



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 01:16 PM EDT

PDB ID : 1TH4 / pdb_00001th4
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

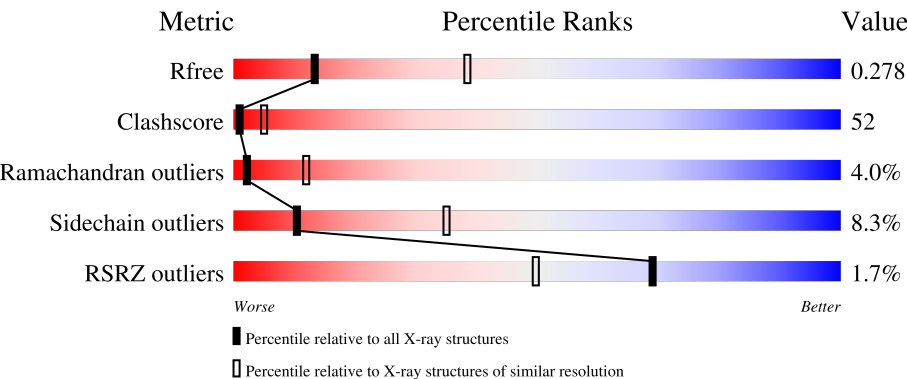
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.98 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2% 30% 57% 10% ..
1	B	506	2% 32% 54% 11% ..
1	C	506	2% 35% 53% 10% ..
1	D	506	2% 35% 54% 9% .

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:

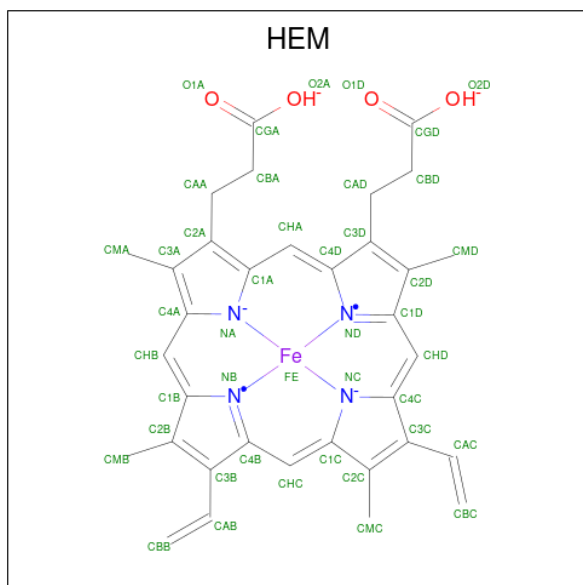
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEM	A	2000	-	-	X	-
2	HEM	B	2001	-	-	X	-
2	HEM	C	2002	-	-	X	-
2	HEM	D	2003	-	-	X	-
3	3TR	D	3074	-	-	X	-

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 4017	C 2548	N 715	O 740	S 14	0	0	0
1	B	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0
1	C	499	Total 4017	C 2548	N 715	O 740	S 14	1	0	0
1	D	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



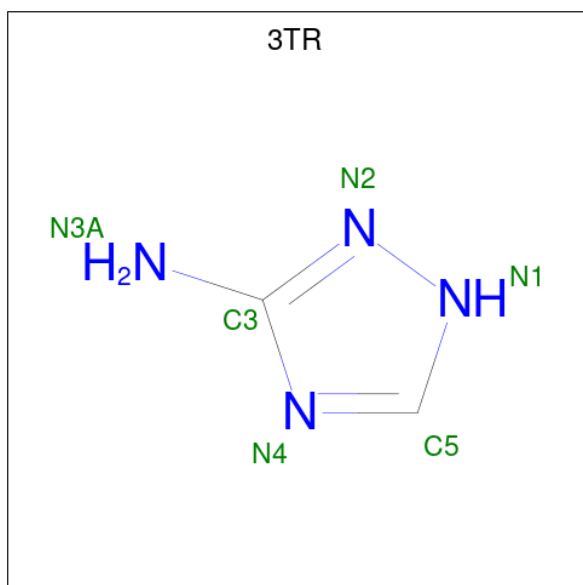
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 3 is 3-AMINO-1,2,4-TRIAZOLE (CCD ID: 3TR) (formula: C₂H₄N₄).



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

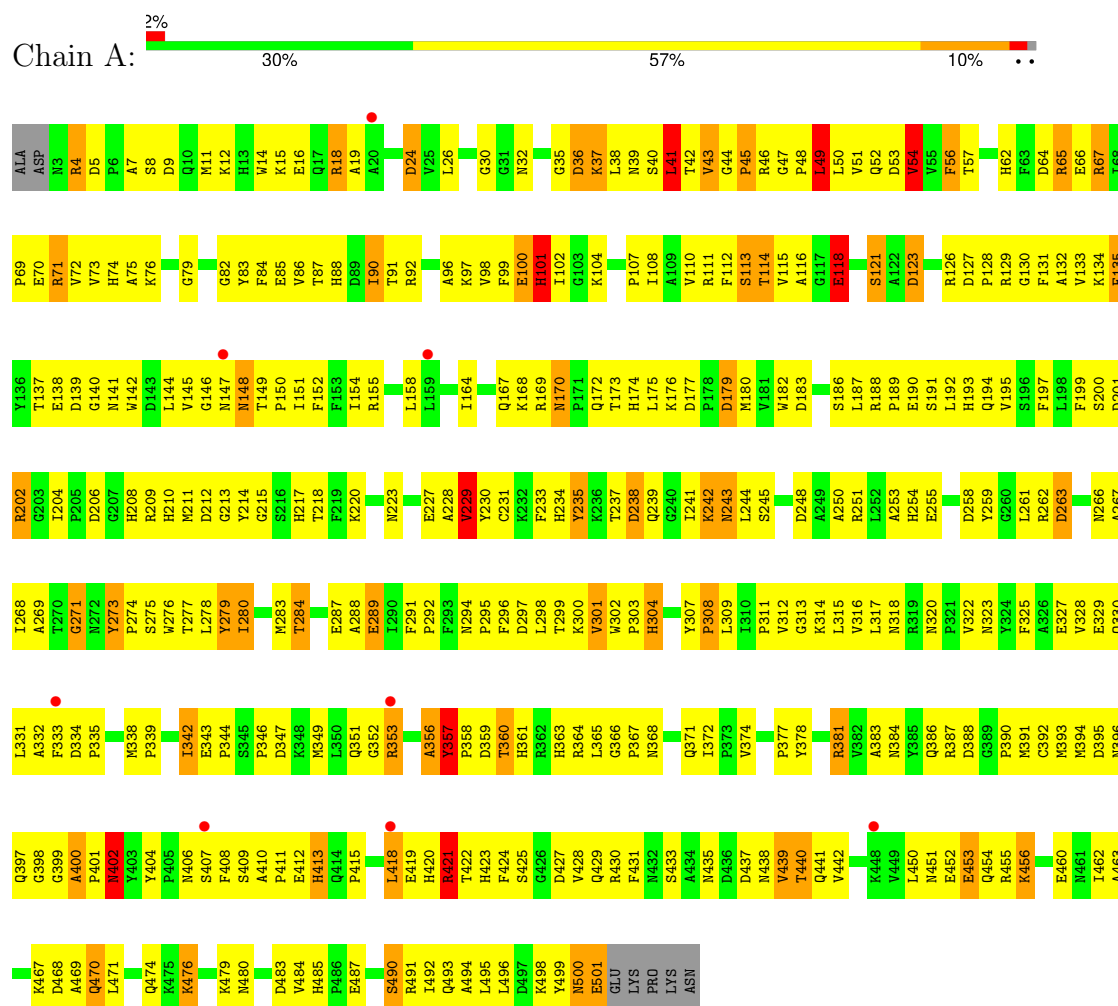
- Molecule 4 is water.

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		

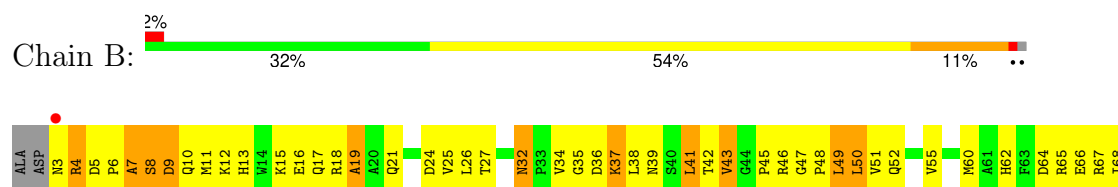
3 Residue-property plots

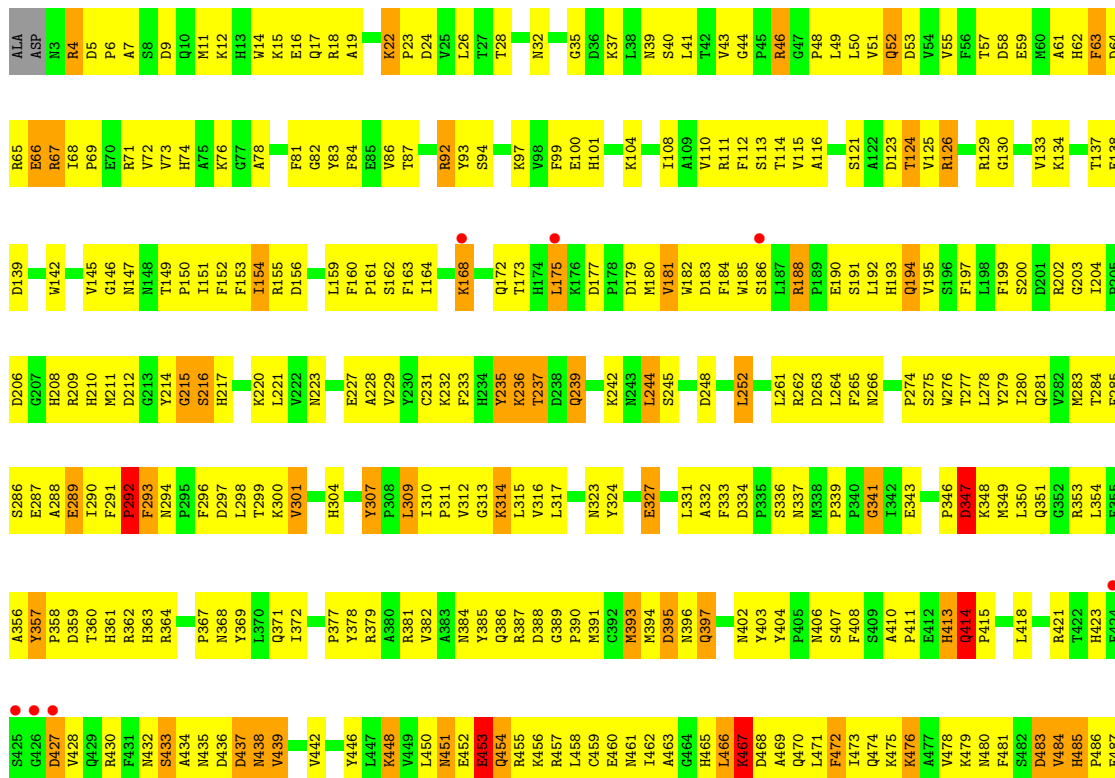
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Catalase



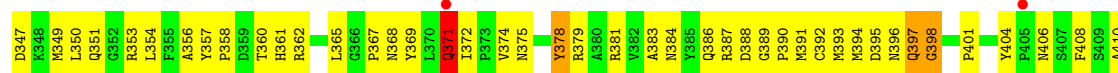
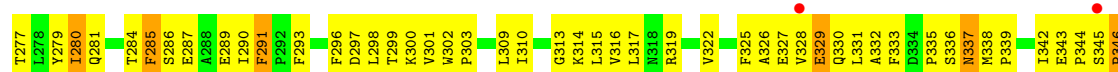
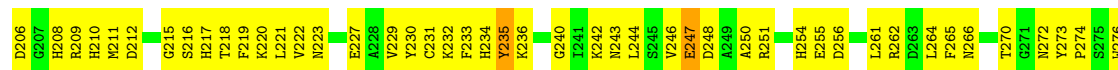
• Molecule 1: Catalase







● Molecule 1: Catalase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.03Å 141.09Å 231.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.98 39.90 – 2.98	Depositor EDS
% Data completeness (in resolution range)	57.6 (39.90-2.98) 57.7 (39.90-2.98)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	0.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.292 0.220 , 0.278	Depositor DCC
R_{free} test set	1001 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16915	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3TR, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.79	7/4137 (0.2%)	1.93	76/5619 (1.4%)
1	B	1.23	7/4137 (0.2%)	1.68	39/5619 (0.7%)
1	C	0.90	10/4137 (0.2%)	1.68	59/5619 (1.1%)
1	D	0.80	1/4137 (0.0%)	1.33	21/5619 (0.4%)
All	All	0.95	25/16548 (0.2%)	1.67	195/22476 (0.9%)

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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CD-NE	59.84	2.30	1.46
1	D	413	HIS	CA-CB	-30.61	1.09	1.53
1	C	202	ARG	NE-CZ	19.98	1.55	1.33
1	B	319	ARG	NE-CZ	18.96	1.53	1.33
1	A	304	HIS	CA-CB	17.70	1.81	1.53
1	C	414	GLN	CA-CB	-16.69	1.32	1.53
1	B	395	ASP	N-CA	-16.50	1.25	1.46
1	C	292	PRO	C-N	16.47	1.55	1.33
1	C	485	HIS	ND1-CE1	-13.91	1.18	1.32
1	B	374	VAL	CA-CB	12.62	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	413	HIS	CB-CG	11.31	1.66	1.50
1	C	292	PRO	CA-C	-10.57	1.35	1.52
1	A	229	VAL	CA-CB	-10.56	1.40	1.54
1	C	485	HIS	CD2-NE2	-10.31	1.26	1.37
1	A	421	ARG	CD-NE	-10.17	1.32	1.46
1	A	280	ILE	CA-CB	9.81	1.67	1.54
1	A	41	LEU	CA-CB	9.33	1.64	1.52
1	B	32	ASN	CB-CG	8.06	1.72	1.52
1	B	395	ASP	CA-C	-7.78	1.42	1.52
1	B	319	ARG	CA-CB	-7.66	1.39	1.53
1	C	485	HIS	CE1-NE2	6.34	1.38	1.32
1	A	49	LEU	CB-CG	-5.95	1.41	1.53
1	C	453	GLU	CA-CB	5.88	1.63	1.53
1	A	243	ASN	N-CA	5.52	1.52	1.45
1	C	454	GLN	CB-CG	-5.07	1.37	1.52

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	413	HIS	CA-CB-CG	42.86	156.66	113.80
1	A	395	ASP	CA-CB-CG	42.70	155.31	112.60
1	B	319	ARG	CG-CD-NE	-39.34	25.46	112.00
1	A	402	ASN	CA-CB-CG	34.44	147.04	112.60
1	C	453	GLU	CB-CG-CD	32.86	168.47	112.60
1	B	487	GLU	CB-CG-CD	28.94	161.79	112.60
1	D	371	GLN	CB-CA-C	28.86	165.13	109.72
1	B	126	ARG	CD-NE-CZ	28.64	164.50	124.40
1	D	453	GLU	CB-CG-CD	28.63	161.27	112.60
1	C	292	PRO	N-CA-C	28.26	153.47	114.18
1	B	395	ASP	CA-C-O	28.10	160.69	120.51
1	C	202	ARG	NE-CZ-NH2	-28.04	93.97	119.20
1	A	41	LEU	CB-CA-C	27.89	158.19	111.05
1	A	435	ASN	CA-CB-CG	27.79	140.39	112.60
1	A	357	TYR	CB-CG-CD2	-27.08	80.18	120.80
1	B	319	ARG	CB-CG-CD	-26.46	50.45	111.30
1	A	418	LEU	N-CA-CB	26.01	149.76	109.71
1	C	483	ASP	N-CA-CB	25.39	153.48	110.32
1	C	395	ASP	CA-CB-CG	-25.15	87.45	112.60
1	C	292	PRO	CA-C-O	24.64	151.63	118.86
1	B	319	ARG	NE-CZ-NH1	-24.50	97.00	121.50
1	B	395	ASP	CA-CB-CG	24.22	136.82	112.60
1	A	456	LYS	CG-CD-CE	24.07	166.65	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	GLU	CB-CG-CD	23.42	152.42	112.60
1	C	52	GLN	CB-CG-CD	23.24	152.11	112.60
1	B	374	VAL	CB-CA-C	-22.96	81.96	112.04
1	B	32	ASN	CA-CB-CG	-22.70	89.90	112.60
1	A	395	ASP	N-CA-CB	22.36	144.01	110.70
1	C	454	GLN	CB-CG-CD	22.25	150.42	112.60
1	A	421	ARG	CB-CG-CD	21.82	161.49	111.30
1	C	292	PRO	O-C-N	-21.47	92.54	122.38
1	C	202	ARG	NE-CZ-NH1	20.85	142.35	121.50
1	B	374	VAL	N-CA-CB	20.60	136.22	110.47
1	A	421	ARG	CG-CD-NE	20.29	156.64	112.00
1	A	357	TYR	CA-CB-CG	20.24	150.33	113.90
1	D	97	LYS	CG-CD-CE	20.23	157.84	111.30
1	B	487	GLU	CA-CB-CG	19.92	153.94	114.10
1	C	501	GLU	CB-CA-C	19.78	147.68	110.10
1	A	229	VAL	CA-CB-CG2	19.50	143.54	110.40
1	A	54	VAL	CA-CB-CG2	-19.37	77.47	110.40
1	A	41	LEU	N-CA-CB	-19.07	82.59	110.24
1	B	319	ARG	CA-CB-CG	19.04	152.17	114.10
1	A	456	LYS	CB-CG-CD	18.96	154.91	111.30
1	C	292	PRO	CB-CA-C	-18.87	80.93	111.31
1	C	453	GLU	N-CA-CB	18.55	141.84	110.49
1	C	414	GLN	CA-CB-CG	18.25	150.59	114.10
1	A	97	LYS	CG-CD-CE	18.00	152.71	111.30
1	A	500	ASN	CA-CB-CG	17.87	130.47	112.60
1	A	453	GLU	CB-CG-CD	17.53	142.40	112.60
1	C	454	GLN	N-CA-CB	-17.52	83.79	110.06
1	C	453	GLU	CA-CB-CG	17.40	148.91	114.10
1	C	414	GLN	CB-CA-C	17.18	134.18	110.13
1	A	118	GLU	N-CA-CB	-17.04	83.30	110.39
1	D	371	GLN	N-CA-CB	-16.54	84.49	110.46
1	B	429	GLN	CA-CB-CG	16.40	146.89	114.10
1	B	277	THR	CB-CA-C	16.39	137.01	110.78
1	C	501	GLU	CB-CG-CD	16.18	140.11	112.60
1	A	435	ASN	CB-CA-C	15.90	137.99	110.64
1	A	501	GLU	CB-CA-C	15.32	139.21	110.10
1	B	412	GLU	N-CA-CB	14.56	134.14	110.85
1	B	478	VAL	N-CA-CB	-14.43	92.43	110.47
1	A	476	LYS	CG-CD-CE	14.35	144.31	111.30
1	A	118	GLU	CB-CG-CD	-14.24	88.40	112.60
1	D	453	GLU	CA-CB-CG	14.15	142.39	114.10
1	A	490	SER	CA-CB-OG	13.76	138.61	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	LEU	CB-CA-C	-13.45	90.08	110.26
1	A	381	ARG	CG-CD-NE	13.27	141.18	112.00
1	B	478	VAL	CB-CA-C	13.26	129.41	112.04
1	A	500	ASN	N-CA-CB	-13.15	88.27	110.49
1	D	74	HIS	CA-CB-CG	13.10	126.90	113.80
1	A	421	ARG	CD-NE-CZ	12.95	142.53	124.40
1	A	284	THR	CA-CB-OG1	12.95	129.02	109.60
1	A	37	LYS	CG-CD-CE	12.68	140.47	111.30
1	C	289	GLU	CB-CA-C	12.45	133.35	110.56
1	A	304	HIS	N-CA-CB	-12.38	91.49	110.06
1	A	357	TYR	CB-CG-CD1	12.16	139.04	120.80
1	A	280	ILE	CB-CA-C	-12.11	91.44	111.29
1	C	289	GLU	CG-CD-OE2	-11.99	90.82	118.40
1	A	421	ARG	CA-CB-CG	11.58	137.26	114.10
1	C	289	GLU	CA-CB-CG	11.50	137.10	114.10
1	B	412	GLU	CA-CB-CG	11.47	137.03	114.10
1	A	49	LEU	CB-CG-CD2	11.42	144.95	110.70
1	B	478	VAL	CA-CB-CG1	-11.42	90.99	110.40
1	B	395	ASP	N-CA-CB	-11.06	91.80	110.49
1	A	476	LYS	CD-CE-NZ	11.04	147.22	111.90
1	A	101	HIS	CB-CA-C	-10.95	88.62	110.42
1	A	456	LYS	CA-CB-CG	10.90	135.90	114.10
1	D	394	MET	CB-CG-SD	10.86	145.29	112.70
1	A	284	THR	CB-CA-C	-10.59	91.40	109.51
1	A	202	ARG	CD-NE-CZ	10.21	138.70	124.40
1	C	454	GLN	CB-CA-C	-10.20	93.34	110.68
1	C	483	ASP	CB-CA-C	-10.12	88.97	110.32
1	C	501	GLU	N-CA-CB	-9.84	93.78	110.50
1	A	356	ALA	N-CA-C	9.74	121.90	111.28
1	A	342	ILE	CB-CA-C	-9.61	99.69	111.32
1	A	342	ILE	N-CA-CB	9.29	123.39	112.15
1	B	478	VAL	CA-CB-CG2	9.12	125.91	110.40
1	A	243	ASN	CB-CA-C	-9.07	90.61	109.94
1	C	478	VAL	CB-CA-C	9.05	125.27	112.05
1	C	413	HIS	CB-CG-ND1	-9.04	109.14	122.70
1	C	413	HIS	CB-CG-CD2	8.97	142.86	131.20
1	A	501	GLU	N-CA-CB	-8.67	95.76	110.50
1	A	41	LEU	CA-CB-CG	-8.64	86.05	116.30
1	A	284	THR	CA-CB-CG2	-8.63	95.83	110.50
1	D	356	ALA	N-CA-C	8.59	121.50	111.02
1	C	292	PRO	CA-C-N	8.55	138.35	123.05
1	C	292	PRO	C-N-CA	8.55	138.35	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ASP	CB-CA-C	-8.42	97.05	110.94
1	A	280	ILE	CA-CB-CG1	8.37	124.62	110.40
1	B	395	ASP	N-CA-C	8.34	128.56	110.80
1	A	176	LYS	CG-CD-CE	8.34	130.47	111.30
1	B	319	ARG	NE-CZ-NH2	8.22	126.60	119.20
1	A	280	ILE	CA-CB-CG2	-8.19	96.58	110.50
1	B	319	ARG	CB-CA-C	-8.13	94.83	109.71
1	C	231	CYS	CA-CB-SG	-8.12	95.71	114.40
1	A	453	GLU	CA-CB-CG	8.01	130.12	114.10
1	B	416	SER	N-CA-CB	-7.98	96.42	110.39
1	A	435	ASN	N-CA-CB	-7.98	97.82	110.98
1	C	123	ASP	N-CA-C	7.63	119.24	111.07
1	C	414	GLN	N-CA-CB	-7.55	96.13	110.17
1	D	89	ASP	CA-CB-CG	7.54	120.14	112.60
1	D	55	VAL	N-CA-C	-7.50	103.92	110.74
1	C	55	VAL	N-CA-C	-7.48	102.50	110.36
1	A	176	LYS	CD-CE-NZ	-7.40	88.21	111.90
1	A	101	HIS	N-CA-CB	7.28	122.78	110.49
1	D	484	VAL	N-CA-C	-7.26	103.39	110.72
1	A	54	VAL	CB-CA-C	7.22	121.83	111.65
1	B	32	ASN	CB-CG-OD1	-7.17	106.45	120.80
1	C	372	ILE	N-CA-C	-7.10	102.53	108.63
1	C	236	LYS	CG-CD-CE	7.07	127.57	111.30
1	C	289	GLU	CB-CG-CD	7.01	124.52	112.60
1	B	32	ASN	CB-CG-ND2	6.88	126.72	116.40
1	B	55	VAL	N-CA-C	-6.82	103.68	110.30
1	A	67	ARG	N-CA-C	6.75	119.69	108.96
1	C	394	MET	CB-CA-C	-6.69	108.13	117.23
1	D	169	ARG	N-CA-C	6.67	120.04	110.10
1	B	394	MET	CA-C-N	6.63	134.20	121.54
1	B	394	MET	C-N-CA	6.63	134.20	121.54
1	A	333	PHE	CA-CB-CG	6.60	120.40	113.80
1	A	229	VAL	CB-CA-C	-6.45	100.71	111.29
1	A	116	ALA	N-CA-C	6.43	119.59	111.69
1	A	90	ILE	N-CA-C	-6.40	106.09	112.17
1	B	374	VAL	CA-CB-CG1	-6.38	99.56	110.40
1	B	319	ARG	N-CA-CB	6.35	121.35	110.68
1	D	115	VAL	N-CA-C	6.22	116.53	111.62
1	C	188	ARG	CA-C-N	6.18	125.80	119.56
1	C	188	ARG	C-N-CA	6.18	125.80	119.56
1	B	374	VAL	CA-CB-CG2	-6.12	99.99	110.40
1	D	67	ARG	N-CA-C	6.10	119.18	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	THR	N-CA-C	-6.03	100.48	109.94
1	C	485	HIS	CA-C-N	5.88	127.19	119.84
1	C	485	HIS	C-N-CA	5.88	127.19	119.84
1	C	484	VAL	N-CA-C	-5.88	105.39	110.74
1	C	324	TYR	N-CA-C	5.87	117.36	111.07
1	C	44	GLY	CA-C-N	5.85	125.99	119.32
1	C	44	GLY	C-N-CA	5.85	125.99	119.32
1	A	304	HIS	CB-CA-C	5.82	120.57	110.68
1	C	154	ILE	N-CA-C	5.76	115.96	108.35
1	B	356	ALA	N-CA-C	5.72	117.98	111.11
1	C	202	ARG	CD-NE-CZ	5.71	132.39	124.40
1	D	182	TRP	N-CA-C	5.69	118.25	111.71
1	A	291	PHE	CA-C-N	5.68	125.39	119.82
1	A	291	PHE	C-N-CA	5.68	125.39	119.82
1	A	353	ARG	CA-CB-CG	5.66	125.41	114.10
1	C	341	GLY	N-CA-C	-5.63	107.78	114.48
1	B	215	GLY	N-CA-C	-5.62	106.00	115.62
1	C	124	THR	N-CA-C	5.60	118.53	108.17
1	A	113	SER	N-CA-C	5.57	116.73	108.60
1	D	371	GLN	CA-CB-CG	-5.55	103.00	114.10
1	C	281	GLN	N-CA-C	-5.55	100.66	109.76
1	A	273	TYR	N-CA-C	5.53	116.62	109.65
1	A	484	VAL	N-CA-C	-5.48	105.77	111.58
1	C	307	TYR	CA-C-N	5.48	125.46	120.03
1	C	307	TYR	C-N-CA	5.48	125.46	120.03
1	A	289	GLU	CB-CG-CD	-5.46	103.32	112.60
1	A	500	ASN	CB-CA-C	5.46	121.28	110.42
1	C	252	LEU	N-CA-C	-5.36	106.00	112.54
1	D	273	TYR	N-CA-C	5.35	116.39	109.65
1	C	327	GLU	N-CA-C	5.35	119.94	113.41
1	D	498	LYS	N-CA-C	-5.35	105.36	111.14
1	A	197	PHE	N-CA-C	-5.30	105.40	111.07
1	B	432	ASN	N-CA-C	5.29	117.37	109.59
1	A	388	ASP	N-CA-C	5.21	117.77	109.02
1	B	378	TYR	N-CA-C	5.18	118.86	112.54
1	C	483	ASP	N-CA-C	-5.17	106.07	112.38
1	C	357	TYR	N-CA-C	5.17	119.20	112.17
1	C	314	LYS	N-CA-C	5.17	117.83	109.40
1	A	121	SER	N-CA-C	5.14	116.92	110.24
1	C	67	ARG	N-CA-C	5.12	118.56	109.96
1	D	18	ARG	N-CA-C	-5.12	104.96	111.11
1	B	195	VAL	N-CA-C	-5.10	105.74	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	434	ALA	N-CA-C	5.09	117.49	111.33
1	C	378	TYR	N-CA-C	5.04	119.05	113.01
1	A	238	ASP	N-CA-C	-5.04	106.83	113.17
1	A	123	ASP	N-CA-C	5.03	116.84	111.36

