



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:57 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

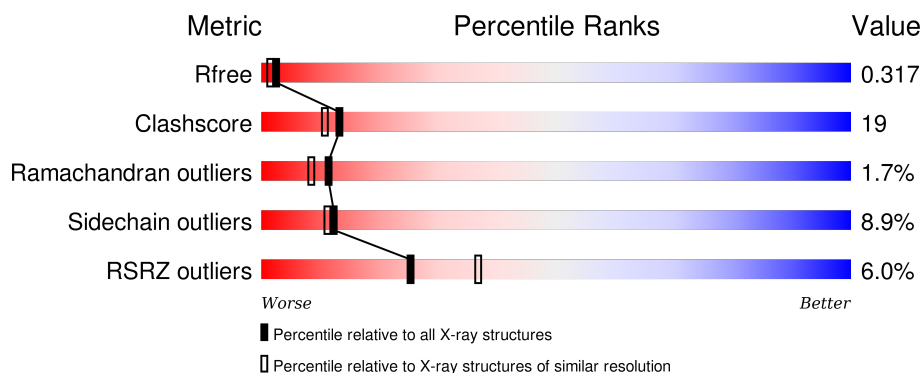
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	<div> <div>5%</div> <div>54%</div> <div>31%</div> <div>•</div> <div>10%</div> </div>
1	B	737	<div> <div>6%</div> <div>58%</div> <div>29%</div> <div>•</div> <div>10%</div> </div>

## 2 Entry composition

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
1	A	663	Total	C	N	O	S	0	0	0
			5201	3257	872	1054	18			
1	B	660	Total	C	N	O	S	0	0	0
			5185	3247	872	1049	17			

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
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		

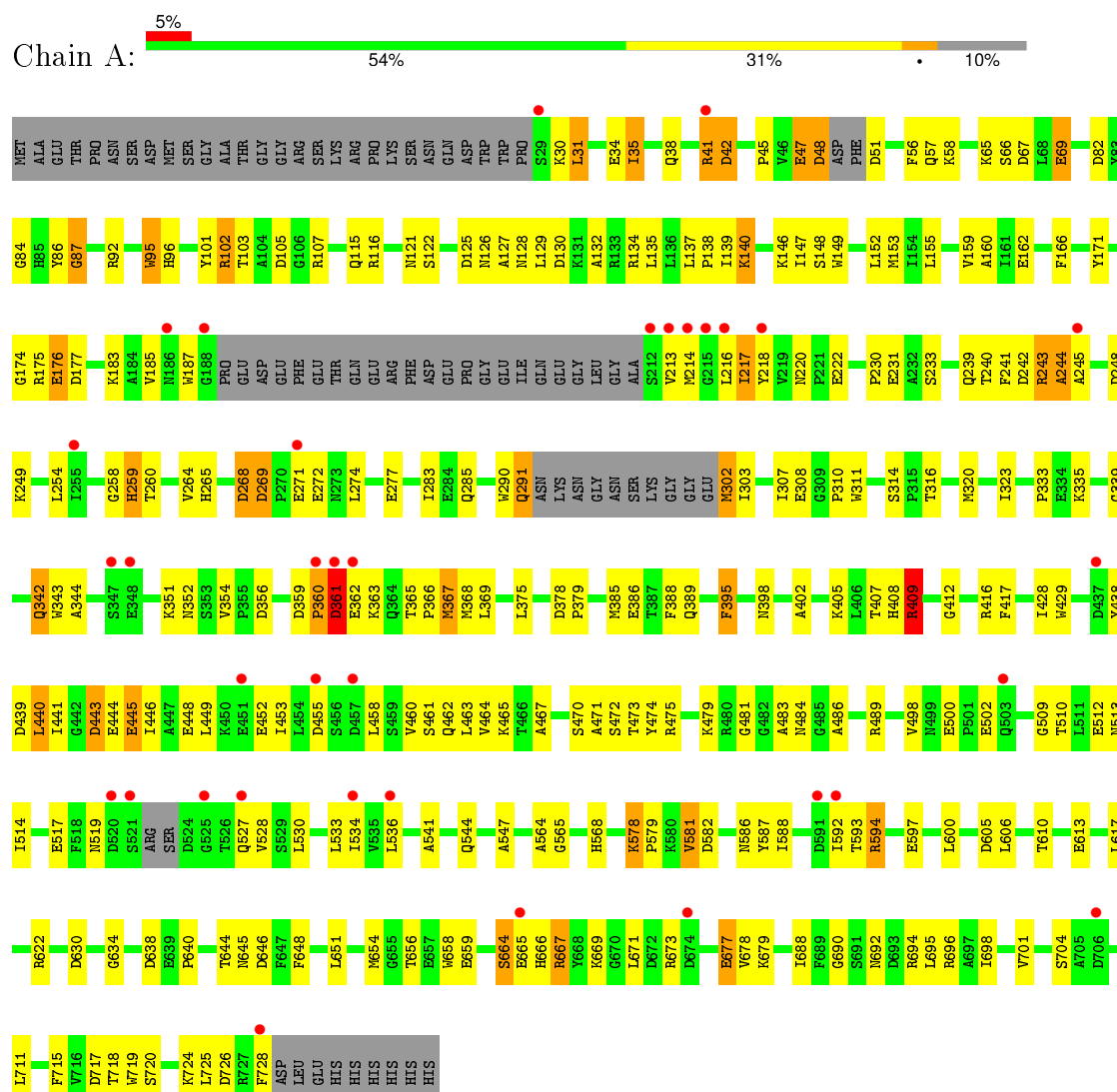
- Molecule 3 is water.

