



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:24 PM GMT

PDB ID : 1TH4  
Title : crystal structure of NADPH depleted bovine liver catalase complexed with 3-amino-1,2,4-triazole  
Authors : Sugadev, R.; Ponnuswamy, M.N.; Kumaran, D.; Swaminathan, S.; Sekar, K.  
Deposited on : 2004-06-01  
Resolution : 2.98 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.

---

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

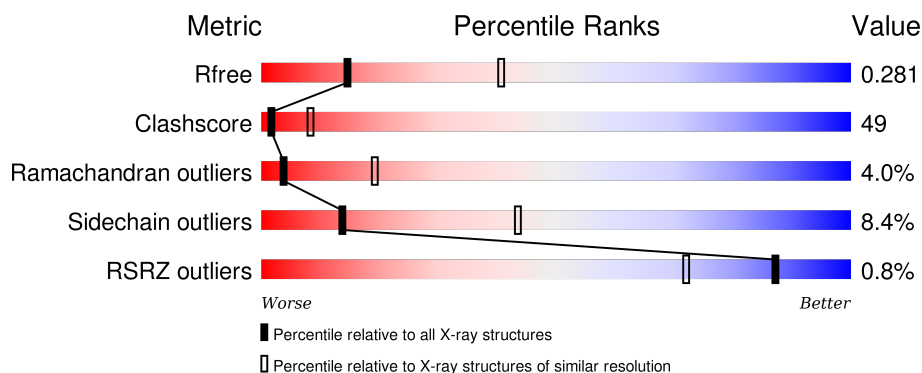
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	506	<div> <div>32%</div> <div>58%</div> <div>8%</div> <div>..</div> </div>
1	B	506	<div> <div>35%</div> <div>53%</div> <div>9%</div> <div>..</div> </div>
1	C	506	<div> <div>38%</div> <div>51%</div> <div>9%</div> <div>..</div> </div>
1	D	506	<div> <div>39%</div> <div>52%</div> <div>7%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3TR	D	3074	-	-	X	-
3	HEM	A	2000	-	-	X	X
3	HEM	B	2001	-	-	X	X
3	HEM	C	2002	-	-	X	X
3	HEM	D	2003	-	-	X	-

## 2 Entry composition [i](#)

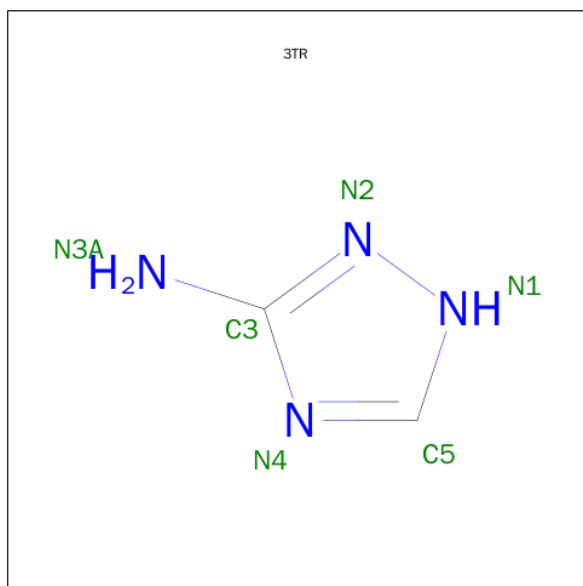
There are 4 unique types of molecules in this entry. The entry contains 16915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	B	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	C	499	Total	C	N	O	S	1	0	0
			4017	2548	715	740	14			
1	D	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			

- Molecule 2 is 3-AMINO-1,2,4-TRIAZOLE (three-letter code: 3TR) (formula:  $C_2H_4N_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	N	0	0
			6	2	4		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

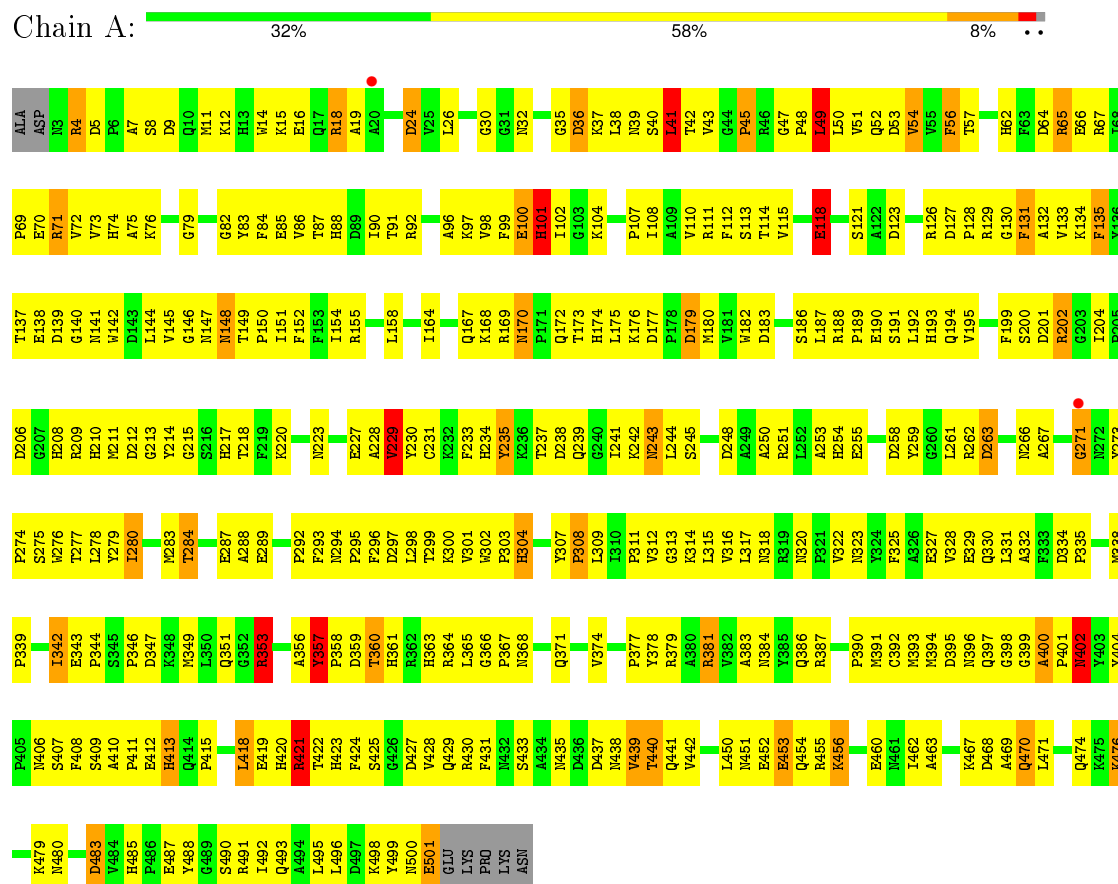
- Molecule 4 is water.

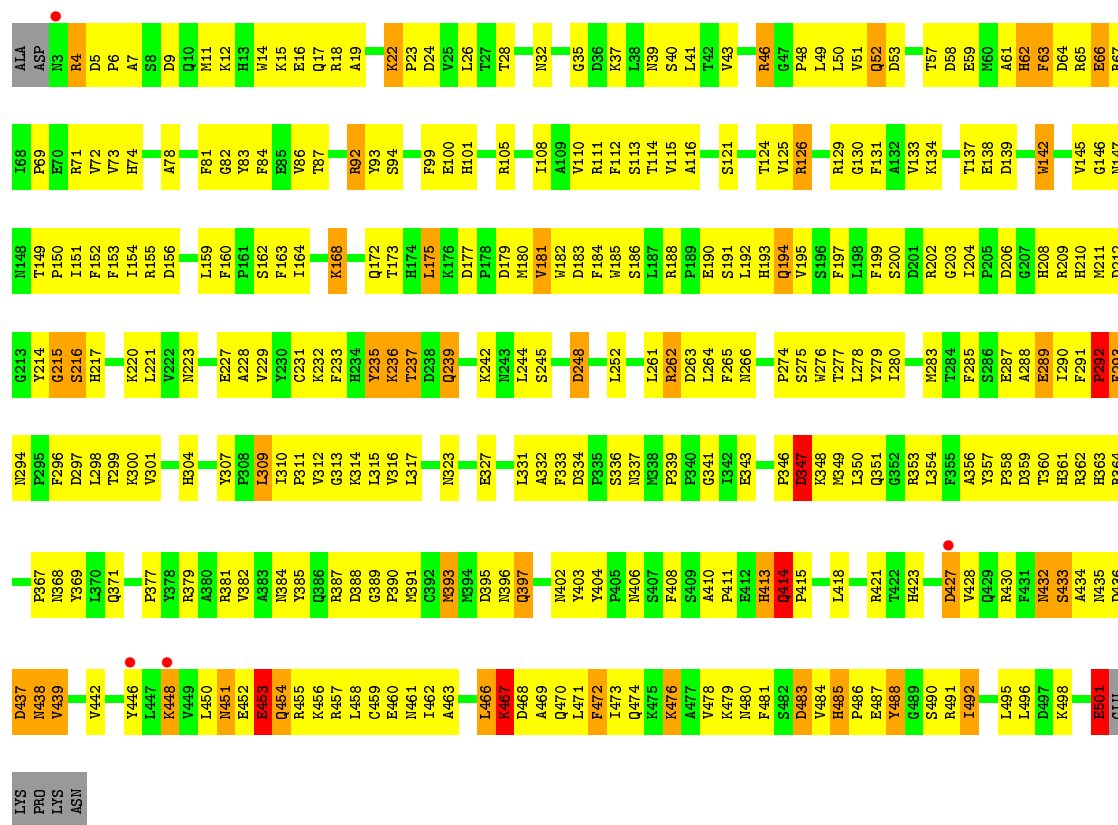
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	145	Total	O	0	0
			145	145		
4	C	188	Total	O	0	0
			188	188		
4	D	182	Total	O	0	0
			182	182		

### 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





T452	P358	S286	H211	V145	V72	ALA
H423	D359	E287	D212	G146	V73	ASP
F424	T360	A288	G215	M147	H74	ARG
H361	H361	E289	S216	M148	A75	ASN
R362	R362	I290	D217	T149	K76	ASP
V427	V427	F291	T218	E150	G77	ASP
Q429	L365	P292	F219	I151	A78	ASP
R430	G366	F293	K220	H153	M11	ASP
F431	P367	F296	L221	D156	K12	ASP
N432	N368	D297	V222	E85	H13	ASP
D436	Y369	L298	N223	T86	K15	ASP
D437	L370	T299	D224	T87	E16	ASP
D437	G371	K300	D225	L158	Q17	ASP
M438	I372	V301	G226	L159	R18	ASP
V439	F373	W302	E227	F160	A19	ASP
T440	V374	P303	A228	S162	I20	ASP
Q441	N375	L309	V229	F163	Q21	ASP
V442	Y378	I310	Y230	I164	R22	ASP
E483	R379	G313	C231	H165	P23	ASP
R457	A380	F233	K232	S166	D24	ASP
L458	R381	K314	F233	Q167	S94	ASP
C459	V382	L315	D234	K168	K95	ASP
E460	A383	V316	Y235	R169	K97	ASP
L466	N384	L317	K236	N170	F99	ASP
K467	V385	R318	G240	P171	E100	ASP
L471	Q386	R319	T241	Q172	H101	ASP
F472	R387	G322	K242	H173	D36	ASP
L473	D388	V322	N243	L175	K37	ASP
K479	P390	F325	L244	K176	L38	ASP
N480	K391	A326	S245	D177	R105	ASP
F481	C392	V246	V246	F178	T106	ASP
S482	M393	E247	E247	D179	P107	ASP
D483	N394	V328	D248	M180	V43	ASP
V484	D395	E329	A249	V181	G44	ASP
H485	N396	Q330	A250	H182	P45	ASP
P486	Q397	L331	R251	D183	R46	ASP
F487	G398	A332	R254	F184	G47	ASP
Y488	P401	F333	E255	L187	L48	ASP
I492	Y404	D334	E255	R188	L50	ASP
L495	P405	S336	L261	P189	V51	ASP
K498	N406	N337	R262	E190	Q52	ASP
E501	F408	M338	D263	S191	D53	ASP
GLU	S409	P339	L264	H193	T57	ASP
LYS	A410	I342	F265	Q194	D58	ASP
PRO	P411	E343	N266	V195	B59	ASP
LYS	A412	S344	P274	D201	N60	ASP
ASN	H413	S345	S275	R202	G130	ASP
	Q414	P346	K276	F131	F63	ASP
	P415	D347	T277	G203	D64	ASP
	S416	K348	L278	I204	R65	ASP
	A417	M349	Y279	P205	B66	ASP
	L418	L350	I280	D206	T137	ASP
	E419	R353	Q281	G207	E138	ASP
	H420	Y357	T284	R208	D139	ASP
	R421		F285	E209	W142	ASP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.03Å 141.09Å 231.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.98 44.37 – 2.98	Depositor EDS
% Data completeness (in resolution range)	57.6 (39.90-2.98) 57.6 (44.37-2.98)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	0.30	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.73 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.235 , 0.292 0.227 , 0.281	Depositor DCC
$R_{free}$ test set	1000 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 57.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 33297 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	16915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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, 3TR

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	0.60	5/4137 (0.1%)	1.78	61/5619 (1.1%)
1	B	0.99	6/4137 (0.1%)	1.45	31/5619 (0.6%)
1	C	0.66	8/4137 (0.2%)	1.49	33/5619 (0.6%)
1	D	0.61	1/4137 (0.0%)	0.92	9/5619 (0.2%)
All	All	0.73	20/16548 (0.1%)	1.44	134/22476 (0.6%)

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	1	2
1	B	1	3
1	C	2	2
1	D	1	0
All	All	5	7

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CD-NE	49.16	2.30	1.46
1	D	413	HIS	CA-CB	-20.41	1.09	1.53
1	C	202	ARG	NE-CZ	16.91	1.55	1.33
1	B	319	ARG	NE-CZ	16.04	1.53	1.33
1	A	304	HIS	CA-CB	12.45	1.81	1.53
1	B	395	ASP	N-CA	-10.72	1.25	1.46
1	C	414	GLN	CA-CB	-9.85	1.32	1.53
1	C	292	PRO	C-N	9.48	1.55	1.34
1	B	32	ASN	CB-CG	9.20	1.72	1.51
1	C	413	HIS	CB-CG	8.85	1.66	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	ARG	CD-NE	-8.49	1.32	1.46
1	C	292	PRO	CA-C	-8.49	1.35	1.52
1	B	374	VAL	CA-CB	7.16	1.69	1.54
1	A	229	VAL	CA-CB	-6.97	1.40	1.54
1	B	319	ARG	CA-CB	-6.49	1.39	1.53
1	C	485	HIS	ND1-CE1	-6.44	1.18	1.34
1	A	176	LYS	CD-CE	6.43	1.67	1.51
1	C	454	GLN	CB-CG	-5.67	1.37	1.52
1	A	280	ILE	CA-CB	5.63	1.67	1.54
1	C	485	HIS	CD2-NE2	-5.20	1.26	1.38

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	TYR	CB-CG-CD2	-68.04	80.18	121.00
1	C	202	ARG	NE-CZ-NH2	-52.67	93.97	120.30
1	B	319	ARG	NE-CZ-NH1	-46.60	97.00	120.30
1	C	202	ARG	NE-CZ-NH1	44.10	142.35	120.30
1	B	319	ARG	CG-CD-NE	-41.12	25.46	111.80
1	A	357	TYR	CB-CG-CD1	30.07	139.04	121.00
1	B	126	ARG	CD-NE-CZ	29.21	164.50	123.60
1	D	371	GLN	CB-CA-C	27.36	165.13	110.40
1	D	413	HIS	CA-CB-CG	25.33	156.66	113.60
1	A	41	LEU	CB-CA-C	25.25	158.19	110.20
1	C	483	ASP	N-CA-CB	23.82	153.48	110.60
1	B	319	ARG	CB-CG-CD	-23.52	50.45	111.60
1	B	395	ASP	CA-C-N	-23.47	65.57	117.20
1	A	54	VAL	CA-CB-CG2	-22.28	77.47	110.90
1	A	229	VAL	CA-CB-CG2	21.76	143.54	110.90
1	A	421	ARG	CG-CD-NE	21.35	156.64	111.80
1	C	453	GLU	CB-CG-CD	20.10	168.47	114.20
1	A	49	LEU	CB-CG-CD2	19.97	144.95	111.00
1	A	418	LEU	N-CA-CB	19.68	149.76	110.40
1	A	357	TYR	CA-CB-CG	19.43	150.33	113.40
1	B	395	ASP	CA-C-O	19.33	160.69	120.10
1	A	421	ARG	CB-CG-CD	19.19	161.49	111.60
1	A	395	ASP	CA-CB-CG	19.05	155.31	113.40
1	C	292	PRO	O-C-N	-18.85	92.54	122.70
1	C	501	GLU	CB-CA-C	18.64	147.68	110.40
1	A	395	ASP	N-CA-CB	18.56	144.01	110.60
1	B	487	GLU	CA-CB-CG	18.43	153.94	113.40
1	A	456	LYS	CG-CD-CE	18.25	166.65	111.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	487	GLU	CB-CG-CD	17.63	161.79	114.20
1	B	319	ARG	CA-CB-CG	17.62	152.17	113.40
1	D	453	GLU	CB-CG-CD	17.43	161.27	114.20
1	C	453	GLU	N-CA-CB	17.36	141.84	110.60
1	C	414	GLN	CA-CB-CG	16.90	150.59	113.40
1	A	456	LYS	CB-CG-CD	16.66	154.91	111.60
1	C	453	GLU	CA-CB-CG	16.14	148.91	113.40
1	C	292	PRO	N-CA-C	15.91	153.47	112.10
1	C	52	GLN	CB-CG-CD	15.58	152.11	111.60
1	B	374	VAL	CB-CA-C	-15.49	81.96	111.40
1	A	476	LYS	CD-CE-NZ	15.44	147.22	111.70
1	D	97	LYS	CG-CD-CE	15.31	157.84	111.90
1	A	402	ASN	CA-CB-CG	15.29	147.04	113.40
1	B	429	GLN	CA-CB-CG	15.22	146.89	113.40
1	A	118	GLU	N-CA-CB	-15.17	83.30	110.60
1	C	454	GLN	CB-CG-CD	14.93	150.42	111.60
1	C	454	GLN	N-CA-CB	-14.90	83.79	110.60
1	D	371	GLN	N-CA-CB	-14.50	84.49	110.60
1	A	501	GLU	CB-CA-C	14.40	139.21	110.40
1	B	412	GLU	CB-CG-CD	14.15	152.42	114.20
1	A	381	ARG	CG-CD-NE	13.99	141.18	111.80
1	A	41	LEU	N-CA-CB	-13.90	82.59	110.40
1	A	435	ASN	CB-CA-C	13.79	137.99	110.40
1	C	289	GLU	CG-CD-OE2	-13.74	90.82	118.30
1	A	97	LYS	CG-CD-CE	13.60	152.71	111.90
1	A	421	ARG	CD-NE-CZ	13.52	142.53	123.60
1	B	478	VAL	CA-CB-CG1	-13.27	90.99	110.90
1	D	453	GLU	CA-CB-CG	13.18	142.39	113.40
1	C	292	PRO	CA-C-O	13.09	151.63	120.20
1	B	412	GLU	N-CA-CB	13.08	134.14	110.60
1	A	41	LEU	CA-CB-CG	-12.72	86.05	115.30
1	B	319	ARG	NE-CZ-NH2	12.60	126.60	120.30
1	C	292	PRO	CB-CA-C	-12.43	80.93	112.00
1	A	500	ASN	N-CA-CB	-12.40	88.27	110.60
1	A	435	ASN	CA-CB-CG	12.27	140.39	113.40
1	C	414	GLN	CB-CA-C	11.89	134.18	110.40
1	A	284	THR	CA-CB-CG2	-11.83	95.83	112.40
1	C	395	ASP	CA-CB-CG	-11.79	87.45	113.40
1	C	289	GLU	CB-CA-C	11.47	133.35	110.40
1	B	374	VAL	N-CA-CB	11.24	136.22	111.50
1	D	394	MET	CB-CG-SD	10.96	145.29	112.40
1	A	101	HIS	CB-CA-C	-10.89	88.62	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ARG	CA-CB-CG	10.85	137.26	113.40
1	A	476	LYS	CG-CD-CE	10.80	144.31	111.90
1	A	202	ARG	CD-NE-CZ	10.79	138.70	123.60
1	C	289	GLU	CA-CB-CG	10.77	137.10	113.40
1	B	412	GLU	CA-CB-CG	10.74	137.03	113.40
1	C	483	ASP	CB-CA-C	-10.71	88.97	110.40
1	B	32	ASN	CA-CB-CG	-10.68	89.90	113.40
1	B	395	ASP	CA-CB-CG	10.64	136.82	113.40
1	A	304	HIS	N-CA-CB	-10.62	91.49	110.60
1	A	418	LEU	CB-CA-C	-10.59	90.08	110.20
1	A	453	GLU	CB-CG-CD	10.45	142.40	114.20
1	B	395	ASP	N-CA-CB	-10.45	91.80	110.60
1	A	456	LYS	CA-CB-CG	10.23	135.90	113.40
1	A	176	LYS	CD-CE-NZ	-10.21	88.21	111.70
1	C	231	CYS	CA-CB-SG	-10.16	95.71	114.00
1	A	490	SER	CA-CB-OG	10.15	138.61	111.20
1	A	280	ILE	CB-CA-C	-10.08	91.44	111.60
1	B	478	VAL	CA-CB-CG2	10.01	125.91	110.90
1	A	243	ASN	CB-CA-C	-9.89	90.61	110.40
1	C	501	GLU	CB-CG-CD	9.60	140.11	114.20
1	A	118	GLU	CB-CG-CD	-9.56	88.40	114.20
1	A	284	THR	CA-CB-OG1	9.54	129.02	109.00
1	A	37	LYS	CG-CD-CE	9.52	140.47	111.90
1	B	478	VAL	CB-CA-C	9.48	129.41	111.40
1	B	277	THR	CB-CA-C	9.41	137.01	111.60
1	B	416	SER	N-CA-CB	-9.39	96.42	110.50
1	C	501	GLU	N-CA-CB	-9.35	93.78	110.60
1	B	478	VAL	N-CA-CB	-8.67	92.43	111.50
1	C	454	GLN	CB-CA-C	-8.53	93.34	110.40
1	A	501	GLU	N-CA-CB	-8.24	95.76	110.60
1	C	414	GLN	N-CA-CB	-8.04	96.13	110.60
1	D	74	HIS	CA-CB-CG	7.82	126.90	113.60
1	B	319	ARG	CB-CA-C	-7.79	94.83	110.40
1	A	500	ASN	CA-CB-CG	7.76	130.47	113.40
1	A	453	GLU	CA-CB-CG	7.60	130.12	113.40
1	C	309	LEU	CB-CG-CD1	7.59	123.91	111.00
1	B	32	ASN	CB-CG-OD1	-7.58	106.45	121.60
1	B	374	VAL	CA-CB-CG1	-7.56	99.56	110.90
1	C	309	LEU	CB-CG-CD2	-7.53	98.20	111.00
1	A	49	LEU	CB-CG-CD1	-7.48	98.28	111.00
1	A	284	THR	CB-CA-C	-7.48	91.40	111.60
1	C	478	VAL	CB-CA-C	7.30	125.27	111.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	VAL	CA-CB-CG2	-7.27	99.99	110.90
1	A	280	ILE	CA-CB-CG1	7.17	124.62	111.00
1	A	280	ILE	CA-CB-CG2	-7.16	96.58	110.90
1	A	435	ASN	N-CA-CB	-7.10	97.82	110.60
1	A	101	HIS	N-CA-CB	6.77	122.78	110.60
1	A	395	ASP	CB-CA-C	-6.67	97.05	110.40
1	C	292	PRO	C-N-CA	6.66	138.35	121.70
1	B	395	ASP	N-CA-C	6.50	128.56	111.00
1	C	202	ARG	CD-NE-CZ	6.28	132.39	123.60
1	A	176	LYS	CG-CD-CE	6.19	130.47	111.90
1	B	319	ARG	N-CA-CB	5.97	121.35	110.60
1	A	342	ILE	CB-CA-C	-5.96	99.69	111.60
1	C	413	HIS	CB-CG-ND1	-5.62	109.14	123.20
1	A	229	VAL	CB-CA-C	-5.62	100.71	111.40
1	A	37	LYS	CD-CE-NZ	-5.54	98.96	111.70
1	A	54	VAL	CB-CA-C	5.49	121.83	111.40
1	A	342	ILE	N-CA-CB	5.47	123.39	110.80
1	A	353	ARG	CA-CB-CG	5.46	125.41	113.40
1	A	500	ASN	CB-CA-C	5.44	121.28	110.40
1	D	20	ALA	N-CA-CB	-5.37	102.58	110.10
1	C	236	LYS	CG-CD-CE	5.22	127.57	111.90
1	A	304	HIS	CB-CA-C	5.08	120.57	110.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	395	ASP	CA
1	B	395	ASP	CA
1	C	453	GLU	CA
1	C	501	GLU	CA
1	D	371	GLN	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	TYR	Sidechain
1	A	421	ARG	Sidechain
1	B	126	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	394	MET	Peptide
1	C	289	GLU	Sidechain
1	C	292	PRO	Peptide