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	489	1
1	B	4017	0	3839	456	0
1	C	4017	0	3840	451	0
1	D	4017	0	3839	415	0
2	A	43	0	30	80	0
2	B	43	0	30	39	0
2	C	43	0	30	51	0
2	D	43	0	30	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	3	12	0
4	A	154	0	0	31	0
4	B	145	0	0	27	0
4	C	188	0	0	17	1
4	D	182	0	0	14	0
All	All	16915	0	15479	1647	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 52.

All (1647) 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
2:A:2000:HEM:CAC	2:A:2000:HEM:CBC	1.87	1.47
1:A:353:ARG:HD2	2:A:2000:HEM:CHC	1.53	1.37
1:C:111:ARG:NE	2:C:2002:HEM:O1D	1.57	1.36
1:A:353:ARG:N	2:A:2000:HEM:HBB2	1.37	1.35
4:B:2096:HOH:O	1:D:38:LEU:HD11	1.16	1.33
1:C:147:ASN:CG	2:C:2002:HEM:HAC	1.55	1.31
1:B:147:ASN:N	2:B:2001:HEM:HBC1	1.45	1.30
1:C:160:PHE:CD1	2: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	2:A:2000:HEM:C3C	2.18	1.26
1:A:353:ARG:HH11	2:A:2000:HEM:CMC	1.48	1.26
1:D:319:ARG:NH2	4:D:3243:HOH:O	1.63	1.26
1:A:100:GLU:O	1:A:101:HIS:ND1	1.65	1.26
1:A:353:ARG:NH1	2:A:2000:HEM:C3C	2.05	1.25
1:A:353:ARG:HD2	2:A:2000:HEM:C1C	1.70	1.24
1:C:147:ASN:OD1	2: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	2:A:2000:HEM:C2C	2.11	1.19
1:A:72:VAL:CG1	2: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	2:A:2000:HEM:HMC3	0.97	1.14
1:A:72:VAL:HG11	2:A:2000:HEM:CMA	1.78	1.12
1:A:145:VAL:HG13	2:A:2000:HEM:HMD3	1.30	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:C	1:A:101:HIS:ND1	2.12	1.08
1:A:72:VAL:CG1	2: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
1:A:398:GLY:HA2	1:C:323:ASN:HB2	1.38	1.06
3:D:3074:3TR:N2	2:D:2003:HEM:C1C	2.23	1.06
1:A:41:LEU:HB2	1:D:430:ARG:HG2	1.39	1.05
1:A:353:ARG:NH1	2:A:2000:HEM:CAC	2.19	1.05
1:C:111:ARG:HE	2: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	2:C:2002:HEM:HAB	1.93	1.04
1:A:353:ARG:N	2:A:2000:HEM:CBB	2.21	1.04
1:A:145:VAL:CG1	2:A:2000:HEM:CMD	2.35	1.03
1:A:145:VAL:CG1	2:A:2000:HEM:HMD3	1.89	1.02
1:C:147:ASN:OD1	2:C:2002:HEM:CAC	2.07	1.01
1:A:353:ARG:NH1	2:A:2000:HEM:CMC	2.19	1.01
1:A:71:ARG:HD3	2: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	2:B:2001:HEM:CBC	2.22	1.01
1:A:145:VAL:HG12	2:A:2000:HEM:CMD	1.90	1.00
1:A:72:VAL:HG11	2: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	2: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	2:A:2000:HEM:C2D	2.46	0.98
1:B:493:GLN:HA	1:B:496:LEU:HD12	1.45	0.98
1:B:147:ASN:HD21	2: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	2:B:2001:HEM:HBC1	1.04	0.96
1:D:261:LEU:O	4:D:3114:HOH:O	1.84	0.95
3:D:3074:3TR:C3	2:D:2003:HEM:NC	2.28	0.95
1:A:353:ARG:H	2:A:2000:HEM:HBB2	1.24	0.95
1:B:129:ARG:HB3	1:B:211:MET:HE1	1.47	0.95
1:A:353:ARG:CD	2:A:2000:HEM:CHC	2.45	0.95
2:A:2000:HEM:HHA	2:A:2000:HEM:HBA2	1.47	0.94
1:A:353:ARG:CA	2:A:2000:HEM:HBB2	1.98	0.94
1:A:300:LYS:HB3	1:A:441:GLN:HE22	1.34	0.93
1:A:208:HIS:HA	1:A:211:MET:HE3	1.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ASN:CG	2:C:2002:HEM:CAC	2.41	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:148:ASN:C	1:A:148:ASN:HD22	1.78	0.92
1:A:353:ARG:NH1	2: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	2:A:2000:HEM:C1C	2.54	0.91
1:B:146:GLY:HA2	2:B:2001:HEM:CBC	2.01	0.91
1:B:404:TYR:CE2	4:B:2096:HOH:O	2.22	0.91
1:C:142:TRP:HB2	1:C:339:PRO:CD	2.01	0.90
1:D:368:ASN:CB	1:D:371:GLN:NE2	2.32	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	2: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	2: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
3:D:3074:3TR:N2	2:D:2003:HEM:NC	2.22	0.88
1:A:235:TYR:HB3	1:A:278:LEU:HD12	1.55	0.88
1:A:353:ARG:HH12	2:A:2000:HEM:CAC	1.84	0.88
1:A:41:LEU:CB	1:D:430:ARG:NH1	2.37	0.88
1:A:322:VAL:HA	1:D:172:GLN:HE21	1.39	0.88
1:A:353:ARG:HG2	1:A:357:TYR:CE1	2.09	0.88
1:A:145:VAL:HG12	2:A:2000:HEM:CHD	2.04	0.88
1:D:43:VAL:HG13	1:D:48:PRO:HD2	1.55	0.88
1:B:450:LEU:HB3	1:B:454:GLN:HG3	1.53	0.87
1:D:291:PHE:HD1	1:D:293:PHE:H	1.15	0.87
1:A:353:ARG:HD2	2: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	2:C:2002:HEM:HAA1	1.55	0.87
1:A:353:ARG:CZ	2: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HD11	1:C:428:VAL:HG12	1.57	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:B:129:ARG:CB	1:B:211:MET:HE1	2.06	0.85
1:D:338:MET:HE2	1:D:342:ILE:HG22	1.59	0.85
1:A:239:GLN:HE22	1:A:275:SER:H	1.21	0.85
1:A:391:MET:HE2	1:C:391:MET:HB2	1.58	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:B:147:ASN:ND2	2: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
2:A:2000:HEM:CBC	2:A:2000:HEM:C3C	2.60	0.84
1:A:145:VAL:HG12	2:A:2000:HEM:HHD	1.58	0.84
2:A:2000:HEM:CBC	2:A:2000:HEM:HHD	2.08	0.84
1:A:145:VAL:CB	2: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	2:A:2000:HEM:C1D	2.12	0.83
1:B:146:GLY:C	2:B:2001:HEM:HBC1	2.02	0.83
1:D:420:HIS:ND1	4:D:3158:HOH:O	2.08	0.83
1:B:495:LEU:HD21	4:B:2081:HOH:O	1.78	0.83
1:C:432:ASN:ND2	1:C:434:ALA:H	1.77	0.83
1:A:11:MET:HE1	1:C:403:TYR:OH	1.78	0.83
1:D:155:ARG:HD3	1:D:297:ASP:CG	2.04	0.82
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:H	1:C:92:ARG:HD3	1.42	0.81
1:C:252:LEU:HD21	4:C:2147:HOH:O	1.80	0.81
1:B:223:ASN:ND2	1:B:227:GLU:HB2	1.93	0.81
1:C:146:GLY:C	2:C:2002:HEM:HBC1	2.06	0.81
1:C:111:ARG:HH21	2:C:2002:HEM:CAD	1.94	0.81
1:B:37:LYS:O	1:B:37:LYS:HG3	1.80	0.81
1:C:177:ASP:HB3	1:C:180:MET:HE2	1.61	0.81
1:B:353:ARG:NH2	2:B:2001:HEM:C2C	2.49	0.80
1:D:439:VAL:HG23	1:D:440:THR:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	2: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	2: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:C:111:ARG:NE	2: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
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
2:B:2001:HEM:HMC1	2:B:2001:HEM:HBC2	1.66	0.78
1:D:43:VAL:CG1	1:D:48:PRO:HD2	2.14	0.78
1:A:180:MET:HE3	1:B:402:ASN:HD21	1.49	0.78
1:B:147:ASN:ND2	2:B:2001:HEM:HMC3	1.99	0.77
1:A:387:ARG:CZ	1:A:397:GLN:HB2	2.13	0.77
1:C:487:GLU:HA	1:C:490:SER:HB3	1.64	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	2: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:O	1:C:466:LEU:HD12	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	2:B:2001:HEM:C3C	2.52	0.76
2:A:2000:HEM:HBA2	2:A:2000:HEM:CHA	2.13	0.76
1:B:92:ARG:NH1	1:B:92:ARG:HB2	2.00	0.76
1:A:366:GLY:HA2	4:A:2013:HOH:O	1.84	0.76
1:B:333:PHE:HD2	2:B:2001:HEM:CGD	1.99	0.76
1:A:353:ARG:H	2: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	2:A:2000:HEM:C2D	2.15	0.76
1:A:145:VAL:CG1	2:A:2000:HEM:CHD	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3074:3TR:C3	2:D:2003:HEM:C1C	2.69	0.76
1:A:66:GLU:HG2	1:C:387:ARG:O	1.85	0.75
1:A:356:ALA:CB	2:A:2000:HEM:HMB2	2.16	0.75
1:A:64:ASP:O	1:D:360:THR:HG23	1.85	0.75
1:B:76:LYS:HE3	1:B:121:SER:O	1.86	0.75
1:D:368:ASN:HB3	1:D:371:GLN:HE21	1.48	0.75
1:A:72:VAL:HG12	2:A:2000:HEM:CMA	2.17	0.74
1:A:413:HIS:O	1:A:415:PRO:HD3	1.87	0.74
4:A:2073:HOH:O	1:C:382:VAL:HG21	1.85	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
1:B:120:GLY:O	4:B:2115:HOH:O	2.04	0.74
1:A:48:PRO:HB2	1:B:50:LEU:HD12	1.68	0.74
1:B:145:VAL:HG12	2:B:2001:HEM:CHD	2.17	0.74
1:A:487:GLU:O	1:A:491:ARG:HG3	1.88	0.74
1:A:148:ASN:C	1:A:148:ASN:ND2	2.43	0.74
1:A:353:ARG:CZ	2:A:2000:HEM:C4C	2.70	0.74
1:A:209:ARG:HG2	1:A:274:PRO:HB3	1.68	0.74
1:B:404:TYR:OH	4:B:2096:HOH:O	2.06	0.74
1:C:18:ARG:HD3	1:C:18:ARG:O	1.87	0.74
1:A:244:LEU:HD11	1:A:259:TYR:HE1	1.51	0.74
1:D:147:ASN:CG	2:D:2003:HEM:HAC	2.13	0.74
1:B:146:GLY:C	2:B:2001:HEM:CBC	2.59	0.73
1:B:353:ARG:NH2	2: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:B:5:ASP:OD2	1:B:7:ALA:HB3	1.88	0.73
1:B:147:ASN:HD21	2:B:2001:HEM:CMC	2.02	0.73
1:C:287:GLU:HA	1:C:290:ILE:HG12	1.70	0.73
1:A:353:ARG:CZ	2:A:2000:HEM:C2C	2.61	0.73
1:A:356:ALA:HB3	2: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
1:A:155:ARG:HD2	1:A:433:SER:O	1.88	0.73
1:A:71:ARG:HD3	2:A:2000:HEM:CGA	2.19	0.73
4:B:2034:HOH:O	1:D:54:VAL:HG21	1.88	0.73
1:A:72:VAL:HG12	2:A:2000:HEM:HMA2	1.69	0.72
1:A:145:VAL:HB	2:A:2000:HEM:CBC	2.19	0.72
1:C:298:LEU:CD2	1:C:349:MET:HG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:208:HIS:HA	1:A:211:MET:CE	2.17	0.72
1:B:146:GLY:C	2:B:2001:HEM:HAC	2.14	0.71
1:C:35:GLY:O	4:C:2038:HOH:O	2.08	0.71
1:D:368:ASN:HB3	1:D:371:GLN:CD	2.13	0.71
1:A:50:LEU:HD12	1:B:48:PRO:HB2	1.70	0.71
1:B:38:LEU:HD13	1:C:188:ARG:NH2	2.06	0.71
1:B:146:GLY:CA	2:B:2001:HEM:CBC	2.68	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:B:147:ASN:ND2	2: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	2:A:2000:HEM:HMA2	2.17	0.71
1:A:14:TRP:CZ3	1:A:18:ARG:HD2	2.26	0.71
1:A:501:GLU:HG3	4:A:2124:HOH:O	1.91	0.71
1:B:439:VAL:O	1:B:442:VAL:HB	1.91	0.71
1:D:274:PRO:HG2	1:D:317:LEU:HB2	1.72	0.71
1:D:439:VAL:HG23	1:D:440:THR:N	2.06	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:51:VAL:HG12	1:B:51:VAL:HA	1.72	0.70
1:A:73:VAL:O	1:A:74:HIS:HB2	1.90	0.70
1:B:146:GLY:HA2	2:B:2001:HEM:HBC1	1.73	0.70
1:A:145:VAL:HG12	2:A:2000:HEM:HMD1	1.74	0.70
1:C:162:SER:HB3	1:D:404:TYR:H	1.55	0.70
1:B:229:VAL:HG23	1:B:284:THR:HA	1.74	0.70
1:D:94:SER:HB2	1:D:221:LEU:HD22	1.72	0.70
3:D:3074:3TR:N2	2:D:2003:HEM:C4C	2.59	0.70
1:B:445:PHE:HA	1:B:449:VAL:HG23	1.73	0.70
1:C:298:LEU:HD22	1:C:349:MET:HG2	1.72	0.70
1:C:360:THR:HG21	2:C:2002:HEM:HMA3	1.74	0.70
1:B:146:GLY:C	2:B:2001:HEM:CAC	2.65	0.70
1:C:396:ASN:O	1:C:397:GLN:HB2	1.91	0.70
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:A:151:ILE:HD13	1:A:193:HIS:CE1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD22	1:B:50:LEU:N	2.07	0.70
1:D:459:CYS:HB3	1:D:492:ILE:HG12	1.74	0.70
4:A:2144:HOH:O	1:B:171:PRO:HG3	1.91	0.69
1:D:169:ARG:HB3	1:D:174:HIS:C	2.17	0.69
1:A:401:PRO:HA	4:A:2144:HOH:O	1.91	0.69
1:D:220:LYS:HG3	1:D:344:PRO:O	1.92	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:A:131:PHE:HD2	1:A:213:GLY:HA3	1.57	0.69
1:A:353:ARG:CG	1:A:357:TYR:CE1	2.75	0.69
4:A:2057:HOH:O	1:B:423:HIS:HE1	1.75	0.69
1:C:346:PRO:O	1:C:347:ASP:C	2.34	0.69
1:C:410:ALA:HB1	1:C:411:PRO:HD2	1.73	0.69
1:A:24:ASP:HB3	1:C:381:ARG:HH12	1.58	0.69
1:A:331:LEU:HD13	1:A:374:VAL:HG22	1.75	0.69
1:B:71:ARG:HE	1:B:111:ARG:CZ	2.06	0.69
1:C:81:PHE:HZ	1:C:327:GLU:HB3	1.58	0.69
1:A:41:LEU:HB2	1:D:430:ARG:NH1	2.07	0.69
1:A:393:MET:SD	1:C:393:MET:HG3	2.32	0.69
1:A:468:ASP:HB3	4:A:2062:HOH:O	1.93	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: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:357:TYR:OH	2:B:2001:HEM:NC	2.26	0.68
1:B:146:GLY:CA	2:B:2001:HEM:HBC1	2.22	0.68
1:C:126:ARG:HG2	1:C:126:ARG:HH11	1.57	0.68
1:C:235:TYR:HA	1:C:277:THR:O	1.93	0.68
1:C:453:GLU:HB3	1:C:457:ARG:NH2	2.08	0.68
1:B:84:PHE:O	1:B:105:ARG:HA	1.94	0.68
1:C:51:VAL:O	4:C:2011:HOH:O	2.11	0.68
1:C:206:ASP:HB2	1:C:244:LEU:HD23	1.76	0.68
1:A:235:TYR:HB3	1:A:278:LEU:CD1	2.23	0.68
1:C:71:ARG:HB3	2:C:2002:HEM:CAA	2.23	0.68
1:C:160:PHE:CE2	2:C:2002:HEM:C2B	2.82	0.68
1:A:41:LEU:HB3	1:D:430:ARG:CZ	2.24	0.68
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:279:TYR:O	1:B:280:ILE:HG23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:PHE:CD1	1:B:292:PRO:HD2	2.29	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: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:B:404:TYR:CZ	4:B:2096:HOH:O	2.43	0.67
1:C:191:SER:O	1:C:195:VAL:HG23	1.93	0.67
1:A:244:LEU:HD11	1:A:259:TYR:CE1	2.28	0.67
2:A:2000:HEM:CBC	2:A:2000:HEM:CHD	2.72	0.67
1:A:353:ARG:NH2	2: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:B:19:ALA:HB3	1:B:21:GLN:HE21	1.59	0.67
1:C:217:HIS:CD2	1:C:350:LEU:HB2	2.30	0.67
1:B:367:PRO:HG2	1:B:390:PRO:CG	2.24	0.67
1:A:242:LYS:HD3	1:A:243:ASN:N	2.10	0.67
2:A:2000:HEM:HBC2	2:A:2000:HEM:HHD	1.76	0.67
1:C:214:TYR:C	1:C:216:SER:H	2.01	0.67
1:D:114:THR:HG22	1:D:127:ASP:OD2	1.94	0.67
2:A:2000:HEM:HBC2	2:A:2000:HEM:CHD	2.25	0.67
1:B:494:ALA:HB1	4:B:2086:HOH:O	1.93	0.67
1:C:72:VAL:HG13	1:C:73:VAL:HG13	1.76	0.67
1:A:323:ASN:ND2	1:C:396:ASN:HB3	2.10	0.67
1:A:439:VAL:O	1:A:440:THR:C	2.38	0.67
1:B:97:LYS:HB2	4:B:2131:HOH:O	1.95	0.67
1:D:116:ALA:O	1:D:168:LYS:NZ	2.28	0.67
1:C:111:ARG:CZ	2: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: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:B:412:GLU:OE2	1:D:23:PRO:HG2	1.95	0.66
1:D:223:ASN:ND2	1:D:227:GLU:HB3	2.02	0.66
1:C:111:ARG:HH21	2: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	2:C:2002:HEM:HAB	2.27	0.66
1:D:155:ARG:HD3	1:D:297:ASP:OD2	1.96	0.66
1:B:295:PRO:HD2	1:C:46:ARG:HH12	1.61	0.66
1:A:71:ARG:HH22	1:A:329:GLU:CD	2.03	0.65
1:A:391:MET:HE2	1:C:391:MET:CB	2.25	0.65
1:C:206:ASP:HB2	1:C:244:LEU:CD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ASN:ND2	1:D:171:PRO:HD3	2.11	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:C:179:ASP:O	1:C:183:ASP:HB2	1.97	0.65
1:D:353:ARG:NH2	2:D:2003:HEM:C4C	2.65	0.65
1:C:487:GLU:OE2	1:C:491:ARG:HD2	1.97	0.65
1:A:363:HIS:CD2	1:D:65:ARG:HA	2.31	0.65
1:C:214:TYR:C	1:C:216:SER:N	2.49	0.65
1:A:24:ASP:HB3	1:C:381:ARG:NH1	2.12	0.65
1:B:183:ASP:O	1:B:187:LEU:HG	1.96	0.65
1:B:404:TYR:HE2	1:D:38:LEU:HG	1.60	0.65
1:B:428:VAL:HG23	1:B:428:VAL:O	1.94	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:C:129:ARG:HG2	1:C:211:MET:HE1	1.79	0.65
1:D:26:LEU:HD22	1:D:34:VAL:HG21	1.78	0.65
1:A:419:GLU:CD	1:A:419:GLU:H	2.05	0.65
1:C:492:ILE:HG22	1:C:496:LEU:HD23	1.79	0.65
1:A:353:ARG:HD3	2:A:2000:HEM:HMC3	1.78	0.64
1:B:64:ASP:HB3	1:C:360:THR:HB	1.77	0.64
1:C:214:TYR:O	1:C:216:SER:N	2.30	0.64
1:D:232:LYS:HE3	1:D:302:TRP:CE2	2.32	0.64
1:A:26:LEU:CD1	1:C:384:ASN:HA	2.28	0.64
1:A:144:LEU:HD11	1:A:233:PHE:CG	2.32	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:D:191:SER:O	1:D:195:VAL:HG23	1.98	0.64
1:A:41:LEU:CB	1:D:430:ARG:CZ	2.75	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:C:472:PHE:C	1:C:472:PHE:CD1	2.75	0.64
1:A:35:GLY:HA2	1:C:414:GLN:O	1.98	0.63
1:A:239:GLN:HE22	1:A:275:SER:N	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PHE:HD1	1:B:142:TRP:O	1.81	0.63
1:A:146:GLY:HA2	1:A:214:TYR:O	1.98	0.63
1:C:160:PHE:CG	2:C:2002:HEM:CAB	2.79	0.63
1:C:208:HIS:HA	1:C:211:MET:CE	2.29	0.63
1:C:310:ILE:N	1:C:310:ILE:HD12	2.14	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:B:62:HIS:HE1	1:D:368:ASN:HD21	1.47	0.63
1:C:110:VAL:HG22	1:C:133:VAL:HG22	1.81	0.63
1:A:132:ALA:HB2	2: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:43:VAL:CG1	1:A:48:PRO:HD2	2.29	0.63
1:A:73:VAL:HG23	1:A:74:HIS:HD2	1.64	0.63
1:C:353:ARG:HD2	1:C:357:TYR:CE1	2.34	0.62
1:C:147:ASN:HB2	2:C:2002:HEM:HBC1	1.80	0.62
1:C:456:LYS:O	1:C:460:GLU:HG3	1.98	0.62
1:A:38:LEU:HD12	4:C:2017:HOH:O	1.99	0.62
1:A:428:VAL:HG11	1:D:50:LEU:HD11	1.81	0.62
1:C:82:GLY:HA3	1:C:316:VAL:O	2.00	0.62
1:C:193:HIS:CA	1:C:442:VAL:HG22	2.29	0.62
1:C:432:ASN:HD22	1:C:433:SER:H	1.46	0.62
1:D:114:THR:HG22	1:D:115:VAL:H	1.64	0.62