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



#### • Molecule 1: Catalase-peroxidase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.283 , 0.325 0.278 , 0.317	Depositor DCC
$R_{free}$ test set	3777 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 116085 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.96	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(°)	Ideal(°)
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 ⓘ

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:O	1:A:581:VAL:HG12	1.85	0.75
1:A:405:LYS:HE3	1:A:429:TRP:CD1	2.22	0.74
1:A:320:MET:HE3	1:A:323:ILE:HB	1.69	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:B:449:LEU:O	1:B:453:ILE:HG13	1.90	0.72
1:A:95:TRP:HH2	1:A:218:TYR:CD1	2.07	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:HG2	1:A:677:GLU:O	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:O	1:B:376:LYS:HG2	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:B:584:VAL:HG13	1:B:621:MET:CG	2.23	0.62
1:A:259:HIS:HB3	1:A:311:TRP:CE2	2.33	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
2:B:800:HEM:HMB1	2:B:800:HEM:HBB2	1.82	0.62
1:A:333:PRO:HD3	1:A:343:TRP:CZ3	2.35	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:594:ARG:HE	1:A:594:ARG:H	1.50	0.60
1:A:65:LYS:HE3	1:A:159:VAL:HG22	1.83	0.60
1:A:474:TYR:HD1	1:A:725:LEU:CB	2.14	0.60
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:A:140:LYS:HG2	1:A:149:TRP:CE2	2.37	0.59
1:B:244:ALA:O	1:B:245:ALA:HB3	2.02	0.59
1:A:474:TYR:HD1	1:A:725:LEU:HB3	1.62	0.59
1:B:368:MET:HG3	1:B:372:ASP:CB	2.33	0.59
1:B:274:LEU:HD22	1:B:290:TRP:HB3	1.85	0.59
1:B:223:GLY:HA3	1:B:227:ASN:O	2.01	0.59
1:A:162:GLU:HA	1:A:166:PHE:O	2.02	0.59
1:B:35:ILE:HG13	1:B:36:LEU:N	2.17	0.59
1:A:102:ARG:HH21	1:A:105:ASP:CG	2.06	0.59
1:A:35:ILE:HD11	1:A:605:ASP:HB2	1.83	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:B:711:LEU:HG	1:B:711:LEU:O	2.03	0.58
1:A:361:ASP:O	1:A:362:GLU:HB2	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
2:B:800:HEM:CMB	2:B:800:HEM:HBB2	2.36	0.56
1:B:330:GLU:HB3	1:B:346:LYS:HE3	1.87	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:B:95:TRP:CE3	1:B:406:LEU:HD21	2.42	0.54
1:A:320:MET:CE	1:A:389:GLN:HA	2.38	0.54
1:B:511:LEU:HA	1:B:514:ILE:HG13	1.89	0.54
1:B:443:ASP:HA	1:B:446:ILE:HD12	1.88	0.54
1:A:463:LEU:HB2	1:A:541:ALA:HB2	1.90	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:B:482:GLY:HA3	1:B:726:ASP:OD2	2.09	0.53
1:B:118:ALA:HB2	1:B:279:GLU:HG3	1.91	0.53
1:A:125:ASP:HB2	1:A:216:LEU:HD23	1.91	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:692:ASN:HD22	1:B:695:LEU:H	1.54	0.53
1:B:161:ILE:HG22	1:B:166:PHE:HB3	1.90	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:458:LEU:HA	1:A:462:GLN:OE1	2.09	0.52
1:A:438:TYR:CD1	1:A:527:GLN:HB2	2.44	0.52
2:A:800:HEM:CMC	2:A:800:HEM:HBC2	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:645:ASN:HA	1:A:711:LEU:CD2	2.38	0.52
1:A:66:SER:O	1:A:69:GLU:HB2	2.10	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: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:35:ILE:CD1	1:A:605:ASP:HB2	2.40	0.51