## 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	4017	0	3838	473	1
1	B	4017	0	3839	431	0
1	C	4017	0	3840	429	0
1	D	4017	0	3839	389	0
2	D	6	0	3	12	0
3	A	43	0	30	79	0
3	B	43	0	30	39	0
3	C	43	0	30	49	0
3	D	43	0	30	25	0
4	A	154	0	0	30	0
4	B	145	0	0	28	0
4	C	188	0	0	17	1
4	D	182	0	0	14	0
All	All	16915	0	15479	1562	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 49.

All (1562) 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:304:HIS:CB	1:A:304:HIS:CA	1.81	1.58
1:A:100:GLU:HG2	1:A:101:HIS:CE1	1.43	1.52
3:A:2000:HEM:CBC	3:A:2000:HEM:CAC	1.87	1.47
1:A:353:ARG:HD2	3:A:2000:HEM:CHC	1.53	1.37
1:C:111:ARG:NE	3:C:2002:HEM:O1D	1.57	1.36
1:A:353:ARG:N	3:A:2000:HEM:HBB2	1.37	1.35
4:B:2096:HOH:O	1:D:38:LEU:HD11	1.16	1.33
1:B:147:ASN:N	3:B:2001:HEM:HBC1	1.45	1.30
1:C:160:PHE:CD1	3:C:2002:HEM:HAB	1.69	1.28
1:D:368:ASN:HB3	1:D:371:GLN:NE2	1.47	1.27
1:A:353:ARG:CZ	3:A:2000:HEM:C3C	2.18	1.26
1:A:353:ARG:HH11	3:A:2000:HEM:CMC	1.48	1.26
1:D:319:ARG:NH2	4:D:3243:HOH:O	1.63	1.26
1:C:147:ASN:CG	3:C:2002:HEM:HAC	1.55	1.26

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:O	1:A:101:HIS:ND1	1.65	1.26
1:A:353:ARG:NH1	3:A:2000:HEM:C3C	2.05	1.25
1:A:353:ARG:HD2	3:A:2000:HEM:C1C	1.70	1.24
1:C:147:ASN:OD1	3:C:2002:HEM:HAC	1.32	1.23
1:A:100:GLU:CG	1:A:101:HIS:CE1	2.24	1.20
1:B:304:HIS:HE1	4:B:2134:HOH:O	1.24	1.20
1:A:353:ARG:NH1	3:A:2000:HEM:C2C	2.11	1.19
1:A:72:VAL:CG1	3:A:2000:HEM:HMA3	1.72	1.17
1:D:368:ASN:O	1:D:371:GLN:HG3	1.43	1.17
1:A:145:VAL:HB	1:A:353:ARG:HH21	1.04	1.15
1:B:137:THR:HB	4:B:2131:HOH:O	1.44	1.15
1:A:353:ARG:HH11	3:A:2000:HEM:HMC3	0.97	1.14
1:A:72:VAL:HG11	3:A:2000:HEM:CMA	1.78	1.12
1:A:145:VAL:HG13	3:A:2000:HEM:HMD3	1.30	1.10
1:A:72:VAL:CG1	3:A:2000:HEM:CMA	2.32	1.07
1:A:100:GLU:HG2	1:A:101:HIS:ND1	1.67	1.07
1:B:223:ASN:HD21	1:B:227:GLU:HB2	1.14	1.07
4:B:2096:HOH:O	1:D:38:LEU:CD1	1.79	1.06
2:D:3074:3TR:N2	3:D:2003:HEM:C1C	2.23	1.06
1:A:398:GLY:HA2	1:C:323:ASN:HB2	1.38	1.06
1:A:353:ARG:NH1	3:A:2000:HEM:CAC	2.19	1.05
1:A:41:LEU:HB2	1:D:430:ARG:HG2	1.39	1.05
1:C:111:ARG:HE	3:C:2002:HEM:CGD	1.69	1.05
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.16	1.05
1:D:223:ASN:HD21	1:D:227:GLU:HB3	1.17	1.04
1:C:160:PHE:CG	3:C:2002:HEM:HAB	1.93	1.04
1:A:353:ARG:N	3:A:2000:HEM:CBB	2.21	1.04
1:A:145:VAL:CG1	3:A:2000:HEM:CMD	2.35	1.03
1:A:100:GLU:C	1:A:101:HIS:ND1	2.12	1.03
1:A:145:VAL:CG1	3:A:2000:HEM:HMD3	1.89	1.02
1:C:147:ASN:OD1	3:C:2002:HEM:CAC	2.07	1.01
1:A:353:ARG:NH1	3:A:2000:HEM:CMC	2.19	1.01
1:A:71:ARG:HD3	3:A:2000:HEM:O2A	1.59	1.01
1:A:145:VAL:HB	1:A:353:ARG:NH2	1.74	1.01
1:B:147:ASN:N	3:B:2001:HEM:CBC	2.22	1.01
1:A:145:VAL:HG12	3:A:2000:HEM:CMD	1.90	1.00
1:A:72:VAL:HG11	3:A:2000:HEM:HMA3	1.03	1.00
1:C:381:ARG:NH1	4:C:2010:HOH:O	1.93	0.99
1:A:145:VAL:HB	3:A:2000:HEM:HBC2	1.41	0.99
1:B:304:HIS:CE1	4:B:2134:HOH:O	2.05	0.99
1:A:145:VAL:CG1	3:A:2000:HEM:C2D	2.46	0.98