1:B:92:ARG:CB	1:B:92:ARG:HH11	2.12	0.62
1:C:155:ARG:NH2	1:C:438:ASN:HD22	1.97	0.62
1:D:71:ARG:HD2	1:D:111:ARG:NH2	2.15	0.62
1:D:231:CYS:HA	1:D:281:GLN:O	1.98	0.62
1:D:419:GLU:H	1:D:419:GLU:CD	2.07	0.62
1:B:94:SER:HA	1:B:222:VAL:O	1.99	0.62
1:A:41:LEU:HD23	1:A:41:LEU:C	2.23	0.62
1:A:126:ARG:HE	1:A:199:PHE:HA	1.65	0.62
1:D:220:LYS:HE3	1:D:343:GLU:HB2	1.82	0.62
1:A:353:ARG:CD	2: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
1:D:397:GLN:C	4:D:3155:HOH:O	2.42	0.61
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:A:367:PRO:HG3	1:C:65:ARG:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ARG:H	1:C:92:ARG:CD	2.13	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:148:ASN:HD22	1:A:149:THR:N	1.97	0.61
1:A:206:ASP:HA	1:A:244:LEU:HG	1.82	0.61
1:A:428:VAL:HG22	1:D:43:VAL:HA	1.83	0.61
1:B:4:ARG:HB2	1:B:4:ARG:HH11	1.63	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:N	1:A:118:GLU:OE1	2.33	0.61
1:B:147:ASN:ND2	2:B:2001:HEM:CMC	2.63	0.61
1:C:46:ARG:CG	1:C:46:ARG:HH11	2.13	0.61
1:D:367:PRO:HG2	1:D:390:PRO:HG2	1.82	0.61
1:A:308:PRO:C	1:A:309:LEU:HD22	2.25	0.61
1:B:71:ARG:HH11	1:B:364:ARG:NH2	1.99	0.61
1:B:245:SER:OG	1:B:247:GLU:HB2	2.01	0.61
1:C:237:THR:HA	1:C:276:TRP:CD1	2.36	0.61
1:D:285:PHE:N	1:D:285:PHE:CD1	2.69	0.61
1:D:290:ILE:O	1:D:291:PHE:C	2.41	0.61
1:A:54:VAL:HG22	4:A:2137:HOH:O	2.01	0.61
1:A:57:THR:CG2	4:C:2006:HOH:O	2.48	0.61
1:C:353:ARG:HD2	1:C:357:TYR:HE1	1.66	0.61
1:D:169:ARG:HD3	1:D:174:HIS:CD2	2.35	0.61
1:D:309:LEU:HD12	1:D:309:LEU:N	2.16	0.61
1:A:57:THR:HG21	4:C:2006:HOH:O	2.01	0.60
1:A:304:HIS:CB	1:A:304:HIS:H	2.13	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
3:D:3074:3TR:N3A	2:D:2003:HEM:NB	2.49	0.60
1:B:444:THR:O	1:B:448:LYS:HB3	2.01	0.60
1:C:432:ASN:HD22	1:C:432:ASN:C	2.08	0.60
1:B:145:VAL:CG1	2:B:2001:HEM:CHD	2.79	0.60
1:D:63:PHE:HA	1:D:66:GLU:HG3	1.83	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:A:83:TYR:CD1	1:A:83:TYR:C	2.79	0.60
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.83	0.60
1:A:351:GLN:HE22	1:C:52:GLN:NE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:PHE:HA	1:C:130:GLY:O	2.02	0.60
1:D:217:HIS:HD1	1:D:298:LEU:HD13	1.65	0.60
1:A:74:HIS:N	4:A:2020:HOH:O	2.35	0.60
1:A:152:PHE:O	1:A:299:THR:HG22	2.01	0.60
1:A:322:VAL:HA	1:D:172:GLN:NE2	2.13	0.60
1:B:217:HIS:NE2	1:B:353:ARG:HD2	2.16	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: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:B:479:LYS:HE2	1:B:483:ASP:OD2	2.01	0.60
1:C:74:HIS:CG	2:C:2002:HEM:C3D	2.89	0.60
1:D:338:MET:HB3	1:D:342:ILE:O	2.01	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:B:4:ARG:NH2	1:C:470:GLN:HG3	2.16	0.60
1:B:34:VAL:HG11	1:B:37:LYS:HB3	1.84	0.60
1:C:74:HIS:O	1:C:111:ARG:NH2	2.28	0.60
1:D:145:VAL:CG1	2:D:2003:HEM:HHD	2.30	0.60
1:A:300:LYS:HE2	1:A:441:GLN:NE2	2.17	0.59
1:A:415:PRO:HA	4:C:2038:HOH:O	2.01	0.59
1:B:26:LEU:HD21	1:B:37:LYS:HD2	1.84	0.59
1:B:147:ASN:CG	2:B:2001:HEM:CBC	2.75	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:D:457:ARG:O	1:D:458:LEU:C	2.45	0.59
1:C:146:GLY:C	2:C:2002:HEM:CBC	2.74	0.59
1:B:145:VAL:HG12	2:B:2001:HEM:C4C	2.38	0.59
1:B:295:PRO:CD	1:C:46:ARG:HH12	2.15	0.59
1:C:356:ALA:O	1:C:360:THR:HG22	2.03	0.59
1:A:76:LYS:HD3	1:A:121:SER:O	2.02	0.59
1:A:131:PHE:HD2	1:A:213:GLY:CA	2.15	0.59
1:B:49:LEU:HD23	1:B:50:LEU:H	1.67	0.59
1:A:412:GLU:O	1:C:26:LEU:HB3	2.01	0.59
1:B:42:THR:HG21	1:C:348:LYS:HE3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:GLU:HG2	1:C:491:ARG:HG3	1.85	0.59
1:B:459:CYS:SG	1:B:491:ARG:HB2	2.42	0.59
1:C:50:LEU:HD22	1:D:48:PRO:HB2	1.82	0.59
1:B:139:ASP:O	1:D:32:ASN:HA	2.02	0.59
1:B:497:ASP:HA	1:B:500:ASN:HB2	1.84	0.59
1:C:186:SER:OG	1:C:476:LYS:HB3	2.02	0.59
1:D:285:PHE:CD1	4:D:3134:HOH:O	2.52	0.59
3:D:3074:3TR:N1	2:D:2003:HEM:C4C	2.70	0.59
1:B:310:ILE:HD12	1:B:310:ILE:N	2.18	0.59
1:C:160:PHE:CZ	2:C:2002:HEM:C3B	2.90	0.59
1:C:364:ARG:NE	2:C:2002:HEM:O1A	2.34	0.59
1:A:175:LEU:HD13	1:D:262:ARG:NH1	2.17	0.59
1:B:479:LYS:O	1:B:482:SER:HB2	2.02	0.59
1:C:402:ASN:OD1	1:D:165:HIS:HB3	2.01	0.59
1:C:487:GLU:O	1:C:491:ARG:HG3	2.03	0.59
1:D:90:ILE:HD11	1:D:99:PHE:CG	2.37	0.59
1:A:65:ARG:HH11	1:A:65:ARG:CG	2.15	0.59
1:B:98:VAL:HG23	1:B:106:THR:OG1	2.03	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:B:276:TRP:HZ3	1:B:317:LEU:HD12	1.68	0.58
1:B:470:GLN:O	1:B:473:ILE:HB	2.03	0.58
1:D:73:VAL:CG1	1:D:164:ILE:HG21	2.32	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
3:D:3074:3TR:N2	2:D:2003:HEM:C2C	2.70	0.58
1:B:191:SER:HB2	1:B:195:VAL:HG23	1.86	0.58
1:B:367:PRO:HG2	1:B:390:PRO:HG2	1.85	0.58
1:C:71:ARG:HD2	1:C:111:ARG:NH2	2.18	0.58
1:C:151:ILE:HG23	1:C:301:VAL:HG12	1.86	0.58
1:A:296:PHE:CD1	1:A:346:PRO:HD2	2.38	0.58
1:B:278:LEU:O	1:B:312:VAL:HG13	2.03	0.58
1:B:381:ARG:HH12	1:D:24:ASP:CG	2.11	0.58
1:B:472:PHE:C	1:B:472:PHE:CD2	2.82	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:A:38:LEU:CD1	4:C:2017:HOH:O	2.51	0.58
1:A:73:VAL:HG11	1:A:164:ILE:HD12	1.85	0.58
1:B:17:GLN:C	1:B:19:ALA:H	2.11	0.58
1:B:359:ASP:OD2	1:C:61:ALA:HA	2.02	0.58
1:A:235:TYR:HA	1:A:277:THR:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2001:HEM:HHA	2:B:2001:HEM:HBA2	1.83	0.58
1:C:215:GLY:HA3	1:C:233:PHE:HB2	1.86	0.58
1:B:233:PHE:C	1:B:234:HIS:HD2	2.11	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:D:192:LEU:HD13	1:D:484:VAL:CG2	2.33	0.58
1:B:443:ARG:HG2	1:B:447:LEU:HD21	1.85	0.58
1:D:26:LEU:C	1:D:26:LEU:HD23	2.29	0.57
1:D:88:HIS:C	1:D:102:ILE:HG12	2.29	0.57
1:D:229:VAL:HA	1:D:285:PHE:HE1	1.68	0.57
1:D:397:GLN:O	1:D:398:GLY:C	2.46	0.57
1:A:9:ASP:HB3	1:A:12:LYS:HE2	1.87	0.57
1:A:302:TRP:HB3	1:A:307:TYR:CD2	2.39	0.57
1:A:50:LEU:C	1:A:52:GLN:H	2.11	0.57
1:A:96:ALA:HB2	1:A:342:ILE:CD1	2.33	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:B:384:ASN:H	1:B:397:GLN:HE22	1.51	0.57
1:D:145:VAL:HG12	2:D:2003:HEM:CHD	2.30	0.57
1:B:43:VAL:CG1	1:B:48:PRO:HD2	2.34	0.57
1:C:147:ASN:ND2	2:C:2002:HEM:HAC	2.14	0.57
1:C:469:ALA:O	1:C:470:GLN:C	2.47	0.57
1:D:217:HIS:ND1	1:D:298:LEU:HD13	2.19	0.57
1:A:65:ARG:HH11	1:A:65:ARG:HG3	1.70	0.57
1:A:254:HIS:HD2	1:D:254:HIS:CD2	2.22	0.57
1:B:35:GLY:HA3	1:D:418:LEU:HD23	1.86	0.57
1:B:146:GLY:CA	2:B:2001:HEM:CAC	2.83	0.57
1:B:404:TYR:CE2	1:D:38:LEU:HG	2.38	0.57
1:A:155:ARG:CZ	1:A:297:ASP:OD2	2.53	0.57
1:A:338:MET:HB3	1:A:342:ILE:O	2.05	0.57
1:B:408:PHE:HA	1:D:15:LYS:HD2	1.86	0.57
1:B:457:ARG:HB2	1:B:457:ARG:NH1	2.20	0.57
1:C:154:ILE:HG13	1:C:349:MET:CE	2.34	0.57
1:C:436:ASP:O	1:C:437:ASP:HB3	2.05	0.57
1:D:233:PHE:C	1:D:234:HIS:HD2	2.12	0.57
1:D:482:SER:HA	1:D:485:HIS:O	2.05	0.57
1:B:151:ILE:HD13	1:B:193:HIS:ND1	2.20	0.57
1:B:204:ILE:HD12	1:B:204:ILE:N	2.19	0.57
1:B:251:ARG:HA	1:B:254:HIS:CE1	2.39	0.57
1:C:367:PRO:HD2	4:C:2007:HOH:O	2.04	0.57
1:C:466:LEU:CD1	1:C:474:GLN:HG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:HIS:CD2	2:D:2003:HEM:O2A	2.57	0.57
1:A:73:VAL:O	2:A:2000:HEM:HAA1	2.05	0.57
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.69	0.57
1:B:81:PHE:HB2	1:B:319:ARG:HG2	1.87	0.57
1:B:98:VAL:HG13	1:B:99:PHE:CD1	2.40	0.57
1:C:46:ARG:NH1	1:C:46:ARG:HG2	2.20	0.56
1:D:265:PHE:HB2	4:D:3114:HOH:O	2.05	0.56
1:A:14:TRP:O	1:A:15:LYS:C	2.48	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
1:B:27:THR:O	1:D:384:ASN:HB3	2.06	0.56
3:D:3074:3TR:H3A1	2:D:2003:HEM:CHC	2.18	0.56
1:B:71:ARG:NH1	1:B:364:ARG:NH2	2.53	0.56
1:B:71:ARG:NH1	1:B:329:GLU:O	2.38	0.56
1:B:333:PHE:CD2	2:B:2001:HEM:CGD	2.86	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:A:141:ASN:OD1	1:A:377:PRO:HA	2.06	0.56
1:A:300:LYS:HE2	1:A:441:GLN:HE21	1.71	0.56
1:B:327:GLU:O	1:B:331:LEU:HG	2.05	0.56
1:A:399:GLY:O	1:A:400:ALA:C	2.48	0.56
1:A:107:PRO:HG2	1:A:378:TYR:OH	2.05	0.55
1:A:210:HIS:HB3	1:A:242:LYS:H	1.70	0.55
1:B:4:ARG:HH22	1:C:470:GLN:HE21	1.51	0.55
1:B:139:ASP:O	1:D:33:PRO:HD3	2.07	0.55
1:B:404:TYR:HE2	1:D:38:LEU:CG	2.19	0.55
1:C:93:TYR:O	1:C:221:LEU:HB3	2.06	0.55
1:C:209:ARG:HB2	1:C:209:ARG:HH11	1.67	0.55
1:D:110:VAL:HG13	1:D:132:ALA:O	2.05	0.55
1:D:166:SER:HB2	1:D:180:MET:O	2.05	0.55
1:D:206:ASP:HA	1:D:244:LEU:HG	1.87	0.55
1:A:69:PRO:HA	4:A:2011:HOH:O	2.05	0.55
1:A:294:ASN:HD21	1:D:46:ARG:HG2	1.71	0.55
1:A:493:GLN:O	1:A:496:LEU:HB2	2.06	0.55
1:B:168:LYS:HE3	1:C:67:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:ASP:OD1	1:C:12:LYS:HD2	2.06	0.55
1:C:193:HIS:CB	1:C:442:VAL:HG22	2.37	0.55
1:A:126:ARG:NH1	1:A:126:ARG:HB2	2.22	0.55
1:B:155:ARG:NH2	1:B:438:ASN:OD1	2.39	0.55
1:C:147:ASN:CB	2:C:2002:HEM:HBC1	2.36	0.55
1:D:18:ARG:O	1:D:19:ALA:HB3	2.06	0.55
1:D:291:PHE:HE1	1:D:293:PHE:HB2	1.71	0.55
1:A:237:THR:HA	1:A:276:TRP:CD1	2.42	0.55
1:C:28:THR:HG23	1:C:32:ASN:O	2.06	0.55
1:C:209:ARG:HH11	1:C:209:ARG:CB	2.20	0.55
1:D:327:GLU:O	1:D:331:LEU:HG	2.07	0.55
1:A:485:HIS:HD2	1:A:487:GLU:HB3	1.72	0.55
1:D:38:LEU:N	1:D:38:LEU:HD12	2.21	0.55
1:D:246:VAL:HG23	1:D:247:GLU:OE1	2.07	0.55
1:B:360:THR:OG1	1:C:64:ASP:CB	2.51	0.55
2:B:2001:HEM:HBC2	2:B:2001:HEM:CMC	2.37	0.55
1:C:155:ARG:NH1	1:C:299:THR:OG1	2.40	0.55
1:D:439:VAL:O	1:D:440:THR:C	2.50	0.55
1:A:40:SER:HB3	1:A:49:LEU:HD21	1.89	0.54
1:A:191:SER:HB2	1:A:195:VAL:HG23	1.89	0.54
1:A:381:ARG:HG3	4:A:2143:HOH:O	2.07	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:50:LEU:C	1:A:52:GLN:N	2.65	0.54
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.42	0.54
1:B:92:ARG:NH1	1:B:92:ARG:CB	2.68	0.54
1:B:186:SER:HB2	1:B:476:LYS:HG3	1.89	0.54
1:C:73:VAL:CG2	2:C:2002:HEM:C1A	2.91	0.54
1:D:212:ASP:OD1	1:D:236:LYS:HA	2.07	0.54
1:B:25:VAL:O	1:B:27:THR:HG23	2.06	0.54
1:B:215:GLY:O	1:B:217:HIS:N	2.39	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:101:HIS:O	1:B:104:LYS:HB2	2.08	0.54
1:B:110:VAL:HG11	1:B:131:PHE:CE1	2.41	0.54
1:A:271:GLY:HA2	1:A:273:TYR:CZ	2.43	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:B:46:ARG:NH2	1:C:294:ASN:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:PHE:CD1	1:C:63:PHE:C	2.85	0.54
1:C:71:ARG:NH1	1:C:111:ARG:NH1	2.54	0.54
1:D:98:VAL:HB	1:D:137:THR:HG21	1.90	0.54
1:D:187:LEU:O	1:D:188:ARG:HD2	2.08	0.54
1:D:347:ASP:OD1	1:D:349:MET:HB2	2.08	0.54
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:B:402:ASN:HD22	1:B:402:ASN:H	1.55	0.54
1:C:160:PHE:CE1	2:C:2002:HEM:CAB	2.89	0.54
1:C:217:HIS:NE2	1:C:350:LEU:HA	2.23	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:160:PHE:HB3	1:D:161:PRO:HD3	1.88	0.54
1:A:96:ALA:CB	1:A:342:ILE:HD11	2.38	0.54
1:A:170:ASN:OD1	1:A:173:THR:N	2.40	0.54
1:B:125:VAL:HG22	1:B:126:ARG:N	2.23	0.54
1:D:293:PHE:HZ	1:D:440:THR:HG21	1.72	0.54
1:D:301:VAL:O	1:D:303:PRO:HD3	2.08	0.54
1:C:74:HIS:ND1	2:C:2002:HEM:C2D	2.76	0.53
1:C:458:LEU:HD21	1:C:488:TYR:OH	2.08	0.53
1:C:481:PHE:O	1:C:484:VAL:HB	2.08	0.53
1:D:115:VAL:N	1:D:127:ASP:OD2	2.40	0.53
1:D:235:TYR:N	1:D:235:TYR:CD1	2.75	0.53
1:A:329:GLU:C	1:A:331:LEU:H	2.16	0.53
1:A:387:ARG:NH2	1:A:397:GLN:HB2	2.23	0.53
1:B:5:ASP:HB2	1:B:6:PRO:HD2	1.90	0.53
1:C:283:MET:HE2	1:C:307:TYR:CZ	2.43	0.53
1:C:472:PHE:CZ	1:C:473:ILE:HG13	2.42	0.53
1:D:90:ILE:O	1:D:90:ILE:HD12	2.08	0.53
1:A:407:SER:C	4:A:2087:HOH:O	2.52	0.53
1:A:217:HIS:CE1	1:A:298:LEU:HD22	2.43	0.53
1:B:160:PHE:N	1:B:161:PRO:HD2	2.24	0.53
1:C:112:PHE:HZ	1:C:276:TRP:CH2	2.26	0.53
1:D:111:ARG:HB3	2:D:2003:HEM:O1D	2.08	0.53
1:A:67:ARG:O	1:D:69:PRO:HB3	2.08	0.53
2:B:2001:HEM:HBA2	2:B:2001:HEM:CHA	2.37	0.53
1:C:160:PHE:CZ	2:C:2002:HEM:C4B	2.97	0.53
1:C:327:GLU:O	1:C:331:LEU:HG	2.08	0.53
1:C:353:ARG:NH1	1:C:357:TYR:OH	2.37	0.53
1:C:459:CYS:HA	1:C:492:ILE:CD1	2.39	0.53
1:B:165:HIS:NE2	1:C:66:GLU:OE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:VAL:O	1:C:43:VAL:HG13	2.09	0.53
1:D:128:PRO:O	1:D:129:ARG:HG2	2.09	0.53
1:D:487:GLU:O	1:D:488:TYR:C	2.50	0.53
1:C:193:HIS:HA	1:C:442:VAL:HG22	1.91	0.53
1:D:208:HIS:HA	1:D:211:MET:CE	2.39	0.53
1:A:429:GLN:NE2	4:A:2135:HOH:O	2.41	0.53
1:D:147:ASN:OD1	2:D:2003:HEM:HAC	2.08	0.53
1:A:115:VAL:N	1:A:127:ASP:OD2	2.36	0.53
1:A:202:ARG:CG	4:A:2140:HOH:O	2.56	0.53
1:A:367:PRO:HD3	4:A:2013:HOH:O	2.09	0.53
1:A:480:ASN:O	1:A:483:ASP:HB2	2.08	0.53
1:B:237:THR:HA	1:B:276:TRP:CD1	2.44	0.53
1:A:96:ALA:HB2	1:A:342:ILE:HD12	1.90	0.53
1:A:129:ARG:HB2	1:A:148:ASN:CB	2.38	0.53
1:A:331:LEU:HD13	1:A:374:VAL:CG2	2.38	0.53
1:B:277:THR:CG2	1:B:314:LYS:HG3	2.39	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:181:VAL:HG12	1:D:182:TRP:N	2.23	0.53
1:D:442:VAL:HG12	1:D:484:VAL:HG11	1.90	0.53
1:A:100:GLU:CG	1:A:101:HIS:ND1	2.54	0.52
1:B:329:GLU:O	1:B:364:ARG:NH2	2.42	0.52
1:C:208:HIS:HA	1:C:211:MET:HE3	1.92	0.52
1:C:403:TYR:N	1:C:403:TYR:CD1	2.78	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:A:304:HIS:CA	1:A:304:HIS:CG	2.80	0.52
1:B:309:LEU:HD23	1:B:309:LEU:N	2.23	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:C:206:ASP:O	1:C:210:HIS:HB2	2.09	0.52
1:D:59:GLU:O	1:D:60:MET:C	2.53	0.52
1:D:127:ASP:HB3	1:D:129:ARG:HH12	1.74	0.52
1:D:291:PHE:CE1	1:D:293:PHE:HB2	2.45	0.52
1:D:485:HIS:CE1	1:D:487:GLU:H	2.27	0.52
1:A:353:ARG:CD	2:A:2000:HEM:C4B	2.88	0.52
1:B:275:SER:HA	1:B:315:LEU:O	2.10	0.52
1:D:280:ILE:CD1	1:D:310:ILE:HB	2.39	0.52
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:74:HIS:HA	1:C:114:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:SER:O	1:D:289:GLU:CB	2.53	0.52
1:B:36:ASP:HB3	1:C:430:ARG:HD3	1.90	0.52
1:C:124:THR:HA	1:C:129:ARG:HH22	1.75	0.52
1:C:126:ARG:HH11	1:C:126:ARG:CG	2.20	0.52
1:C:22:LYS:HD3	1:C:23:PRO:N	2.24	0.52
1:C:49:LEU:HG	1:D:51:VAL:HG21	1.92	0.52
1:C:73:VAL:HG23	2:C:2002:HEM:C1A	2.45	0.52
1:C:446:TYR:CE1	1:C:455:ARG:HG3	2.45	0.52
1:D:297:ASP:CG	1:D:300:LYS:HD3	2.35	0.52
1:D:367:PRO:HG2	1:D:390:PRO:CG	2.39	0.52
1:A:145:VAL:HG11	2:A:2000:HEM:C2D	2.34	0.52
1:B:187:LEU:O	1:B:188:ARG:HD2	2.10	0.52
1:B:345:SER:C	1:B:347:ASP:H	2.18	0.52
1:C:154:ILE:HG13	1:C:349:MET:HE1	1.92	0.52
1:D:86:VAL:O	1:D:102:ILE:HG23	2.09	0.52
1:D:173:THR:O	1:D:174:HIS:CB	2.58	0.52
1:A:100:GLU:HG3	1:A:101:HIS:CE1	2.35	0.52
1:A:146:GLY:HA3	1:A:235:TYR:OH	2.10	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:B:413:HIS:CE1	1:B:415:PRO:HD3	2.45	0.52
1:C:191:SER:C	1:C:195:VAL:HG23	2.35	0.52
1:C:235:TYR:N	1:C:235:TYR:CD1	2.77	0.52
1:A:84:PHE:HD1	1:A:314:LYS:O	1.92	0.51
1:A:188:ARG:HB3	1:A:190:GLU:CD	2.35	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:B:419:GLU:CD	1:B:419:GLU:H	2.18	0.51
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:30:GLY:O	1:C:377:PRO:HB3	2.11	0.51
1:B:109:ALA:HB3	1:B:134:LYS:HB3	1.92	0.51
1:C:146:GLY:O	2:C:2002:HEM:CBC	2.58	0.51
1:D:151:ILE:HG23	1:D:301:VAL:HG13	1.93	0.51
1:D:386:GLN:HA	4:D:3075:HOH:O	2.09	0.51
1:A:301:VAL:O	1:A:303:PRO:HD3	2.10	0.51
1:B:439:VAL:HG23	1:B:440:THR:H	1.75	0.51
1:C:43:VAL:CG1	1:C:48:PRO:HD2	2.40	0.51
1:C:460:GLU:HA	1:C:495:LEU:HD13	1.91	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

