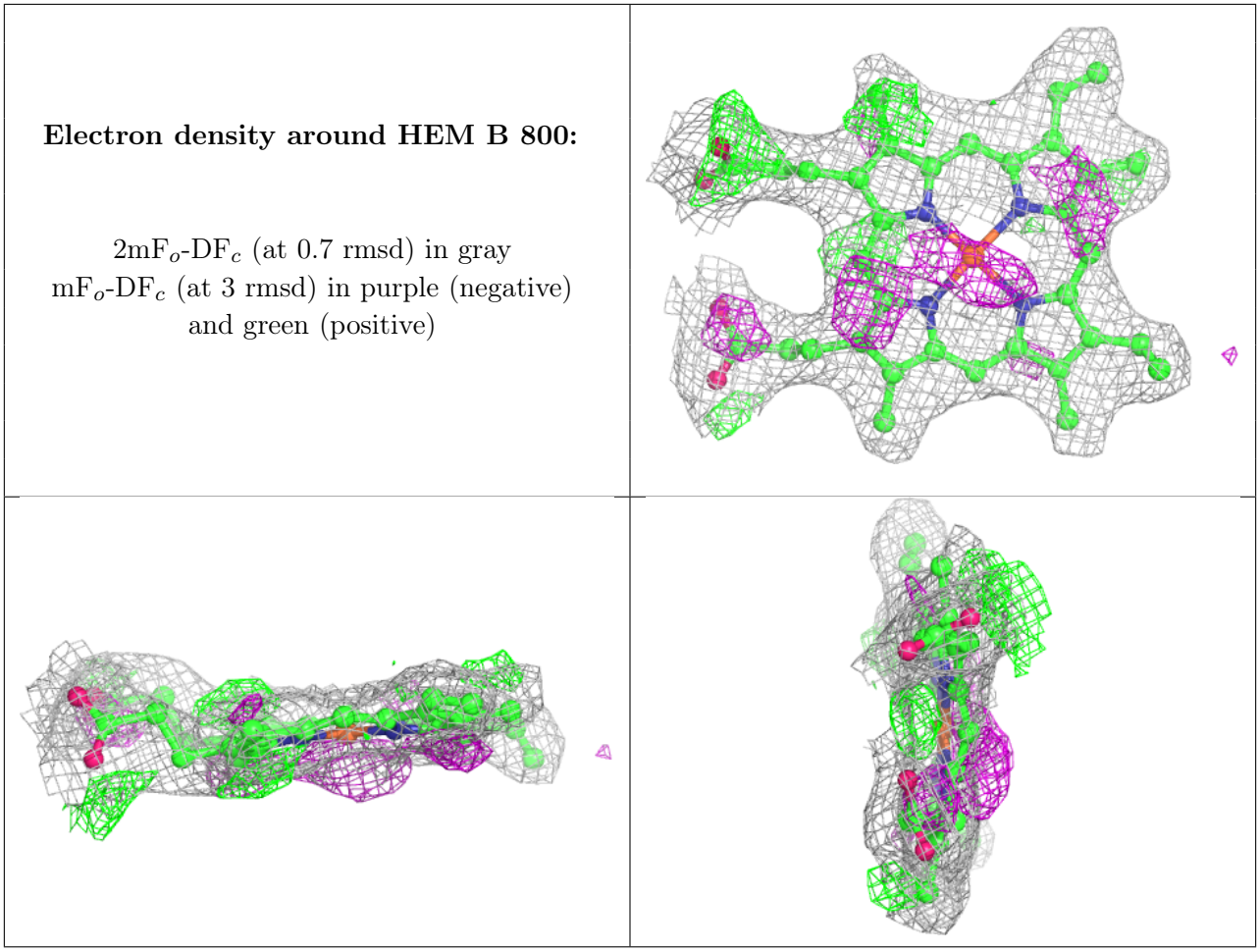
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	HEM	B	800	43/43	0.91	0.19	16,18,19,20	0