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:GLN:HA	1:B:496:LEU:HD12	1.45	0.98
1:B:147:ASN:HD21	3:B:2001:HEM:HMC3	1.26	0.97
1:C:142:TRP:HB2	1:C:339:PRO:HD3	1.45	0.97
1:A:335:PRO:HG2	1:A:353:ARG:HG2	1.46	0.96
1:B:147:ASN:H	3:B:2001:HEM:HBC1	1.04	0.96
2:D:3074:3TR:C3	3:D:2003:HEM:NC	2.28	0.95
1:D:261:LEU:O	4:D:3114:HOH:O	1.84	0.95
1:A:353:ARG:H	3:A:2000:HEM:HBB2	1.24	0.95
1:A:353:ARG:CD	3:A:2000:HEM:CHC	2.45	0.95
3:A:2000:HEM:HHA	3:A:2000:HEM:HBA2	1.47	0.94
1:A:353:ARG:CA	3:A:2000:HEM:HBB2	1.98	0.94
1:A:300:LYS:HB3	1:A:441:GLN:HE22	1.34	0.93
1:D:368:ASN:O	1:D:371:GLN:CG	2.15	0.93
1:A:433:SER:HB3	4:A:2003:HOH:O	1.68	0.92
1:A:353:ARG:NH1	3:A:2000:HEM:HMC3	1.82	0.92
1:A:92:ARG:HD2	4:A:2023:HOH:O	1.70	0.91
1:A:353:ARG:CD	3:A:2000:HEM:C1C	2.54	0.91
1:B:404:TYR:CE2	4:B:2096:HOH:O	2.22	0.91
1:B:146:GLY:HA2	3:B:2001:HEM:CBC	2.01	0.91
1:D:368:ASN:CB	1:D:371:GLN:NE2	2.32	0.90
1:C:142:TRP:HB2	1:C:339:PRO:CD	2.01	0.90
1:C:18:ARG:HH12	1:C:23:PRO:HA	1.36	0.90
1:A:262:ARG:HD2	4:A:2044:HOH:O	1.71	0.90
1:D:17:GLN:NE2	4:D:3179:HOH:O	2.02	0.90
1:A:404:TYR:H	1:B:162:SER:HB3	1.37	0.89
1:A:100:GLU:CG	1:A:101:HIS:HE1	1.81	0.89
1:D:145:VAL:HG12	3:D:2003:HEM:HHD	1.54	0.89
1:A:392:CYS:SG	1:A:396:ASN:ND2	2.45	0.89
1:C:406:ASN:ND2	1:C:410:ALA:HB3	1.87	0.89
1:A:145:VAL:CG1	3:A:2000:HEM:C1D	2.55	0.89
1:C:432:ASN:HD22	1:C:433:SER:N	1.69	0.89
1:A:304:HIS:CB	1:A:304:HIS:N	2.35	0.89
1:A:353:ARG:HE	1:A:357:TYR:HE1	1.18	0.88
2:D:3074:3TR:N2	3:D:2003:HEM:NC	2.22	0.88
1:A:353:ARG:HH12	3:A:2000:HEM:CAC	1.84	0.88
1:C:147:ASN:CG	3:C:2002:HEM:CAC	2.41	0.88
1:A:235:TYR:HB3	1:A:278:LEU:HD12	1.55	0.88
1:A:41:LEU:CB	1:D:430:ARG:NH1	2.37	0.88
1:A:353:ARG:HG2	1:A:357:TYR:CE1	2.09	0.88
1:A:322:VAL:HA	1:D:172:GLN:HE21	1.39	0.88
1:A:145:VAL:HG12	3:A:2000:HEM:CHD	2.04	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:VAL:HG13	1:D:48:PRO:HD2	1.55	0.88
1:D:291:PHE:HD1	1:D:293:PHE:H	1.15	0.87
1:B:450:LEU:HB3	1:B:454:GLN:HG3	1.53	0.87
1:A:353:ARG:HD2	3:A:2000:HEM:C4B	2.09	0.87
1:D:177:ASP:HB3	1:D:180:MET:HB2	1.53	0.87
1:D:406:ASN:HD21	1:D:410:ALA:HB3	1.38	0.87
1:C:71:ARG:HB3	3:C:2002:HEM:HAA1	1.55	0.87
1:A:353:ARG:CZ	3:A:2000:HEM:CAC	2.53	0.87
1:D:170:ASN:ND2	1:D:172:GLN:H	1.73	0.86
1:A:41:LEU:HB3	1:D:430:ARG:NH1	1.90	0.86
1:A:384:ASN:OD1	1:A:386:GLN:HB2	1.76	0.86
1:B:41:LEU:HD11	1:C:428:VAL:HG12	1.57	0.86
1:A:148:ASN:C	1:A:148:ASN:HD22	1.78	0.86
1:D:22:LYS:HE3	1:D:22:LYS:HA	1.57	0.85
1:B:443:ARG:NH2	4:B:2018:HOH:O	2.08	0.85
1:D:420:HIS:ND1	4:D:3158:HOH:O	2.08	0.85
1:B:112:PHE:HA	1:B:130:GLY:O	1.77	0.85
1:C:332:ALA:HB1	1:C:361:HIS:CE1	2.12	0.85
1:A:239:GLN:HE22	1:A:275:SER:H	1.21	0.85
1:B:147:ASN:ND2	3:B:2001:HEM:CBC	2.40	0.84
1:D:285:PHE:HD1	1:D:285:PHE:H	1.25	0.84
1:B:323:ASN:HD21	1:D:396:ASN:HD22	1.21	0.84
3:A:2000:HEM:CBC	3:A:2000:HEM:C3C	2.60	0.84
1:A:145:VAL:HG12	3:A:2000:HEM:HHD	1.58	0.84
3:A:2000:HEM:CBC	3:A:2000:HEM:HHD	2.08	0.84
1:A:145:VAL:CB	3:A:2000:HEM:HBC2	2.08	0.83
1:B:85:GLU:HG3	1:B:105:ARG:HG2	1.59	0.83
1:A:145:VAL:HG11	3:A:2000:HEM:C1D	2.12	0.83
1:A:208:HIS:HA	1:A:211:MET:HE3	1.57	0.83
1:C:432:ASN:ND2	1:C:434:ALA:H	1.77	0.83
1:B:495:LEU:HD21	4:B:2081:HOH:O	1.78	0.83
1:C:190:GLU:HA	1:C:438:ASN:HB3	1.61	0.82
1:B:360:THR:OG1	1:C:64:ASP:HB3	1.78	0.82
1:A:15:LYS:HD2	1:C:408:PHE:HA	1.59	0.82
1:A:402:ASN:ND2	1:B:165:HIS:HB3	1.94	0.82
1:D:286:SER:O	1:D:289:GLU:HB3	1.80	0.82
1:A:129:ARG:HB2	1:A:148:ASN:HB3	1.62	0.81
1:D:189:PRO:HG3	1:D:480:ASN:HD21	1.43	0.81
1:A:39:ASN:ND2	1:D:432:ASN:HA	1.96	0.81
1:C:92:ARG:HD3	1:C:92:ARG:H	1.42	0.81
1:C:252:LEU:HD21	4:C:2147:HOH:O	1.80	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASN:ND2	1:B:227:GLU:HB2	1.93	0.81
1:C:111:ARG:HH21	3:C:2002:HEM:CAD	1.94	0.81
1:B:37:LYS:HG3	1:B:37:LYS:O	1.80	0.81
1:B:353:ARG:NH2	3:B:2001:HEM:C2C	2.49	0.80
1:D:439:VAL:HG23	1:D:440:THR:H	1.46	0.80
1:A:52:GLN:HG3	1:C:351:GLN:HE22	1.47	0.80
1:A:186:SER:HB2	1:A:476:LYS:HG2	1.64	0.80
1:C:116:ALA:HA	1:C:168:LYS:HE2	1.64	0.80
1:B:323:ASN:ND2	1:D:396:ASN:HB3	1.96	0.80
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.46	0.80
1:B:353:ARG:NH2	3:B:2001:HEM:C1C	2.50	0.80
1:B:451:ASN:O	1:B:455:ARG:HB2	1.81	0.80
1:C:160:PHE:CD1	3:C:2002:HEM:CAB	2.61	0.79
1:B:177:ASP:O	1:B:181:VAL:HG23	1.82	0.79
1:A:427:ASP:OD1	1:B:423:HIS:HB2	1.83	0.79
1:C:151:ILE:HD13	1:C:193:HIS:ND1	1.98	0.79
1:B:146:GLY:C	3:B:2001:HEM:HBC1	2.02	0.78
1:C:111:ARG:NE	3:C:2002:HEM:CGD	2.36	0.78
1:B:323:ASN:HD21	1:D:396:ASN:ND2	1.80	0.78
1:B:444:THR:HG22	4:B:2094:HOH:O	1.82	0.78
3:B:2001:HEM:HMC1	3:B:2001:HEM:HBC2	1.66	0.78
1:A:150:PRO:HB3	1:A:214:TYR:CD1	2.18	0.78
1:A:183:ASP:O	1:A:187:LEU:HG	1.81	0.78
1:D:155:ARG:HD3	1:D:297:ASP:CG	2.04	0.78
1:D:43:VAL:CG1	1:D:48:PRO:HD2	2.14	0.78
1:B:147:ASN:ND2	3:B:2001:HEM:HMC3	1.99	0.77
1:C:487:GLU:HA	1:C:490:SER:HB3	1.64	0.77
1:A:387:ARG:CZ	1:A:397:GLN:HB2	2.13	0.77
1:A:41:LEU:HB2	1:D:430:ARG:CG	2.14	0.77
1:C:488:TYR:O	1:C:492:ILE:HG12	1.85	0.77
1:B:190:GLU:HA	1:B:438:ASN:HB3	1.64	0.77
1:A:145:VAL:HG12	3:A:2000:HEM:C1D	2.20	0.77
1:D:358:PRO:O	1:D:362:ARG:HG3	1.85	0.77
1:C:466:LEU:HD12	1:C:466:LEU:O	1.84	0.77
1:D:129:ARG:HB2	1:D:148:ASN:OD1	1.85	0.77
1:C:209:ARG:NH1	1:C:209:ARG:HB2	2.00	0.76
1:C:239:GLN:HE22	1:C:275:SER:H	1.30	0.76
1:B:353:ARG:NH2	3:B:2001:HEM:C3C	2.52	0.76
3:A:2000:HEM:HBA2	3:A:2000:HEM:CHA	2.13	0.76
1:B:92:ARG:NH1	1:B:92:ARG:HB2	2.00	0.76
1:B:333:PHE:HD2	3:B:2001:HEM:CGD	1.99	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLY:HA2	4:A:2013:HOH:O	1.84	0.76
1:A:353:ARG:H	3:A:2000:HEM:CBB	1.88	0.76
1:B:457:ARG:HH11	1:B:457:ARG:HB2	1.51	0.76
1:B:74:HIS:CE1	1:B:115:VAL:HG22	2.21	0.76
1:A:145:VAL:HG12	3:A:2000:HEM:C2D	2.15	0.76
1:A:145:VAL:CG1	3:A:2000:HEM:CHD	2.64	0.76
2:D:3074:3TR:C3	3:D:2003:HEM:C1C	2.69	0.76
1:A:66:GLU:HG2	1:C:387:ARG:O	1.85	0.75
1:C:146:GLY:C	3:C:2002:HEM:HBC1	2.06	0.75
1:A:356:ALA:CB	3:A:2000:HEM:HMB2	2.16	0.75
1:A:64:ASP:O	1:D:360:THR:HG23	1.85	0.75
1:D:368:ASN:HB3	1:D:371:GLN:HE21	1.48	0.75
1:B:76:LYS:HE3	1:B:121:SER:O	1.86	0.75
1:A:72:VAL:HG12	3:A:2000:HEM:CMA	2.17	0.74
1:B:212:ASP:OD1	1:B:236:LYS:HA	1.86	0.74
1:B:336:SER:O	4:B:2034:HOH:O	2.05	0.74
4:A:2073:HOH:O	1:C:382:VAL:HG21	1.85	0.74
1:A:413:HIS:O	1:A:415:PRO:HD3	1.87	0.74
1:B:120:GLY:O	4:B:2115:HOH:O	2.04	0.74
1:B:145:VAL:HG12	3:B:2001:HEM:CHD	2.17	0.74
1:A:48:PRO:HB2	1:B:50:LEU:HD12	1.68	0.74
1:A:487:GLU:O	1:A:491:ARG:HG3	1.88	0.74
1:A:353:ARG:CZ	3:A:2000:HEM:C4C	2.70	0.74
1:B:404:TYR:OH	4:B:2096:HOH:O	2.06	0.74
1:C:18:ARG:O	1:C:18:ARG:HD3	1.87	0.74
1:A:209:ARG:HG2	1:A:274:PRO:HB3	1.68	0.74
1:A:244:LEU:HD11	1:A:259:TYR:HE1	1.51	0.74
1:B:129:ARG:HB3	1:B:211:MET:HE1	1.69	0.74
1:B:353:ARG:NH2	3:B:2001:HEM:C4C	2.56	0.73
1:A:223:ASN:ND2	1:A:227:GLU:HB2	2.03	0.73
1:B:145:VAL:HG21	1:B:335:PRO:HD3	1.70	0.73
1:A:208:HIS:HA	1:A:211:MET:CE	2.17	0.73
1:B:147:ASN:HD21	3:B:2001:HEM:CMC	2.02	0.73
1:B:5:ASP:OD2	1:B:7:ALA:HB3	1.88	0.73
1:C:287:GLU:HA	1:C:290:ILE:HG12	1.70	0.73
1:A:353:ARG:CZ	3:A:2000:HEM:C2C	2.61	0.73
1:A:356:ALA:HB3	3:A:2000:HEM:HMB2	1.71	0.73
1:B:466:LEU:HD22	1:B:474:GLN:HG2	1.70	0.73
1:D:209:ARG:HG2	1:D:274:PRO:HB3	1.70	0.73
1:A:49:LEU:O	1:B:51:VAL:HG22	1.88	0.73
1:A:228:ALA:O	1:A:229:VAL:HG13	1.89	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:HD2	1:A:433:SER:O	1.88	0.73
1:A:71:ARG:HD3	3:A:2000:HEM:CGA	2.19	0.73
4:B:2034:HOH:O	1:D:54:VAL:HG21	1.88	0.73
1:A:145:VAL:HB	3:A:2000:HEM:CBC	2.19	0.72
1:A:72:VAL:HG12	3:A:2000:HEM:HMA2	1.69	0.72
1:C:298:LEU:CD2	1:C:349:MET:HG2	2.19	0.72
1:A:223:ASN:HD21	1:A:227:GLU:HB2	1.52	0.72
1:C:336:SER:HA	1:C:354:LEU:HD22	1.71	0.72
1:B:331:LEU:HD23	1:B:374:VAL:HB	1.72	0.72
1:D:338:MET:CE	1:D:342:ILE:HG22	2.19	0.72
1:C:35:GLY:O	4:C:2038:HOH:O	2.08	0.71
1:A:50:LEU:HD12	1:B:48:PRO:HB2	1.70	0.71
1:B:146:GLY:CA	3:B:2001:HEM:CBC	2.68	0.71
1:B:38:LEU:HD13	1:C:188:ARG:NH2	2.06	0.71
1:A:239:GLN:NE2	1:A:275:SER:H	1.88	0.71
1:D:189:PRO:HG3	1:D:480:ASN:ND2	2.03	0.71
1:D:43:VAL:O	1:D:47:GLY:HA3	1.91	0.71
1:A:148:ASN:C	1:A:148:ASN:ND2	2.43	0.71
1:B:147:ASN:ND2	3:B:2001:HEM:HBC2	2.06	0.71
1:B:454:GLN:HA	1:B:457:ARG:NH1	2.04	0.71
1:A:72:VAL:CG1	3:A:2000:HEM:HMA2	2.17	0.71
1:D:439:VAL:HG23	1:D:440:THR:N	2.06	0.71
1:B:439:VAL:O	1:B:442:VAL:HB	1.91	0.71
1:A:14:TRP:CZ3	1:A:18:ARG:HD2	2.26	0.71
1:D:274:PRO:HG2	1:D:317:LEU:HB2	1.72	0.71
1:A:501:GLU:HG3	4:A:2124:HOH:O	1.91	0.71
1:A:87:THR:OG1	1:A:313:GLY:HA2	1.91	0.70
1:B:404:TYR:HE2	4:B:2096:HOH:O	1.68	0.70
1:C:347:ASP:HB3	1:C:350:LEU:HB3	1.74	0.70
1:A:73:VAL:O	1:A:74:HIS:HB2	1.90	0.70
1:B:146:GLY:HA2	3:B:2001:HEM:HBC1	1.73	0.70
1:A:51:VAL:HG12	1:B:51:VAL:HA	1.72	0.70
1:A:145:VAL:HG12	3:A:2000:HEM:HMD1	1.74	0.70
1:C:162:SER:HB3	1:D:404:TYR:H	1.55	0.70
1:D:94:SER:HB2	1:D:221:LEU:HD22	1.72	0.70
1:B:229:VAL:HG23	1:B:284:THR:HA	1.74	0.70
2:D:3074:3TR:N2	3:D:2003:HEM:C4C	2.59	0.70
1:C:360:THR:HG21	3:C:2002:HEM:HMA3	1.74	0.70
1:C:298:LEU:HD22	1:C:349:MET:HG2	1.72	0.70
1:B:445:PHE:HA	1:B:449:VAL:HG23	1.73	0.70
1:C:396:ASN:O	1:C:397:GLN:HB2	1.91	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PRO:HD3	4:A:2048:HOH:O	1.91	0.70
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.73	0.70
1:B:50:LEU:N	1:B:50:LEU:HD22	2.07	0.70
1:D:459:CYS:HB3	1:D:492:ILE:HG12	1.74	0.70
1:A:151:ILE:HD13	1:A:193:HIS:CE1	2.26	0.70
4:A:2144:HOH:O	1:B:171:PRO:HG3	1.91	0.69
1:D:338:MET:HE2	1:D:342:ILE:HG22	1.73	0.69
1:D:220:LYS:HG3	1:D:344:PRO:O	1.92	0.69
1:A:401:PRO:HA	4:A:2144:HOH:O	1.91	0.69
1:D:192:LEU:HD13	1:D:484:VAL:HG23	1.74	0.69
1:B:80:ALA:HA	1:B:321:PRO:HD3	1.75	0.69
1:A:71:ARG:HD2	1:A:111:ARG:NH2	2.08	0.69
1:D:147:ASN:CG	3:D:2003:HEM:HAC	2.13	0.69
1:A:353:ARG:CG	1:A:357:TYR:CE1	2.75	0.69
1:B:146:GLY:C	3:B:2001:HEM:CBC	2.59	0.69
1:C:410:ALA:HB1	1:C:411:PRO:HD2	1.73	0.69
4:A:2057:HOH:O	1:B:423:HIS:HE1	1.75	0.69
1:A:131:PHE:HD2	1:A:213:GLY:HA3	1.57	0.69
1:A:331:LEU:HD13	1:A:374:VAL:HG22	1.75	0.69
1:A:24:ASP:HB3	1:C:381:ARG:HH12	1.58	0.69
1:C:81:PHE:HZ	1:C:327:GLU:HB3	1.58	0.69
1:B:71:ARG:HE	1:B:111:ARG:CZ	2.06	0.69
1:A:41:LEU:HB2	1:D:430:ARG:NH1	2.07	0.69
1:C:280:ILE:HG23	1:C:312:VAL:HG21	1.74	0.69
1:D:86:VAL:HG23	1:D:104:LYS:O	1.92	0.69
1:A:468:ASP:HB3	4:A:2062:HOH:O	1.93	0.69
1:A:393:MET:SD	1:C:393:MET:HG3	2.32	0.69
1:B:357:TYR:OH	3:B:2001:HEM:NC	2.26	0.68
1:A:41:LEU:O	1:A:41:LEU:HD23	1.93	0.68
1:B:150:PRO:HA	1:B:216:SER:HA	1.75	0.68
1:B:146:GLY:CA	3:B:2001:HEM:HBC1	2.22	0.68
1:C:126:ARG:HH11	1:C:126:ARG:HG2	1.57	0.68
1:C:453:GLU:HB3	1:C:457:ARG:NH2	2.08	0.68
1:C:235:TYR:HA	1:C:277:THR:O	1.93	0.68
1:B:84:PHE:O	1:B:105:ARG:HA	1.94	0.68
1:C:206:ASP:HB2	1:C:244:LEU:HD23	1.76	0.68
1:C:51:VAL:O	4:C:2011:HOH:O	2.11	0.68
1:A:235:TYR:HB3	1:A:278:LEU:CD1	2.23	0.68
1:C:160:PHE:CE2	3:C:2002:HEM:C2B	2.82	0.68
1:C:71:ARG:HB3	3:C:2002:HEM:CAA	2.23	0.68
1:A:41:LEU:HB3	1:D:430:ARG:CZ	2.24	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ASN:ND2	1:B:410:ALA:HB3	2.09	0.68
1:D:281:GLN:OE1	1:D:302:TRP:HB2	1.94	0.68
1:D:347:ASP:HB3	1:D:350:LEU:HB3	1.75	0.68
1:B:291:PHE:CD1	1:B:292:PRO:HD2	2.29	0.68
1:B:279:TYR:O	1:B:280:ILE:HG23	1.94	0.68
1:C:211:MET:O	1:C:237:THR:HB	1.94	0.68
1:C:404:TYR:OH	1:C:413:HIS:HD2	1.77	0.68
1:B:404:TYR:CZ	4:B:2096:HOH:O	2.43	0.67
1:A:131:PHE:CD2	1:A:213:GLY:HA3	2.30	0.67
1:A:168:LYS:HE3	1:D:67:ARG:HH21	1.59	0.67
1:C:191:SER:O	1:C:195:VAL:HG23	1.93	0.67
3:A:2000:HEM:CBC	3:A:2000:HEM:CHD	2.72	0.67
1:A:244:LEU:HD11	1:A:259:TYR:CE1	2.28	0.67
1:A:353:ARG:NH2	3:A:2000:HEM:CAC	2.58	0.67
1:C:78:ALA:HB2	1:C:261:LEU:HD22	1.76	0.67
1:C:100:GLU:HG2	4:C:2008:HOH:O	1.95	0.67
1:C:217:HIS:CD2	1:C:350:LEU:HB2	2.30	0.67
1:B:19:ALA:HB3	1:B:21:GLN:HE21	1.59	0.67
1:B:367:PRO:HG2	1:B:390:PRO:CG	2.24	0.67
3:A:2000:HEM:HBC2	3:A:2000:HEM:HHD	1.76	0.67
1:B:146:GLY:C	3:B:2001:HEM:HAC	2.14	0.67
1:D:368:ASN:HB3	1:D:371:GLN:CD	2.13	0.67
1:D:114:THR:HG22	1:D:127:ASP:OD2	1.94	0.67
1:A:242:LYS:HD3	1:A:243:ASN:N	2.10	0.67
3:A:2000:HEM:CHD	3:A:2000:HEM:HBC2	2.25	0.67
1:C:72:VAL:HG13	1:C:73:VAL:HG13	1.76	0.67
1:B:494:ALA:HB1	4:B:2086:HOH:O	1.93	0.67
1:B:97:LYS:HB2	4:B:2131:HOH:O	1.95	0.67
1:A:323:ASN:ND2	1:C:396:ASN:HB3	2.10	0.67
1:D:116:ALA:O	1:D:168:LYS:NZ	2.28	0.67
1:C:111:ARG:CZ	3:C:2002:HEM:O1D	2.43	0.66
1:A:383:ALA:O	1:C:26:LEU:HA	1.95	0.66
1:C:212:ASP:OD1	1:C:236:LYS:HA	1.94	0.66
1:D:223:ASN:ND2	1:D:227:GLU:HB3	2.02	0.66
1:B:412:GLU:OE2	1:D:23:PRO:HG2	1.95	0.66
1:A:258:ASP:HB3	1:A:261:LEU:HD12	1.76	0.66
1:A:450:LEU:HA	1:A:454:GLN:NE2	2.11	0.66
1:C:111:ARG:HH21	3:C:2002:HEM:HAD1	1.60	0.66
1:C:239:GLN:HE22	1:C:275:SER:N	1.93	0.66
1:C:160:PHE:CE1	3:C:2002:HEM:HAB	2.27	0.66
1:D:155:ARG:HD3	1:D:297:ASP:OD2	1.96	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PRO:HD2	1:C:46:ARG:HH12	1.61	0.66
1:C:154:ILE:HG13	1:C:349:MET:HE2	1.78	0.66
1:C:206:ASP:HB2	1:C:244:LEU:CD2	2.26	0.65
1:C:402:ASN:ND2	1:D:171:PRO:HD3	2.11	0.65
1:B:146:GLY:C	3:B:2001:HEM:CAC	2.65	0.65
1:B:466:LEU:HB3	1:B:496:LEU:HD21	1.78	0.65
1:C:423:HIS:HA	1:D:427:ASP:HA	1.77	0.65
1:B:94:SER:HB2	1:B:221:LEU:HD22	1.77	0.65
1:D:353:ARG:NH2	3:D:2003:HEM:C4C	2.65	0.65
1:C:179:ASP:O	1:C:183:ASP:HB2	1.97	0.65
1:C:487:GLU:OE2	1:C:491:ARG:HD2	1.97	0.65
1:D:169:ARG:HB3	1:D:174:HIS:C	2.17	0.65
1:A:363:HIS:CD2	1:D:65:ARG:HA	2.31	0.65
1:B:404:TYR:HE2	1:D:38:LEU:HG	1.60	0.65
1:A:24:ASP:HB3	1:C:381:ARG:NH1	2.12	0.65
1:C:18:ARG:NH1	1:C:23:PRO:HA	2.10	0.65
1:D:170:ASN:HD22	1:D:172:GLN:H	1.43	0.65
1:B:183:ASP:O	1:B:187:LEU:HG	1.96	0.65
1:B:428:VAL:O	1:B:428:VAL:HG23	1.94	0.65
1:D:26:LEU:HD22	1:D:34:VAL:HG21	1.78	0.65
1:C:492:ILE:HG22	1:C:496:LEU:HD23	1.79	0.65
1:A:353:ARG:HD3	3:A:2000:HEM:HMC3	1.78	0.64
1:B:64:ASP:HB3	1:C:360:THR:HB	1.77	0.64
1:D:232:LYS:HE3	1:D:302:TRP:CE2	2.32	0.64
1:C:214:TYR:O	1:C:216:SER:N	2.30	0.64
1:A:26:LEU:CD1	1:C:384:ASN:HA	2.28	0.64
1:D:191:SER:O	1:D:195:VAL:HG23	1.98	0.64
1:A:206:ASP:H	1:A:243:ASN:HA	1.61	0.64
1:D:26:LEU:HD22	1:D:34:VAL:CG2	2.27	0.64
1:C:214:TYR:C	1:C:216:SER:N	2.49	0.64
1:A:144:LEU:HD11	1:A:233:PHE:CG	2.32	0.64
1:A:41:LEU:CB	1:D:430:ARG:CZ	2.75	0.64
1:C:346:PRO:O	1:C:347:ASP:C	2.34	0.64
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.78	0.64
1:B:464:GLY:O	1:B:467:LYS:HE3	1.98	0.64
1:C:439:VAL:HG12	1:C:484:VAL:HG22	1.80	0.64
1:A:192:LEU:HD12	1:A:438:ASN:O	1.98	0.64
1:D:112:PHE:HA	1:D:130:GLY:O	1.96	0.64
1:D:138:GLU:HA	1:D:379:ARG:O	1.97	0.64
1:B:251:ARG:HH11	1:B:251:ARG:HG2	1.62	0.64
1:A:239:GLN:HE22	1:A:275:SER:N	1.92	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:HIS:HA	1:C:211:MET:HE3	1.79	0.63
1:A:35:GLY:HA2	1:C:414:GLN:O	1.98	0.63
1:D:12:LYS:HG2	1:D:16:GLU:OE1	1.97	0.63
1:D:299:THR:OG1	1:D:300:LYS:HD2	1.98	0.63
1:B:135:PHE:HD1	1:B:142:TRP:O	1.81	0.63
1:C:160:PHE:CG	3:C:2002:HEM:CAB	2.79	0.63
1:A:146:GLY:HA2	1:A:214:TYR:O	1.98	0.63
1:C:208:HIS:HA	1:C:211:MET:CE	2.29	0.63
1:C:310:ILE:HD12	1:C:310:ILE:N	2.14	0.63
1:C:110:VAL:HG22	1:C:133:VAL:HG22	1.81	0.63
1:B:62:HIS:HE1	1:D:368:ASN:HD21	1.47	0.63
1:A:189:PRO:O	1:A:192:LEU:HG	1.98	0.63
1:A:368:ASN:HB3	1:A:371:GLN:NE2	2.14	0.63
1:A:132:ALA:HB2	3:A:2000:HEM:HMD3	1.81	0.63
1:C:43:VAL:HG21	1:D:43:VAL:HG21	1.79	0.63
1:B:408:PHE:CD1	1:D:11:MET:HB3	2.33	0.63
1:A:170:ASN:OD1	1:A:172:GLN:N	2.32	0.63
1:A:73:VAL:HG23	1:A:74:HIS:HD2	1.64	0.63
1:A:43:VAL:CG1	1:A:48:PRO:HD2	2.29	0.63
1:C:353:ARG:HD2	1:C:357:TYR:CE1	2.34	0.62
1:C:147:ASN:HB2	3:C:2002:HEM:HBC1	1.80	0.62
1:C:456:LYS:O	1:C:460:GLU:HG3	1.98	0.62
1:C:432:ASN:HD22	1:C:433:SER:H	1.46	0.62
1:A:428:VAL:HG11	1:D:50:LEU:HD11	1.81	0.62
1:C:193:HIS:CA	1:C:442:VAL:HG22	2.29	0.62
1:D:114:THR:HG22	1:D:115:VAL:H	1.64	0.62
1:C:82:GLY:HA3	1:C:316:VAL:O	2.00	0.62
1:A:38:LEU:HD12	4:C:2017:HOH:O	1.99	0.62
1:B:92:ARG:CB	1:B:92:ARG:HH11	2.12	0.62
1:C:214:TYR:C	1:C:216:SER:H	2.01	0.62
1:D:71:ARG:HD2	1:D:111:ARG:NH2	2.15	0.62
1:C:155:ARG:NH2	1:C:438:ASN:HD22	1.97	0.62
1:D:231:CYS:HA	1:D:281:GLN:O	1.98	0.62
1:B:94:SER:HA	1:B:222:VAL:O	1.99	0.62
1:A:439:VAL:O	1:A:440:THR:C	2.38	0.62
1:D:220:LYS:HE3	1:D:343:GLU:HB2	1.82	0.62
1:A:126:ARG:HE	1:A:199:PHE:HA	1.65	0.62
1:A:353:ARG:CD	3:A:2000:HEM:C2C	2.82	0.61
1:A:353:ARG:NE	1:A:357:TYR:HE1	1.94	0.61
1:B:323:ASN:ND2	1:D:396:ASN:HD22	1.94	0.61
1:C:404:TYR:OH	1:C:413:HIS:CD2	2.52	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:PHE:O	1:C:299:THR:HG22	1.99	0.61
1:C:466:LEU:HD11	1:C:474:GLN:HG2	1.81	0.61
1:C:92:ARG:H	1:C:92:ARG:CD	2.13	0.61
1:A:367:PRO:HG3	1:C:65:ARG:HD3	1.81	0.61