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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:B:250:ALA:O	1:B:253:ALA:HB3	2.09	0.51
1:B:442:VAL:HG12	1:B:484:VAL:HG11	1.92	0.51
1:C:457:ARG:O	1:C:461:ASN:CG	2.53	0.51
1:D:160:PHE:CD1	2:D:2003:HEM:HAB	2.46	0.51
1:D:206:ASP:CA	1:D:244:LEU:HG	2.40	0.51
1:D:208:HIS:HA	1:D:211:MET:HE3	1.92	0.51
1:A:126:ARG:HA	1:A:204:ILE:HG12	1.92	0.51
1:B:235:TYR:N	1:B:235:TYR:CD1	2.79	0.51
1:D:297:ASP:OD1	1:D:297:ASP:C	2.54	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:48:PRO:HD3	1:D:424:PHE:CE2	2.46	0.51
1:A:173:THR:O	1:A:174:HIS:CB	2.58	0.51
1:A:384:ASN:OD1	1:A:386:GLN:CB	2.53	0.51
1:B:6:PRO:HG2	1:B:266:ASN:OD1	2.11	0.51
1:B:26:LEU:HD21	1:B:37:LYS:CG	2.41	0.51
1:B:49:LEU:HD23	1:B:50:LEU:N	2.26	0.51
1:B:232:LYS:O	1:B:280:ILE:HA	2.09	0.51
1:B:493:GLN:CA	1:B:496:LEU:HD12	2.29	0.51
1:C:265:PHE:C	1:C:265:PHE:CD1	2.88	0.51
1:D:148:ASN:O	1:D:148:ASN:ND2	2.43	0.51
1:D:210:HIS:CD2	1:D:242:LYS:HB2	2.46	0.51
1:A:201:ASP:CG	4:A:2084:HOH:O	2.53	0.51
1:B:353:ARG:NH2	2:B:2001:HEM:NC	2.57	0.51
1:A:202:ARG:HG3	4:A:2140:HOH:O	2.11	0.51
1:A:492:ILE:HG22	1:A:496:LEU:HD13	1.92	0.51
1:C:291:PHE:CD2	1:C:293:PHE:O	2.64	0.51
1:A:217:HIS:HD2	1:A:353:ARG:NH1	2.06	0.50
1:A:275:SER:HA	1:A:315:LEU:O	2.12	0.50
1:B:67:ARG:NH2	1:C:168:LYS:HZ1	2.10	0.50
1:B:265:PHE:CD1	1:B:320:ASN:CG	2.89	0.50
1:C:191:SER:HB2	1:C:195:VAL:CG2	2.41	0.50
1:C:206:ASP:OD2	1:C:242:LYS:HE3	2.10	0.50
1:C:239:GLN:CD	1:C:239:GLN:H	2.17	0.50
1:C:310:ILE:N	1:C:310:ILE:CD1	2.74	0.50
1:C:369:TYR:C	1:C:371:GLN:H	2.19	0.50
1:D:353:ARG:HB3	1:D:357:TYR:CE1	2.46	0.50
1:D:372:ILE:HG22	1:D:374:VAL:HG12	1.92	0.50
1:A:67:ARG:C	1:D:69:PRO:HB3	2.36	0.50
1:A:110:VAL:HG12	1:A:133:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ARG:HG3	2: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:B:325:PHE:CD1	1:D:388:ASP:OD2	2.64	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:A:74:HIS:ND1	1:A:114:THR:O	2.45	0.50
1:A:296:PHE:CE1	1:A:346:PRO:HD2	2.47	0.50
1:B:74:HIS:NE2	1:B:115:VAL:HG22	2.25	0.50
1:D:74:HIS:O	1:D:111:ARG:NH2	2.43	0.50
1:A:283:MET:SD	1:A:288:ALA:HA	2.51	0.50
1:B:404:TYR:OH	1:B:413:HIS:HD2	1.95	0.50
1:C:350:LEU:O	1:C:353:ARG:N	2.44	0.50
1:D:26:LEU:C	1:D:26:LEU:CD2	2.84	0.50
1:A:85:GLU:HA	1:A:104:LYS:O	2.11	0.50
1:A:182:TRP:CH2	1:A:462:ILE:HG23	2.46	0.50
1:B:439:VAL:O	1:B:442:VAL:CB	2.58	0.50
1:C:264:LEU:HD12	1:C:264:LEU:O	2.11	0.50
1:D:251:ARG:O	1:D:254:HIS:CD2	2.65	0.50
1:A:43:VAL:O	1:A:47:GLY:HA3	2.11	0.50
1:A:145:VAL:CG1	2:A:2000:HEM:HBC2	2.42	0.50
1:A:353:ARG:CB	2:A:2000:HEM:HBB2	2.41	0.50
1:B:393:MET:HG2	1:D:393:MET:SD	2.51	0.50
1:C:211:MET:HB2	4:C:2048:HOH:O	2.10	0.50
1:D:160:PHE:CG	2:D:2003:HEM:HAB	2.46	0.50
1:A:70:GLU:O	1:A:71:ARG:C	2.52	0.50
1:A:233:PHE:C	1:A:234:HIS:HD2	2.19	0.50
1:B:191:SER:O	1:B:192:LEU:C	2.54	0.50
1:B:284:THR:HG23	1:B:287:GLU:OE1	2.11	0.50
1:C:111:ARG:HH21	2: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: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
1:D:148:ASN:C	1:D:148:ASN:HD22	2.20	0.50
1:A:54:VAL:CG2	4:A:2137:HOH:O	2.59	0.50
2:A:2000:HEM:CHA	2:A:2000:HEM:CBA	2.88	0.50
1:B:50:LEU:N	1:B:50:LEU:CD2	2.74	0.50
1:B:83:TYR:HA	1:B:108:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:PHE:HA	1:B:449:VAL:CG2	2.40	0.50
1:C:83:TYR:CD1	1:C:83:TYR:C	2.89	0.50
1:D:115:VAL:HG21	1:D:128:PRO:HB2	1.93	0.50
1:D:179:ASP:OD1	1:D:473:ILE:HD12	2.12	0.50
1:A:408:PHE:CD1	1:C:11:MET:HB3	2.47	0.49
1:A:471:LEU:HD23	1:A:474:GLN:NE2	2.26	0.49
1:B:72:VAL:HG11	1:C:63:PHE:CE1	2.47	0.49
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.93	0.49
1:B:251:ARG:HG2	1:B:251:ARG:NH1	2.26	0.49
1:D:170:ASN:HA	1:D:180:MET:SD	2.52	0.49
1:D:182:TRP:CD2	1:D:466:LEU:HD13	2.47	0.49
1:A:220:LYS:HD2	1:A:420:HIS:HD2	1.78	0.49
1:B:135:PHE:HB2	1:B:142:TRP:HB3	1.94	0.49
1:C:387:ARG:HG2	1:C:387:ARG:HH11	1.77	0.49
1:D:129:ARG:HB2	1:D:148:ASN:CG	2.36	0.49
1:D:287:GLU:C	1:D:289:GLU:N	2.69	0.49
1:A:32:ASN:N	1:A:32:ASN:HD22	2.08	0.49
1:C:155:ARG:HH22	1:C:438:ASN:HD22	1.60	0.49
1:C:160:PHE:CE2	1:C:164:ILE:HG13	2.47	0.49
1:D:218:THR:O	1:D:345:SER:HB3	2.12	0.49
3:D:3074:3TR:N3A	2:D:2003:HEM:C1C	2.79	0.49
1:A:300:LYS:HB3	1:A:441:GLN:NE2	2.16	0.49
1:B:74:HIS:ND1	1:B:114:THR:O	2.45	0.49
1:B:189:PRO:O	1:B:192:LEU:HG	2.13	0.49
1:B:332:ALA:HB3	1:B:375:ASN:OD1	2.12	0.49
1:C:74:HIS:CE1	2:C:2002:HEM:C2D	3.00	0.49
1:A:492:ILE:O	1:A:493:GLN:C	2.55	0.49
1:B:340:PRO:HG3	4:B:2035:HOH:O	2.13	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:D:6:PRO:HD2	1:D:266:ASN:OD1	2.13	0.49
1:D:114:THR:HG21	4:D:3081:HOH:O	2.12	0.49
1:A:180:MET:HG3	1:D:11:MET:HE2	1.93	0.49
1:C:151:ILE:HD13	1:C:193:HIS:CE1	2.47	0.49
1:C:434:ALA:C	1:C:435:ASN:HD22	2.21	0.49
1:D:145:VAL:CG1	2:D:2003:HEM:CHD	2.89	0.49
1:D:170:ASN:HD22	1:D:173:THR:H	1.60	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:B:219:PHE:CD1	1:B:338:MET:HE1	2.47	0.49
1:B:396:ASN:HB2	1:D:326:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PHE:CE1	1:C:278:LEU:HD23	2.48	0.49
1:C:467:LYS:HD2	1:C:467:LYS:O	2.12	0.49
1:D:166:SER:HA	1:D:180:MET:HE2	1.95	0.49
1:D:209:ARG:CG	1:D:274:PRO:HB3	2.42	0.49
1:D:372:ILE:HB	1:D:375:ASN:HD22	1.78	0.49
1:A:353:ARG:NH2	2:A:2000:HEM:C3C	2.72	0.49
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.95	0.49
2:A:2000:HEM:CBC	2:A:2000:HEM:C4C	2.96	0.49
1:C:160:PHE:CE1	2:C:2002:HEM:C3B	3.01	0.49
1:C:361:HIS:C	1:C:363:HIS:H	2.20	0.49
1:A:98:VAL:HB	1:A:137:THR:HG21	1.95	0.49
1:B:41:LEU:CD1	1:C:428:VAL:HG12	2.37	0.49
1:B:71:ARG:HE	1:B:111:ARG:NH1	2.09	0.49
1:B:177:ASP:CG	1:B:180:MET:HG3	2.37	0.49
1:C:111:ARG:CZ	2:C:2002:HEM:CGD	2.91	0.49
1:C:485:HIS:CE1	1:C:487:GLU:H	2.31	0.49
1:A:311:PRO:HD2	4:A:2009:HOH:O	2.12	0.49
1:B:416:SER:HB3	4:B:2075:HOH:O	2.12	0.49
1:C:193:HIS:HB2	1:C:442:VAL:HG22	1.95	0.49
1:D:204:ILE:HD12	1:D:204:ILE:N	2.28	0.49
1:D:332:ALA:HB1	1:D:361:HIS:ND1	2.28	0.49
1:D:414:GLN:O	1:D:416:SER:N	2.46	0.49
1:A:245:SER:HB3	4:A:2141:HOH:O	2.12	0.48
1:A:352:GLY:C	2:A:2000:HEM:CBB	2.86	0.48
1:B:62:HIS:CE1	1:D:368:ASN:HD21	2.30	0.48
1:B:86:VAL:HB	1:B:103:GLY:H	1.78	0.48
1:B:443:ARG:HG3	1:B:484:VAL:O	2.14	0.48
1:D:218:THR:O	1:D:345:SER:OG	2.28	0.48
3:D:3074:3TR:N3A	2:D:2003:HEM:C4B	2.78	0.48
1:B:347:ASP:O	1:B:350:LEU:N	2.46	0.48
1:C:153:PHE:CD2	1:C:153:PHE:N	2.81	0.48
1:C:99:PHE:O	1:C:100:GLU:C	2.56	0.48
1:C:108:ILE:HA	1:C:134:LYS:O	2.12	0.48
1:C:492:ILE:CG2	1:C:496:LEU:HD23	2.43	0.48
1:D:97:LYS:HA	1:D:100:GLU:HG3	1.96	0.48
1:A:38:LEU:CD2	1:D:159:LEU:HD11	2.44	0.48
1:A:155:ARG:NE	1:A:297:ASP:OD2	2.46	0.48
1:A:368:ASN:ND2	1:A:390:PRO:O	2.42	0.48
1:A:451:ASN:H	1:A:454:GLN:HE21	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:THR:O	1:D:345:SER:CB	2.62	0.48
1:A:86:VAL:HG21	1:A:99:PHE:HA	1.96	0.48
1:A:137:THR:OG1	1:A:140:GLY:O	2.30	0.48
1:A:238:ASP:HB2	1:A:275:SER:OG	2.14	0.48
1:A:329:GLU:C	1:A:331:LEU:N	2.71	0.48
1:A:430:ARG:HB3	1:D:39:ASN:HB2	1.95	0.48
1:B:25:VAL:O	1:B:26:LEU:C	2.56	0.48
1:B:32:ASN:HD22	1:D:339:PRO:HA	1.79	0.48
1:B:60:MET:HE1	1:C:161:PRO:HD3	1.95	0.48
1:B:65:ARG:HA	1:C:363:HIS:CD2	2.49	0.48
1:C:82:GLY:C	1:C:108:ILE:HG12	2.39	0.48
1:B:37:LYS:O	1:B:37:LYS:CG	2.57	0.48
1:B:116:ALA:O	1:B:168:LYS:NZ	2.46	0.48
1:B:451:ASN:OD1	1:B:453:GLU:HB2	2.14	0.48
1:C:110:VAL:CG2	1:C:133:VAL:HG22	2.44	0.48
1:A:72:VAL:HG12	2:A:2000:HEM:HAA2	1.96	0.48
1:B:18:ARG:O	1:B:19:ALA:C	2.55	0.48
1:B:71:ARG:HD2	1:B:364:ARG:NH1	2.29	0.48
1:B:479:LYS:HE2	1:B:483:ASP:CG	2.39	0.48
1:D:73:VAL:HG12	1:D:164:ILE:HG21	1.96	0.48
1:D:232:LYS:HZ2	1:D:302:TRP:CD1	2.32	0.48
1:D:254:HIS:O	1:D:255:GLU:C	2.56	0.48
1:A:248:ASP:HA	1:A:251:ARG:HH12	1.79	0.48
1:A:450:LEU:HA	1:A:454:GLN:HE22	1.75	0.48
1:A:487:GLU:HG2	1:A:491:ARG:CD	2.44	0.48
1:A:495:LEU:O	1:A:498:LYS:HB3	2.13	0.48
1:B:337:ASN:N	1:B:337:ASN:ND2	2.60	0.48
1:C:111:ARG:HH21	2:C:2002:HEM:CGD	2.26	0.48
1:D:345:SER:C	1:D:347:ASP:H	2.22	0.48
1:A:101:HIS:O	1:A:104:LYS:HB2	2.14	0.48
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:41:LEU:HB2	1:D:430:ARG:CZ	2.41	0.48
1:A:266:ASN:O	1:A:267:ALA:C	2.57	0.48
1:A:329:GLU:O	1:A:331:LEU:N	2.47	0.48
1:B:332:ALA:N	1:B:375:ASN:OD1	2.47	0.48
1:B:393:MET:HG2	1:D:393:MET:HG3	1.96	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:C:297:ASP:CG	1:C:300:LYS:HG2	2.38	0.48
1:D:142:TRP:HA	1:D:337:ASN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:CYS:C	1:D:393:MET:HE2	2.39	0.48
1:A:251:ARG:HG2	1:A:255:GLU:CD	2.39	0.47
1:A:276:TRP:HB2	1:A:315:LEU:HB2	1.96	0.47
1:A:295:PRO:HD3	1:D:46:ARG:NH1	2.28	0.47
1:B:107:PRO:O	1:B:136:TYR:HD1	1.97	0.47
1:C:129:ARG:HG2	1:C:211:MET:CE	2.43	0.47
1:D:160:PHE:CE1	1:D:164:ILE:HD11	2.48	0.47
1:A:56:PHE:O	1:A:57:THR:C	2.57	0.47
1:C:147:ASN:N	2:C:2002:HEM:HBC1	2.28	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:A:126:ARG:NE	1:A:199:PHE:HA	2.28	0.47
1:B:379:ARG:HD3	4:B:2073:HOH:O	2.14	0.47
1:C:410:ALA:HB1	1:C:411:PRO:CD	2.40	0.47
1:D:414:GLN:O	1:D:417:ALA:N	2.41	0.47
1:D:439:VAL:CG2	1:D:440:THR:N	2.76	0.47
1:A:167:GLN:HE21	1:A:167:GLN:HB3	1.54	0.47
1:A:439:VAL:O	1:A:442:VAL:N	2.46	0.47
1:B:165:HIS:HE2	1:C:66:GLU:CD	2.22	0.47
1:C:206:ASP:HA	1:C:244:LEU:HG	1.96	0.47
1:C:448:LYS:NZ	4:C:2184:HOH:O	2.36	0.47
1:A:67:ARG:HH21	1:D:168:LYS:HE3	1.79	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:D:247:GLU:O	1:D:251:ARG:HB2	2.14	0.47
1:A:396:ASN:C	1:A:398:GLY:H	2.21	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:C:297:ASP:OD1	1:C:299:THR:N	2.41	0.47
1:D:57:THR:O	1:D:58:ASP:C	2.55	0.47
1:D:368:ASN:CG	1:D:371:GLN:NE2	2.73	0.47
1:D:395:ASP:O	1:D:396:ASN:HB3	2.15	0.47
1:B:69:PRO:HD3	1:C:69:PRO:HG3	1.97	0.47
1:B:160:PHE:CZ	1:B:164:ILE:HD11	2.50	0.47
1:B:351:GLN:HA	1:B:354:LEU:HD12	1.96	0.47
1:B:357:TYR:HB2	1:B:358:PRO:HD3	1.96	0.47
1:B:472:PHE:CZ	1:B:473:ILE:HG13	2.50	0.47
1:C:291:PHE:HD2	1:C:293:PHE:O	1.96	0.47
1:C:414:GLN:HA	1:C:415:PRO:HD2	1.81	0.47
1:C:452:GLU:O	1:C:455:ARG:HB3	2.15	0.47
1:C:466:LEU:HD11	1:C:474:GLN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:PRO:O	1:D:391:MET:HB2	2.14	0.47
1:D:419:GLU:CD	1:D:419:GLU:N	2.72	0.47
1:D:440:THR:HG22	1:D:441:GLN:N	2.29	0.47
1:A:45:PRO:HD3	1:D:431:PHE:CE2	2.50	0.47
1:A:179:ASP:O	1:A:183:ASP:HB2	2.14	0.47
1:A:353:ARG:HD3	2:A:2000:HEM:CMC	2.45	0.47
1:B:71:ARG:N	1:B:364:ARG:HH11	2.13	0.47
1:B:454:GLN:HA	1:B:457:ARG:HH12	1.78	0.47
1:C:432:ASN:HD21	1:C:434:ALA:H	1.57	0.47
1:A:54:VAL:HG22	1:A:54:VAL:H	1.44	0.47
1:A:179:ASP:OD2	1:A:470:GLN:HG3	2.15	0.47
1:A:308:PRO:O	1:A:309:LEU:HD22	2.15	0.47
1:A:325:PHE:O	1:A:329:GLU:HB3	2.15	0.47
1:C:81:PHE:N	1:C:81:PHE:CD1	2.83	0.47
1:D:95:LYS:HG2	1:D:222:VAL:O	2.15	0.47
1:D:358:PRO:HB2	1:D:362:ARG:CZ	2.45	0.47
1:A:36:ASP:HB3	1:C:418:LEU:HD21	1.96	0.47
1:A:110:VAL:CG1	1:A:133:VAL:HG13	2.45	0.47
1:A:110:VAL:HG21	1:A:317:LEU:HD11	1.97	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:A:325:PHE:CD2	1:C:388:ASP:HA	2.50	0.47
1:B:65:ARG:O	1:D:389:GLY:HA2	2.15	0.47
1:B:245:SER:C	1:B:247:GLU:N	2.70	0.47
1:B:367:PRO:HD2	4:B:2004:HOH:O	2.15	0.47
1:B:386:GLN:C	1:B:387:ARG:HG2	2.40	0.47
1:C:111:ARG:NH2	2:C:2002:HEM:CGD	2.78	0.47
1:C:296:PHE:O	1:C:297:ASP:C	2.58	0.47
1:C:451:ASN:H	1:C:454:GLN:HE21	1.63	0.47
1:C:470:GLN:O	1:C:471:LEU:C	2.57	0.47
1:D:189:PRO:C	1:D:191:SER:N	2.68	0.47
1:D:221:LEU:HB2	1:D:229:VAL:HG23	1.96	0.47
1:A:169:ARG:HD2	1:A:174:HIS:O	2.15	0.46
1:B:279:TYR:O	1:B:280:ILE:CG2	2.63	0.46
1:B:333:PHE:CD2	2:B:2001:HEM:O1D	2.68	0.46
1:C:385:TYR:CE2	1:C:404:TYR:HB2	2.49	0.46
1:D:73:VAL:O	1:D:74:HIS:HB2	2.14	0.46
1:D:99:PHE:O	1:D:100:GLU:C	2.57	0.46
1:D:127:ASP:C	1:D:128:PRO:O	2.58	0.46
1:D:128:PRO:C	1:D:129:ARG:HG2	2.40	0.46
1:A:87:THR:HG1	1:A:313:GLY:HA2	1.79	0.46

