Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 11:58 PM EST

PDB ID	:	1TGU
Title	:	The crystal structure of bovine liver catalase without NADPH
Authors	:	Sugadev, R.; Balasundaresan, D.; Ponnuswamy, M.N.; Kumaran, D.; Swaminathan, S.; Sekar, K.
Deposited on	:	2004-05-31
Resolution	:	2.80 Å(reported)

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

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

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

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

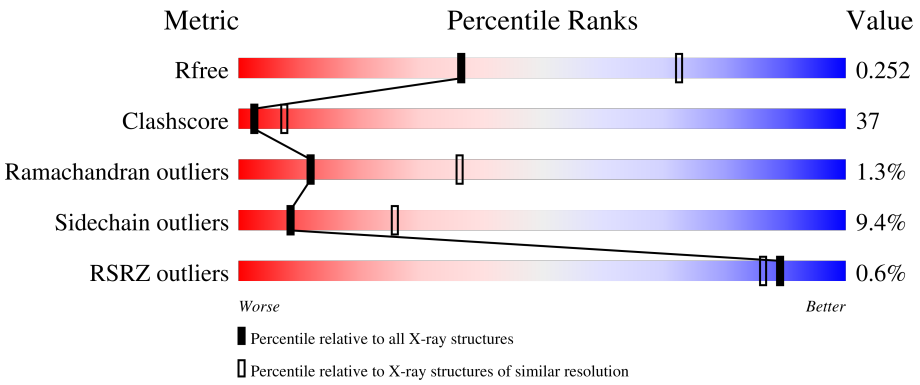
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	506	% 54% 38% 6% ••
1	B	506	% 38% 51% 8% ••
1	C	506	46% 43% 8% ••
1	D	506	% 41% 53% • •

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	D	2003	-	-	X	-

2 Entry composition (i)

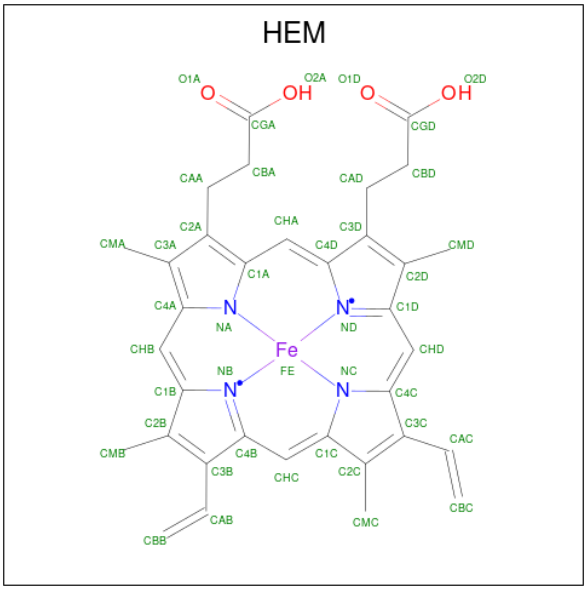
There are 3 unique types of molecules in this entry. The entry contains 17173 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catalase.

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

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 3 is water.