1:C:94:SER:HB2	1:C:221:LEU:HD22	1.82	0.61
1:A:71:ARG:HG3	1:A:75:ALA:HA	1.81	0.61
1:A:428:VAL:HG22	1:D:43:VAL:HA	1.83	0.61
1:A:148:ASN:HD22	1:A:149:THR:N	1.97	0.61
1:B:4:ARG:HB2	1:B:4:ARG:HH11	1.63	0.61
1:A:206:ASP:HA	1:A:244:LEU:HG	1.82	0.61
1:D:279:TYR:HB3	1:D:309:LEU:HB3	1.81	0.61
1:C:262:ARG:HG3	1:C:266:ASN:ND2	2.16	0.61
1:A:118:GLU:OE1	1:A:118:GLU:N	2.33	0.61
1:B:147:ASN:ND2	3:B:2001:HEM:CMC	2.63	0.61
1:C:46:ARG:HH11	1:C:46:ARG:CG	2.13	0.61
1:D:367:PRO:HG2	1:D:390:PRO:HG2	1.82	0.61
1:A:71:ARG:HH22	1:A:329:GLU:CD	2.03	0.61
1:D:285:PHE:CD1	1:D:285:PHE:N	2.69	0.61
1:B:71:ARG:HH11	1:B:364:ARG:NH2	1.99	0.61
1:C:237:THR:HA	1:C:276:TRP:CD1	2.36	0.61
1:B:245:SER:OG	1:B:247:GLU:HB2	2.01	0.61
1:D:169:ARG:HD3	1:D:174:HIS:CD2	2.35	0.61
1:C:353:ARG:HD2	1:C:357:TYR:HE1	1.66	0.61
1:A:54:VAL:HG22	4:A:2137:HOH:O	2.01	0.61
1:D:309:LEU:HD12	1:D:309:LEU:N	2.16	0.61
1:A:57:THR:CG2	4:C:2006:HOH:O	2.48	0.61
1:A:304:HIS:CB	1:A:304:HIS:H	2.13	0.60
2:D:3074:3TR:N3A	3:D:2003:HEM:NB	2.49	0.60
1:B:26:LEU:HD21	1:B:37:LYS:CD	2.31	0.60
1:D:427:ASP:HB2	1:D:429:GLN:HE21	1.66	0.60
1:A:57:THR:HG21	4:C:2006:HOH:O	2.01	0.60
1:B:444:THR:O	1:B:448:LYS:HB3	2.01	0.60
1:B:145:VAL:CG1	3:B:2001:HEM:CHD	2.79	0.60
1:D:406:ASN:ND2	1:D:410:ALA:HB3	2.13	0.60
1:D:485:HIS:CE1	1:D:486:PRO:HG2	2.36	0.60
1:D:63:PHE:HA	1:D:66:GLU:HG3	1.83	0.60
1:A:386:GLN:HB3	1:C:62:HIS:CD2	2.36	0.60
4:A:2144:HOH:O	1:B:171:PRO:CG	2.50	0.60
1:B:71:ARG:HH21	1:B:111:ARG:CZ	2.15	0.60
1:C:112:PHE:HA	1:C:130:GLY:O	2.02	0.60
1:A:351:GLN:HE22	1:C:52:GLN:NE2	1.99	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:HIS:HD1	1:D:298:LEU:HD13	1.65	0.60
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.83	0.60
1:A:152:PHE:O	1:A:299:THR:HG22	2.01	0.60
1:A:74:HIS:N	4:A:2020:HOH:O	2.35	0.60
1:B:217:HIS:NE2	1:B:353:ARG:HD2	2.16	0.60
1:A:322:VAL:HA	1:D:172:GLN:NE2	2.13	0.60
1:B:266:ASN:O	1:B:270:THR:HG23	2.00	0.60
1:B:391:MET:HG2	1:D:365:LEU:O	2.01	0.60
1:A:384:ASN:OD1	1:A:386:GLN:N	2.32	0.60
1:B:71:ARG:HB3	1:B:73:VAL:O	2.01	0.60
1:D:183:ASP:O	1:D:187:LEU:HG	2.02	0.60
1:C:74:HIS:CG	3:C:2002:HEM:C3D	2.89	0.60
1:B:479:LYS:HE2	1:B:483:ASP:OD2	2.01	0.60
1:A:487:GLU:HG2	1:A:491:ARG:HD2	1.84	0.60
1:B:206:ASP:OD1	1:B:244:LEU:HD21	2.01	0.60
1:D:338:MET:HB3	1:D:342:ILE:O	2.01	0.60
1:A:419:GLU:H	1:A:419:GLU:CD	2.05	0.60
1:A:332:ALA:HB1	1:A:361:HIS:CE1	2.36	0.60
1:B:71:ARG:HH21	1:B:111:ARG:NE	2.00	0.60
1:A:217:HIS:CD2	1:A:353:ARG:NH1	2.70	0.60
1:C:74:HIS:O	1:C:111:ARG:NH2	2.28	0.60
1:D:145:VAL:CG1	3:D:2003:HEM:HHD	2.30	0.60
1:B:34:VAL:HG11	1:B:37:LYS:HB3	1.84	0.60
1:B:4:ARG:NH2	1:C:470:GLN:HG3	2.16	0.60
1:A:300:LYS:HE2	1:A:441:GLN:NE2	2.17	0.59
1:B:26:LEU:HD21	1:B:37:LYS:HD2	1.84	0.59
1:A:415:PRO:HA	4:C:2038:HOH:O	2.01	0.59
1:B:208:HIS:O	1:B:211:MET:HG2	2.02	0.59
1:B:387:ARG:HG2	1:B:387:ARG:HH11	1.66	0.59
1:C:356:ALA:O	1:C:360:THR:HG22	2.03	0.59
1:B:145:VAL:HG12	3:B:2001:HEM:C4C	2.38	0.59
1:B:295:PRO:CD	1:C:46:ARG:HH12	2.15	0.59
1:B:49:LEU:HD23	1:B:50:LEU:H	1.67	0.59
1:A:131:PHE:HD2	1:A:213:GLY:CA	2.15	0.59
1:A:76:LYS:HD3	1:A:121:SER:O	2.02	0.59
1:B:42:THR:HG21	1:C:348:LYS:HE3	1.84	0.59
1:C:487:GLU:HG2	1:C:491:ARG:HG3	1.85	0.59
1:B:149:THR:HB	1:B:197:PHE:CE2	2.37	0.59
1:C:453:GLU:HB3	1:C:457:ARG:HH22	1.67	0.59
1:A:412:GLU:O	1:C:26:LEU:HB3	2.01	0.59
1:C:50:LEU:HD22	1:D:48:PRO:HB2	1.82	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:CYS:SG	1:B:491:ARG:HB2	2.42	0.59
1:B:139:ASP:O	1:D:32:ASN:HA	2.02	0.59
2:D:3074:3TR:N1	3:D:2003:HEM:C4C	2.70	0.59
1:B:497:ASP:HA	1:B:500:ASN:HB2	1.84	0.59
1:D:285:PHE:CD1	4:D:3134:HOH:O	2.52	0.59
1:C:186:SER:OG	1:C:476:LYS:HB3	2.02	0.59
1:C:160:PHE:CZ	3:C:2002:HEM:C3B	2.90	0.59
1:C:364:ARG:NE	3:C:2002:HEM:O1A	2.34	0.59
1:C:472:PHE:C	1:C:472:PHE:CD1	2.75	0.59
1:B:310:ILE:HD12	1:B:310:ILE:N	2.18	0.59
1:B:479:LYS:O	1:B:482:SER:HB2	2.02	0.59
1:C:487:GLU:O	1:C:491:ARG:HG3	2.03	0.59
1:C:402:ASN:OD1	1:D:165:HIS:HB3	2.01	0.59
1:D:90:ILE:HD11	1:D:99:PHE:CG	2.37	0.59
1:A:175:LEU:HD13	1:D:262:ARG:NH1	2.17	0.59
1:B:98:VAL:HG23	1:B:106:THR:OG1	2.03	0.59
1:A:65:ARG:HH11	1:A:65:ARG:CG	2.15	0.59
1:B:64:ASP:HB3	1:C:360:THR:CB	2.33	0.58
1:C:239:GLN:NE2	1:C:275:SER:H	2.01	0.58
1:D:73:VAL:CG1	1:D:164:ILE:HG21	2.32	0.58
1:B:276:TRP:HZ3	1:B:317:LEU:HD12	1.68	0.58
1:C:402:ASN:HB2	1:D:165:HIS:HD1	1.68	0.58
1:B:470:GLN:O	1:B:473:ILE:HB	2.03	0.58
1:D:280:ILE:HD11	1:D:310:ILE:HB	1.86	0.58
1:B:145:VAL:HG12	1:B:353:ARG:HH22	1.68	0.58
2:D:3074:3TR:N2	3:D:2003:HEM:C2C	2.70	0.58
1:C:71:ARG:HD2	1:C:111:ARG:NH2	2.18	0.58
1:B:191:SER:HB2	1:B:195:VAL:HG23	1.86	0.58
1:C:151:ILE:HG23	1:C:301:VAL:HG12	1.86	0.58
1:B:367:PRO:HG2	1:B:390:PRO:HG2	1.85	0.58
1:C:217:HIS:HE1	1:C:349:MET:HB3	1.67	0.58
1:C:423:HIS:HB2	1:D:427:ASP:OD1	2.03	0.58
1:B:278:LEU:O	1:B:312:VAL:HG13	2.03	0.58
1:A:296:PHE:CD1	1:A:346:PRO:HD2	2.38	0.58
1:A:73:VAL:HG11	1:A:164:ILE:HD12	1.85	0.58
1:A:38:LEU:CD1	4:C:2017:HOH:O	2.51	0.58
1:B:359:ASP:OD2	1:C:61:ALA:HA	2.02	0.58
3:B:2001:HEM:HHA	3:B:2001:HEM:HBA2	1.83	0.58
1:A:235:TYR:HA	1:A:277:THR:O	2.02	0.58
1:C:215:GLY:HA3	1:C:233:PHE:HB2	1.86	0.58
1:A:391:MET:HE3	1:C:391:MET:HB3	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:HD13	1:D:484:VAL:CG2	2.33	0.58
1:B:71:ARG:HH21	1:B:111:ARG:CD	2.16	0.58
1:D:76:LYS:HE3	1:D:121:SER:O	2.03	0.58
1:B:443:ARG:HG2	1:B:447:LEU:HD21	1.85	0.58
1:D:229:VAL:HA	1:D:285:PHE:HE1	1.68	0.57
1:B:242:LYS:NZ	4:B:2008:HOH:O	2.35	0.57
1:A:302:TRP:HB3	1:A:307:TYR:CD2	2.39	0.57
1:A:9:ASP:HB3	1:A:12:LYS:HE2	1.87	0.57
1:D:145:VAL:HG12	3:D:2003:HEM:CHD	2.30	0.57
1:B:43:VAL:O	1:B:47:GLY:HA3	2.04	0.57
1:B:81:PHE:HB2	1:B:319:ARG:HE	1.69	0.57
1:A:96:ALA:HB2	1:A:342:ILE:CD1	2.33	0.57
1:B:384:ASN:H	1:B:397:GLN:HE22	1.51	0.57
1:D:419:GLU:H	1:D:419:GLU:CD	2.07	0.57
1:C:147:ASN:ND2	3:C:2002:HEM:HAC	2.14	0.57
1:B:43:VAL:CG1	1:B:48:PRO:HD2	2.34	0.57
1:D:397:GLN:C	4:D:3155:HOH:O	2.42	0.57
1:D:217:HIS:ND1	1:D:298:LEU:HD13	2.19	0.57
1:A:41:LEU:HD23	1:A:41:LEU:C	2.23	0.57
1:B:404:TYR:CE2	1:D:38:LEU:HG	2.38	0.57
1:B:146:GLY:CA	3:B:2001:HEM:CAC	2.83	0.57
1:A:65:ARG:HH11	1:A:65:ARG:HG3	1.70	0.57
1:B:35:GLY:HA3	1:D:418:LEU:HD23	1.86	0.57
1:A:254:HIS:HD2	1:D:254:HIS:CD2	2.22	0.57
1:A:155:ARG:CZ	1:A:297:ASP:OD2	2.53	0.57
1:B:457:ARG:NH1	1:B:457:ARG:HB2	2.20	0.57
1:C:154:ILE:HG13	1:C:349:MET:CE	2.34	0.57
1:B:408:PHE:HA	1:D:15:LYS:HD2	1.86	0.57
1:D:482:SER:HA	1:D:485:HIS:O	2.05	0.57
1:A:338:MET:HB3	1:A:342:ILE:O	2.05	0.57
1:C:436:ASP:O	1:C:437:ASP:HB3	2.05	0.57
1:C:466:LEU:CD1	1:C:474:GLN:HG2	2.35	0.57
1:B:251:ARG:HA	1:B:254:HIS:CE1	2.39	0.57
1:B:151:ILE:HD13	1:B:193:HIS:ND1	2.20	0.57
1:C:367:PRO:HD2	4:C:2007:HOH:O	2.04	0.57
1:B:204:ILE:N	1:B:204:ILE:HD12	2.19	0.57
1:D:361:HIS:CD2	3:D:2003:HEM:O2A	2.57	0.57
1:A:73:VAL:O	3:A:2000:HEM:HAA1	2.05	0.57
1:B:98:VAL:HG13	1:B:99:PHE:CD1	2.40	0.57
1:B:81:PHE:HB2	1:B:319:ARG:HG2	1.87	0.57
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.69	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:PHE:HB2	4:D:3114:HOH:O	2.05	0.56
1:C:46:ARG:NH1	1:C:46:ARG:HG2	2.20	0.56
1:B:110:VAL:HG11	1:B:131:PHE:HE1	1.70	0.56
1:C:463:ALA:HB1	1:C:496:LEU:HD22	1.86	0.56
1:D:310:ILE:HD12	1:D:310:ILE:N	2.20	0.56
1:A:71:ARG:NH2	1:A:329:GLU:O	2.38	0.56
2:D:3074:3TR:H3A1	3:D:2003:HEM:CHC	2.18	0.56
1:B:27:THR:O	1:D:384:ASN:HB3	2.06	0.56
1:B:71:ARG:NH1	1:B:329:GLU:O	2.38	0.56
1:B:71:ARG:NH1	1:B:364:ARG:NH2	2.53	0.56
1:B:333:PHE:CD2	3:B:2001:HEM:CGD	2.86	0.56
1:D:290:ILE:O	1:D:291:PHE:C	2.41	0.56
1:A:308:PRO:C	1:A:309:LEU:HD22	2.25	0.56
1:D:219:PHE:O	1:D:230:TYR:HA	2.04	0.56
1:B:358:PRO:O	1:B:362:ARG:HG3	2.05	0.56
1:D:420:HIS:CE1	4:D:3158:HOH:O	2.53	0.56
1:B:487:GLU:O	1:B:491:ARG:HG3	2.06	0.56
1:C:294:ASN:ND2	4:C:2049:HOH:O	2.39	0.56
1:D:386:GLN:HG2	4:D:3075:HOH:O	2.05	0.56
1:B:327:GLU:O	1:B:331:LEU:HG	2.05	0.56
1:A:300:LYS:HE2	1:A:441:GLN:HE21	1.71	0.56
1:A:141:ASN:OD1	1:A:377:PRO:HA	2.06	0.56
1:D:18:ARG:O	1:D:19:ALA:HB3	2.06	0.56
1:A:83:TYR:CD1	1:A:83:TYR:C	2.79	0.56
1:A:210:HIS:HB3	1:A:242:LYS:H	1.70	0.55
1:A:107:PRO:HG2	1:A:378:TYR:OH	2.05	0.55
1:B:404:TYR:HE2	1:D:38:LEU:CG	2.19	0.55
1:B:139:ASP:O	1:D:33:PRO:HD3	2.07	0.55
1:D:166:SER:HB2	1:D:180:MET:O	2.05	0.55
1:B:4:ARG:HH22	1:C:470:GLN:HE21	1.51	0.55
1:C:209:ARG:HB2	1:C:209:ARG:HH11	1.67	0.55
1:C:93:TYR:O	1:C:221:LEU:HB3	2.06	0.55
1:D:110:VAL:HG13	1:D:132:ALA:O	2.05	0.55
1:D:206:ASP:HA	1:D:244:LEU:HG	1.87	0.55
1:B:168:LYS:HE3	1:C:67:ARG:HH21	1.71	0.55
1:A:69:PRO:HA	4:A:2011:HOH:O	2.05	0.55
1:A:493:GLN:O	1:A:496:LEU:HB2	2.06	0.55
1:A:294:ASN:HD21	1:D:46:ARG:HG2	1.71	0.55
1:A:381:ARG:HB3	4:A:2070:HOH:O	2.06	0.55
1:A:100:GLU:HG3	1:A:101:HIS:HE1	1.66	0.55
1:C:193:HIS:CB	1:C:442:VAL:HG22	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ASP:OD1	1:C:12:LYS:HD2	2.06	0.55
1:C:147:ASN:CB	3:C:2002:HEM:HBC1	2.36	0.55
1:B:147:ASN:CG	3:B:2001:HEM:CBC	2.75	0.55
1:D:291:PHE:HE1	1:D:293:PHE:HB2	1.71	0.55
1:B:155:ARG:NH2	1:B:438:ASN:OD1	2.39	0.55
1:A:126:ARG:NH1	1:A:126:ARG:HB2	2.22	0.55
1:D:457:ARG:O	1:D:458:LEU:C	2.45	0.55
1:A:237:THR:HA	1:A:276:TRP:CD1	2.42	0.55
1:C:209:ARG:CB	1:C:209:ARG:HH11	2.20	0.55
1:C:28:THR:HG23	1:C:32:ASN:O	2.06	0.55
1:D:327:GLU:O	1:D:331:LEU:HG	2.07	0.55
1:D:38:LEU:N	1:D:38:LEU:HD12	2.21	0.55
1:A:485:HIS:HD2	1:A:487:GLU:HB3	1.72	0.55
1:D:246:VAL:HG23	1:D:247:GLU:OE1	2.07	0.55
3:B:2001:HEM:CMC	3:B:2001:HEM:HBC2	2.37	0.55
1:C:155:ARG:NH1	1:C:299:THR:OG1	2.40	0.55
1:B:360:THR:OG1	1:C:64:ASP:CB	2.51	0.55
1:A:40:SER:HB3	1:A:49:LEU:HD21	1.89	0.54
1:A:415:PRO:CA	4:C:2038:HOH:O	2.56	0.54
1:B:13:HIS:O	1:B:17:GLN:HG2	2.08	0.54
1:A:381:ARG:HG3	4:A:2143:HOH:O	2.07	0.54
1:A:191:SER:HB2	1:A:195:VAL:HG23	1.89	0.54
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.42	0.54
1:C:73:VAL:CG2	3:C:2002:HEM:C1A	2.91	0.54
1:B:92:ARG:CB	1:B:92:ARG:NH1	2.68	0.54
1:D:212:ASP:OD1	1:D:236:LYS:HA	2.07	0.54
1:B:186:SER:HB2	1:B:476:LYS:HG3	1.89	0.54
1:B:215:GLY:O	1:B:217:HIS:N	2.39	0.54
1:B:25:VAL:O	1:B:27:THR:HG23	2.06	0.54
1:C:279:TYR:HD1	1:C:311:PRO:HA	1.73	0.54
1:C:480:ASN:O	1:C:483:ASP:N	2.41	0.54
1:B:110:VAL:HG11	1:B:131:PHE:CE1	2.41	0.54
1:B:101:HIS:O	1:B:104:LYS:HB2	2.08	0.54
1:B:447:LEU:HD22	1:B:485:HIS:CD2	2.43	0.54
1:C:190:GLU:HA	1:C:438:ASN:CB	2.35	0.54
1:A:271:GLY:HA2	1:A:273:TYR:CZ	2.43	0.54
1:C:71:ARG:NH1	1:C:111:ARG:NH1	2.54	0.54
1:B:46:ARG:NH2	1:C:294:ASN:HA	2.22	0.54
1:D:347:ASP:OD1	1:D:349:MET:HB2	2.08	0.54
1:D:187:LEU:O	1:D:188:ARG:HD2	2.08	0.54
1:D:98:VAL:HB	1:D:137:THR:HG21	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:MET:CE	1:C:180:MET:HG2	2.38	0.54
1:B:83:TYR:CA	1:B:108:ILE:HG12	2.37	0.54
1:C:160:PHE:CE1	3:C:2002:HEM:CAB	2.89	0.54
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.88	0.54
1:C:217:HIS:NE2	1:C:350:LEU:HA	2.23	0.54
1:B:402:ASN:H	1:B:402:ASN:HD22	1.55	0.54
1:C:476:LYS:O	1:C:479:LYS:HB3	2.08	0.54
1:D:70:GLU:OE1	1:D:118:GLU:HB3	2.08	0.54
1:D:293:PHE:HZ	1:D:440:THR:HG21	1.72	0.54
1:A:170:ASN:OD1	1:A:173:THR:N	2.40	0.54
1:A:96:ALA:CB	1:A:342:ILE:HD11	2.38	0.54
1:D:301:VAL:O	1:D:303:PRO:HD3	2.08	0.54
1:B:125:VAL:HG22	1:B:126:ARG:N	2.23	0.54
1:C:74:HIS:ND1	3:C:2002:HEM:C2D	2.76	0.53
1:C:458:LEU:HD21	1:C:488:TYR:OH	2.08	0.53
1:D:115:VAL:N	1:D:127:ASP:OD2	2.40	0.53
1:C:481:PHE:O	1:C:484:VAL:HB	2.08	0.53
1:D:235:TYR:CD1	1:D:235:TYR:N	2.75	0.53
1:B:472:PHE:C	1:B:472:PHE:CD2	2.82	0.53
1:C:146:GLY:C	3:C:2002:HEM:CBC	2.74	0.53
1:A:387:ARG:NH2	1:A:397:GLN:HB2	2.23	0.53
1:C:472:PHE:CZ	1:C:473:ILE:HG13	2.42	0.53
1:B:5:ASP:HB2	1:B:6:PRO:HD2	1.90	0.53
1:B:17:GLN:C	1:B:19:ALA:H	2.11	0.53
1:D:90:ILE:HD12	1:D:90:ILE:O	2.08	0.53
1:B:233:PHE:C	1:B:234:HIS:HD2	2.11	0.53
1:A:217:HIS:CE1	1:A:298:LEU:HD22	2.43	0.53
1:D:111:ARG:HB3	3:D:2003:HEM:O1D	2.08	0.53
1:C:112:PHE:HZ	1:C:276:TRP:CH2	2.26	0.53
1:A:180:MET:HA	1:D:11:MET:HE1	1.90	0.53
1:B:160:PHE:N	1:B:161:PRO:HD2	2.24	0.53
1:C:160:PHE:CZ	3:C:2002:HEM:C4B	2.97	0.53
3:B:2001:HEM:CHA	3:B:2001:HEM:HBA2	2.37	0.53
1:C:459:CYS:HA	1:C:492:ILE:CD1	2.39	0.53
1:C:353:ARG:NH1	1:C:357:TYR:OH	2.37	0.53
1:C:327:GLU:O	1:C:331:LEU:HG	2.08	0.53
1:A:67:ARG:O	1:D:69:PRO:HB3	2.08	0.53
1:C:43:VAL:O	1:C:43:VAL:HG13	2.09	0.53
1:B:165:HIS:NE2	1:C:66:GLU:OE2	2.40	0.53
1:D:128:PRO:O	1:D:129:ARG:HG2	2.09	0.53
1:C:193:HIS:HA	1:C:442:VAL:HG22	1.91	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:HIS:C	1:D:102:ILE:HG12	2.29	0.53
1:D:208:HIS:HA	1:D:211:MET:CE	2.39	0.53
1:D:147:ASN:OD1	3:D:2003:HEM:HAC	2.08	0.53
1:D:397:GLN:O	1:D:398:GLY:C	2.46	0.53
1:D:26:LEU:HD23	1:D:26:LEU:C	2.29	0.53
1:A:429:GLN:NE2	4:A:2135:HOH:O	2.41	0.53
1:A:115:VAL:N	1:A:127:ASP:OD2	2.36	0.53
1:A:367:PRO:HD3	4:A:2013:HOH:O	2.09	0.53
1:B:237:THR:HA	1:B:276:TRP:CD1	2.44	0.53
1:A:480:ASN:O	1:A:483:ASP:HB2	2.08	0.53
1:A:202:ARG:CG	4:A:2140:HOH:O	2.56	0.53
1:A:331:LEU:HD13	1:A:374:VAL:CG2	2.38	0.53
1:B:330:GLN:O	1:B:331:LEU:O	2.27	0.53
1:B:331:LEU:HD13	1:B:333:PHE:CE2	2.44	0.53
1:D:442:VAL:HG12	1:D:484:VAL:HG11	1.90	0.53
1:A:129:ARG:HB2	1:A:148:ASN:CB	2.38	0.53
1:A:96:ALA:HB2	1:A:342:ILE:HD12	1.90	0.53
1:B:277:THR:CG2	1:B:314:LYS:HG3	2.39	0.53
1:D:181:VAL:HG12	1:D:182:TRP:N	2.23	0.53
1:A:100:GLU:CG	1:A:101:HIS:ND1	2.54	0.52
1:C:403:TYR:N	1:C:403:TYR:CD1	2.78	0.52
1:C:469:ALA:O	1:C:470:GLN:C	2.47	0.52
1:B:329:GLU:O	1:B:364:ARG:NH2	2.42	0.52
1:A:50:LEU:C	1:A:52:GLN:H	2.11	0.52
1:B:381:ARG:HH12	1:D:24:ASP:CG	2.11	0.52
1:A:65:ARG:CG	1:A:65:ARG:NH1	2.71	0.52
1:A:456:LYS:O	1:A:460:GLU:HG3	2.09	0.52
1:D:233:PHE:C	1:D:234:HIS:HD2	2.12	0.52
1:A:304:HIS:CA	1:A:304:HIS:CG	2.80	0.52
1:B:331:LEU:HD23	1:B:374:VAL:CB	2.38	0.52
1:C:50:LEU:HD23	1:D:50:LEU:HD23	1.91	0.52
1:D:291:PHE:CE1	1:D:293:PHE:HB2	2.45	0.52
1:D:127:ASP:HB3	1:D:129:ARG:HH12	1.74	0.52
1:C:206:ASP:O	1:C:210:HIS:HB2	2.09	0.52
1:D:485:HIS:CE1	1:D:487:GLU:H	2.27	0.52
1:B:309:LEU:N	1:B:309:LEU:HD23	2.23	0.52
1:A:353:ARG:CD	3:A:2000:HEM:C4B	2.88	0.52
1:D:280:ILE:CD1	1:D:310:ILE:HB	2.39	0.52
1:B:275:SER:HA	1:B:315:LEU:O	2.10	0.52
1:C:74:HIS:HA	1:C:114:THR:O	2.10	0.52
1:D:286:SER:O	1:D:289:GLU:CB	2.53	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLN:HG3	1:C:351:GLN:NE2	2.22	0.52
1:C:46:ARG:HH11	1:C:46:ARG:HG2	1.74	0.52
1:C:126:ARG:HH11	1:C:126:ARG:CG	2.20	0.52
1:C:124:THR:HA	1:C:129:ARG:HH22	1.75	0.52
1:B:36:ASP:HB3	1:C:430:ARG:HD3	1.90	0.52
1:C:73:VAL:HG23	3:C:2002:HEM:C1A	2.45	0.52
1:C:22:LYS:HD3	1:C:23:PRO:N	2.24	0.52
1:A:14:TRP:O	1:A:15:LYS:C	2.48	0.52
1:D:367:PRO:HG2	1:D:390:PRO:CG	2.39	0.52
1:C:49:LEU:HG	1:D:51:VAL:HG21	1.92	0.52
1:C:446:TYR:CE1	1:C:455:ARG:HG3	2.45	0.52
1:A:145:VAL:HG11	3:A:2000:HEM:C2D	2.34	0.52
1:D:173:THR:O	1:D:174:HIS:CB	2.58	0.52
1:D:86:VAL:O	1:D:102:ILE:HG23	2.09	0.52
1:B:187:LEU:O	1:B:188:ARG:HD2	2.10	0.52
1:A:100:GLU:HG3	1:A:101:HIS:CE1	2.35	0.52
1:B:413:HIS:CE1	1:B:415:PRO:HD3	2.45	0.52
1:A:146:GLY:HA3	1:A:235:TYR:OH	2.10	0.52
1:C:235:TYR:CD1	1:C:235:TYR:N	2.77	0.52
1:A:284:THR:OG1	1:A:287:GLU:HG3	2.10	0.52
1:B:32:ASN:ND2	1:D:339:PRO:HA	2.24	0.52
1:C:14:TRP:O	1:C:18:ARG:HB2	2.10	0.51
1:C:41:LEU:HG	1:C:50:LEU:HD12	1.92	0.51
1:A:451:ASN:H	1:A:454:GLN:NE2	2.09	0.51
1:B:39:ASN:HA	1:C:156:ASP:OD2	2.10	0.51
1:A:84:PHE:HD1	1:A:314:LYS:O	1.92	0.51
1:C:146:GLY:O	3:C:2002:HEM:CBC	2.58	0.51
1:B:109:ALA:HB3	1:B:134:LYS:HB3	1.92	0.51
1:D:386:GLN:HA	4:D:3075:HOH:O	2.09	0.51
1:D:151:ILE:HG23	1:D:301:VAL:HG13	1.93	0.51
1:A:30:GLY:O	1:C:377:PRO:HB3	2.11	0.51
1:C:43:VAL:CG1	1:C:48:PRO:HD2	2.40	0.51
1:B:439:VAL:HG23	1:B:440:THR:H	1.75	0.51
1:C:469:ALA:O	1:C:474:GLN:HG3	2.10	0.51
1:D:148:ASN:O	1:D:149:THR:HB	2.10	0.51
1:C:460:GLU:HA	1:C:495:LEU:HD13	1.91	0.51
1:A:301:VAL:O	1:A:303:PRO:HD3	2.10	0.51
1:D:160:PHE:CD1	3:D:2003:HEM:HAB	2.46	0.51
1:B:442:VAL:HG12	1:B:484:VAL:HG11	1.92	0.51
1:D:206:ASP:CA	1:D:244:LEU:HG	2.40	0.51
1:B:250:ALA:O	1:B:253:ALA:HB3	2.09	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASN:HA	1:C:139:ASP:O	2.10	0.51
1:A:126:ARG:HA	1:A:204:ILE:HG12	1.92	0.51
1:B:235:TYR:CD1	1:B:235:TYR:N	2.79	0.51
1:D:460:GLU:HA	1:D:495:LEU:HD13	1.92	0.51
1:A:108:ILE:HA	1:A:134:LYS:O	2.11	0.51
1:A:384:ASN:OD1	1:A:386:GLN:CB	2.53	0.51
1:A:48:PRO:HD3	1:D:424:PHE:CE2	2.46	0.51
1:B:26:LEU:HD21	1:B:37:LYS:CG	2.41	0.51
1:A:399:GLY:O	1:A:400:ALA:C	2.48	0.51
1:B:6:PRO:HG2	1:B:266:ASN:OD1	2.11	0.51
1:A:173:THR:O	1:A:174:HIS:CB	2.58	0.51
1:B:493:GLN:CA	1:B:496:LEU:HD12	2.29	0.51
1:B:49:LEU:HD23	1:B:50:LEU:N	2.26	0.51
1:D:148:ASN:O	1:D:148:ASN:ND2	2.43	0.51