2	HEM	A	800	43/43	0.93	0.18	22,24,28,31	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.

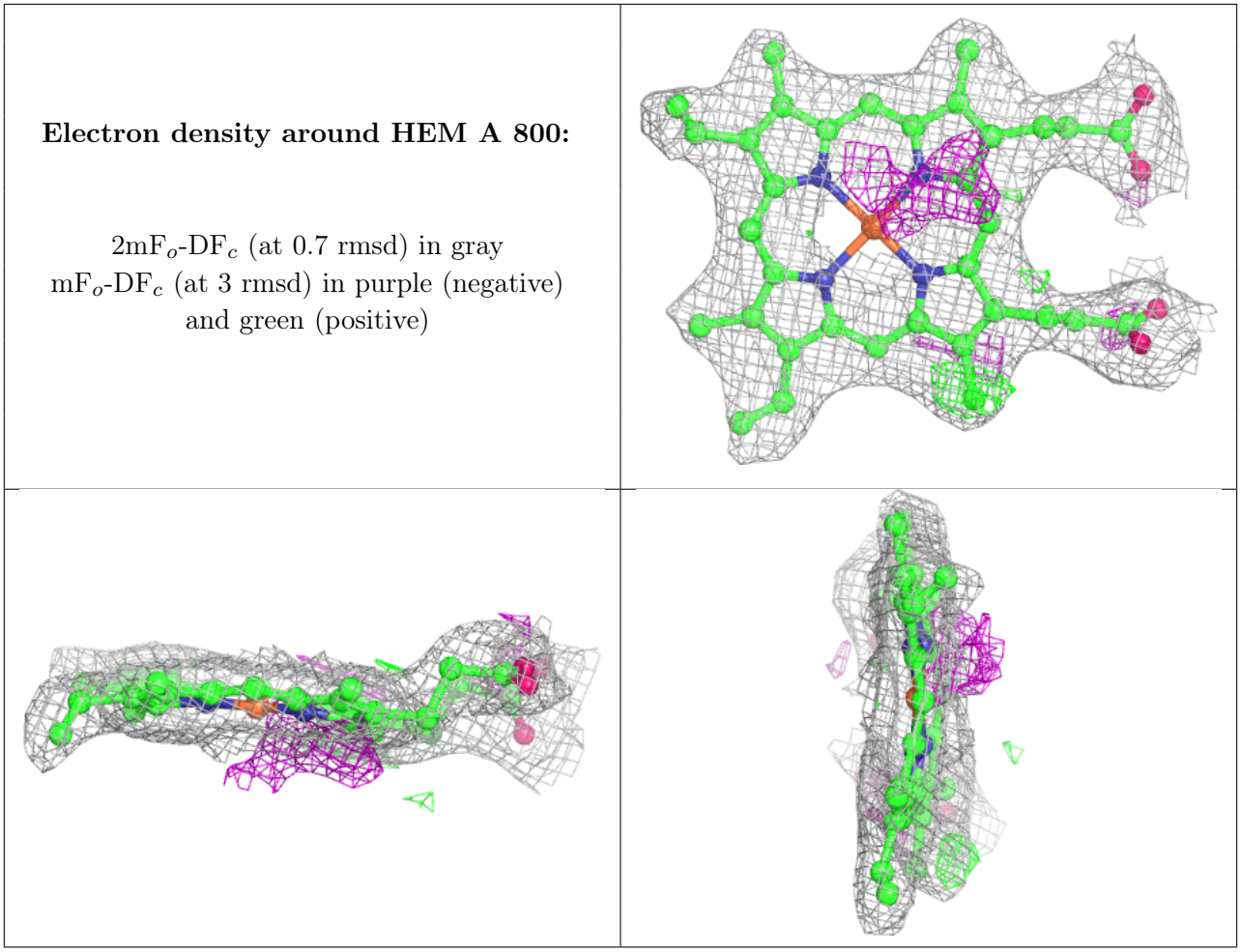
Electron density around HEM B 800:

$2mF_o$-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.