1:A:95:TRP:CD1	1:A:96:HIS:HD2	2.29	0.51
1:A:486:ALA:O	1:A:489:ARG:HG2	2.10	0.51
1:A:149:TRP:O	1:A:153:MET:HG3	2.11	0.51
1:A:213:VAL:HB	1:A:216:LEU:HD12	1.93	0.50
1:A:82:ASP:OD1	1:A:265:HIS:NE2	2.43	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: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:B:159:VAL:O	1:B:160:ALA:C	2.49	0.50
1:A:582:ASP:C	1:A:582:ASP:OD1	2.50	0.50
1:B:95:TRP:CD1	1:B:96:HIS:CD2	3.00	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:270:PRO:C	1:B:272:GLU:H	2.15	0.49
1:B:474:TYR:CD2	1:B:726:ASP:HB3	2.47	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: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:B:311:TRP:NE1	1:B:372:ASP:OD2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:THR:H	1:A:594:ARG:HH21	1.59	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:264:VAL:HG23	1:A:264:VAL:O	2.12	0.49
1:A:125:ASP:O	1:A:125:ASP:OD2	2.30	0.49
1:A:665:GLU:HB3	1:A:666:HIS:CE1	2.48	0.49
1:A:644:THR:OG1	1:A:646:ASP:HB2	2.13	0.49
1:A:82:ASP:C	1:A:84:GLY:H	2.16	0.48
1:B:158:ASN:ND2	1:B:171:TYR:HB2	2.28	0.48
1:A:254:LEU:HG	1:A:402:ALA:HB1	1.95	0.48
1:A:694:ARG:O	1:A:698:ILE:HG13	2.14	0.48
1:B:409:ARG:NH2	1:B:409:ARG:HG3	2.28	0.48
1:B:265:HIS:HD2	1:B:302:MET:HG2	1.77	0.48
1:A:470:SER:HG	1:A:483:ALA:HB1	1.77	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:473:THR:O	1:A:481:GLY:HA3	2.13	0.48
1:B:648:PHE:O	1:B:652:LEU:HG	2.13	0.48
1:A:519:ASN:HD21	1:A:528:VAL:H	1.62	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:B:329:TYR:O	1:B:376:LYS:NZ	2.46	0.48
1:B:241:PHE:O	1:B:244:ALA:HB3	2.14	0.48
1:A:449:LEU:O	1:A:453:ILE:HG13	2.13	0.48
1:B:252:ALA:HB1	1:B:385:MET:SD	2.54	0.47
1:B:373:ILE:O	1:B:376:LYS:N	2.47	0.47
1:A:386:GLU:CD	3:A:761:HOH:O	2.53	0.47
1:A:352:ASN:HB3	1:A:363:LYS:HB2	1.96	0.47
1:B:424:ASP:OD1	1:B:424:ASP:N	2.47	0.47
1:B:474:TYR:CD1	1:B:474:TYR:C	2.88	0.47
1:A:409:ARG:NH2	1:A:409:ARG:HG3	2.30	0.47
1:B:320:MET:HB2	1:B:324:ASN:ND2	2.30	0.47
1:A:48:ASP:N	1:A:48:ASP:OD2	2.47	0.47
1:A:218:TYR:HA	1:A:218:TYR:HD2	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:B:524:ASP:C	1:B:524:ASP:OD2	2.53	0.47
1:A:673:ARG:HD3	1:B:78:TRP:HB3	1.97	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:B:134:ARG:NH1	1:B:288:LEU:HD21	2.29	0.46
1:B:111:ALA:O	1:B:175:ARG:HB3	2.14	0.46
1:A:175:ARG:NH2	1:A:407:THR:O	2.41	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:B:95:TRP:CZ3	1:B:218:TYR:OH	2.67	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: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:CD1	1:A:395:PHE:O	2.68	0.46
1:B:242:ASP:C	1:B:244:ALA:H	2.19	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:42:ASP:N	1:A:42:ASP:OD1	2.49	0.46
1:B:474:TYR:HD2	1:B:726:ASP:HB3	1.81	0.46
1:A:502:GLU:H	1:A:502:GLU:CD	2.18	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:471:ALA:CA	1:A:483:ALA:HB2	2.47	0.45
1:A:56:PHE:C	1:A:58:LYS:H	2.19	0.45
1:A:509:GLY:O	1:A:513:ASN:OD1	2.34	0.45