1:B:232:LYS:O	1:B:280:ILE:HA	2.09	0.51
1:D:210:HIS:CD2	1:D:242:LYS:HB2	2.46	0.51
1:B:353:ARG:NH2	3:B:2001:HEM:NC	2.57	0.51
1:C:291:PHE:CD2	1:C:293:PHE:O	2.64	0.51
1:A:492:ILE:HG22	1:A:496:LEU:HD13	1.92	0.51
1:A:202:ARG:HG3	4:A:2140:HOH:O	2.11	0.51
1:A:217:HIS:HD2	1:A:353:ARG:NH1	2.06	0.50
1:D:353:ARG:HB3	1:D:357:TYR:CE1	2.46	0.50
1:A:275:SER:HA	1:A:315:LEU:O	2.12	0.50
1:C:206:ASP:OD2	1:C:242:LYS:HE3	2.10	0.50
1:C:191:SER:HB2	1:C:195:VAL:CG2	2.41	0.50
1:C:310:ILE:CD1	1:C:310:ILE:N	2.74	0.50
1:D:372:ILE:HG22	1:D:374:VAL:HG12	1.92	0.50
1:A:353:ARG:HG3	3:A:2000:HEM:C4B	2.46	0.50
1:B:62:HIS:HE1	1:D:368:ASN:ND2	2.07	0.50
1:B:95:LYS:HG3	1:B:222:VAL:O	2.12	0.50
1:C:151:ILE:HG13	1:C:194:GLN:HG2	1.92	0.50
1:C:209:ARG:HB3	1:C:239:GLN:HG3	1.93	0.50
1:D:26:LEU:O	1:D:34:VAL:HG22	2.12	0.50
1:D:208:HIS:HA	1:D:211:MET:HE2	1.93	0.50
1:B:325:PHE:CD1	1:D:388:ASP:OD2	2.64	0.50
1:A:110:VAL:HG12	1:A:133:VAL:HA	1.93	0.50
1:A:74:HIS:ND1	1:A:114:THR:O	2.45	0.50
1:D:74:HIS:O	1:D:111:ARG:NH2	2.43	0.50
1:B:74:HIS:NE2	1:B:115:VAL:HG22	2.25	0.50
1:A:296:PHE:CE1	1:A:346:PRO:HD2	2.47	0.50
1:B:404:TYR:OH	1:B:413:HIS:HD2	1.95	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:LEU:O	1:C:353:ARG:N	2.44	0.50
1:A:283:MET:SD	1:A:288:ALA:HA	2.51	0.50
1:A:85:GLU:HA	1:A:104:LYS:O	2.11	0.50
1:B:439:VAL:O	1:B:442:VAL:CB	2.58	0.50
1:D:251:ARG:O	1:D:254:HIS:CD2	2.65	0.50
1:A:182:TRP:CH2	1:A:462:ILE:HG23	2.46	0.50
1:C:264:LEU:O	1:C:264:LEU:HD12	2.11	0.50
1:A:145:VAL:CG1	3:A:2000:HEM:HBC2	2.42	0.50
1:A:353:ARG:CB	3:A:2000:HEM:HBB2	2.41	0.50
1:D:160:PHE:CG	3:D:2003:HEM:HAB	2.46	0.50
1:A:43:VAL:O	1:A:47:GLY:HA3	2.11	0.50
1:C:211:MET:HB2	4:C:2048:HOH:O	2.10	0.50
1:B:393:MET:HG2	1:D:393:MET:SD	2.51	0.50
1:C:111:ARG:HH21	3:C:2002:HEM:HAD2	1.76	0.50
1:C:142:TRP:HB2	1:C:339:PRO:CG	2.42	0.50
1:D:189:PRO:O	1:D:191:SER:N	2.45	0.50
1:B:284:THR:HG23	1:B:287:GLU:OE1	2.11	0.50
1:D:439:VAL:O	1:D:440:THR:C	2.50	0.50
1:A:43:VAL:HG21	1:B:43:VAL:HG21	1.93	0.50
1:B:218:THR:OG1	1:B:232:LYS:HE3	2.11	0.50
1:C:367:PRO:HG2	1:C:390:PRO:CG	2.41	0.50
3:A:2000:HEM:CBA	3:A:2000:HEM:CHA	2.88	0.50
1:B:50:LEU:N	1:B:50:LEU:CD2	2.74	0.50
1:D:115:VAL:HG21	1:D:128:PRO:HB2	1.93	0.50
1:A:54:VAL:CG2	4:A:2137:HOH:O	2.59	0.50
1:B:445:PHE:HA	1:B:449:VAL:CG2	2.40	0.50
1:B:83:TYR:HA	1:B:108:ILE:HG12	1.93	0.50
1:D:179:ASP:OD1	1:D:473:ILE:HD12	2.12	0.50
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.93	0.49
1:D:170:ASN:HA	1:D:180:MET:SD	2.52	0.49
1:A:50:LEU:C	1:A:52:GLN:N	2.65	0.49
1:B:72:VAL:HG11	1:C:63:PHE:CE1	2.47	0.49
1:A:408:PHE:CD1	1:C:11:MET:HB3	2.47	0.49
1:B:251:ARG:HG2	1:B:251:ARG:NH1	2.26	0.49
1:B:393:MET:HE3	1:D:372:ILE:HA	1.93	0.49
1:D:182:TRP:CD2	1:D:466:LEU:HD13	2.47	0.49
1:A:471:LEU:HD23	1:A:474:GLN:NE2	2.26	0.49
1:C:387:ARG:HH11	1:C:387:ARG:HG2	1.77	0.49
1:B:135:PHE:HB2	1:B:142:TRP:HB3	1.94	0.49
1:A:220:LYS:HD2	1:A:420:HIS:HD2	1.78	0.49
1:C:160:PHE:CE2	1:C:164:ILE:HG13	2.47	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3074:3TR:N3A	3:D:2003:HEM:C1C	2.79	0.49
1:C:155:ARG:HH22	1:C:438:ASN:HD22	1.60	0.49
1:D:218:THR:O	1:D:345:SER:HB3	2.12	0.49
1:A:32:ASN:N	1:A:32:ASN:HD22	2.08	0.49
1:C:74:HIS:CE1	3:C:2002:HEM:C2D	3.00	0.49
1:A:300:LYS:HB3	1:A:441:GLN:NE2	2.16	0.49
1:B:189:PRO:O	1:B:192:LEU:HG	2.13	0.49
1:B:74:HIS:ND1	1:B:114:THR:O	2.45	0.49
1:B:332:ALA:HB3	1:B:375:ASN:OD1	2.12	0.49
1:C:63:PHE:C	1:C:63:PHE:CD1	2.85	0.49
1:D:114:THR:HG21	4:D:3081:HOH:O	2.12	0.49
1:B:428:VAL:O	1:B:428:VAL:CG2	2.58	0.49
1:C:134:LYS:HB2	1:C:333:PHE:CE2	2.47	0.49
1:B:340:PRO:HG3	4:B:2035:HOH:O	2.13	0.49
1:D:6:PRO:HD2	1:D:266:ASN:OD1	2.13	0.49
1:D:145:VAL:CG1	3:D:2003:HEM:CHD	2.89	0.49
1:D:170:ASN:HD22	1:D:173:THR:H	1.60	0.49
1:C:151:ILE:HD13	1:C:193:HIS:CE1	2.47	0.49
1:D:209:ARG:CG	1:D:274:PRO:HB3	2.42	0.49
1:A:173:THR:O	1:A:174:HIS:HB3	2.13	0.49
1:A:254:HIS:CD2	1:D:254:HIS:CD2	3.00	0.49
1:D:372:ILE:HB	1:D:375:ASN:HD22	1.78	0.49
1:C:467:LYS:HD2	1:C:467:LYS:O	2.12	0.49
1:B:396:ASN:HB2	1:D:326:ALA:HB2	1.94	0.49
1:C:84:PHE:CE1	1:C:278:LEU:HD23	2.48	0.49
1:A:353:ARG:NH2	3:A:2000:HEM:C3C	2.72	0.49
3:A:2000:HEM:CBC	3:A:2000:HEM:C4C	2.96	0.49
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.95	0.49
1:C:160:PHE:CE1	3:C:2002:HEM:C3B	3.01	0.49
1:C:111:ARG:CZ	3:C:2002:HEM:CGD	2.91	0.49
1:B:41:LEU:CD1	1:C:428:VAL:HG12	2.37	0.49
1:C:485:HIS:CE1	1:C:487:GLU:H	2.31	0.49
1:B:71:ARG:HE	1:B:111:ARG:NH1	2.09	0.49
1:A:98:VAL:HB	1:A:137:THR:HG21	1.95	0.49
1:A:329:GLU:C	1:A:331:LEU:H	2.16	0.49
1:D:332:ALA:HB1	1:D:361:HIS:ND1	2.28	0.49
1:C:193:HIS:HB2	1:C:442:VAL:HG22	1.95	0.49
1:B:416:SER:HB3	4:B:2075:HOH:O	2.12	0.49
1:D:414:GLN:O	1:D:416:SER:N	2.46	0.49
1:D:204:ILE:N	1:D:204:ILE:HD12	2.28	0.49
1:A:311:PRO:HD2	4:A:2009:HOH:O	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:HIS:CE1	1:D:368:ASN:HD21	2.30	0.48
2:D:3074:3TR:N3A	3:D:2003:HEM:C4B	2.78	0.48
1:B:443:ARG:HG3	1:B:484:VAL:O	2.14	0.48
1:B:86:VAL:HB	1:B:103:GLY:H	1.78	0.48
1:A:245:SER:HB3	4:A:2141:HOH:O	2.12	0.48
1:A:407:SER:C	4:A:2087:HOH:O	2.52	0.48
1:B:347:ASP:O	1:B:350:LEU:N	2.46	0.48
1:C:153:PHE:N	1:C:153:PHE:CD2	2.81	0.48
1:C:492:ILE:CG2	1:C:496:LEU:HD23	2.43	0.48
1:C:108:ILE:HA	1:C:134:LYS:O	2.12	0.48
1:D:97:LYS:HA	1:D:100:GLU:HG3	1.96	0.48
1:A:155:ARG:NE	1:A:297:ASP:OD2	2.46	0.48
1:D:218:THR:O	1:D:345:SER:CB	2.62	0.48
1:A:451:ASN:H	1:A:454:GLN:HE21	1.60	0.48
1:A:368:ASN:ND2	1:A:390:PRO:O	2.42	0.48
1:A:38:LEU:CD2	1:D:159:LEU:HD11	2.44	0.48
1:D:487:GLU:O	1:D:488:TYR:C	2.50	0.48
1:A:391:MET:HE3	1:C:391:MET:CB	2.43	0.48
1:B:393:MET:CE	1:D:372:ILE:HA	2.43	0.48
1:B:430:ARG:HG3	1:B:430:ARG:HH11	1.79	0.48
1:B:65:ARG:HA	1:C:363:HIS:CD2	2.49	0.48
1:A:238:ASP:HB2	1:A:275:SER:OG	2.14	0.48
1:D:390:PRO:O	1:D:391:MET:HB2	2.14	0.48
1:B:32:ASN:HD22	1:D:339:PRO:HA	1.79	0.48
1:A:137:THR:OG1	1:A:140:GLY:O	2.30	0.48
1:A:86:VAL:HG21	1:A:99:PHE:HA	1.96	0.48
1:A:430:ARG:HB3	1:D:39:ASN:HB2	1.95	0.48
1:C:110:VAL:CG2	1:C:133:VAL:HG22	2.44	0.48
1:B:37:LYS:CG	1:B:37:LYS:O	2.57	0.48
1:B:451:ASN:OD1	1:B:453:GLU:HB2	2.14	0.48
1:C:129:ARG:HG2	1:C:211:MET:CE	2.43	0.48
1:A:72:VAL:HG12	3:A:2000:HEM:HAA2	1.96	0.48
1:D:73:VAL:HG12	1:D:164:ILE:HG21	1.96	0.48
1:B:71:ARG:HD2	1:B:364:ARG:NH1	2.29	0.48
1:C:111:ARG:HH21	3:C:2002:HEM:CGD	2.26	0.48
1:A:487:GLU:HG2	1:A:491:ARG:CD	2.44	0.48
1:A:450:LEU:HA	1:A:454:GLN:HE22	1.75	0.48
1:A:495:LEU:O	1:A:498:LYS:HB3	2.13	0.48
1:A:248:ASP:HA	1:A:251:ARG:HH12	1.79	0.48
1:B:337:ASN:N	1:B:337:ASN:ND2	2.60	0.48
1:A:101:HIS:O	1:A:104:LYS:HB2	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ILE:HG13	1:C:291:PHE:N	2.29	0.48
1:D:151:ILE:HD12	1:D:151:ILE:O	2.14	0.48
1:A:329:GLU:O	1:A:331:LEU:N	2.47	0.48
1:A:41:LEU:HB2	1:D:430:ARG:CZ	2.41	0.48
1:C:126:ARG:HE	1:C:203:GLY:HA3	1.78	0.48
1:C:221:LEU:O	1:C:228:ALA:HA	2.14	0.48
1:B:393:MET:HG2	1:D:393:MET:HG3	1.96	0.48
1:B:332:ALA:N	1:B:375:ASN:OD1	2.47	0.48
1:D:142:TRP:HA	1:D:337:ASN:O	2.14	0.48
1:D:160:PHE:CE1	1:D:164:ILE:HD11	2.48	0.47
1:A:276:TRP:HB2	1:A:315:LEU:HB2	1.96	0.47
1:B:107:PRO:O	1:B:136:TYR:HD1	1.97	0.47
1:A:295:PRO:HD3	1:D:46:ARG:NH1	2.28	0.47
1:C:147:ASN:N	3:C:2002:HEM:HBC1	2.28	0.47
1:D:59:GLU:O	1:D:60:MET:C	2.53	0.47
1:D:85:GLU:O	1:D:313:GLY:HA3	2.13	0.47
1:A:73:VAL:HG12	1:A:164:ILE:HG21	1.96	0.47
1:C:410:ALA:HB1	1:C:411:PRO:CD	2.40	0.47
1:D:439:VAL:CG2	1:D:440:THR:N	2.76	0.47
1:A:126:ARG:NE	1:A:199:PHE:HA	2.28	0.47
1:D:414:GLN:O	1:D:417:ALA:N	2.41	0.47
1:B:379:ARG:HD3	4:B:2073:HOH:O	2.14	0.47
1:C:206:ASP:HA	1:C:244:LEU:HG	1.96	0.47
1:A:439:VAL:O	1:A:442:VAL:N	2.46	0.47
1:A:167:GLN:HB3	1:A:167:GLN:HE21	1.54	0.47
1:A:332:ALA:HB2	1:A:365:LEU:HD11	1.97	0.47
1:B:71:ARG:HE	1:B:111:ARG:NH2	2.11	0.47
1:A:67:ARG:HH21	1:D:168:LYS:HE3	1.79	0.47
1:D:247:GLU:O	1:D:251:ARG:HB2	2.14	0.47
1:D:297:ASP:CG	1:D:300:LYS:HD3	2.35	0.47
1:D:395:ASP:O	1:D:396:ASN:HB3	2.15	0.47
1:C:297:ASP:OD1	1:C:299:THR:N	2.41	0.47
1:D:189:PRO:C	1:D:191:SER:N	2.68	0.47
1:A:408:PHE:O	1:A:409:SER:HB2	2.15	0.47
1:B:236:LYS:O	1:B:276:TRP:HA	2.15	0.47
1:B:357:TYR:HB2	1:B:358:PRO:HD3	1.96	0.47
1:D:440:THR:HG22	1:D:441:GLN:N	2.29	0.47
1:C:466:LEU:HD11	1:C:474:GLN:HA	1.96	0.47
1:C:291:PHE:HD2	1:C:293:PHE:O	1.96	0.47
1:C:191:SER:C	1:C:195:VAL:HG23	2.35	0.47
1:C:414:GLN:HA	1:C:415:PRO:HD2	1.81	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:MET:CE	1:B:402:ASN:HD21	2.27	0.47
1:B:472:PHE:CZ	1:B:473:ILE:HG13	2.50	0.47
1:B:160:PHE:CZ	1:B:164:ILE:HD11	2.50	0.47
1:C:452:GLU:O	1:C:455:ARG:HB3	2.15	0.47
1:B:69:PRO:HD3	1:C:69:PRO:HG3	1.97	0.47
1:B:351:GLN:HA	1:B:354:LEU:HD12	1.96	0.47
1:A:353:ARG:HD3	3:A:2000:HEM:CMC	2.45	0.47
1:C:432:ASN:HD21	1:C:434:ALA:H	1.57	0.47
1:B:454:GLN:HA	1:B:457:ARG:HH12	1.78	0.47
1:A:179:ASP:O	1:A:183:ASP:HB2	2.14	0.47
1:B:71:ARG:N	1:B:364:ARG:HH11	2.13	0.47
1:B:345:SER:C	1:B:347:ASP:H	2.18	0.47
1:B:419:GLU:CD	1:B:419:GLU:H	2.18	0.47
1:A:45:PRO:HD3	1:D:431:PHE:CE2	2.50	0.47
1:A:325:PHE:O	1:A:329:GLU:HB3	2.15	0.47
1:A:179:ASP:OD2	1:A:470:GLN:HG3	2.15	0.47
1:D:358:PRO:HB2	1:D:362:ARG:CZ	2.45	0.47
1:C:239:GLN:H	1:C:239:GLN:CD	2.17	0.47
1:A:54:VAL:HG22	1:A:54:VAL:H	1.44	0.47
1:C:81:PHE:CD1	1:C:81:PHE:N	2.83	0.47
1:A:308:PRO:O	1:A:309:LEU:HD22	2.15	0.47
1:D:95:LYS:HG2	1:D:222:VAL:O	2.15	0.47
1:A:325:PHE:CD2	1:C:388:ASP:HA	2.50	0.47
1:C:111:ARG:NH2	3:C:2002:HEM:CGD	2.78	0.47
1:B:65:ARG:O	1:D:389:GLY:HA2	2.15	0.47
1:D:221:LEU:HB2	1:D:229:VAL:HG23	1.96	0.47
1:B:367:PRO:HD2	4:B:2004:HOH:O	2.15	0.47
1:A:110:VAL:HG21	1:A:317:LEU:HD11	1.97	0.47
1:A:110:VAL:CG1	1:A:133:VAL:HG13	2.45	0.47
1:A:36:ASP:HB3	1:C:418:LEU:HD21	1.96	0.47
1:C:451:ASN:H	1:C:454:GLN:HE21	1.63	0.47
1:C:181:VAL:HG12	1:C:182:TRP:N	2.29	0.47
1:A:135:PHE:CD1	1:A:135:PHE:N	2.83	0.47
1:A:218:THR:CG2	1:A:230:TYR:HB3	2.45	0.47
1:B:333:PHE:CD2	3:B:2001:HEM:O1D	2.68	0.46
1:D:73:VAL:O	1:D:74:HIS:HB2	2.14	0.46
1:A:188:ARG:HB3	1:A:190:GLU:CD	2.35	0.46
1:C:457:ARG:O	1:C:461:ASN:CG	2.53	0.46
1:B:279:TYR:O	1:B:280:ILE:CG2	2.63	0.46
1:C:385:TYR:CE2	1:C:404:TYR:HB2	2.49	0.46
1:A:169:ARG:HD2	1:A:174:HIS:O	2.15	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:CZ	1:A:365:LEU:HD21	2.45	0.46
1:D:71:ARG:HB3	3:D:2003:HEM:HBA1	1.97	0.46
1:D:297:ASP:OD1	1:D:297:ASP:C	2.54	0.46
1:B:155:ARG:NH1	1:B:299:THR:OG1	2.49	0.46
1:D:115:VAL:HG21	1:D:128:PRO:HD2	1.97	0.46
1:B:114:THR:HB	1:B:115:VAL:H	1.58	0.46
1:D:296:PHE:HB3	1:D:347:ASP:HA	1.96	0.46
1:B:393:MET:HE1	1:D:372:ILE:HG13	1.96	0.46
1:B:249:ALA:O	1:B:253:ALA:HB2	2.14	0.46
1:A:325:PHE:CE2	1:C:388:ASP:HA	2.50	0.46
1:B:454:GLN:CA	1:B:457:ARG:HH12	2.28	0.46
1:C:463:ALA:CB	1:C:496:LEU:HD22	2.45	0.46
1:C:228:ALA:O	1:C:229:VAL:HG13	2.15	0.46
1:B:277:THR:HG22	1:B:314:LYS:HG3	1.97	0.46
1:A:26:LEU:HD12	1:C:384:ASN:HA	1.97	0.46
1:B:41:LEU:HD13	1:B:42:THR:N	2.31	0.46
1:B:491:ARG:O	1:B:494:ALA:HB3	2.15	0.46
1:B:446:TYR:O	1:B:455:ARG:NH1	2.49	0.46
1:B:389:GLY:HA2	1:D:65:ARG:O	2.15	0.46
1:D:110:VAL:HA	1:D:132:ALA:O	2.15	0.46
1:B:462:ILE:HD13	1:B:481:PHE:CZ	2.50	0.46
1:B:471:LEU:CD2	4:B:2097:HOH:O	2.64	0.46
1:D:329:GLU:HA	1:D:329:GLU:OE1	2.14	0.46
1:B:149:THR:OG1	1:B:150:PRO:HD2	2.16	0.46
1:B:294:ASN:HA	1:C:46:ARG:NH1	2.30	0.46
1:B:402:ASN:N	1:B:402:ASN:HD22	2.13	0.46
1:C:87:THR:OG1	1:C:313:GLY:HA2	2.16	0.46
1:B:10:GLN:NE2	1:C:172:GLN:NE2	2.64	0.46
1:C:265:PHE:C	1:C:265:PHE:CD1	2.88	0.46
1:A:356:ALA:HB3	3:A:2000:HEM:CMB	2.43	0.46
1:A:72:VAL:HG13	1:A:73:VAL:N	2.30	0.46
1:A:129:ARG:O	1:A:147:ASN:OD1	2.33	0.46
1:C:275:SER:HA	1:C:315:LEU:O	2.15	0.46
1:C:150:PRO:HG3	1:C:214:TYR:CD1	2.50	0.46
1:A:202:ARG:HG2	4:A:2140:HOH:O	2.16	0.46
1:B:340:PRO:HD3	4:B:2035:HOH:O	2.15	0.46
1:B:388:ASP:HA	1:D:325:PHE:CE2	2.51	0.46
1:B:24:ASP:O	1:D:411:PRO:HA	2.15	0.46
1:A:67:ARG:C	1:D:69:PRO:HB3	2.36	0.46
1:A:430:ARG:NE	1:B:419:GLU:OE1	2.47	0.46
1:A:423:HIS:CE1	1:A:425:SER:HB2	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:HB3	1:A:344:PRO:CD	2.46	0.46
1:C:498:LYS:O	1:C:501:GLU:HB3	2.16	0.46
1:B:122:ALA:HB2	1:B:257:PRO:HB3	1.98	0.46
1:C:369:TYR:C	1:C:371:GLN:H	2.19	0.46
1:A:96:ALA:CB	1:A:342:ILE:CD1	2.94	0.46
1:C:32:ASN:HD22	1:C:32:ASN:N	2.14	0.46
1:B:156:ASP:OD2	1:C:39:ASN:HA	2.16	0.46
1:A:201:ASP:CG	4:A:2084:HOH:O	2.53	0.46
1:A:334:ASP:HA	1:A:357:TYR:CG	2.51	0.46
1:D:442:VAL:HG11	1:D:484:VAL:HG21	1.98	0.46
1:D:209:ARG:HG2	1:D:274:PRO:CB	2.43	0.46
1:D:331:LEU:HD21	1:D:374:VAL:HG22	1.98	0.46
1:A:42:THR:O	1:D:431:PHE:HE1	1.99	0.46
1:B:95:LYS:HG2	1:B:224:ALA:N	2.31	0.46
2:D:3074:3TR:N3A	3:D:2003:HEM:NC	2.65	0.46
1:C:406:ASN:HD21	1:C:410:ALA:CB	2.06	0.46
1:C:194:GLN:OE1	1:C:197:PHE:HB3	2.16	0.46
1:A:187:LEU:O	1:A:188:ARG:HD2	2.16	0.46
1:B:116:ALA:O	1:B:168:LYS:NZ	2.46	0.46
1:B:11:MET:SD	1:C:180:MET:HG2	2.56	0.46
1:C:427:ASP:OD1	1:D:423:HIS:HB2	2.16	0.46
1:C:245:SER:OG	1:C:248:ASP:HB2	2.15	0.46
1:C:173:THR:O	1:C:175:LEU:HG	2.16	0.46
1:C:74:HIS:CE1	3:C:2002:HEM:C1D	3.05	0.45
1:B:447:LEU:HD22	1:B:485:HIS:HD2	1.79	0.45
1:D:115:VAL:HG23	1:D:127:ASP:OD2	2.16	0.45
1:A:410:ALA:HB1	1:A:411:PRO:HD2	1.98	0.45
1:B:66:GLU:HG2	1:D:387:ARG:O	2.16	0.45
1:B:67:ARG:NH2	1:C:168:LYS:NZ	2.63	0.45
1:D:155:ARG:CG	1:D:299:THR:HG23	2.46	0.45
1:C:396:ASN:O	1:C:397:GLN:CB	2.61	0.45
1:D:26:LEU:HD11	1:D:37:LYS:HD3	1.98	0.45
1:A:439:VAL:HG23	1:A:440:THR:N	2.31	0.45
1:B:388:ASP:H	1:B:396:ASN:HD21	1.64	0.45
1:C:283:MET:HE2	1:C:307:TYR:CZ	2.52	0.45
1:C:432:ASN:HD22	1:C:432:ASN:C	2.08	0.45
1:D:290:ILE:O	1:D:291:PHE:O	2.33	0.45
1:D:358:PRO:HB2	1:D:362:ARG:NH2	2.31	0.45
1:D:338:MET:HE2	1:D:342:ILE:C	2.37	0.45
1:D:26:LEU:C	1:D:26:LEU:CD2	2.84	0.45
1:D:60:MET:O	1:D:63:PHE:HB3	2.15	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASN:O	1:C:430:ARG:HB3	2.15	0.45
1:A:343:GLU:HB3	1:A:344:PRO:HD2	1.97	0.45
1:B:422:THR:HB	1:B:424:PHE:HE1	1.81	0.45
1:C:285:PHE:O	1:C:288:ALA:HB3	2.16	0.45
1:B:265:PHE:CD1	1:B:320:ASN:CG	2.89	0.45
1:A:327:GLU:O	1:A:331:LEU:HD22	2.16	0.45
1:A:70:GLU:O	1:A:71:ARG:C	2.52	0.45
1:B:191:SER:O	1:B:192:LEU:C	2.54	0.45
1:B:491:ARG:O	1:B:495:LEU:HD23	2.16	0.45
1:C:199:PHE:CB	1:C:458:LEU:HD12	2.46	0.45
1:B:329:GLU:OE1	1:B:329:GLU:HA	2.16	0.45
1:C:212:ASP:OD1	1:C:237:THR:HG22	2.17	0.45
1:A:65:ARG:O	1:C:389:GLY:HA2	2.16	0.45
1:B:88:HIS:HB2	1:B:312:VAL:HA	1.98	0.45
1:D:206:ASP:HB2	1:D:244:LEU:HG	1.97	0.45
1:C:138:GLU:HA	1:C:379:ARG:O	2.17	0.45
1:B:144:LEU:HD11	1:B:215:GLY:HA2	1.97	0.45
1:C:485:HIS:HA	1:C:486:PRO:HD2	1.67	0.45
1:A:144:LEU:HD11	1:A:233:PHE:CD1	2.51	0.45
1:A:177:ASP:HB3	1:A:180:MET:HB2	1.98	0.45
1:D:372:ILE:CG2	1:D:374:VAL:HG12	2.46	0.45
1:C:223:ASN:HD21	1:C:227:GLU:HB2	1.82	0.45
1:A:298:LEU:HD12	1:A:298:LEU:O	2.16	0.45
1:C:71:ARG:HG2	3:C:2002:HEM:O1A	2.17	0.45
1:A:90:ILE:HD13	1:A:312:VAL:HG22	1.97	0.45
1:D:287:GLU:C	1:D:289:GLU:N	2.69	0.45
1:D:126:ARG:O	1:D:127:ASP:HB2	2.17	0.45
1:C:83:TYR:CD1	1:C:83:TYR:C	2.89	0.45
1:D:202:ARG:HG2	1:D:202:ARG:H	1.57	0.45
1:B:97:LYS:HG3	1:B:139:ASP:OD2	2.16	0.45
1:A:51:VAL:CG2	1:B:49:LEU:HB3	2.47	0.45
1:B:84:PHE:CE1	1:B:313:GLY:HA3	2.52	0.45
1:D:148:ASN:C	1:D:148:ASN:HD22	2.20	0.45
1:A:273:TYR:HA	1:A:274:PRO:HD3	1.87	0.45
1:B:129:ARG:HB3	1:B:211:MET:CE	2.41	0.45
1:B:482:SER:O	1:B:485:HIS:N	2.50	0.45
1:B:177:ASP:CG	1:B:180:MET:HG3	2.37	0.45
1:C:470:GLN:O	1:C:473:ILE:HB	2.16	0.45
1:C:113:SER:O	1:C:130:GLY:N	2.31	0.45
1:B:81:PHE:HB2	1:B:319:ARG:NE	2.31	0.45
1:A:411:PRO:HA	1:C:24:ASP:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:HH12	1:A:397:GLN:NE2	2.15	0.45
1:D:129:ARG:HB2	1:D:148:ASN:CG	2.36	0.45
1:B:38:LEU:HD13	1:C:188:ARG:HH21	1.79	0.45
1:A:126:ARG:HH11	1:A:126:ARG:HB2	1.80	0.45
1:B:387:ARG:HG2	1:B:387:ARG:NH1	2.31	0.45
1:D:151:ILE:HG12	1:D:193:HIS:CD2	2.52	0.45
1:D:234:HIS:N	1:D:234:HIS:CD2	2.85	0.45
1:B:388:ASP:HA	1:D:325:PHE:CD2	2.52	0.45
1:C:37:LYS:HD2	1:C:59:GLU:OE1	2.17	0.45
1:D:274:PRO:HD2	1:D:317:LEU:O	2.17	0.45
1:C:402:ASN:HB2	1:D:165:HIS:ND1	2.31	0.45
1:A:233:PHE:C	1:A:234:HIS:HD2	2.19	0.45
1:D:14:TRP:CH2	1:D:18:ARG:HD3	2.52	0.45
1:C:220:LYS:HG2	1:C:221:LEU:N	2.31	0.45
1:D:485:HIS:ND1	1:D:487:GLU:N	2.63	0.45
1:B:151:ILE:HD12	1:B:194:GLN:HB2	1.98	0.45
1:B:132:ALA:HB2	3:B:2001:HEM:HMD2	1.98	0.44
1:C:334:ASP:HB2	1:C:337:ASN:OD1	2.17	0.44
1:A:492:ILE:O	1:A:493:GLN:C	2.55	0.44
1:B:83:TYR:N	1:B:108:ILE:HG12	2.32	0.44
1:C:467:LYS:HE2	1:C:468:ASP:OD2	2.17	0.44
1:B:10:GLN:HE21	1:C:172:GLN:NE2	2.15	0.44
1:B:26:LEU:HD21	1:B:37:LYS:HG2	1.98	0.44
1:C:126:ARG:HB2	1:C:126:ARG:CZ	2.47	0.44
1:D:97:LYS:O	1:D:100:GLU:HG3	2.17	0.44
1:D:106:THR:HG21	1:D:137:THR:HG22	1.99	0.44