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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:A:469:ALA:O	1:A:470:GLN:C	2.56	0.46
1:B:114:THR:HB	1:B:115:VAL:H	1.58	0.46
1:B:155:ARG:NH1	1:B:299:THR:OG1	2.49	0.46
1:B:198:LEU:C	1:B:200:SER:H	2.22	0.46
1:B:249:ALA:O	1:B:253:ALA:HB2	2.14	0.46
1:D:71:ARG:HB3	2:D:2003:HEM:HBA1	1.97	0.46
1:D:115:VAL:HG21	1:D:128:PRO:HD2	1.97	0.46
1:D:296:PHE:HB3	1:D:347:ASP:HA	1.96	0.46
1:A:53:ASP:OD1	1:A:53:ASP:C	2.58	0.46
1:A:127:ASP:C	1:A:128:PRO:O	2.56	0.46
1:A:325:PHE:CE2	1:C:388:ASP:HA	2.50	0.46
1:B:277:THR:HG22	1:B:314:LYS:HG3	1.97	0.46
1:B:454:GLN:CA	1:B:457:ARG:HH12	2.28	0.46
1:C:228:ALA:O	1:C:229:VAL:HG13	2.15	0.46
1:C:463:ALA:CB	1:C:496:LEU:HD22	2.45	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:389:GLY:HA2	1:D:65:ARG:O	2.15	0.46
1:B:446:TYR:O	1:B:455:ARG:NH1	2.49	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:B:491:ARG:O	1:B:494:ALA:HB3	2.15	0.46
1:D:110:VAL:HA	1:D:132:ALA:O	2.15	0.46
1:D:329:GLU:HA	1:D:329:GLU:OE1	2.14	0.46
1:B:10:GLN:NE2	1:C:172:GLN:NE2	2.64	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:HD22	1:B:402:ASN:N	2.13	0.46
1:C:87:THR:OG1	1:C:313:GLY:HA2	2.16	0.46
1:D:188:ARG:HB3	1:D:190:GLU:CD	2.41	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:A:202:ARG:HG2	4:A:2140:HOH:O	2.16	0.46
1:A:356:ALA:HB3	2:A:2000:HEM:CMB	2.43	0.46
1:B:233:PHE:C	1:B:234:HIS:CD2	2.92	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:C:150:PRO:HG3	1:C:214:TYR:CD1	2.50	0.46
1:C:275:SER:HA	1:C:315:LEU:O	2.15	0.46
1:C:432:ASN:ND2	1:C:432:ASN:C	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:LEU:O	1:C:472:PHE:C	2.59	0.46
1:A:343:GLU:HB3	1:A:344:PRO:CD	2.46	0.46
1:A:423:HIS:CE1	1:A:425:SER:HB2	2.51	0.46
1:A:430:ARG:NE	1:B:419:GLU:OE1	2.47	0.46
1:B:24:ASP:O	1:D:411:PRO:HA	2.15	0.46
1:B:122:ALA:HB2	1:B:257:PRO:HB3	1.98	0.46
1:B:492:ILE:O	1:B:493:GLN:C	2.58	0.46
1:C:498:LYS:O	1:C:501:GLU:HB3	2.16	0.46
1:A:96:ALA:CB	1:A:342:ILE:CD1	2.94	0.46
1:B:156:ASP:OD2	1:C:39:ASN:HA	2.16	0.46
1:C:32:ASN:N	1:C:32:ASN:HD22	2.14	0.46
1:A:42:THR:O	1:D:431:PHE:HE1	1.99	0.46
1:A:334:ASP:HA	1:A:357:TYR:CG	2.51	0.46
1:C:17:GLN:C	1:C:19:ALA:H	2.24	0.46
1:C:181:VAL:HG12	1:C:182:TRP:N	2.29	0.46
1:C:485:HIS:ND1	1:C:485:HIS:C	2.74	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:D:442:VAL:HG11	1:D:484:VAL:HG21	1.98	0.46
1:A:51:VAL:HG13	1:B:50:LEU:C	2.40	0.46
1:A:53:ASP:CG	1:D:430:ARG:HH22	2.23	0.46
1:A:187:LEU:O	1:A:188:ARG:HD2	2.16	0.46
1:B:11:MET:SD	1:C:180:MET:HG2	2.56	0.46
1:B:95:LYS:HG2	1:B:224:ALA:N	2.31	0.46
1:C:173:THR:O	1:C:175:LEU:HG	2.16	0.46
1:C:194:GLN:OE1	1:C:197:PHE:HB3	2.16	0.46
1:C:245:SER:OG	1:C:248:ASP:HB2	2.15	0.46
1:C:406:ASN:HD21	1:C:410:ALA:CB	2.06	0.46
1:C:427:ASP:OD1	1:D:423:HIS:HB2	2.16	0.46
1:D:264:LEU:O	1:D:265:PHE:C	2.58	0.46
3:D:3074:3TR:N3A	2:D:2003:HEM:NC	2.65	0.46
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:95:LYS:HG2	1:B:223:ASN:C	2.41	0.45
1:B:447:LEU:HD22	1:B:485:HIS:HD2	1.79	0.45
1:C:57:THR:O	1:C:58:ASP:C	2.58	0.45
1:C:74:HIS:CE1	2:C:2002:HEM:C1D	3.05	0.45
1:D:115:VAL:HG23	1:D:127:ASP:OD2	2.16	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:396:ASN:O	1:C:397:GLN:CB	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LEU:HD11	1:D:37:LYS:HD3	1.98	0.45
1:D:155:ARG:CG	1:D:299:THR:HG23	2.46	0.45
1:D:338:MET:HE1	1:D:343:GLU:C	2.41	0.45
1:A:343:GLU:HB3	1:A:344:PRO:HD2	1.97	0.45
1:A:396:ASN:C	1:A:398:GLY:N	2.72	0.45
1:B:39:ASN:O	1:C:430:ARG:HB3	2.15	0.45
1:B:67:ARG:NH2	1:C:168:LYS:NZ	2.63	0.45
1:B:422:THR:HB	1:B:424:PHE:HE1	1.81	0.45
1:C:22:LYS:HD3	1:C:22:LYS:C	2.41	0.45
1:C:197:PHE:CD1	1:C:197:PHE:C	2.94	0.45
1:C:285:PHE:O	1:C:288:ALA:HB3	2.16	0.45
1:C:361:HIS:C	1:C:363:HIS:N	2.71	0.45
1:D:60:MET:O	1:D:63:PHE:HB3	2.15	0.45
1:D:358:PRO:HB2	1:D:362:ARG:NH2	2.31	0.45
1:A:65:ARG:O	1:C:389:GLY:HA2	2.16	0.45
1:A:327:GLU:O	1:A:331:LEU:HD22	2.16	0.45
1:A:452:GLU:O	1:A:453:GLU:C	2.59	0.45
1:B:88:HIS:HB2	1:B:312:VAL:HA	1.98	0.45
1:B:329:GLU:OE1	1:B:329:GLU:HA	2.16	0.45
1:B:332:ALA:HB3	1:B:375:ASN:CG	2.41	0.45
1:B:423:HIS:C	1:B:423:HIS:CD2	2.94	0.45
1:B:491:ARG:O	1:B:495:LEU:HD23	2.16	0.45
1:C:138:GLU:HA	1:C:379:ARG:O	2.17	0.45
1:C:199:PHE:CB	1:C:458:LEU:HD12	2.46	0.45
1:C:212:ASP:OD1	1:C:237:THR:HG22	2.17	0.45
1:D:206:ASP:HB2	1:D:244:LEU:HG	1.97	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:A:263:ASP:OD1	1:A:263:ASP:C	2.59	0.45
1:B:50:LEU:C	1:B:52:GLN:N	2.72	0.45
1:B:144:LEU:HD11	1:B:215:GLY:HA2	1.97	0.45
1:C:223:ASN:HD21	1:C:227:GLU:HB2	1.82	0.45
1:C:485:HIS:HA	1:C:486:PRO:HD2	1.67	0.45
1:D:372:ILE:CG2	1:D:374:VAL:HG12	2.46	0.45
1:A:90:ILE:HD13	1:A:312:VAL:HG22	1.97	0.45
1:A:298:LEU:O	1:A:298:LEU:HD12	2.16	0.45
1:C:71:ARG:HG2	2:C:2002:HEM:O1A	2.17	0.45
1:D:90:ILE:HD12	1:D:90:ILE:C	2.41	0.45
1:D:126:ARG:O	1:D:127:ASP:HB2	2.17	0.45
1:D:202:ARG:H	1:D:202:ARG:HG2	1.57	0.45
1:D:290:ILE:O	1:D:291:PHE:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:VAL:CG2	1:B:49:LEU:HB3	2.47	0.45
1:A:273:TYR:HA	1:A:274:PRO:HD3	1.87	0.45
1:B:84:PHE:CE1	1:B:313:GLY:HA3	2.52	0.45
1:B:97:LYS:HG3	1:B:139:ASP:OD2	2.16	0.45
1:B:393:MET:HE1	1:D:372:ILE:HG13	1.99	0.45
1:C:125:VAL:O	1:C:126:ARG:C	2.60	0.45
1:A:411:PRO:HA	1:C:24:ASP:O	2.17	0.45
1:B:81:PHE:HB2	1:B:319:ARG:NE	2.31	0.45
1:B:482:SER:O	1:B:485:HIS:N	2.50	0.45
1:C:113:SER:O	1:C:130:GLY:N	2.31	0.45
1:C:290:ILE:O	1:C:291:PHE:C	2.58	0.45
1:C:470:GLN:O	1:C:473:ILE:HB	2.16	0.45
1:A:126:ARG:HB2	1:A:126:ARG:HH11	1.80	0.45
1:A:387:ARG:HH12	1:A:397:GLN:NE2	2.15	0.45
1:B:38:LEU:HD13	1:C:188:ARG:HH21	1.79	0.45
1:B:387:ARG:HG2	1:B:387:ARG:NH1	2.31	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: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:151:ILE:HD12	1:B:194:GLN:HB2	1.98	0.45
1:C:220:LYS:HG2	1:C:221:LEU:N	2.31	0.45
1:C:402:ASN:HB2	1:D:165:HIS:ND1	2.31	0.45
1:D:14:TRP:CH2	1:D:18:ARG:HD3	2.52	0.45
1:D:274:PRO:HD2	1:D:317:LEU:O	2.17	0.45
1:D:485:HIS:ND1	1:D:487:GLU:N	2.63	0.45
1:D:492:ILE:O	1:D:493:GLN:C	2.59	0.45
1:B:10:GLN:HE21	1:C:172:GLN:NE2	2.15	0.44
1:B:83:TYR:N	1:B:108:ILE:HG12	2.32	0.44
1:B:132:ALA:HB2	2:B:2001:HEM:HMD2	1.98	0.44
1:B:236:LYS:C	1:B:276:TRP:HD1	2.24	0.44
1:C:334:ASP:HB2	1:C:337:ASN:OD1	2.17	0.44
1:C:467:LYS:HE2	1:C:468:ASP:OD2	2.17	0.44
1:A:248:ASP:HA	1:A:251:ARG:NH1	2.33	0.44
1:B:26:LEU:HD21	1:B:37:LYS:HG2	1.98	0.44
1:B:265:PHE:HB2	4:B:2025:HOH:O	2.17	0.44
1:B:403:TYR:CD1	1:B:403:TYR:N	2.85	0.44
1:B:418:LEU:HD21	1:D:36:ASP:HB3	1.99	0.44
1:C:126:ARG:HB2	1:C:126:ARG:CZ	2.47	0.44
1:D:83:TYR:CZ	1:D:316:VAL:HG21	2.52	0.44
1:D:87:THR:OG1	1:D:313:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:ILE:O	4:A:2026:HOH:O	2.20	0.44
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.48	0.44
1:B:15:LYS:O	1:B:18:ARG:HB2	2.17	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:D:167:GLN:HE21	1:D:167:GLN:HB3	1.55	0.44
1:A:490:SER:O	1:A:491:ARG:C	2.60	0.44
1:B:8:SER:C	1:B:10:GLN:H	2.26	0.44
1:B:98:VAL:HG13	1:B:99:PHE:CE1	2.52	0.44
1:C:217:HIS:NE2	1:C:350:LEU:CA	2.80	0.44
1:C:386:GLN:C	1:C:387:ARG:HG2	2.43	0.44
1:D:27:THR:HB	1:D:31:GLY:C	2.42	0.44
1:D:78:ALA:HB2	1:D:261:LEU:HG	2.00	0.44
1:D:84:PHE:O	1:D:105:ARG:HA	2.17	0.44
1:D:300:LYS:HA	1:D:441:GLN:OE1	2.18	0.44
1:D:439:VAL:CG2	1:D:440:THR:H	2.23	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:278:LEU:HG	1:B:312:VAL:HG13	2.00	0.44
1:B:279:TYR:HA	1:B:310:ILE:O	2.17	0.44
1:B:454:GLN:N	1:B:457:ARG:HH12	2.16	0.44
1:B:480:ASN:O	1:B:481:PHE:C	2.59	0.44
1:C:214:TYR:O	1:C:215:GLY:C	2.58	0.44
1:C:350:LEU:O	1:C:351:GLN:C	2.60	0.44
1:D:322:VAL:HB	1:D:327:GLU:OE2	2.17	0.44
1:A:50:LEU:N	1:A:50:LEU:HD22	2.32	0.44
1:A:73:VAL:CG1	1:A:164:ILE:HG21	2.48	0.44
1:A:320:ASN:HD22	1:A:320:ASN:HA	1.63	0.44
1:A:396:ASN:HB3	1:C:323:ASN:ND2	2.33	0.44
1:B:323:ASN:HB2	1:D:398:GLY:HA2	2.00	0.44
1:B:372:ILE:HG12	1:D:393:MET:HE1	1.99	0.44
1:D:350:LEU:O	1:D:351:GLN:C	2.60	0.44
1:A:353:ARG:HB2	2:A:2000:HEM:HBB2	1.99	0.44
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.83	0.44
1:B:95:LYS:HB3	1:B:224:ALA:N	2.32	0.44
1:B:295:PRO:HD2	1:C:46:ARG:NH1	2.29	0.44
1:B:393:MET:HE3	1:D:372:ILE:HA	1.99	0.44
1:B:439:VAL:O	1:B:442:VAL:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:PHE:CE2	1:B:473:ILE:HG13	2.52	0.44
1:C:369:TYR:C	1:C:371:GLN:N	2.75	0.44
1:D:148:ASN:O	1:D:149:THR:CB	2.66	0.44
1:D:170:ASN:HD22	1:D:172:GLN:N	2.12	0.44
1:D:335:PRO:HD3	1:D:357:TYR:CG	2.53	0.44
1:A:215:GLY:O	1:A:217:HIS:N	2.50	0.44
1:B:103:GLY:O	1:B:105:ARG:HG3	2.18	0.44
1:B:332:ALA:HA	1:B:361:HIS:NE2	2.33	0.44
1:B:447:LEU:O	1:B:447:LEU:HG	2.18	0.44
1:B:496:LEU:O	1:B:500:ASN:N	2.45	0.44
1:D:15:LYS:O	1:D:18:ARG:HB3	2.17	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:D:470:GLN:O	1:D:471:LEU:C	2.61	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
1:B:134:LYS:HB2	1:B:333:PHE:CE1	2.53	0.44
1:B:290:ILE:O	1:B:291:PHE:C	2.61	0.44
1:B:408:PHE:N	1:B:408:PHE:CD2	2.86	0.44
1:C:65:ARG:O	1:C:66:GLU:C	2.61	0.44
1:C:86:VAL:HG11	1:C:101:HIS:O	2.18	0.44
1:C:199:PHE:HB2	1:C:458:LEU:HD12	2.00	0.44
1:D:97:LYS:HA	1:D:100:GLU:CG	2.48	0.44
1:A:26:LEU:HD13	1:C:411:PRO:HB2	1.99	0.43
1:A:430:ARG:HH11	1:A:430:ARG:HG2	1.82	0.43
1:A:431:PHE:CD1	1:D:45:PRO:HB3	2.53	0.43
1:A:455:ARG:HB2	1:A:491:ARG:HH12	1.83	0.43
1:C:142:TRP:CB	1:C:339:PRO:HD3	2.33	0.43
1:A:217:HIS:HE1	1:A:349:MET:HB3	1.82	0.43
1:B:114:THR:C	1:B:115:VAL:HG23	2.43	0.43
1:B:393:MET:O	1:B:394:MET:C	2.61	0.43
1:B:439:VAL:O	1:B:440:THR:C	2.61	0.43
1:B:492:ILE:HG22	1:B:496:LEU:HD11	2.00	0.43
1:C:154:ILE:HG13	1:C:349:MET:HE2	2.00	0.43
1:C:334:ASP:OD1	1:C:361:HIS:CE1	2.71	0.43
1:D:297:ASP:OD2	1:D:300:LYS:HD3	2.18	0.43
1:D:414:GLN:C	1:D:416:SER:N	2.74	0.43
1:D:455:ARG:O	1:D:456:LYS:C	2.60	0.43
1:A:44:GLY:C	1:A:46:ARG:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LEU:HD22	1:C:484:VAL:HG21	2.00	0.43
1:C:287:GLU:HA	1:C:290:ILE:CG1	2.44	0.43
1:C:358:PRO:HA	1:C:369:TYR:OH	2.18	0.43
1:D:86:VAL:HG12	1:D:88:HIS:O	2.19	0.43
1:D:162:SER:CB	4:D:3076:HOH:O	2.67	0.43
1:D:482:SER:O	1:D:485:HIS:N	2.52	0.43
1:B:192:LEU:HD12	1:B:438:ASN:O	2.17	0.43
1:C:12:LYS:O	1:C:16:GLU:HG3	2.17	0.43
1:C:387:ARG:HG2	1:C:387:ARG:NH1	2.33	0.43
1:C:453:GLU:CG	1:C:457:ARG:HH22	2.31	0.43
1:C:465:HIS:ND1	1:C:465:HIS:C	2.76	0.43
1:D:220:LYS:HA	1:D:229:VAL:O	2.18	0.43
1:D:235:TYR:HA	1:D:277:THR:O	2.18	0.43
1:A:39:ASN:CG	1:D:432:ASN:HA	2.42	0.43
1:B:4:ARG:NH1	1:B:9:ASP:OD1	2.51	0.43
1:B:106:THR:HG23	1:B:136:TYR:O	2.18	0.43
4:B:2096:HOH:O	1:D:38:LEU:HD12	1.81	0.43
1:D:296:PHE:CE1	1:D:346:PRO:HD2	2.54	0.43
1:A:210:HIS:HB3	1:A:242:LYS:N	2.34	0.43
4:A:2054:HOH:O	1:C:22:LYS:HE2	2.18	0.43
1:B:443:ARG:C	1:B:445:PHE:H	2.25	0.43
1:C:97:LYS:C	1:C:99:PHE:N	2.76	0.43
1:C:285:PHE:O	1:C:286:SER:C	2.61	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: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
1:C:252:LEU:CD2	4:C:2147:HOH:O	2.51	0.43
1:C:475:LYS:O	1:C:476:LYS:C	2.61	0.43
1:D:189:PRO:O	1:D:190:GLU:C	2.60	0.43
1:D:233:PHE:C	1:D:234:HIS:CD2	2.94	0.43
1:D:287:GLU:O	1:D:290:ILE:N	2.51	0.43
1:D:328:VAL:O	1:D:329:GLU:C	2.61	0.43
1:B:404:TYR:HE2	1:D:38:LEU:CD1	2.32	0.43
1:C:111:ARG:NH2	2:C:2002:HEM:CAD	2.75	0.43
1:C:304:HIS:CD2	1:C:309:LEU:HD13	2.53	0.43