1:B:34:GLU:N	1:B:34:GLU:OE1	2.50	0.45
1:B:312:THR:OG1	1:B:315:PRO:HA	2.16	0.45
1:A:440:LEU:HA	1:A:440:LEU:HD23	1.81	0.45
1:A:269:ASP:OD1	1:A:271:GLU:HB2	2.17	0.45
1:A:379:PRO:HD2	3:A:832:HOH:O	2.17	0.45
1:B:42:ASP:N	1:B:42:ASP:OD1	2.50	0.45
1:A:258:GLY:O	1:A:260:THR: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:B:555:ILE:CG2	1:B:556:PRO:HD2	2.48	0.44
1:A:264:VAL:HG23	1:A:307:ILE:C	2.38	0.44
1:A:213:VAL:HG12	1:A:214:MET:N	2.33	0.44
1:B:82:ASP:OD2	1:B:358:HIS:CE1	2.70	0.44
1:A:67:ASP:HB3	1:A:139:ILE:HD13	2.00	0.44
1:A:67:ASP:HB3	1:A:139:ILE:CD1	2.47	0.44
1:A:47:GLU:HG2	1:A:47:GLU:H	1.55	0.44
1:A:147:ILE:O	1:A:147:ILE:HG23	2.18	0.44
1:B:603:ASN:C	1:B:605:ASP:N	2.71	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:A:230:PRO:HG2	1:A:231:GLU:OE2	2.18	0.44
1:B:659:GLU:OE1	1:B:671:LEU:HD11	2.18	0.44
1:B:405:LYS:O	1:B:409:ARG:HB2	2.17	0.44
1:A:408:HIS:HB3	1:A:417:PHE:CE1	2.52	0.44
1:A:134:ARG:CZ	1:B:696:ARG:NH2	2.81	0.44
1:B:166:PHE:CD1	1:B:318:TRP:CD2	3.05	0.43
1:B:45:PRO:HD2	1:B:179:PHE:CZ	2.52	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:B:166:PHE:HD2	1:B:167:LYS:H	1.59	0.43
1:A:412:GLY:HA3	1:A:479:LYS:CB	2.46	0.43
1:B:603:ASN:O	1:B:604:ALA:C	2.57	0.43
1:A:656:THR:HA	1:A:671:LEU:O	2.18	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: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:715:PHE:C	1:A:715:PHE:CD2	2.91	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:56:PHE:C	1:A:58:LYS:N	2.72	0.43
1:A:30:LYS:O	1:A:31:LEU:C	2.56	0.43
1:B:103:THR:O	1:B:475:ARG:NH2	2.51	0.43
1:A:285:GLN:NE2	1:A:291:GLN:HE22	2.17	0.43
1:A:41:ARG:HD2	1:B:41:ARG:CD	2.43	0.43
1:B:166:PHE:CD2	1:B:167:LYS:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:800:HEM:HBC2	2:A:800:HEM:HMC1	2.01	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:A:265:HIS:N	1:A:265:HIS:ND1	2.67	0.42
1:A:443:ASP:HA	1:A:446:ILE:HD12	2.01	0.42
1:A:302:MET:N	3:A:811:HOH:O	2.51	0.42
1:B:595:PRO:O	1:B:598:GLU:HB2	2.19	0.42
1:B:419:GLY:O	1:B:422:VAL:HG23	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:B:702:TYR:O	1:B:707:ALA:HB3	2.19	0.42
1:A:665:GLU:HB3	1:A:666:HIS:ND1	2.34	0.42
1:B:503:GLN:O	1:B:506:THR:HB	2.20	0.42
1:B:230:PRO:O	1:B:231:GLU:C	2.58	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:B:95:TRP:HZ3	1:B:406:LEU:HD11	1.84	0.42
1:A:354:VAL:CG2	1:A:366:PRO:HD3	2.50	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:B:688:ILE:C	1:B:690:GLY:H	2.23	0.42
1:B:463:LEU:HB2	1:B:541:ALA:HB2	2.01	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:B:313:GLN:C	1:B:315:PRO:HD3	2.40	0.41
1:A:127:ALA:HA	1:A:290:TRP:CH2	2.54	0.41
1:A:107:ARG:CZ	1:A:606:LEU:HD21	2.51	0.41
1:B:73:THR:OG1	1:B:73:THR:O	2.38	0.41
1:B:376:LYS:CG	1:B:376:LYS:O	2.66	0.41
1:A:536:LEU:HD12	1:A:536:LEU:HA	1.88	0.41
1:A:220:ASN:OD1	1:A:222:GLU:HB2	2.21	0.41
1:A:405:LYS:HE3	1:A:429:TRP:CG	2.53	0.41
1:A:264:VAL:HG12	2:A:800:HEM:HAA1	2.01	0.41
1:B:217:ILE:N	1:B:217:ILE:HD13	2.36	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