1:A:248:ASP:HA	1:A:251:ARG:NH1	2.33	0.44
1:D:87:THR:OG1	1:D:313:GLY:HA2	2.17	0.44
1:B:265:PHE:HB2	4:B:2025:HOH:O	2.17	0.44
1:B:418:LEU:HD21	1:D:36:ASP:HB3	1.99	0.44
1:D:83:TYR:CZ	1:D:316:VAL:HG21	2.52	0.44
1:B:403:TYR:CD1	1:B:403:TYR:N	2.85	0.44
1:B:41:LEU:HD12	1:B:50:LEU:HD23	1.99	0.44
1:B:180:MET:HG2	1:C:11:MET:CE	2.47	0.44
1:C:368:ASN:O	1:C:371:GLN:HB2	2.17	0.44
1:B:15:LYS:O	1:B:18:ARG:HB2	2.17	0.44
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.48	0.44
1:A:102:ILE:O	4:A:2026:HOH:O	2.20	0.44
1:D:167:GLN:HB3	1:D:167:GLN:HE21	1.55	0.44
1:D:78:ALA:HB2	1:D:261:LEU:HG	2.00	0.44
1:D:439:VAL:CG2	1:D:440:THR:H	2.23	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:LYS:HA	1:D:441:GLN:OE1	2.18	0.44
1:C:361:HIS:C	1:C:363:HIS:N	2.71	0.44
1:C:217:HIS:NE2	1:C:350:LEU:CA	2.80	0.44
1:B:98:VAL:HG13	1:B:99:PHE:CE1	2.52	0.44
1:D:84:PHE:O	1:D:105:ARG:HA	2.17	0.44
1:B:454:GLN:N	1:B:457:ARG:HH12	2.16	0.44
1:A:209:ARG:CG	1:A:274:PRO:HB3	2.42	0.44
1:A:242:LYS:HD3	1:A:243:ASN:H	1.82	0.44
1:B:279:TYR:HA	1:B:310:ILE:O	2.17	0.44
1:B:278:LEU:HG	1:B:312:VAL:HG13	2.00	0.44
1:D:322:VAL:HB	1:D:327:GLU:OE2	2.17	0.44
1:A:73:VAL:CG1	1:A:164:ILE:HG21	2.48	0.44
1:A:396:ASN:HB3	1:C:323:ASN:ND2	2.33	0.44
1:A:50:LEU:N	1:A:50:LEU:HD22	2.32	0.44
1:B:323:ASN:HB2	1:D:398:GLY:HA2	2.00	0.44
1:A:320:ASN:HD22	1:A:320:ASN:HA	1.63	0.44
1:A:353:ARG:HB2	3:A:2000:HEM:HBB2	1.99	0.44
1:B:95:LYS:HB3	1:B:224:ALA:N	2.32	0.44
1:D:335:PRO:HD3	1:D:357:TYR:CG	2.53	0.44
1:D:170:ASN:HD22	1:D:172:GLN:N	2.12	0.44
1:B:439:VAL:O	1:B:442:VAL:N	2.49	0.44
1:D:148:ASN:O	1:D:149:THR:CB	2.66	0.44
1:C:99:PHE:O	1:C:100:GLU:C	2.56	0.44
1:B:295:PRO:HD2	1:C:46:ARG:NH1	2.29	0.44
1:D:60:MET:HE3	1:D:63:PHE:HD2	1.83	0.44
1:B:472:PHE:CE2	1:B:473:ILE:HG13	2.52	0.44
1:A:471:LEU:HA	1:A:471:LEU:HD23	1.83	0.44
1:A:215:GLY:O	1:A:217:HIS:N	2.50	0.44
1:B:496:LEU:O	1:B:500:ASN:N	2.45	0.44
1:D:155:ARG:HD3	1:D:297:ASP:OD1	2.17	0.44
1:D:439:VAL:O	1:D:442:VAL:N	2.50	0.44
1:B:447:LEU:O	1:B:447:LEU:HG	2.18	0.44
1:B:103:GLY:O	1:B:105:ARG:HG3	2.18	0.44
1:D:15:LYS:O	1:D:18:ARG:HB3	2.17	0.44
1:B:332:ALA:HA	1:B:361:HIS:NE2	2.33	0.44
1:B:134:LYS:HB2	1:B:333:PHE:CE1	2.53	0.44
1:C:199:PHE:HB2	1:C:458:LEU:HD12	2.00	0.44
1:B:408:PHE:CD2	1:B:408:PHE:N	2.86	0.44
1:D:97:LYS:HA	1:D:100:GLU:CG	2.48	0.44
1:A:96:ALA:HB2	1:A:342:ILE:HD11	2.00	0.44
1:A:98:VAL:HG13	1:A:99:PHE:CD1	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:VAL:HG11	1:C:101:HIS:O	2.18	0.44
1:A:26:LEU:HD13	1:C:411:PRO:HB2	1.99	0.43
1:C:142:TRP:CB	1:C:339:PRO:HD3	2.33	0.43
1:A:455:ARG:HB2	1:A:491:ARG:HH12	1.83	0.43
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.82	0.43
1:A:431:PHE:CD1	1:D:45:PRO:HB3	2.53	0.43
1:A:217:HIS:HE1	1:A:349:MET:HB3	1.82	0.43
1:B:492:ILE:HG22	1:B:496:LEU:HD11	2.00	0.43
1:D:297:ASP:OD2	1:D:300:LYS:HD3	2.18	0.43
1:C:334:ASP:OD1	1:C:361:HIS:CE1	2.71	0.43
1:B:25:VAL:O	1:B:26:LEU:C	2.56	0.43
1:C:82:GLY:C	1:C:108:ILE:HG12	2.39	0.43
1:A:329:GLU:C	1:A:331:LEU:N	2.71	0.43
1:C:287:GLU:HA	1:C:290:ILE:CG1	2.44	0.43
1:D:86:VAL:HG12	1:D:88:HIS:O	2.19	0.43
1:C:358:PRO:HA	1:C:369:TYR:OH	2.18	0.43
1:C:192:LEU:HD22	1:C:484:VAL:HG21	2.00	0.43
1:D:482:SER:O	1:D:485:HIS:N	2.52	0.43
1:D:419:GLU:CD	1:D:419:GLU:N	2.72	0.43
1:A:421:ARG:CG	1:B:429:GLN:HG2	2.47	0.43
1:B:68:ILE:HA	1:C:69:PRO:HG3	2.00	0.43
1:D:162:SER:CB	4:D:3076:HOH:O	2.67	0.43
1:B:192:LEU:HD12	1:B:438:ASN:O	2.17	0.43
1:D:220:LYS:HA	1:D:229:VAL:O	2.18	0.43
1:C:387:ARG:NH1	1:C:387:ARG:HG2	2.33	0.43
1:C:453:GLU:CG	1:C:457:ARG:HH22	2.31	0.43
1:B:18:ARG:O	1:B:19:ALA:C	2.55	0.43
1:D:235:TYR:HA	1:D:277:THR:O	2.18	0.43
1:D:254:HIS:O	1:D:255:GLU:C	2.56	0.43
1:C:12:LYS:O	1:C:16:GLU:HG3	2.17	0.43
4:B:2096:HOH:O	1:D:38:LEU:HD12	1.81	0.43
1:B:4:ARG:NH1	1:B:9:ASP:OD1	2.51	0.43
1:D:296:PHE:CE1	1:D:346:PRO:HD2	2.54	0.43
1:D:345:SER:C	1:D:347:ASP:H	2.22	0.43
1:B:106:THR:HG23	1:B:136:TYR:O	2.18	0.43
4:A:2054:HOH:O	1:C:22:LYS:HE2	2.18	0.43
1:C:459:CYS:HA	1:C:492:ILE:HD11	2.00	0.43
1:C:472:PHE:CE1	1:C:473:ILE:HG13	2.54	0.43
1:A:210:HIS:HB3	1:A:242:LYS:N	2.34	0.43
1:D:276:TRP:HB2	1:D:315:LEU:HB2	2.01	0.43
1:C:160:PHE:CZ	1:C:164:ILE:HG13	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:ALA:C	1:C:435:ASN:HD22	2.21	0.43
1:D:287:GLU:O	1:D:290:ILE:N	2.51	0.43
1:C:252:LEU:CD2	4:C:2147:HOH:O	2.51	0.43
1:A:391:MET:CE	1:C:391:MET:HB2	2.49	0.43
1:C:111:ARG:NH2	3:C:2002:HEM:CAD	2.75	0.43
1:B:404:TYR:HE2	1:D:38:LEU:CD1	2.32	0.43
1:A:396:ASN:C	1:A:398:GLY:H	2.21	0.43
1:C:361:HIS:C	1:C:363:HIS:H	2.20	0.43
1:C:297:ASP:CG	1:C:300:LYS:HG2	2.38	0.43
1:C:453:GLU:HG3	1:C:457:ARG:HH22	1.84	0.43
1:A:251:ARG:HG2	1:A:255:GLU:CD	2.39	0.43
1:C:304:HIS:CD2	1:C:309:LEU:HD13	2.53	0.43
1:A:266:ASN:O	1:A:267:ALA:C	2.57	0.43
1:C:74:HIS:NE2	1:C:115:VAL:HG22	2.33	0.43
1:B:479:LYS:HE2	1:B:483:ASP:CG	2.39	0.43
1:C:199:PHE:HB2	1:C:458:LEU:CD1	2.49	0.43
1:C:336:SER:HA	1:C:354:LEU:CD2	2.45	0.43
1:B:381:ARG:HH12	1:D:24:ASP:CB	2.32	0.43
1:A:56:PHE:O	1:A:57:THR:C	2.57	0.43
1:A:287:GLU:OE1	1:A:307:TYR:HE1	2.01	0.43
1:A:4:ARG:HD2	1:A:9:ASP:OD1	2.18	0.43
1:C:177:ASP:HB3	1:C:180:MET:CE	2.49	0.43
1:B:160:PHE:H	1:B:161:PRO:HD2	1.84	0.43
1:C:304:HIS:CE1	4:C:2083:HOH:O	2.72	0.43
3:B:2001:HEM:HHD	3:B:2001:HEM:HMD2	1.74	0.43
1:B:46:ARG:HH21	1:C:294:ASN:HA	1.83	0.43
1:A:62:HIS:HE1	1:C:387:ARG:O	2.02	0.43
1:D:208:HIS:O	1:D:211:MET:HG2	2.19	0.43
1:D:210:HIS:HD2	1:D:242:LYS:HB2	1.82	0.43
1:B:165:HIS:HE2	1:C:66:GLU:CD	2.22	0.42
1:B:280:ILE:O	1:B:310:ILE:HD13	2.19	0.42
1:B:384:ASN:N	1:B:397:GLN:HE22	2.14	0.42
1:A:422:THR:HB	1:A:424:PHE:CE1	2.54	0.42
1:D:357:TYR:N	1:D:357:TYR:CD1	2.86	0.42
1:C:291:PHE:CE2	1:C:293:PHE:HD1	2.37	0.42
1:C:371:GLN:OE1	1:C:393:MET:HB2	2.19	0.42
1:C:150:PRO:HG3	1:C:214:TYR:CE1	2.54	0.42
1:D:159:LEU:HD23	1:D:184:PHE:CE1	2.54	0.42
1:C:221:LEU:HA	1:C:341:GLY:O	2.19	0.42
1:A:279:TYR:O	1:A:280:ILE:HG23	2.19	0.42
1:B:141:ASN:OD1	1:B:377:PRO:HB3	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:ARG:HG2	1:D:381:ARG:HH11	1.84	0.42
1:A:353:ARG:CD	3:A:2000:HEM:CMC	2.97	0.42
1:A:71:ARG:HH21	1:A:364:ARG:HH22	1.67	0.42
1:C:71:ARG:HG2	3:C:2002:HEM:CGA	2.49	0.42
1:D:368:ASN:CG	1:D:371:GLN:NE2	2.73	0.42
1:D:284:THR:O	1:D:287:GLU:N	2.52	0.42
1:D:410:ALA:HB1	1:D:411:PRO:HD2	2.02	0.42
1:A:112:PHE:HA	1:A:130:GLY:O	2.19	0.42
1:C:280:ILE:HG23	1:C:312:VAL:CG2	2.47	0.42
1:C:82:GLY:HA3	1:C:317:LEU:HA	2.01	0.42
1:D:57:THR:O	1:D:58:ASP:C	2.55	0.42
1:C:71:ARG:NE	3:C:2002:HEM:O2D	2.52	0.42
1:B:414:GLN:HA	1:B:415:PRO:HD2	1.89	0.42
1:A:293:PHE:HB3	1:A:300:LYS:HZ3	1.84	0.42
1:A:235:TYR:CD1	1:A:235:TYR:N	2.86	0.42
1:B:192:LEU:HD13	1:B:484:VAL:CG2	2.49	0.42
1:B:179:ASP:OD1	1:C:4:ARG:NH2	2.41	0.42
1:A:397:GLN:O	1:A:400:ALA:HB3	2.19	0.42
1:B:294:ASN:ND2	1:C:46:ARG:HD2	2.34	0.42
1:D:277:THR:HB	1:D:279:TYR:CE1	2.54	0.42
1:A:492:ILE:CG2	1:A:496:LEU:HD13	2.48	0.42
1:C:446:TYR:CE1	1:C:455:ARG:CG	3.03	0.42
1:A:421:ARG:HG2	1:B:429:GLN:HG2	2.01	0.42
1:C:84:PHE:HA	1:C:314:LYS:O	2.19	0.42
1:A:104:LYS:NZ	1:A:138:GLU:OE2	2.50	0.42
1:A:74:HIS:HA	1:A:114:THR:O	2.19	0.42
1:A:51:VAL:HG12	1:B:51:VAL:CA	2.45	0.42
1:A:408:PHE:HA	1:C:15:LYS:HD2	2.01	0.42
1:C:209:ARG:HD2	1:C:274:PRO:HB3	2.01	0.42
1:B:74:HIS:N	4:B:2029:HOH:O	2.52	0.42
1:A:206:ASP:CA	1:A:244:LEU:HG	2.49	0.42
1:B:81:PHE:CD1	1:B:81:PHE:N	2.87	0.42
1:B:154:ILE:CD1	1:B:160:PHE:HA	2.49	0.42
1:B:265:PHE:O	1:B:320:ASN:ND2	2.51	0.42
1:A:353:ARG:NE	3:A:2000:HEM:C4C	2.87	0.42
1:D:127:ASP:C	1:D:128:PRO:O	2.58	0.42
1:B:71:ARG:HB2	1:B:75:ALA:HA	2.02	0.42
1:A:363:HIS:NE2	1:D:65:ARG:HA	2.34	0.42
1:A:76:LYS:NZ	1:A:123:ASP:OD1	2.53	0.42
1:B:11:MET:O	1:D:408:PHE:HD2	2.02	0.42
1:A:460:GLU:HA	1:A:495:LEU:HD13	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:NE2	1:C:172:GLN:HE21	2.18	0.42
1:A:327:GLU:O	1:A:374:VAL:HG21	2.20	0.42
1:B:144:LEU:HD11	1:B:215:GLY:CA	2.49	0.42
1:D:157:ALA:O	1:D:160:PHE:N	2.34	0.42
1:D:437:ASP:OD2	1:D:440:THR:HB	2.18	0.42
1:C:155:ARG:NH2	1:C:438:ASN:ND2	2.66	0.42
1:C:471:LEU:O	1:C:473:ILE:N	2.53	0.42
1:D:128:PRO:C	1:D:129:ARG:HG2	2.40	0.42
1:C:145:VAL:CG1	1:C:353:ARG:HH12	2.32	0.42
1:A:151:ILE:HD13	1:A:193:HIS:ND1	2.35	0.42
1:D:132:ALA:HB1	1:D:333:PHE:CD2	2.55	0.42
1:D:206:ASP:CB	1:D:244:LEU:HG	2.50	0.42
1:A:145:VAL:HG13	3:A:2000:HEM:CMD	2.07	0.42
1:D:361:HIS:HB3	1:D:369:TYR:CE2	2.55	0.42
1:A:396:ASN:C	1:A:398:GLY:N	2.72	0.42
1:C:62:HIS:O	1:C:62:HIS:ND1	2.49	0.42
1:D:229:VAL:HA	1:D:285:PHE:CE1	2.53	0.42
1:C:296:PHE:O	1:C:297:ASP:C	2.58	0.42
1:C:470:GLN:O	1:C:471:LEU:C	2.57	0.42
1:C:78:ALA:CB	1:C:261:LEU:HD13	2.49	0.42
1:C:220:LYS:HD2	1:C:343:GLU:HB2	2.02	0.42
1:A:351:GLN:NE2	1:C:52:GLN:NE2	2.67	0.42
1:B:386:GLN:C	1:B:387:ARG:HG2	2.40	0.42
1:A:152:PHE:CB	1:A:298:LEU:HG	2.49	0.42
1:B:414:GLN:HB2	1:D:25:VAL:HG13	2.02	0.42
1:D:93:TYR:O	1:D:223:ASN:HB3	2.20	0.42
1:A:278:LEU:O	1:A:312:VAL:HB	2.20	0.42
1:C:63:PHE:HA	1:C:66:GLU:HG3	2.01	0.42
1:C:199:PHE:CD2	1:C:462:ILE:HA	2.54	0.42
1:A:67:ARG:O	1:D:69:PRO:CB	2.68	0.42
1:A:67:ARG:HG3	1:D:72:VAL:HA	2.02	0.42
1:B:245:SER:C	1:B:247:GLU:N	2.70	0.42
1:D:99:PHE:O	1:D:100:GLU:C	2.57	0.42
1:B:393:MET:CG	1:D:393:MET:HG3	2.50	0.42
1:B:198:LEU:C	1:B:200:SER:H	2.22	0.42
1:B:3:ASN:HD21	1:B:12:LYS:NZ	2.17	0.42
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.93	0.42
1:B:146:GLY:HA2	3:B:2001:HEM:CAC	2.44	0.42
1:A:40:SER:HB3	1:A:49:LEU:CD2	2.50	0.42
1:B:50:LEU:C	1:B:52:GLN:N	2.72	0.42
1:A:469:ALA:O	1:A:470:GLN:C	2.56	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ARG:HG2	1:C:211:MET:HE1	2.01	0.42
1:A:110:VAL:HG12	1:A:133:VAL:HG22	2.02	0.42
1:A:279:TYR:CD1	1:A:279:TYR:N	2.88	0.42
1:A:127:ASP:C	1:A:128:PRO:O	2.56	0.41
1:C:115:VAL:HG12	1:C:116:ALA:N	2.35	0.41
1:B:67:ARG:HH21	1:C:168:LYS:NZ	2.17	0.41
1:B:131:PHE:O	1:B:146:GLY:O	2.38	0.41
1:A:53:ASP:C	1:A:53:ASP:OD1	2.58	0.41
1:A:262:ARG:NH1	1:D:175:LEU:HD13	2.35	0.41
1:C:294:ASN:HD21	1:C:296:PHE:HB2	1.85	0.41
1:C:487:GLU:HG2	1:C:491:ARG:CG	2.48	0.41
1:C:65:ARG:O	1:C:67:ARG:N	2.53	0.41
1:D:151:ILE:HG12	1:D:193:HIS:HD2	1.85	0.41
1:B:125:VAL:CG2	1:B:126:ARG:N	2.83	0.41
1:B:233:PHE:CD1	1:B:233:PHE:N	2.88	0.41
1:C:163:PHE:HB2	1:C:184:PHE:CZ	2.54	0.41
1:B:365:LEU:HD12	1:B:369:TYR:HB2	2.01	0.41
1:A:353:ARG:CG	3:A:2000:HEM:C4B	3.03	0.41
1:C:110:VAL:HG12	1:C:111:ARG:N	2.35	0.41
1:A:273:TYR:CD1	1:A:318:ASN:HA	2.55	0.41
1:C:32:ASN:ND2	1:C:32:ASN:N	2.68	0.41
1:D:162:SER:HB2	4:D:3076:HOH:O	2.20	0.41
1:B:146:GLY:CA	3:B:2001:HEM:HAC	2.50	0.41
1:D:383:ALA:HB1	1:D:411:PRO:HG3	2.02	0.41
1:A:54:VAL:HG11	1:C:336:SER:HB3	2.02	0.41
1:B:78:ALA:HB1	1:B:264:LEU:HD23	2.03	0.41
1:D:188:ARG:HB3	1:D:190:GLU:CD	2.41	0.41
1:D:91:THR:HG21	1:D:100:GLU:O	2.20	0.41
1:B:233:PHE:C	1:B:234:HIS:CD2	2.92	0.41
1:A:250:ALA:O	1:A:253:ALA:HB3	2.19	0.41
1:B:175:LEU:HD12	1:C:7:ALA:HB1	2.03	0.41
1:D:146:GLY:O	1:D:147:ASN:OD1	2.38	0.41
1:A:53:ASP:CG	1:D:430:ARG:HH22	2.23	0.41
1:D:264:LEU:O	1:D:265:PHE:C	2.58	0.41
1:A:155:ARG:HB3	1:A:155:ARG:HE	1.68	0.41
1:B:43:VAL:HG13	1:B:43:VAL:O	2.20	0.41
1:B:443:ARG:O	1:B:447:LEU:HD23	2.20	0.41
1:A:399:GLY:O	1:A:400:ALA:O	2.38	0.41
1:C:471:LEU:O	1:C:472:PHE:C	2.59	0.41
1:C:287:GLU:CA	1:C:290:ILE:HG12	2.45	0.41
1:A:112:PHE:CE1	1:A:131:PHE:CE1	3.08	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:GLY:HA3	1:C:317:LEU:HD23	2.02	0.41
1:D:248:ASP:HA	1:D:251:ARG:NH1	2.36	0.41
1:A:496:LEU:O	1:A:499:TYR:N	2.53	0.41
1:A:479:LYS:HG3	1:A:480:ASN:N	2.35	0.41
1:A:360:THR:CG2	1:A:361:HIS:N	2.84	0.41
1:A:188:ARG:HB3	1:A:190:GLU:OE2	2.20	0.41
1:B:129:ARG:CB	1:B:211:MET:CE	2.98	0.41
1:D:34:VAL:O	1:D:34:VAL:HG23	2.21	0.41
1:B:108:ILE:HD13	1:B:315:LEU:HD22	2.03	0.41
1:B:138:GLU:HA	1:B:379:ARG:O	2.20	0.41
1:D:498:LYS:O	1:D:501:GLU:N	2.46	0.41
1:B:492:ILE:O	1:B:493:GLN:C	2.58	0.41
1:B:195:VAL:HG13	1:B:199:PHE:CE1	2.56	0.41
1:D:285:PHE:CE1	4:D:3134:HOH:O	2.74	0.41
1:A:11:MET:CE	1:C:403:TYR:OH	2.69	0.41
1:A:387:ARG:NH1	1:A:397:GLN:NE2	2.69	0.41
1:A:177:ASP:O	1:A:180:MET:HB2	2.21	0.41
1:A:4:ARG:HD3	1:A:8:SER:HB2	2.03	0.41
1:A:294:ASN:ND2	1:D:46:ARG:HG2	2.34	0.41
1:A:420:HIS:CG	1:A:421:ARG:N	2.89	0.41
1:C:359:ASP:HA	1:C:362:ARG:HD2	2.01	0.41
1:B:145:VAL:HG12	1:B:353:ARG:NH2	2.33	0.41
1:B:95:LYS:H	1:B:95:LYS:HG3	1.74	0.41
1:A:154:ILE:HA	1:A:190:GLU:HG3	2.02	0.41
1:C:485:HIS:C	1:C:485:HIS:ND1	2.74	0.41
1:B:4:ARG:CB	1:B:4:ARG:HH11	2.32	0.41
1:C:290:ILE:O	1:C:291:PHE:C	2.58	0.41
1:B:287:GLU:O	1:B:290:ILE:HG22	2.21	0.41
1:C:232:LYS:O	1:C:280:ILE:HA	2.21	0.41
1:B:381:ARG:NH1	1:D:24:ASP:HB3	2.36	0.41
1:D:97:LYS:CA	1:D:100:GLU:HG3	2.50	0.41
1:C:17:GLN:C	1:C:19:ALA:H	2.24	0.41
1:A:5:ASP:OD2	1:A:7:ALA:HB3	2.21	0.41
1:A:88:HIS:CE1	4:A:2109:HOH:O	2.74	0.41
1:A:79:GLY:HA3	1:A:328:VAL:HG13	2.03	0.41
1:D:335:PRO:CD	1:D:357:TYR:CG	3.03	0.41
1:A:212:ASP:HB2	1:A:214:TYR:CE2	2.55	0.41
1:B:454:GLN:CA	1:B:457:ARG:NH1	2.79	0.41
1:A:51:VAL:HG13	1:B:50:LEU:C	2.40	0.41
1:C:298:LEU:HD23	1:C:349:MET:HG2	1.99	0.41
1:C:421:ARG:HD2	1:D:429:GLN:OE1	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HA	1:D:40:SER:O	2.21	0.41
1:A:423:HIS:HE1	1:A:425:SER:HB2	1.85	0.41
1:B:334:ASP:N	1:B:334:ASP:OD1	2.54	0.41
1:A:353:ARG:NE	3:A:2000:HEM:C2C	2.89	0.41
1:B:95:LYS:HG2	1:B:223:ASN:C	2.41	0.41
1:D:173:THR:O	1:D:174:HIS:HB3	2.20	0.41
1:B:43:VAL:HG13	1:B:48:PRO:HD2	2.01	0.41
1:A:209:ARG:HG2	1:A:274:PRO:CB	2.45	0.41
1:D:338:MET:HE3	1:D:342:ILE:HG22	2.02	0.41
1:C:126:ARG:CG	1:C:126:ARG:NH1	2.78	0.41
1:C:262:ARG:HG3	1:C:266:ASN:HD22	1.85	0.41
1:D:215:GLY:O	1:D:217:HIS:N	2.54	0.41
1:B:393:MET:HB3	1:B:394:MET:H	1.49	0.41
1:D:460:GLU:HG2	1:D:495:LEU:HD11	2.03	0.41
1:C:57:THR:O	1:C:58:ASP:C	2.58	0.41
1:C:5:ASP:HB2	1:C:6:PRO:HD2	2.02	0.41
1:C:147:ASN:HB2	3:C:2002:HEM:CBC	2.48	0.41
1:C:160:PHE:CE2	3:C:2002:HEM:C3B	3.08	0.41
1:D:368:ASN:HA	1:D:368:ASN:HD22	1.69	0.41
1:D:353:ARG:NH2	3:D:2003:HEM:CHD	2.84	0.41
1:A:300:LYS:CB	1:A:441:GLN:HE22	2.19	0.41
1:C:22:LYS:HD3	1:C:22:LYS:C	2.41	0.41
1:C:432:ASN:ND2	1:C:432:ASN:C	2.74	0.41
1:B:177:ASP:OD1	1:B:179:ASP:HB2	2.20	0.41
1:C:197:PHE:CD1	1:C:197:PHE:C	2.94	0.41
1:B:78:ALA:O	1:B:111:ARG:HG3	2.21	0.41
1:D:201:ASP:O	1:D:243:ASN:HB3	2.21	0.41
1:A:70:GLU:OE2	1:A:118:GLU:HA	2.21	0.40
1:A:334:ASP:OD1	1:A:361:HIS:ND1	2.54	0.40
1:C:74:HIS:CG	3:C:2002:HEM:C4D	3.10	0.40
1:C:73:VAL:CG2	3:C:2002:HEM:NA	2.84	0.40
1:B:423:HIS:C	1:B:423:HIS:CD2	2.94	0.40
1:B:236:LYS:C	1:B:276:TRP:HD1	2.24	0.40
1:C:217:HIS:CG	1:C:350:LEU:HB2	2.56	0.40
1:C:350:LEU:O	1:C:353:ARG:HB2	2.21	0.40
1:C:367:PRO:HG2	1:C:390:PRO:HG2	2.03	0.40
1:D:374:VAL:CG1	1:D:375:ASN:N	2.84	0.40
1:B:11:MET:HB3	1:D:408:PHE:CD2	2.56	0.40
1:C:153:PHE:HD1	1:C:185:TRP:HE1	1.68	0.40
1:D:107:PRO:HG2	1:D:136:TYR:HB2	2.02	0.40
1:C:194:GLN:OE1	1:C:194:GLN:O	2.39	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:THR:O	1:D:345:SER:OG	2.28	0.40
1:D:218:THR:HG23	1:D:302:TRP:CZ2	2.56	0.40
1:B:332:ALA:HB3	1:B:375:ASN:CG	2.41	0.40
1:A:251:ARG:O	1:A:255:GLU:HG3	2.21	0.40
1:A:452:GLU:O	1:A:453:GLU:C	2.59	0.40
1:C:448:LYS:NZ	4:C:2184:HOH:O	2.36	0.40
1:A:263:ASP:C	1:A:263:ASP:OD1	2.59	0.40
1:A:217:HIS:CD2	1:A:353:ARG:HH11	2.35	0.40
1:B:494:ALA:CB	4:B:2086:HOH:O	2.59	0.40
1:B:45:PRO:O	1:B:46:ARG:HD2	2.21	0.40
1:C:214:TYR:O	1:C:215:GLY:C	2.58	0.40
1:D:90:ILE:C	1:D:90:ILE:HD12	2.41	0.40
1:B:393:MET:O	1:B:394:MET:O	2.39	0.40
1:D:98:VAL:O	1:D:98:VAL:HG22	2.21	0.40
1:C:450:LEU:HG	1:C:454:GLN:HB3	2.03	0.40
1:A:11:MET:HE3	1:C:408:PHE:CE1	2.56	0.40
1:A:400:ALA:HA	1:A:401:PRO:HD3	1.99	0.40
1:B:148:ASN:HA	1:B:212:ASP:O	2.22	0.40
1:C:291:PHE:CG	1:C:292:PRO:HD2	2.57	0.40
1:B:290:ILE:CG2	1:B:291:PHE:N	2.84	0.40
1:C:125:VAL:O	1:C:126:ARG:C	2.60	0.40
1:A:391:MET:HE2	1:C:391:MET:HB2	2.02	0.40
1:D:246:VAL:O	1:D:250:ALA:CB	2.70	0.40
1:D:331:LEU:HD23	1:D:331:LEU:HA	1.91	0.40
1:A:463:ALA:O	1:A:467:LYS:HB3	2.21	0.40
1:A:82:GLY:HA3	1:A:316:VAL:O	2.22	0.40
1:B:146:GLY:HA3	1:B:214:TYR:O	2.21	0.40
1:A:41:LEU:N	1:D:430:ARG:NH1	2.69	0.40
1:D:18:ARG:NH2	1:D:24:ASP:OD1	2.55	0.40
1:C:153:PHE:HD2	1:C:153:PHE:H	1.69	0.40
1:B:252:LEU:CD1	1:B:252:LEU:N	2.84	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:289:GLU:OE1	4:C:2061:HOH:O[3_655]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	497/506 (98%)	400 (80%)	80 (16%)	17 (3%)	5	23
1	B	497/506 (98%)	408 (82%)	65 (13%)	24 (5%)	3	15
1	C	497/506 (98%)	398 (80%)	82 (16%)	17 (3%)	5	23
1	D	497/506 (98%)	402 (81%)	74 (15%)	21 (4%)	3	18
All	All	1988/2024 (98%)	1608 (81%)	301 (15%)	79 (4%)	4	19