1:C:453:GLU:HG3	1:C:457:ARG:HH22	1.84	0.43
1:A:4:ARG:HD2	1:A:9:ASP:OD1	2.18	0.43
1:A:287:GLU:OE1	1:A:307:TYR:HE1	2.01	0.43
1:B:160:PHE:H	1:B:161:PRO:HD2	1.84	0.43
1:B:381:ARG:HH12	1:D:24:ASP:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:HIS:NE2	1:C:115:VAL:HG22	2.33	0.43
1:C:199:PHE:HB2	1:C:458:LEU:CD1	2.49	0.43
1:C:304:HIS:CE1	4:C:2083:HOH:O	2.72	0.43
1:C:336:SER:HA	1:C:354:LEU:CD2	2.45	0.43
1:A:62:HIS:HE1	1:C:387:ARG:O	2.02	0.43
1:B:46:ARG:HH21	1:C:294:ASN:HA	1.83	0.43
2:B:2001:HEM:HMD2	2:B:2001:HEM:HHD	1.74	0.43
1:C:349:MET:HE3	2:C:2002:HEM:HBB1	2.00	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:A:287:GLU:C	1:A:289:GLU:N	2.76	0.42
1:A:422:THR:HB	1:A:424:PHE:CE1	2.54	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:D:482:SER:O	1:D:485:HIS:C	2.62	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
1:B:481:PHE:O	1:B:482:SER:C	2.62	0.42
1:C:150:PRO:HG3	1:C:214:TYR:CE1	2.54	0.42
1:C:221:LEU:HA	1:C:341:GLY:O	2.19	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:D:28:THR:O	1:D:29:GLY:C	2.61	0.42
1:D:159:LEU:HD23	1:D:184:PHE:CE1	2.54	0.42
1:D:357:TYR:CD1	1:D:357:TYR:N	2.86	0.42
1:D:381:ARG:HH11	1:D:381:ARG:HG2	1.84	0.42
1:A:71:ARG:HH21	1:A:364:ARG:HH22	1.67	0.42
1:A:83:TYR:C	1:A:83:TYR:HD1	2.25	0.42
1:A:112:PHE:HA	1:A:130:GLY:O	2.19	0.42
1:A:353:ARG:CD	2:A:2000:HEM:CMC	2.97	0.42
1:C:71:ARG:HG2	2:C:2002:HEM:CGA	2.49	0.42
1:C:82:GLY:HA3	1:C:317:LEU:HA	2.01	0.42
1:C:280:ILE:HG23	1:C:312:VAL:CG2	2.47	0.42
1:C:284:THR:O	1:C:285:PHE:C	2.62	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:235:TYR:CD1	1:A:235:TYR:N	2.86	0.42
1:A:397:GLN:O	1:A:400:ALA:HB3	2.19	0.42
1:A:421:ARG:HG2	1:B:429:GLN:HG2	2.01	0.42
1:A:492:ILE:CG2	1:A:496:LEU:HD13	2.48	0.42
1:B:179:ASP:OD1	1:C:4:ARG:NH2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:HD13	1:B:484:VAL:CG2	2.49	0.42
1:B:294:ASN:ND2	1:C:46:ARG:HD2	2.34	0.42
1:B:414:GLN:HA	1:B:415:PRO:HD2	1.89	0.42
1:C:71:ARG:NE	2:C:2002:HEM:O2D	2.52	0.42
1:C:84:PHE:HA	1:C:314:LYS:O	2.19	0.42
1:C:446:TYR:CE1	1:C:455:ARG:CG	3.03	0.42
1:D:165:HIS:O	1:D:166:SER:C	2.63	0.42
1:D:277:THR:HB	1:D:279:TYR:CE1	2.54	0.42
1:A:51:VAL:HG12	1:B:51:VAL:CA	2.45	0.42
1:A:74:HIS:HA	1:A:114:THR:O	2.19	0.42
1:A:104:LYS:NZ	1:A:138:GLU:OE2	2.50	0.42
1:A:206:ASP:CA	1:A:244:LEU:HG	2.49	0.42
1:A:408:PHE:HA	1:C:15:LYS:HD2	2.01	0.42
1:A:496:LEU:C	1:A:500:ASN:HD22	2.28	0.42
1:B:17:GLN:C	1:B:19:ALA:N	2.76	0.42
1:B:39:ASN:CG	1:C:432:ASN:HA	2.44	0.42
1:B:74:HIS:N	4:B:2029:HOH:O	2.52	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:C:209:ARG:HD2	1:C:274:PRO:HB3	2.01	0.42
1:C:395:ASP:O	1:C:395:ASP:CG	2.62	0.42
1:D:11:MET:O	1:D:12:LYS:C	2.60	0.42
1:D:60:MET:HE1	1:D:63:PHE:CD2	2.54	0.42
1:D:353:ARG:O	1:D:354:LEU:C	2.62	0.42
1:A:76:LYS:NZ	1:A:123:ASP:OD1	2.53	0.42
1:A:169:ARG:HB3	1:A:174:HIS:C	2.45	0.42
1:A:353:ARG:NE	2:A:2000:HEM:C4C	2.87	0.42
1:A:363:HIS:NE2	1:D:65:ARG:HA	2.34	0.42
1:A:460:GLU:HA	1:A:495:LEU:HD13	2.02	0.42
1:B:10:GLN:NE2	1:C:172:GLN:HE21	2.18	0.42
1:B:11:MET:O	1:D:408:PHE:HD2	2.02	0.42
1:B:71:ARG:HB2	1:B:75:ALA:HA	2.02	0.42
1:C:208:HIS:HA	1:C:211:MET:HE2	2.02	0.42
1:D:284:THR:O	1:D:285:PHE:C	2.63	0.42
1:A:151:ILE:HD13	1:A:193:HIS:ND1	2.35	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:C:145:VAL:CG1	1:C:353:ARG:HH12	2.32	0.42
1:C:147:ASN:CG	2:C:2002:HEM:CBC	2.93	0.42
1:C:155:ARG:NH2	1:C:438:ASN:ND2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:LEU:O	1:C:473:ILE:N	2.53	0.42
1:D:132:ALA:HB1	1:D:333:PHE:CD2	2.55	0.42
1:D:157:ALA:O	1:D:158:LEU:C	2.61	0.42
1:D:157:ALA:O	1:D:160:PHE:N	2.34	0.42
1:D:206:ASP:CB	1:D:244:LEU:HG	2.50	0.42
1:D:330:GLN:O	1:D:331:LEU:C	2.61	0.42
1:D:437:ASP:OD2	1:D:440:THR:HB	2.18	0.42
1:A:145:VAL:HG13	2:A:2000:HEM:CMD	2.07	0.42
1:A:351:GLN:NE2	1:C:52:GLN:NE2	2.67	0.42
1:C:62:HIS:O	1:C:62:HIS:ND1	2.49	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:D:229:VAL:HA	1:D:285:PHE:CE1	2.53	0.42
1:D:361:HIS:HB3	1:D:369:TYR:CE2	2.55	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:A:152:PHE:CB	1:A:298:LEU:HG	2.49	0.42
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.93	0.42
1:A:278:LEU:O	1:A:312:VAL:HB	2.20	0.42
1:B:3:ASN:HD21	1:B:12:LYS:NZ	2.17	0.42
1:B:393:MET:CG	1:D:393:MET:HG3	2.50	0.42
1:B:414:GLN:HB2	1:D:25:VAL:HG13	2.02	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:D:93:TYR:O	1:D:223:ASN:HB3	2.20	0.42
1:A:40:SER:HB3	1:A:49:LEU:CD2	2.50	0.42
1:A:110:VAL:HG12	1:A:133:VAL:HG22	2.02	0.42
1:A:268:ILE:O	1:A:269:ALA:C	2.63	0.42
1:A:279:TYR:CD1	1:A:279:TYR:N	2.88	0.42
1:B:146:GLY:HA2	2:B:2001:HEM:CAC	2.44	0.42
1:A:262:ARG:NH1	1:D:175:LEU:HD13	2.35	0.41
1:B:67:ARG:HH21	1:C:168:LYS:NZ	2.17	0.41
1:B:125:VAL:CG2	1:B:126:ARG:N	2.83	0.41
1:B:131:PHE:O	1:B:146:GLY:O	2.38	0.41
1:B:233:PHE:CD1	1:B:233:PHE:N	2.88	0.41
1:B:365:LEU:HD12	1:B:369:TYR:HB2	2.01	0.41
1:C:65:ARG:O	1:C:67:ARG:N	2.53	0.41
1:C:163:PHE:HB2	1:C:184:PHE:CZ	2.54	0.41
1:C:294:ASN:HD21	1:C:296:PHE:HB2	1.85	0.41
1:C:407:SER:C	1:C:408:PHE:CD1	2.98	0.41
1:C:487:GLU:HG2	1:C:491:ARG:CG	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ILE:HG12	1:D:193:HIS:HD2	1.85	0.41
1:A:273:TYR:CD1	1:A:318:ASN:HA	2.55	0.41
1:A:353:ARG:CG	2:A:2000:HEM:C4B	3.03	0.41
1:C:32:ASN:N	1:C:32:ASN:ND2	2.68	0.41
1:C:110:VAL:HG12	1:C:111:ARG:N	2.35	0.41
1:C:466:LEU:C	1:C:468:ASP:H	2.27	0.41
1:D:162:SER:HB2	4:D:3076:HOH:O	2.20	0.41
1:A:54:VAL:HG11	1:C:336:SER:HB3	2.02	0.41
1:A:250:ALA:O	1:A:253:ALA:HB3	2.19	0.41
1:B:78:ALA:HB1	1:B:264:LEU:HD23	2.03	0.41
1:B:146:GLY:CA	2:B:2001:HEM:HAC	2.50	0.41
1:B:175:LEU:HD12	1:C:7:ALA:HB1	2.03	0.41
1:D:91:THR:HG21	1:D:100:GLU:O	2.20	0.41
1:D:270:THR:C	1:D:272:ASN:H	2.27	0.41
1:D:383:ALA:HB1	1:D:411:PRO:HG3	2.02	0.41
1:A:112:PHE:CE1	1:A:131:PHE:CE1	3.08	0.41
1:A:155:ARG:HE	1:A:155:ARG:HB3	1.68	0.41
1:A:399:GLY:O	1:A:400:ALA:O	2.38	0.41
1:A:479:LYS:HG3	1:A:480:ASN:N	2.35	0.41
1:A:496:LEU:O	1:A:499:TYR:N	2.53	0.41
1:B:43:VAL:O	1:B:43:VAL:HG13	2.20	0.41
1:B:443:ARG:O	1:B:447:LEU:HD23	2.20	0.41
1:B:471:LEU:C	1:B:473:ILE:N	2.77	0.41
1:C:82:GLY:HA3	1:C:317:LEU:HD23	2.02	0.41
1:C:287:GLU:CA	1:C:290:ILE:HG12	2.45	0.41
1:D:146:GLY:O	1:D:147:ASN:OD1	2.38	0.41
1:D:248:ASP:HA	1:D:251:ARG:NH1	2.36	0.41
1:D:451:ASN:OD1	1:D:451:ASN:C	2.63	0.41
1:A:82:GLY:C	1:A:108:ILE:HG12	2.45	0.41
1:A:188:ARG:HB3	1:A:190:GLU:OE2	2.20	0.41
1:A:360:THR:CG2	1:A:361:HIS:N	2.84	0.41
1:B:70:GLU:O	1:B:71:ARG:C	2.64	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:C:63:PHE:C	1:C:65:ARG:N	2.79	0.41
1:D:34:VAL:O	1:D:34:VAL:HG23	2.21	0.41
1:D:256:ASP:OD1	1:D:256:ASP:C	2.63	0.41
1:D:498:LYS:O	1:D:501:GLU:N	2.46	0.41
1:A:4:ARG:HD3	1:A:8:SER:HB2	2.03	0.41
1:A:24:ASP:CG	1:C:381:ARG:HH22	2.28	0.41
1:A:177:ASP:O	1:A:180:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:ND2	1:D:46:ARG:HG2	2.34	0.41
1:A:297:ASP:OD1	1:A:299:THR:OG1	2.34	0.41
1:A:387:ARG:NH1	1:A:397:GLN:NE2	2.69	0.41
1:A:420:HIS:CG	1:A:421:ARG:N	2.89	0.41
1:B:67:ARG:C	1:C:69:PRO:HB3	2.46	0.41
1:B:195:VAL:HG13	1:B:199:PHE:CE1	2.56	0.41
1:B:219:PHE:HD1	1:B:338:MET:HE1	1.85	0.41
1:C:180:MET:O	1:C:181:VAL:C	2.63	0.41
1:C:359:ASP:HA	1:C:362:ARG:HD2	2.01	0.41
1:D:285:PHE:CE1	4:D:3134:HOH:O	2.74	0.41
1:A:5:ASP:OD2	1:A:7:ALA:HB3	2.21	0.41
1:A:79:GLY:HA3	1:A:328:VAL:HG13	2.03	0.41
1:A:88:HIS:CE1	4:A:2109:HOH:O	2.74	0.41
1:A:154:ILE:HA	1:A:190:GLU:HG3	2.02	0.41
1:B:4:ARG:HH11	1:B:4:ARG:CB	2.32	0.41
1:B:95:LYS:HG3	1:B:95:LYS:H	1.74	0.41
1:B:145:VAL:HG12	1:B:353:ARG:NH2	2.33	0.41
1:B:287:GLU:O	1:B:290:ILE:HG22	2.21	0.41
1:B:381:ARG:NH1	1:D:24:ASP:HB3	2.36	0.41
1:B:475:LYS:C	1:B:477:ALA:N	2.78	0.41
1:C:232:LYS:O	1:C:280:ILE:HA	2.21	0.41
1:C:421:ARG:HD2	1:D:429:GLN:CD	2.46	0.41
1:D:97:LYS:CA	1:D:100:GLU:HG3	2.50	0.41
1:A:212:ASP:HB2	1:A:214:TYR:CE2	2.55	0.41
1:A:423:HIS:HE1	1:A:425:SER:HB2	1.85	0.41
1:A:430:ARG:HA	1:D:40:SER:O	2.21	0.41
1:B:99:PHE:O	1:B:100:GLU:C	2.63	0.41
1:B:334:ASP:OD1	1:B:334:ASP:N	2.54	0.41
1:B:454:GLN:CA	1:B:457:ARG:NH1	2.79	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
1:D:201:ASP:O	1:D:243:ASN:CG	2.63	0.41
1:D:335:PRO:CD	1:D:357:TYR:CG	3.03	0.41
1:A:209:ARG:HG2	1:A:274:PRO:CB	2.45	0.41
1:A:223:ASN:CG	1:A:227:GLU:HB2	2.45	0.41
1:A:353:ARG:NE	2:A:2000:HEM:C2C	2.89	0.41
1:A:371:GLN:O	1:A:372:ILE:C	2.63	0.41
1:B:43:VAL:HG13	1:B:48:PRO:HD2	2.01	0.41
1:B:141:ASN:CG	1:B:377:PRO:HB3	2.46	0.41
1:B:302:TRP:O	1:B:303:PRO:C	2.64	0.41
1:B:393:MET:HB3	1:B:394:MET:H	1.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:THR:C	1:B:442:VAL:N	2.76	0.41
1:C:5:ASP:HB2	1:C:6:PRO:HD2	2.02	0.41
1:C:63:PHE:C	1:C:65:ARG:H	2.29	0.41
1:C:115:VAL:HG12	1:C:116:ALA:N	2.35	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:173:THR:O	1:D:174:HIS:HB3	2.20	0.41
1:D:215:GLY:O	1:D:217:HIS:N	2.54	0.41
1:D:460:GLU:HG2	1:D:495:LEU:HD11	2.03	0.41
1:A:300:LYS:CB	1:A:441:GLN:HE22	2.19	0.41
1:A:368:ASN:C	4:A:2004:HOH:O	2.63	0.41
1:B:78:ALA:O	1:B:111:ARG:HG3	2.21	0.41
1:B:177:ASP:OD1	1:B:179:ASP:HB2	2.20	0.41
1:C:147:ASN:HB2	2:C:2002:HEM:CBC	2.48	0.41
1:C:160:PHE:CE2	2:C:2002:HEM:C3B	3.08	0.41
1:D:201:ASP:O	1:D:243:ASN:HB3	2.21	0.41
1:D:353:ARG:NH2	2:D:2003:HEM:CHD	2.84	0.41
1:D:368:ASN:HD22	1:D:368:ASN:HA	1.69	0.41
1:A:70:GLU:OE2	1:A:118:GLU:HA	2.21	0.40
1:A:283:MET:HE3	1:A:302:TRP:CD2	2.56	0.40
1:A:334:ASP:OD1	1:A:361:HIS:ND1	2.54	0.40
1:B:11:MET:HB3	1:D:408:PHE:CD2	2.56	0.40
1:B:245:SER:O	1:B:246:VAL:C	2.65	0.40
1:C:73:VAL:CG2	2:C:2002:HEM:NA	2.84	0.40
1:C:74:HIS:CG	2:C:2002:HEM:C4D	3.10	0.40
1:C:153:PHE:HD1	1:C:185:TRP:HE1	1.68	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:107:PRO:HG2	1:D:136:TYR:HB2	2.02	0.40
1:D:374:VAL:CG1	1:D:375:ASN:N	2.84	0.40
1:A:251:ARG:O	1:A:255:GLU:HG3	2.21	0.40
1:B:223:ASN:C	1:B:225:ASP:N	2.79	0.40
1:B:291:PHE:C	1:B:293:PHE:H	2.29	0.40
1:C:194:GLN:OE1	1:C:194:GLN:O	2.39	0.40
1:D:218:THR:HG23	1:D:302:TRP:CZ2	2.56	0.40
1:A:147:ASN:C	1:A:149:THR:H	2.28	0.40
1:A:217:HIS:CD2	1:A:353:ARG:HH11	2.35	0.40
1:A:297:ASP:OD1	1:A:297:ASP:C	2.64	0.40
1:A:493:GLN:O	1:A:494:ALA:C	2.64	0.40
1:B:45:PRO:O	1:B:46:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:MET:O	1:B:394:MET:O	2.39	0.40
1:B:494:ALA:CB	4:B:2086:HOH:O	2.59	0.40
1:C:450:LEU:HG	1:C:454:GLN:HB3	2.03	0.40
1:D:98:VAL:HG22	1:D:98:VAL:O	2.21	0.40
1:A:82:GLY:HA3	1:A:316:VAL:O	2.22	0.40
1:A:400:ALA:HA	1:A:401:PRO:HD3	1.99	0.40
1:A:463:ALA:O	1:A:467:LYS:HB3	2.21	0.40
1:B:148:ASN:HA	1:B:212:ASP:O	2.22	0.40
1:B:290:ILE:CG2	1:B:291:PHE:N	2.84	0.40
1:C:291:PHE:CG	1:C:292:PRO:HD2	2.57	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:41:LEU:N	1:D:430:ARG:NH1	2.69	0.40
1:B:146:GLY:HA3	1:B:214:TYR:O	2.21	0.40
1:B:248:ASP:C	1:B:250:ALA:N	2.78	0.40
1:B:252:LEU:N	1:B:252:LEU:CD1	2.84	0.40
1:C:153:PHE:H	1:C:153:PHE:HD2	1.69	0.40
1:C:262:ARG:O	1:C:263:ASP:C	2.65	0.40
1:D:18:ARG:NH2	1:D:24:ASP:OD1	2.55	0.40
1:D:95:LYS:HB3	1:D:223:ASN:C	2.47	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%)	3 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	497/506 (98%)	408 (82%)	65 (13%)	24 (5%)	2	9
1	C	497/506 (98%)	398 (80%)	82 (16%)	17 (3%)	3	15
1	D	497/506 (98%)	402 (81%)	74 (15%)	21 (4%)	2	11
All	All	1988/2024 (98%)	1608 (81%)	301 (15%)	79 (4%)	2	12