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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: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:428:ILE:HA	1:A:428:ILE:HD12	1.80	0.41
1:B:555:ILE:HG22	1:B:556:PRO:HD2	2.01	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:95:TRP:HZ3	1:B:218:TYR:HH	1.58	0.41
1:A:724:LYS:HZ3	1:A:724:LYS:HG3	1.64	0.41
1:A:147:ILE:HD13	1:A:152:LEU:HD13	2.03	0.41
1:B:375:LEU:HA	1:B:375:LEU:HD23	1.90	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:433:LEU:HA	1:B:434:PRO:HD2	1.68	0.41
1:B:34:GLU:HA	1:B:37:ASP:OD2	2.21	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: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:HD23	1:B:31:LEU:HA	1.65	0.40
1:A:654:MET:HE1	1:B:288:LEU:HD11	2.04	0.40
1:A:375:LEU:HD22	1:A:385:MET:HE1	2.04	0.40
1:A:132:ALA:O	1:A:135:LEU:HB2	2.21	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
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

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%)	11	7
1	B	652/737 (88%)	558 (86%)	84 (13%)	10 (2%)	13	10
All	All	1305/1474 (88%)	1131 (87%)	152 (12%)	22 (2%)	11	8

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%)	12	11
1	B	543/607 (90%)	494 (91%)	49 (9%)	12	11
All	All	1088/1214 (90%)	991 (91%)	97 (9%)	12	11

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

Some 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 ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	30,50,50	2.48	6 (20%)	24,82,82	3.09	12 (50%)
2	HEM	B	800	1	30,50,50	2.29	6 (20%)	24,82,82	2.87	9 (37%)

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	-	0/10/54/54	0/0/8/8
2	HEM	B	800	1	-	0/10/54/54	0/0/8/8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	C3B-C4B	-7.33	1.45	1.51
2	A	800	HEM	C3D-C4D	-7.27	1.42	1.51
2	B	800	HEM	C3D-C4D	-7.09	1.42	1.51
2	A	800	HEM	C3B-C4B	-6.57	1.46	1.51
2	A	800	HEM	C2C-C1C	-5.65	1.41	1.52
2	B	800	HEM	C2C-C1C	-3.40	1.46	1.52
2	B	800	HEM	C2B-C1B	-2.38	1.44	1.51
2	A	800	HEM	C2A-C3A	-2.25	1.31	1.37
2	B	800	HEM	CMA-C3A	2.09	1.56	1.51
2	B	800	HEM	FE-NC	2.26	2.04	1.95
2	A	800	HEM	C3C-CAC	2.46	1.55	1.51
2	A	800	HEM	FE-NC	4.62	2.14	1.95