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLU
1	B	19	ALA
1	B	100	GLU
1	B	331	LEU
1	B	394	MET
1	C	181	VAL
1	D	149	THR
1	D	401	PRO
1	A	56	PHE
1	A	229	VAL
1	A	308	PRO
1	A	347	ASP
1	B	124	THR
1	B	169	ARG
1	B	216	SER
1	B	393	MET
1	B	440	THR
1	B	448	LYS
1	C	168	LYS
1	C	427	ASP
1	D	100	GLU
1	D	121	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	398	GLY
1	D	411	PRO
1	D	440	THR
1	A	440	THR
1	B	115	VAL
1	B	348	LYS
1	B	437	ASP
1	C	66	GLU
1	C	121	SER
1	C	216	SER
1	C	347	ASP
1	D	12	LYS
1	D	19	ALA
1	D	52	GLN
1	D	59	GLU
1	D	216	SER
1	D	378	TYR
1	A	19	ALA
1	A	101	HIS
1	A	330	GLN
1	A	470	GLN
1	B	192	LEU
1	B	199	PHE
1	B	203	GLY
1	B	259	TYR
1	B	332	ALA
1	B	395	ASP
1	C	215	GLY
1	C	397	GLN
1	D	190	GLU
1	D	337	ASN
1	A	91	THR
1	A	359	ASP
1	A	437	ASP
1	B	7	ALA
1	B	16	GLU
1	C	53	ASP
1	C	200	SER
1	C	393	MET
1	C	437	ASP
1	C	448	LYS
1	C	466	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	467	LYS
1	D	437	ASP
1	A	271	GLY
1	A	400	ALA
1	B	9	ASP
1	B	388	ASP
1	B	492	ILE
1	D	471	LEU
1	A	45	PRO
1	D	240	GLY
1	D	291	PHE
1	A	439	VAL
1	C	492	ILE
1	D	346	PRO
1	D	128	PRO