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	395 (92%)	36 (8%)	10	35
1	B	431/437 (99%)	387 (90%)	44 (10%)	7	27
1	C	431/437 (99%)	397 (92%)	34 (8%)	11	37
1	D	431/437 (99%)	402 (93%)	29 (7%)	15	44
All	All	1724/1748 (99%)	1581 (92%)	143 (8%)	10	35

All (143) 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	37	LYS
1	A	41	LEU
1	A	43	VAL
1	A	49	LEU
1	A	54	VAL
1	A	65	ARG
1	A	71	ARG
1	A	101	HIS
1	A	113	SER
1	A	118	GLU
1	A	135	PHE
1	A	139	ASP

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Mol	Chain	Res	Type
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	242	LYS
1	A	263	ASP
1	A	279	TYR
1	A	301	VAL
1	A	360	THR
1	A	394	MET
1	A	402	ASN
1	A	413	HIS
1	A	418	LEU
1	A	421	ARG
1	B	4	ARG
1	B	8	SER
1	B	37	LYS
1	B	41	LEU
1	B	43	VAL
1	B	49	LEU
1	B	50	LEU
1	B	92	ARG
1	B	95	LYS
1	B	104	LYS
1	B	114	THR
1	B	126	ARG
1	B	127	ASP
1	B	144	LEU
1	B	149	THR
1	B	151	ILE
1	B	179	ASP
1	B	204	ILE
1	B	232	LYS
1	B	235	TYR
1	B	237	THR
1	B	239	GLN
1	B	246	VAL

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Mol	Chain	Res	Type
1	B	290	ILE
1	B	309	LEU
1	B	312	VAL
1	B	320	ASN
1	B	330	GLN
1	B	334	ASP
1	B	336	SER
1	B	337	ASN
1	B	364	ARG
1	B	374	VAL
1	B	395	ASP
1	B	402	ASN
1	B	412	GLU
1	B	429	GLN
1	B	438	ASN
1	B	441	GLN
1	B	454	GLN
1	B	457	ARG
1	B	466	LEU
1	B	473	ILE
1	B	498	LYS
1	C	4	ARG
1	C	22	LYS
1	C	40	SER
1	C	46	ARG
1	C	63	PHE
1	C	68	ILE
1	C	76	LYS
1	C	92	ARG
1	C	104	LYS
1	C	126	ARG
1	C	137	THR
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	244	LEU
1	C	293	PHE

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Mol	Chain	Res	Type
1	C	301	VAL
1	C	309	LEU
1	C	347	ASP
1	C	414	GLN
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	501	GLU
1	D	3	ASN
1	D	22	LYS
1	D	26	LEU
1	D	43	VAL
1	D	111	ARG
1	D	138	GLU
1	D	139	ASP
1	D	148	ASN
1	D	159	LEU
1	D	167	GLN
1	D	170	ASN
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	329	GLU
1	D	336	SER
1	D	371	GLN
1	D	378	TYR
1	D	397	GLN
1	D	412	GLU
1	D	414	GLN
1	D	453	GLU
1	D	457	ARG
1	D	479	LYS
1	D	498	LYS
1	D	501	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	52	GLN
1	A	148	ASN
1	A	167	GLN
1	A	239	GLN
1	A	254	HIS
1	A	320	ASN
1	A	337	ASN
1	A	351	GLN
1	A	363	HIS
1	A	396	ASN
1	A	402	ASN
1	A	413	HIS
1	A	429	GLN
1	A	435	ASN
1	A	438	ASN
1	A	454	GLN
1	A	470	GLN
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	101	HIS
1	B	147	ASN
1	B	167	GLN
1	B	234	HIS
1	B	254	HIS
1	B	272	ASN
1	B	281	GLN
1	B	323	ASN
1	B	337	ASN
1	B	363	HIS
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

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Mol	Chain	Res	Type
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	101	HIS
1	C	172	GLN
1	C	239	GLN
1	C	337	ASN
1	C	363	HIS
1	C	413	HIS
1	C	414	GLN
1	C	420	HIS
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	32	ASN
1	D	52	GLN
1	D	148	ASN
1	D	167	GLN
1	D	170	ASN
1	D	210	HIS
1	D	254	HIS
1	D	294	ASN
1	D	337	ASN
1	D	368	ASN
1	D	371	GLN
1	D	413	HIS
1	D	429	GLN
1	D	480	ASN
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 oligosaccharides 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$
2	HEM	D	2003	1,3	50,50,50	3.41	8 (16%)	67,82,82	2.88	12 (17%)
2	HEM	B	2001	-	50,50,50	2.47	7 (14%)	67,82,82	2.62	7 (10%)
2	HEM	C	2002	-	50,50,50	1.18	4 (8%)	67,82,82	1.14	4 (5%)
2	HEM	A	2000	1	50,50,50	2.71	7 (14%)	67,82,82	1.32	5 (7%)
3	3TR	D	3074	1,2	6,6,6	2.21	3 (50%)	6,7,7	1.22	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	2003	1,3	-	9/14/54/54	-
2	HEM	B	2001	-	-	6/14/54/54	-
2	HEM	C	2002	-	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	2000	1	-	6/14/54/54	-
3	3TR	D	3074	1,2	-	-	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2003	HEM	CHD-C4C	14.71	1.67	1.38
2	D	2003	HEM	CHC-C4B	-12.61	1.10	1.39
2	A	2000	HEM	CBC-CAC	11.93	1.87	1.30
2	B	2001	HEM	FE-NC	11.11	2.31	1.95
2	A	2000	HEM	FE-NB	10.34	2.26	1.94
2	D	2003	HEM	CHD-C1D	-9.39	1.17	1.39
2	B	2001	HEM	CHB-C4A	8.27	1.58	1.39
2	A	2000	HEM	FE-NA	7.02	2.18	1.95
2	B	2001	HEM	CHD-C1D	6.17	1.53	1.39
2	D	2003	HEM	FE-NC	-5.67	1.76	1.95
2	B	2001	HEM	CBC-CAC	4.85	1.53	1.30
2	C	2002	HEM	CBC-CAC	4.55	1.52	1.30
2	D	2003	HEM	CBC-CAC	4.24	1.50	1.30
2	D	2003	HEM	CHA-C1A	-3.82	1.30	1.39
3	D	3074	3TR	C3-N4	-3.69	1.32	1.37
2	A	2000	HEM	FE-ND	3.36	2.05	1.94
2	B	2001	HEM	CAB-C3B	-3.26	1.38	1.47
2	D	2003	HEM	CAB-C3B	-3.24	1.38	1.47
2	C	2002	HEM	CAB-C3B	-3.21	1.38	1.47
2	A	2000	HEM	CAB-C3B	-3.15	1.39	1.47
2	A	2000	HEM	CAC-C3C	-3.01	1.39	1.47
2	D	2003	HEM	CBB-CAB	2.57	1.42	1.30
2	B	2001	HEM	CBB-CAB	2.56	1.42	1.30
2	C	2002	HEM	CBB-CAB	2.55	1.42	1.30
3	D	3074	3TR	C3-N2	-2.54	1.29	1.33
2	A	2000	HEM	CBB-CAB	2.54	1.42	1.30
2	B	2001	HEM	CHC-C1C	2.47	1.43	1.38
2	C	2002	HEM	FE-NB	2.20	2.01	1.94
3	D	3074	3TR	C5-N1	2.20	1.38	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2003	HEM	CBA-CAA-C2A	18.16	162.74	112.53
2	B	2001	HEM	CHD-C1D-C2D	-12.76	104.89	125.03
2	B	2001	HEM	CHD-C1D-ND	11.77	137.09	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	HEM	C4C-CHD-C1D	-8.25	108.49	126.02
2	D	2003	HEM	CHC-C4B-NB	-6.53	117.40	124.42
2	A	2000	HEM	CMC-C2C-C1C	-6.03	114.10	124.73
2	D	2003	HEM	C4C-CHD-C1D	-5.09	115.20	126.02
2	D	2003	HEM	CHA-C1A-NA	4.96	132.86	123.86
2	D	2003	HEM	CHD-C4C-NC	-4.63	119.41	124.45
2	D	2003	HEM	CHA-C1A-C2A	-4.63	115.16	125.30
2	A	2000	HEM	CBC-CAC-C3C	-4.53	104.92	127.53
2	B	2001	HEM	C1C-CHC-C4B	-4.47	116.52	126.02
2	C	2002	HEM	CAC-C3C-C4C	-4.45	114.20	124.82
2	D	2003	HEM	C1C-CHC-C4B	3.37	133.19	126.02
2	D	2003	HEM	C1A-CHA-C4D	-3.36	118.35	126.25
2	C	2002	HEM	CAC-C3C-C2C	3.33	139.27	128.43
2	B	2001	HEM	CHC-C1C-NC	-3.31	120.85	124.45
2	D	2003	HEM	CHC-C4B-C3B	2.81	130.67	125.07
2	A	2000	HEM	CMC-C2C-C3C	2.63	134.79	128.43
2	B	2001	HEM	CHB-C4A-NA	-2.53	119.27	123.86
2	C	2002	HEM	CMB-C2B-C1B	2.46	128.88	125.03
2	D	2003	HEM	CMB-C2B-C1B	2.45	128.86	125.03
3	D	3074	3TR	N3A-C3-N4	-2.44	117.62	121.53
2	B	2001	HEM	CMB-C2B-C1B	2.42	128.82	125.03
2	A	2000	HEM	CMB-C2B-C1B	2.42	128.82	125.03
2	D	2003	HEM	CHD-C1D-ND	-2.34	121.91	124.42
2	C	2002	HEM	CHC-C1C-C2C	-2.05	121.22	125.49
2	D	2003	HEM	CHC-C1C-C2C	-2.03	121.27	125.49
2	A	2000	HEM	CHC-C1C-C2C	-2.02	121.28	125.49

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	HEM	C1A-C2A-CAA-CBA
2	A	2000	HEM	C2B-C3B-CAB-CBB
2	A	2000	HEM	C4B-C3B-CAB-CBB
2	C	2002	HEM	C2B-C3B-CAB-CBB
2	C	2002	HEM	C4B-C3B-CAB-CBB
2	C	2002	HEM	C2C-C3C-CAC-CBC
2	C	2002	HEM	C4C-C3C-CAC-CBC
2	D	2003	HEM	C3A-C2A-CAA-CBA
2	D	2003	HEM	C2B-C3B-CAB-CBB
2	D	2003	HEM	C4B-C3B-CAB-CBB
2	D	2003	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	D	2003	HEM	C1A-C2A-CAA-CBA
2	A	2000	HEM	C3A-C2A-CAA-CBA
2	B	2001	HEM	C1A-C2A-CAA-CBA
2	B	2001	HEM	C2B-C3B-CAB-CBB
2	D	2003	HEM	CAD-CBD-CGD-O2D
2	D	2003	HEM	CAD-CBD-CGD-O1D
2	A	2000	HEM	CAD-CBD-CGD-O1D
2	D	2003	HEM	CAA-CBA-CGA-O2A
2	A	2000	HEM	CAD-CBD-CGD-O2D
2	C	2002	HEM	CAD-CBD-CGD-O2D
2	B	2001	HEM	CAA-CBA-CGA-O2A
2	D	2003	HEM	CAA-CBA-CGA-O1A
2	B	2001	HEM	CAD-CBD-CGD-O2D
2	B	2001	HEM	CAA-CBA-CGA-O1A
2	C	2002	HEM	CAD-CBD-CGD-O1D
2	C	2002	HEM	CAA-CBA-CGA-O2A
2	B	2001	HEM	CAD-CBD-CGD-O1D
2	C	2002	HEM	CAA-CBA-CGA-O1A

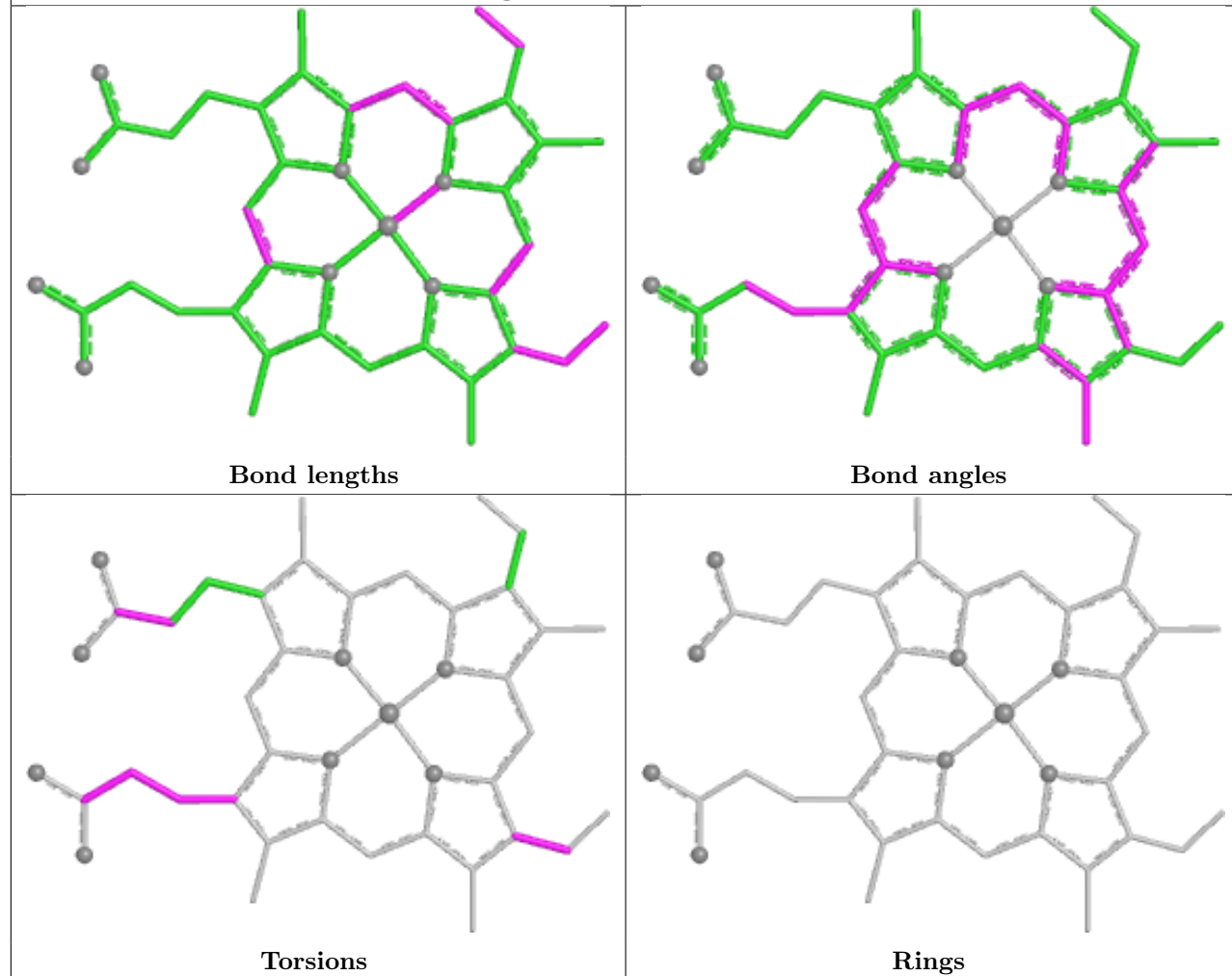
There are no ring outliers.