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	CAA-CBA-CGA	-7.03	99.86	112.75
2	A	800	HEM	C3C-CAC-CBC	-5.83	115.51	124.46
2	A	800	HEM	CAA-CBA-CGA	-4.70	104.14	112.75
2	A	800	HEM	C4B-CHC-C1C	-3.05	120.73	125.82
2	A	800	HEM	CAD-CBD-CGD	-2.32	103.53	113.02
2	B	800	HEM	C2D-C3D-C4D	2.03	104.94	101.50
2	A	800	HEM	CMD-C2D-C3D	2.16	123.89	114.35
2	A	800	HEM	CAA-C2A-C1A	2.18	129.38	127.01
2	B	800	HEM	CMD-C2D-C3D	2.57	125.71	114.35
2	B	800	HEM	C3B-C4B-CHC	2.73	127.01	123.16
2	A	800	HEM	C2D-C3D-C4D	2.82	106.28	101.50
2	A	800	HEM	CAD-C3D-C4D	3.27	124.00	112.47
2	B	800	HEM	CAD-C3D-C4D	3.75	125.71	112.47
2	A	800	HEM	C1D-CHD-C4C	4.07	132.62	125.82
2	B	800	HEM	CBA-CAA-C2A	4.22	120.09	112.53
2	B	800	HEM	CMC-C2C-C3C	4.60	128.02	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	HEM	CMB-C2B-C3B	4.87	128.68	116.53
2	B	800	HEM	CMB-C2B-C3B	5.04	129.12	116.53
2	B	800	HEM	CAD-C3D-C2D	5.61	129.35	113.22
2	A	800	HEM	CAD-C3D-C2D	5.71	129.64	113.22
2	A	800	HEM	CMC-C2C-C3C	7.01	134.03	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

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

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	663/737 (89%)	0.26	35 (5%)	30 43	14, 35, 55, 68	0
1	B	660/737 (89%)	0.50	45 (6%)	20 30	24, 43, 60, 71	0
All	All	1323/1474 (89%)	0.38	80 (6%)	25 37	14, 39, 58, 71	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	MET	5.4
1	A	360	PRO	5.2
1	B	663	ASP	4.8
1	B	348	GLU	4.8
1	A	361	ASP	4.5
1	B	361	ASP	4.3
1	B	592	ILE	4.2
1	A	591	ASP	4.2
1	B	239	GLN	4.2
1	A	525	GLY	4.2
1	A	186	ASN	4.1
1	B	271	GLU	4.0
1	B	665	GLU	3.9
1	B	29	SER	3.8
1	B	591	ASP	3.8
1	B	662	ALA	3.7
1	A	188	GLY	3.4
1	A	437	ASP	3.4
1	A	29	SER	3.2
1	B	311	TRP	3.1
1	B	534	ILE	3.1
1	A	245	ALA	3.1
1	B	523	SER	3.1
1	A	213	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	520	ASP	3.1
1	B	77	ASP	3.1
1	B	264	VAL	3.1
1	B	347	SER	3.1
1	B	360	PRO	3.0
1	B	276	PRO	2.9
1	A	271	GLU	2.9
1	B	437	ASP	2.9
1	A	521	SER	2.8
1	A	215	GLY	2.8
1	A	706	ASP	2.8
1	B	242	ASP	2.7
1	A	216	LEU	2.7
1	B	618	ILE	2.7
1	B	558	GLU	2.7
1	A	362	GLU	2.7
1	B	215	GLY	2.7
1	B	187	TRP	2.7
1	B	620	GLY	2.6
1	A	457	ASP	2.6
1	A	218	TYR	2.6
1	B	259	HIS	2.5
1	A	348	GLU	2.5
1	B	369	LEU	2.5
1	A	455	ASP	2.5
1	B	341	TRP	2.5
1	B	584	VAL	2.5
1	B	728	PHE	2.5
1	A	255	ILE	2.4
1	A	728	PHE	2.4
1	B	379	PRO	2.4
1	B	255	ILE	2.3
1	A	347	SER	2.3
1	A	503	GLN	2.3
1	A	534	ILE	2.3
1	A	674	ASP	2.3
1	B	457	ASP	2.3
1	B	186	ASN	2.3
1	B	552	ASP	2.2
1	B	349	GLU	2.2
1	A	536	LEU	2.2
1	A	527	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	531	ALA	2.2
1	A	41	ARG	2.2
1	B	228	PRO	2.2
1	A	212	SER	2.2
1	B	329	TYR	2.2
1	B	254	LEU	2.2
1	A	451	GLU	2.1
1	B	225	ASP	2.1
1	A	592	ILE	2.1
1	B	165	GLY	2.0
1	B	455	ASP	2.0
1	A	665	GLU	2.0
1	B	227	ASN	2.0
1	B	685	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEM	B	800	43/43	0.93	0.23	0.92	39,42,46,48	0
2	HEM	A	800	43/43	0.94	0.18	0.44	17,22,25,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.