### 5.3.2 Protein sidechains ⓘ

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	431/437 (99%)	396 (92%)	35 (8%)	15	45
1	B	431/437 (99%)	387 (90%)	44 (10%)	9	32
1	C	431/437 (99%)	394 (91%)	37 (9%)	13	42
1	D	431/437 (99%)	403 (94%)	28 (6%)	21	57
All	All	1724/1748 (99%)	1580 (92%)	144 (8%)	14	43

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	16	GLU
1	A	18	ARG
1	A	24	ASP
1	A	36	ASP
1	A	41	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	49	LEU
1	A	65	ARG
1	A	71	ARG
1	A	101	HIS
1	A	113	SER
1	A	118	GLU
1	A	131	PHE
1	A	135	PHE
1	A	139	ASP
1	A	148	ASN
1	A	158	LEU
1	A	170	ASN
1	A	179	ASP
1	A	194	GLN
1	A	200	SER
1	A	229	VAL
1	A	231	CYS
1	A	235	TYR
1	A	263	ASP
1	A	353	ARG
1	A	360	THR
1	A	379	ARG
1	A	394	MET
1	A	402	ASN
1	A	413	HIS
1	A	418	LEU
1	A	421	ARG
1	A	483	ASP
1	A	488	TYR
1	B	4	ARG
1	B	8	SER
1	B	37	LYS
1	B	41	LEU
1	B	46	ARG
1	B	49	LEU
1	B	50	LEU
1	B	92	ARG
1	B	95	LYS
1	B	114	THR
1	B	126	ARG
1	B	127	ASP
1	B	131	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	144	LEU
1	B	149	THR
1	B	151	ILE
1	B	179	ASP
1	B	201	ASP
1	B	202	ARG
1	B	204	ILE
1	B	232	LYS
1	B	235	TYR
1	B	237	THR
1	B	239	GLN
1	B	272	ASN
1	B	290	ILE
1	B	312	VAL
1	B	330	GLN
1	B	334	ASP
1	B	337	ASN
1	B	374	VAL
1	B	393	MET
1	B	395	ASP
1	B	396	ASN
1	B	402	ASN
1	B	412	GLU
1	B	427	ASP
1	B	429	GLN
1	B	438	ASN
1	B	441	GLN
1	B	457	ARG
1	B	466	LEU
1	B	472	PHE
1	B	498	LYS
1	C	4	ARG
1	C	22	LYS
1	C	40	SER
1	C	46	ARG
1	C	62	HIS
1	C	63	PHE
1	C	92	ARG
1	C	105	ARG
1	C	126	ARG
1	C	131	PHE
1	C	137	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	142	TRP
1	C	149	THR
1	C	159	LEU
1	C	175	LEU
1	C	194	GLN
1	C	204	ILE
1	C	235	TYR
1	C	237	THR
1	C	239	GLN
1	C	248	ASP
1	C	262	ARG
1	C	263	ASP
1	C	293	PHE
1	C	347	ASP
1	C	414	GLN
1	C	432	ASN
1	C	433	SER
1	C	438	ASN
1	C	439	VAL
1	C	451	ASN
1	C	453	GLU
1	C	467	LYS
1	C	472	PHE
1	C	476	LYS
1	C	488	TYR
1	C	501	GLU
1	D	3	ASN
1	D	22	LYS
1	D	111	ARG
1	D	131	PHE
1	D	138	GLU
1	D	139	ASP
1	D	148	ASN
1	D	159	LEU
1	D	167	GLN
1	D	202	ARG
1	D	235	TYR
1	D	247	GLU
1	D	280	ILE
1	D	285	PHE
1	D	314	LYS
1	D	336	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	371	GLN
1	D	378	TYR
1	D	388	ASP
1	D	397	GLN
1	D	413	HIS
1	D	414	GLN
1	D	436	ASP
1	D	453	GLU
1	D	467	LYS
1	D	479	LYS
1	D	488	TYR
1	D	501	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	167	GLN
1	A	234	HIS
1	A	239	GLN
1	A	254	HIS
1	A	320	ASN
1	A	337	ASN
1	A	363	HIS
1	A	396	ASN
1	A	402	ASN
1	A	413	HIS
1	A	429	GLN
1	A	454	GLN
1	A	470	GLN
1	A	480	ASN
1	A	485	HIS
1	A	500	ASN
1	B	3	ASN
1	B	21	GLN
1	B	32	ASN
1	B	62	HIS
1	B	147	ASN
1	B	167	GLN
1	B	210	HIS
1	B	234	HIS
1	B	272	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	337	ASN
1	B	386	GLN
1	B	396	ASN
1	B	397	GLN
1	B	402	ASN
1	B	413	HIS
1	B	423	HIS
1	B	429	GLN
1	B	435	ASN
1	B	461	ASN
1	B	474	GLN
1	C	3	ASN
1	C	13	HIS
1	C	17	GLN
1	C	21	GLN
1	C	32	ASN
1	C	52	GLN
1	C	172	GLN
1	C	239	GLN
1	C	413	HIS
1	C	414	GLN
1	C	432	ASN
1	C	435	ASN
1	C	438	ASN
1	C	454	GLN
1	C	461	ASN
1	C	470	GLN
1	C	474	GLN
1	C	500	ASN
1	D	3	ASN
1	D	32	ASN
1	D	52	GLN
1	D	148	ASN
1	D	167	GLN
1	D	170	ASN
1	D	193	HIS
1	D	210	HIS
1	D	234	HIS
1	D	254	HIS
1	D	330	GLN
1	D	337	ASN
1	D	368	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	371	GLN
1	D	396	ASN
1	D	429	GLN
1	D	480	ASN
1	D	493	GLN
1	D	500	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 ⓘ

5 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	$\# Z  > 2$
3	HEM	A	2000	1	30,50,50	3.58	12 (40%)	24,82,82	3.55	9 (37%)
3	HEM	B	2001	1	30,50,50	3.57	15 (50%)	24,82,82	3.37	12 (50%)
3	HEM	C	2002	1	30,50,50	2.73	10 (33%)	24,82,82	2.35	9 (37%)
3	HEM	D	2003	1,2	30,50,50	4.44	16 (53%)	24,82,82	6.41	13 (54%)
2	3TR	D	3074	1,3	4,6,6	2.33	2 (50%)	1,7,7	4.31	1 (100%)

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
3	HEM	A	2000	1	-	0/10/54/54	0/0/8/8
3	HEM	B	2001	1	-	0/10/54/54	0/0/8/8
3	HEM	C	2002	1	-	0/10/54/54	0/0/8/8
3	HEM	D	2003	1,2	-	0/10/54/54	0/0/8/8
2	3TR	D	3074	1,3	-	0/0/0/0	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2003	HEM	CHC-C4B	-10.25	1.10	1.38
3	D	2003	HEM	CHD-C1D	-7.60	1.17	1.38
3	C	2002	HEM	C3B-C4B	-6.97	1.45	1.51
3	A	2000	HEM	C3B-C4B	-6.83	1.45	1.51
3	D	2003	HEM	C3B-C4B	-6.82	1.45	1.51
3	B	2001	HEM	C3B-C4B	-6.76	1.45	1.51
3	B	2001	HEM	C3B-CAB	-6.73	1.38	1.51
3	D	2003	HEM	C3B-CAB	-6.71	1.38	1.51
3	C	2002	HEM	C3B-CAB	-6.66	1.38	1.51
3	A	2000	HEM	C3B-CAB	-6.57	1.39	1.51
3	A	2000	HEM	C3C-CAC	-6.38	1.39	1.51
3	D	2003	HEM	C2D-C3D	-6.19	1.36	1.54
3	A	2000	HEM	C2D-C3D	-6.17	1.36	1.54
3	C	2002	HEM	C2D-C3D	-6.17	1.36	1.54
3	B	2001	HEM	C2D-C3D	-6.17	1.36	1.54
3	D	2003	HEM	FE-NC	-4.96	1.76	1.95
3	A	2000	HEM	C3D-C4D	-4.60	1.45	1.51
3	D	2003	HEM	C3D-C4D	-4.44	1.45	1.51
3	C	2002	HEM	C3D-C4D	-4.43	1.45	1.51
3	B	2001	HEM	C3D-C4D	-4.37	1.46	1.51
3	A	2000	HEM	C2C-C1C	-3.34	1.46	1.52
3	C	2002	HEM	C2C-C1C	-3.29	1.46	1.52
3	D	2003	HEM	C2C-C1C	-3.29	1.46	1.52
3	D	2003	HEM	C1A-CHA	-3.26	1.30	1.39
3	B	2001	HEM	C2C-C1C	-3.07	1.46	1.52
3	C	2002	HEM	C2B-C1B	-2.09	1.45	1.51
3	D	2003	HEM	C2B-C1B	-2.07	1.45	1.51
3	B	2001	HEM	C2D-C1D	-2.07	1.45	1.51
3	A	2000	HEM	C2B-C1B	-2.06	1.45	1.51
3	B	2001	HEM	C2B-C1B	-2.03	1.45	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2003	HEM	C2D-C1D	-2.00	1.45	1.51
3	A	2000	HEM	CBB-CAB	2.30	1.42	1.29
3	C	2002	HEM	CBB-CAB	2.31	1.42	1.29
3	B	2001	HEM	CBB-CAB	2.31	1.42	1.29
3	D	2003	HEM	CBB-CAB	2.32	1.42	1.29
2	D	3074	3TR	C3-N3A	2.50	1.39	1.34
3	B	2001	HEM	CHC-C1C	2.90	1.43	1.36
3	B	2001	HEM	C1C-NC	3.07	1.39	1.36
3	D	2003	HEM	C1C-NC	3.21	1.40	1.36
3	C	2002	HEM	C1C-NC	3.21	1.40	1.36
2	D	3074	3TR	C5-N1	3.24	1.38	1.32
3	A	2000	HEM	C1C-NC	3.29	1.40	1.36
3	D	2003	HEM	CBC-CAC	3.71	1.50	1.29
3	C	2002	HEM	CBC-CAC	3.98	1.52	1.29
3	C	2002	HEM	C4C-NC	4.01	1.41	1.36
3	A	2000	HEM	C4C-NC	4.03	1.41	1.36
3	B	2001	HEM	C4C-NC	4.03	1.41	1.36
3	D	2003	HEM	C4C-NC	4.06	1.41	1.36
3	B	2001	HEM	CBC-CAC	4.22	1.53	1.29
3	B	2001	HEM	CHD-C1D	5.18	1.53	1.38
3	A	2000	HEM	FE-NB	5.52	2.26	1.97
3	B	2001	HEM	C4A-CHB	6.57	1.58	1.39
3	B	2001	HEM	FE-NC	9.17	2.31	1.95
3	A	2000	HEM	CBC-CAC	10.13	1.87	1.29
3	D	2003	HEM	CHD-C4C	13.30	1.67	1.36

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	HEM	C3C-CAC-CBC	-12.74	104.92	124.46
3	B	2001	HEM	C1D-CHD-C4C	-10.37	108.49	125.82
3	D	2003	HEM	C1D-CHD-C4C	-6.36	115.20	125.82
3	B	2001	HEM	C4B-CHC-C1C	-5.57	116.52	125.82
2	D	3074	3TR	N3A-C3-N4	-4.31	117.62	123.05
3	D	2003	HEM	CHC-C4B-NB	-2.96	117.40	124.52
3	A	2000	HEM	CAA-C2A-C1A	-2.62	124.17	127.01
3	B	2001	HEM	C3C-CAC-CBC	-2.58	120.50	124.46
3	B	2001	HEM	CAA-C2A-C1A	-2.57	124.22	127.01
3	C	2002	HEM	CAA-C2A-C1A	-2.56	124.22	127.01
3	B	2001	HEM	CBA-CAA-C2A	-2.50	108.05	112.53
3	C	2002	HEM	CBA-CAA-C2A	-2.43	108.17	112.53
3	A	2000	HEM	CBA-CAA-C2A	-2.42	108.19	112.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2003	HEM	CAA-C2A-C1A	-2.42	124.38	127.01
3	D	2003	HEM	C2D-C3D-C4D	2.10	105.06	101.50
3	C	2002	HEM	C2D-C3D-C4D	2.11	105.07	101.50
3	B	2001	HEM	C2D-C3D-C4D	2.13	105.11	101.50
3	A	2000	HEM	C2D-C3D-C4D	2.13	105.11	101.50
3	D	2003	HEM	C3C-CAC-CBC	2.15	127.75	124.46
3	C	2002	HEM	CMD-C2D-C3D	2.53	125.56	114.35
3	D	2003	HEM	CMD-C2D-C3D	2.54	125.58	114.35
3	B	2001	HEM	CMD-C2D-C3D	2.54	125.58	114.35
3	A	2000	HEM	CMD-C2D-C3D	2.54	125.60	114.35
3	C	2002	HEM	CMB-C2B-C3B	3.27	124.70	116.53
3	D	2003	HEM	CMB-C2B-C3B	3.29	124.75	116.53
3	A	2000	HEM	CMB-C2B-C3B	3.30	124.77	116.53
3	B	2001	HEM	CMB-C2B-C3B	3.31	124.78	116.53
3	B	2001	HEM	CAD-C3D-C4D	3.76	125.73	112.47
3	D	2003	HEM	CAD-C3D-C4D	3.77	125.75	112.47
3	A	2000	HEM	CAD-C3D-C4D	3.78	125.79	112.47
3	C	2002	HEM	CAD-C3D-C4D	3.79	125.83	112.47
3	B	2001	HEM	CMC-C2C-C3C	4.27	127.18	116.53
3	D	2003	HEM	C4B-CHC-C1C	4.41	133.19	125.82
3	C	2002	HEM	CMC-C2C-C3C	4.59	127.98	116.53
3	D	2003	HEM	CMC-C2C-C3C	4.70	128.26	116.53
3	C	2002	HEM	C3C-CAC-CBC	4.99	132.11	124.46
3	B	2001	HEM	CHD-C1D-ND	5.22	137.09	124.52
3	D	2003	HEM	C3B-C4B-CHC	5.33	130.67	123.16
3	A	2000	HEM	CAD-C3D-C2D	5.41	128.78	113.22
3	C	2002	HEM	CAD-C3D-C2D	5.42	128.79	113.22
3	B	2001	HEM	CAD-C3D-C2D	5.43	128.84	113.22
3	D	2003	HEM	CAD-C3D-C2D	5.45	128.88	113.22
3	A	2000	HEM	CMC-C2C-C3C	7.32	134.79	116.53
3	D	2003	HEM	CBA-CAA-C2A	28.01	162.74	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 192 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	HEM	79	0
3	B	2001	HEM	39	0
3	C	2002	HEM	49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2003	HEM	25	0
2	D	3074	3TR	12	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(Å²)	Q<0.9
1	A	499/506 (98%)	-0.37	2 (0%)	93	83	10, 40, 76, 97	0
1	B	499/506 (98%)	-0.29	5 (1%)	84	66	16, 44, 78, 102	0
1	C	499/506 (98%)	-0.16	4 (0%)	87	72	16, 41, 81, 100	1 (0%)
1	D	499/506 (98%)	-0.28	5 (1%)	84	66	15, 45, 84, 101	0
All	All	1996/2024 (98%)	-0.27	16 (0%)	87	72	10, 43, 80, 102	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	ARG	3.3
1	D	422	THR	3.2
1	B	19	ALA	3.1
1	B	20	ALA	3.0
1	C	448	LYS	2.9
1	D	224	ALA	2.8
1	A	271	GLY	2.6
1	B	14	TRP	2.4
1	C	3	ASN	2.4
1	A	20	ALA	2.3
1	D	409	SER	2.3
1	C	446	TYR	2.1
1	C	427	ASP	2.1
1	D	225	ASP	2.1
1	D	428	VAL	2.1
1	B	292	PRO	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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( $\text{\AA}^2$ )	Q<0.9
3	HEM	A	2000	43/43	0.80	0.42	6.46	80,94,101,101	0
3	HEM	C	2002	43/43	0.83	0.38	4.51	41,58,72,92	0
3	HEM	B	2001	43/43	0.89	0.29	4.13	21,56,83,101	0
2	3TR	D	3074	6/6	0.94	0.20	0.59	89,96,99,101	0
3	HEM	D	2003	43/43	0.96	0.17	0.25	20,38,56,59	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.