5 monomers are involved in 195 short contacts:

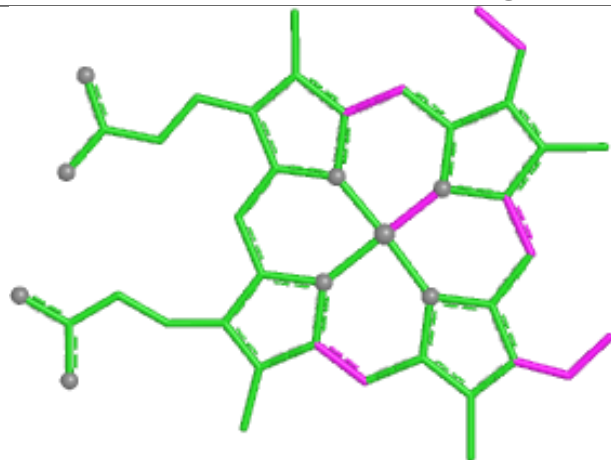
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2003	HEM	25	0
2	B	2001	HEM	39	0
2	C	2002	HEM	51	0
2	A	2000	HEM	80	0
3	D	3074	3TR	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

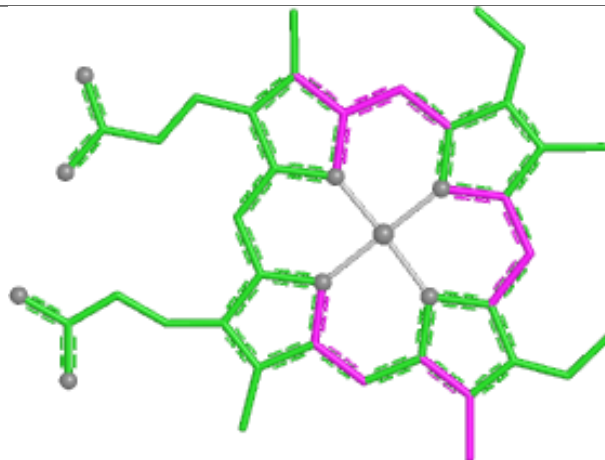
Ligand HEM D 2003



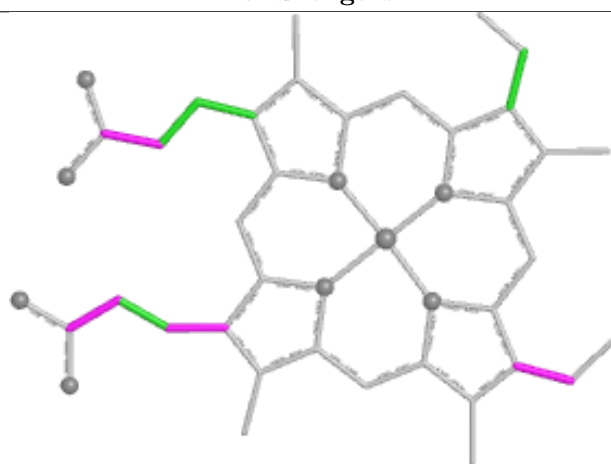
Ligand HEM B 2001



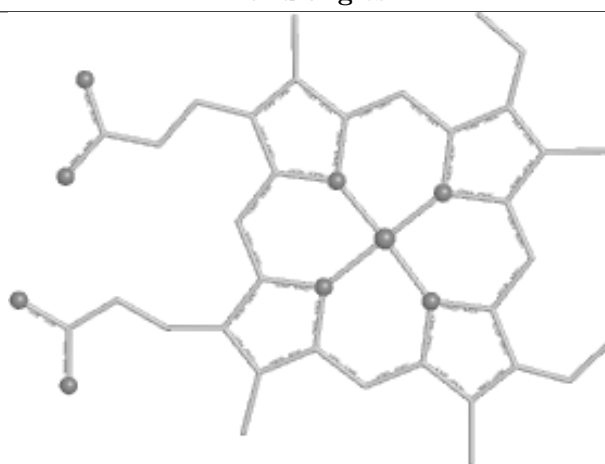
Bond lengths



Bond angles

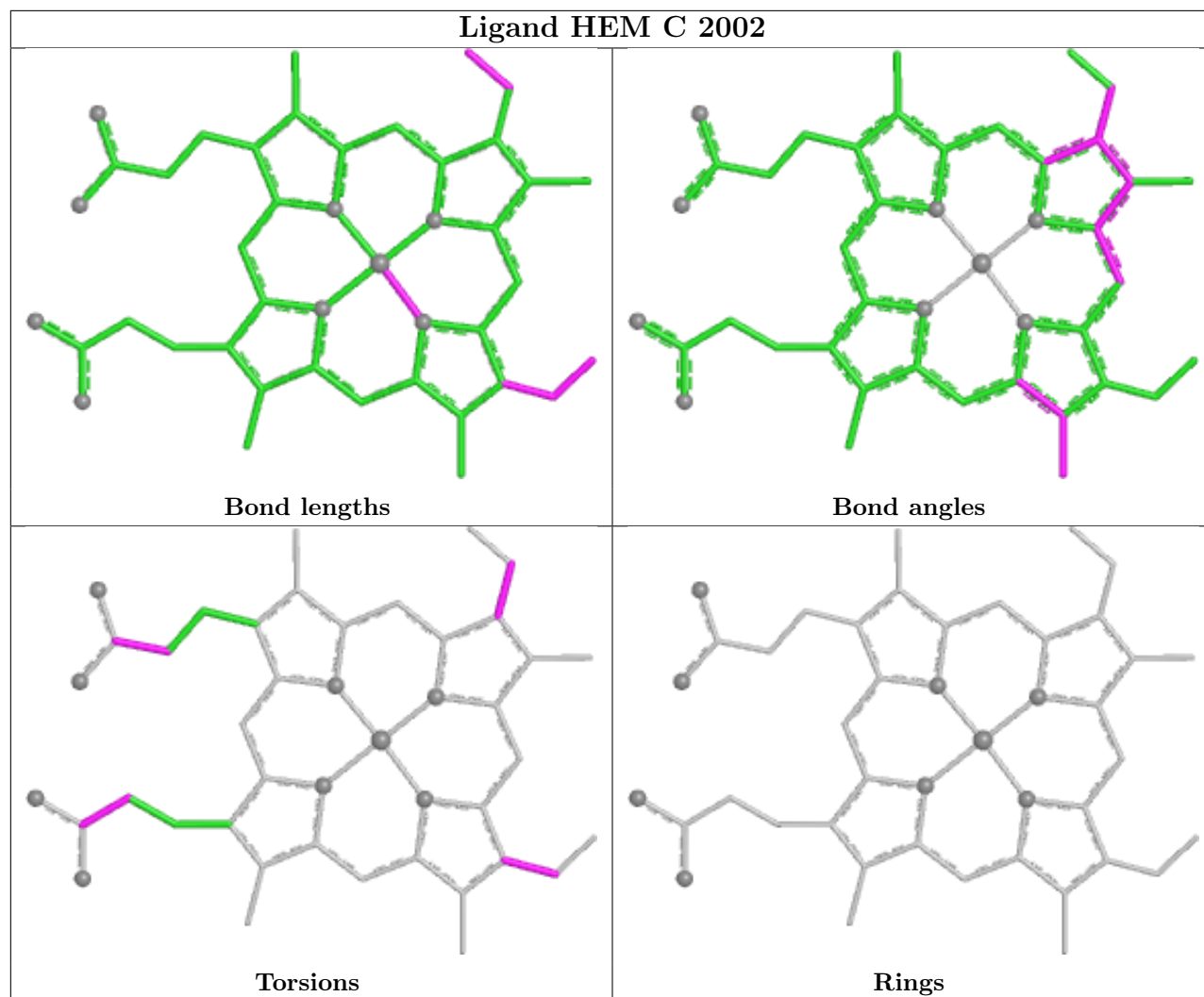


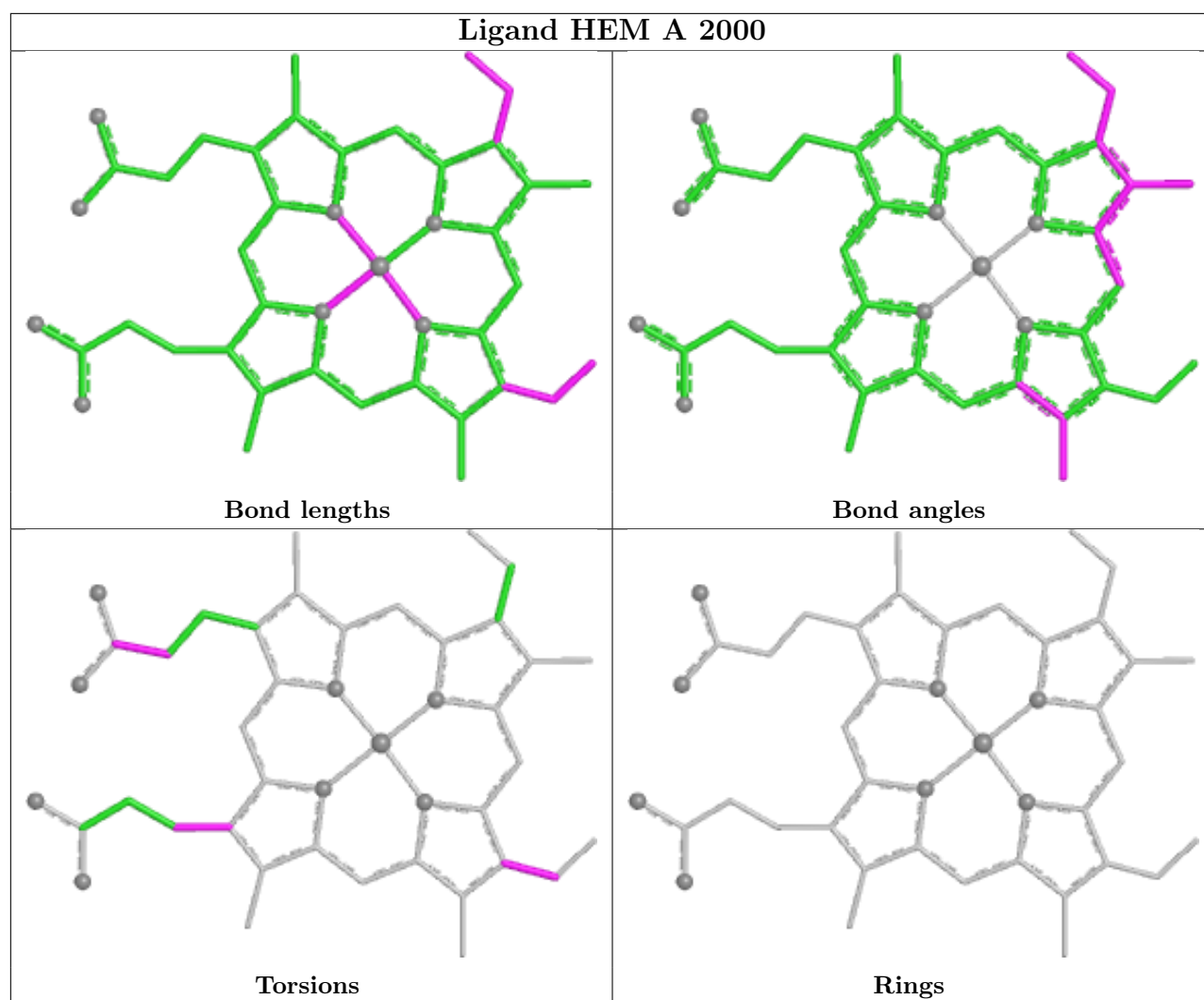
Torsions



Rings

Ligand HEM C 2002





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	499/506 (98%)	0.28	8 (1%) 70 51	10, 40, 76, 97	0
1	B	499/506 (98%)	0.31	8 (1%) 70 51	16, 44, 78, 102	0
1	C	499/506 (98%)	0.26	8 (1%) 70 51	16, 41, 81, 100	1 (0%)
1	D	499/506 (98%)	0.32	10 (2%) 65 45	15, 45, 84, 101	0
All	All	1996/2024 (98%)	0.29	34 (1%) 69 50	10, 43, 80, 102	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	ARG	5.7
1	D	371	GLN	3.8
1	C	424	PHE	3.2
1	C	175	LEU	3.0
1	C	501	GLU	2.9
1	A	418	LEU	2.7
1	D	422	THR	2.6
1	B	3	ASN	2.5
1	B	165	HIS	2.5
1	C	168	LYS	2.4
1	A	159	LEU	2.4
1	A	407	SER	2.4
1	D	425	SER	2.4
1	C	426	GLY	2.3
1	B	175	LEU	2.3
1	D	459	CYS	2.3
1	A	20	ALA	2.3
1	D	20	ALA	2.3
1	C	427	ASP	2.3
1	D	159	LEU	2.3
1	A	147	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	328	VAL	2.2
1	A	448	LYS	2.2
1	B	501	GLU	2.2
1	B	122	ALA	2.2
1	B	228	ALA	2.2
1	B	412	GLU	2.2
1	C	186	SER	2.1
1	D	345	SER	2.1
1	C	425	SER	2.1
1	D	424	PHE	2.1
1	D	405	PRO	2.0
1	B	203	GLY	2.0
1	A	333	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

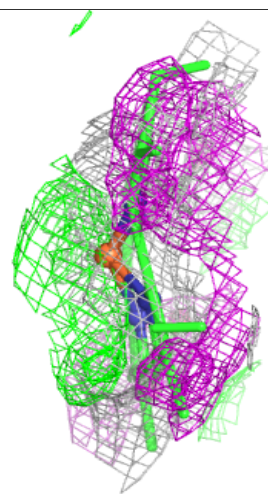
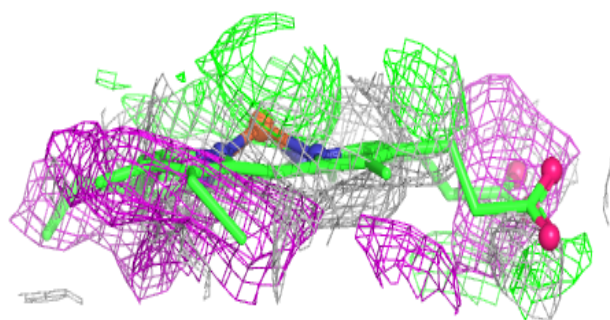
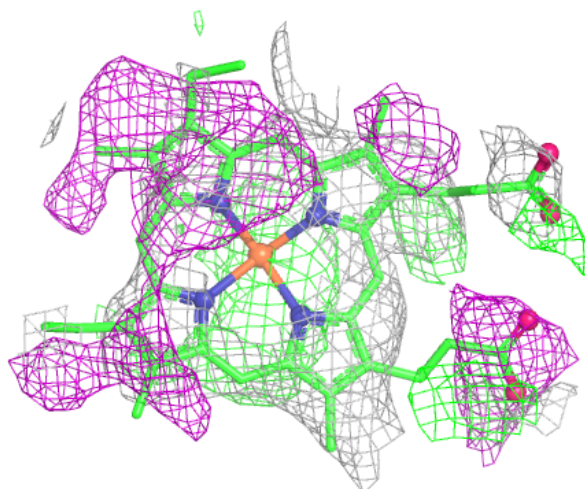
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	2000	43/43	0.77	0.30	80,94,101,101	0
2	HEM	C	2002	43/43	0.81	0.23	41,58,72,92	0
2	HEM	B	2001	43/43	0.88	0.20	21,56,83,101	0
3	3TR	D	3074	6/6	0.89	0.26	89,96,99,101	0
2	HEM	D	2003	43/43	0.95	0.11	20,38,56,59	0

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

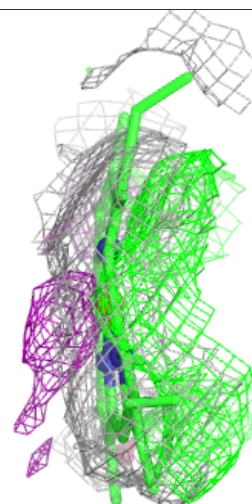
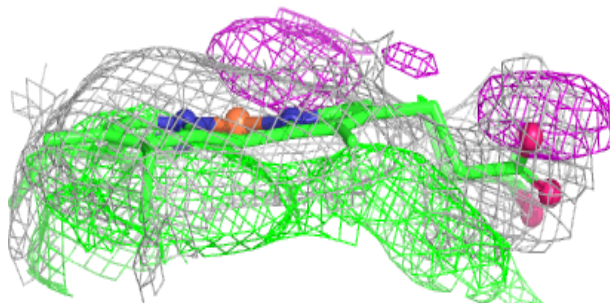
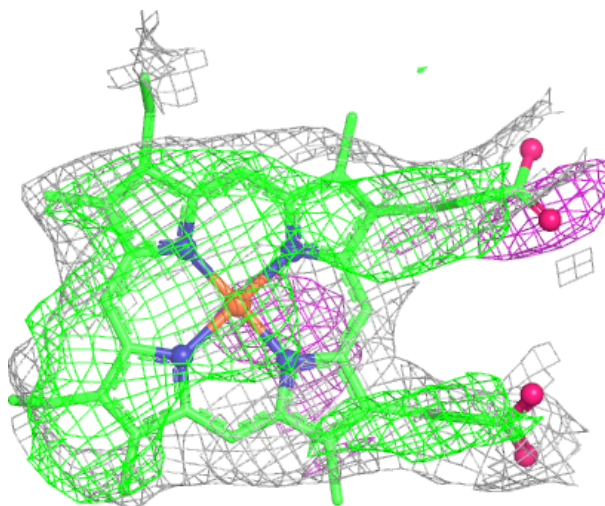
Electron density around HEM A 2000:

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



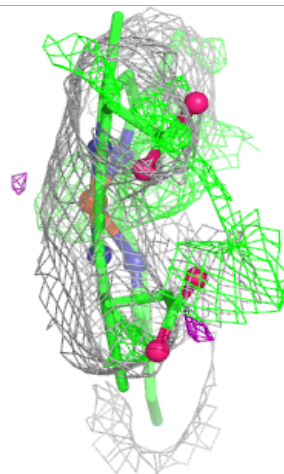
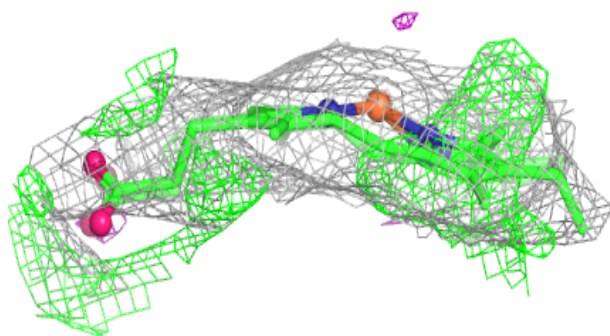
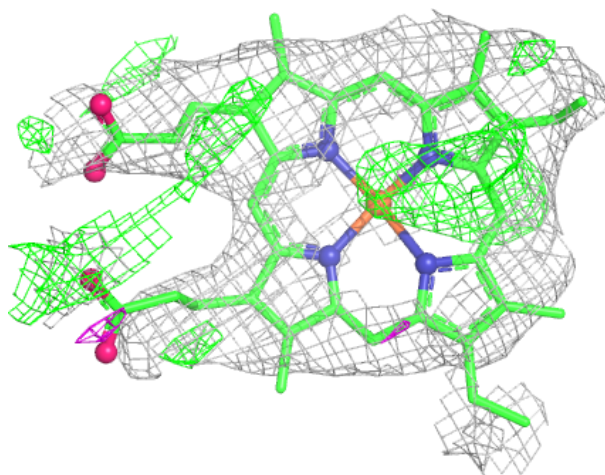
Electron density around HEM C 2002:

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



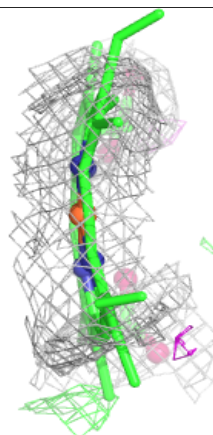
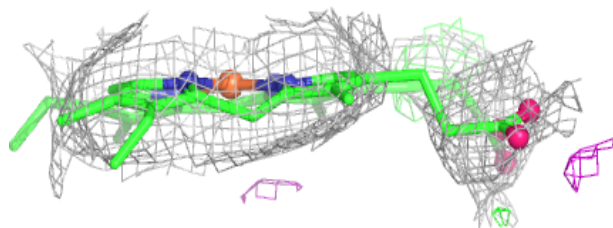
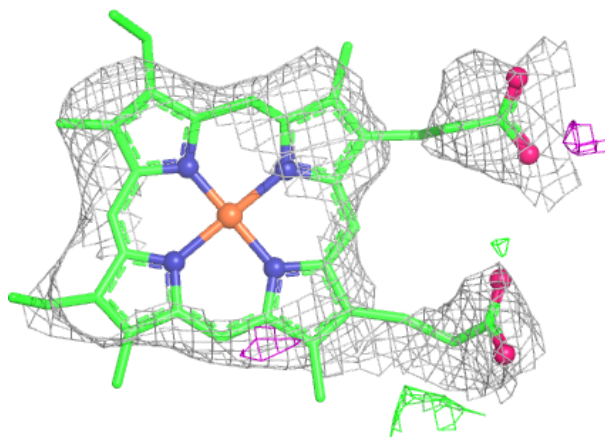
Electron density around HEM B 2001:

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



Electron density around HEM D 2003:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.