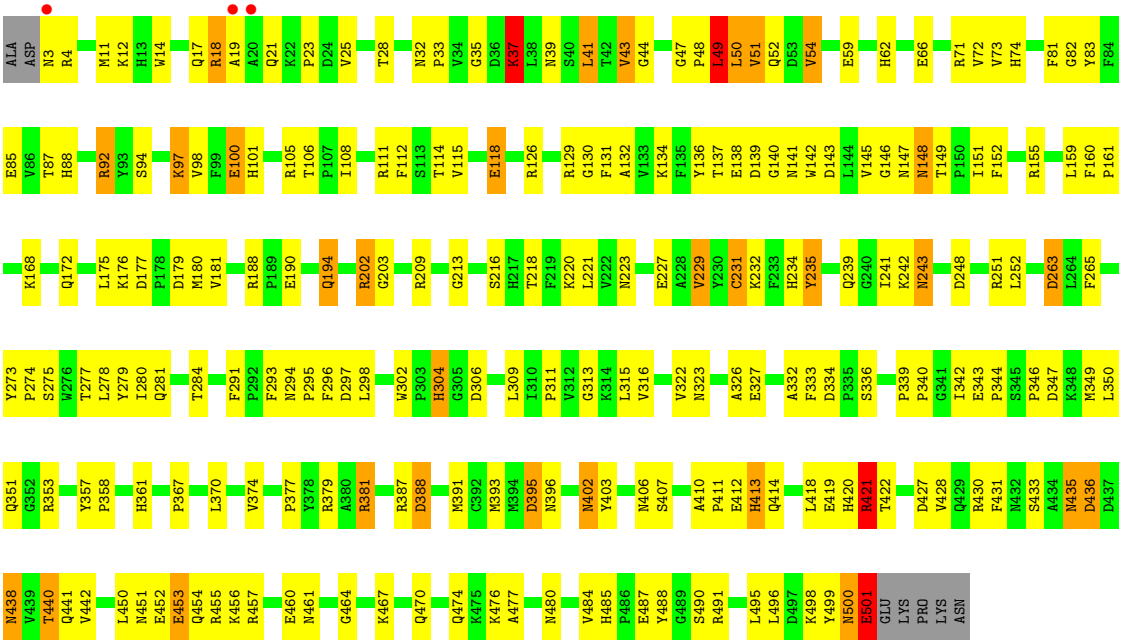
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	229	229	229	0	0
			Total	O		
3	B	236	236	236	0	0
			Total	O		
3	C	236	236	236	0	0
			Total	O		
3	D	232	232	232	0	0

3 Residue-property plots (i)

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

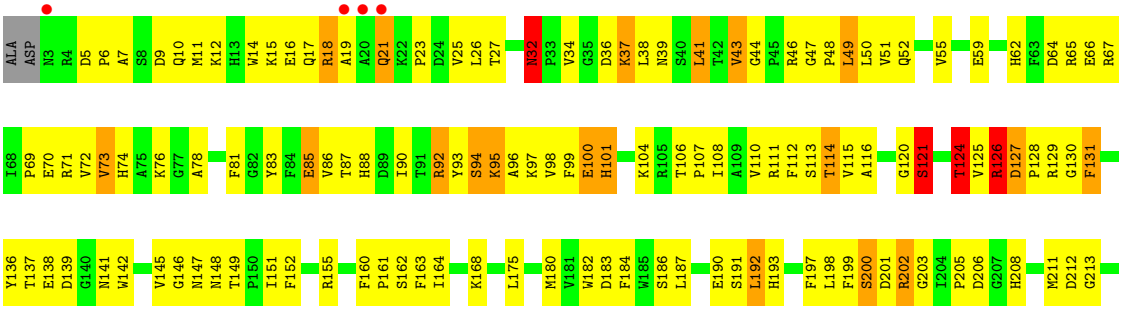
- Molecule 1: Catalase

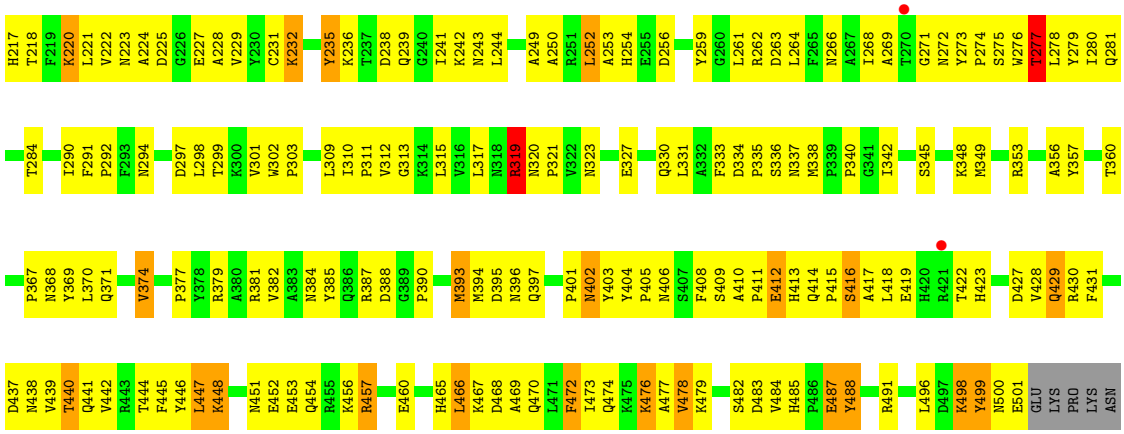
Chain A:



- Molecule 1: Catalase

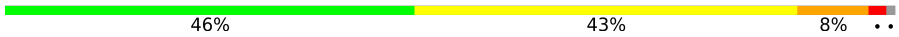
Chain B:

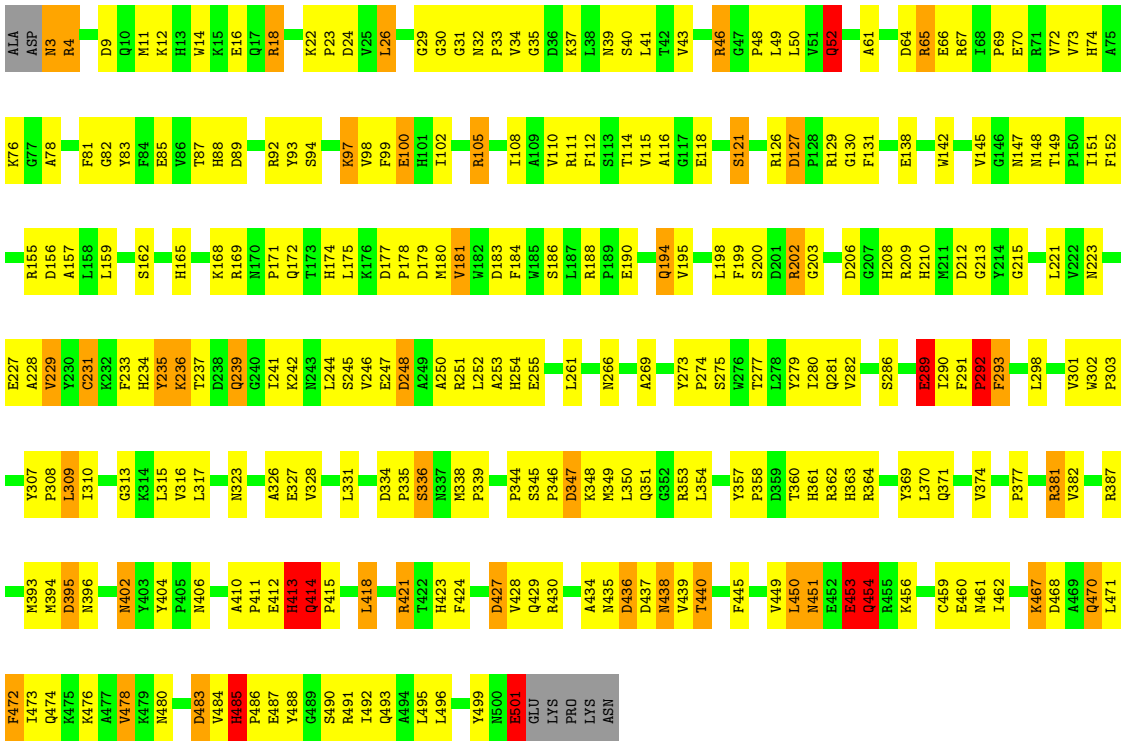




- Molecule 1: Catalase

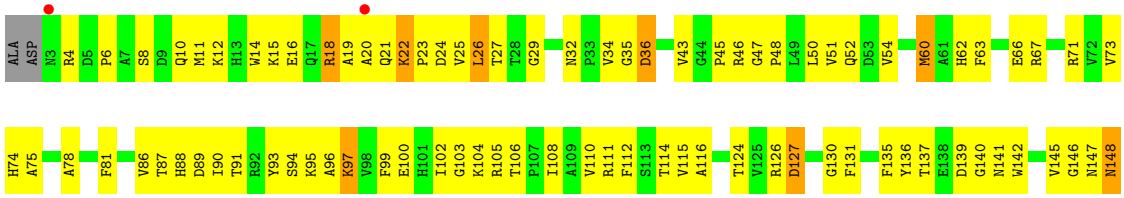
Chain C:

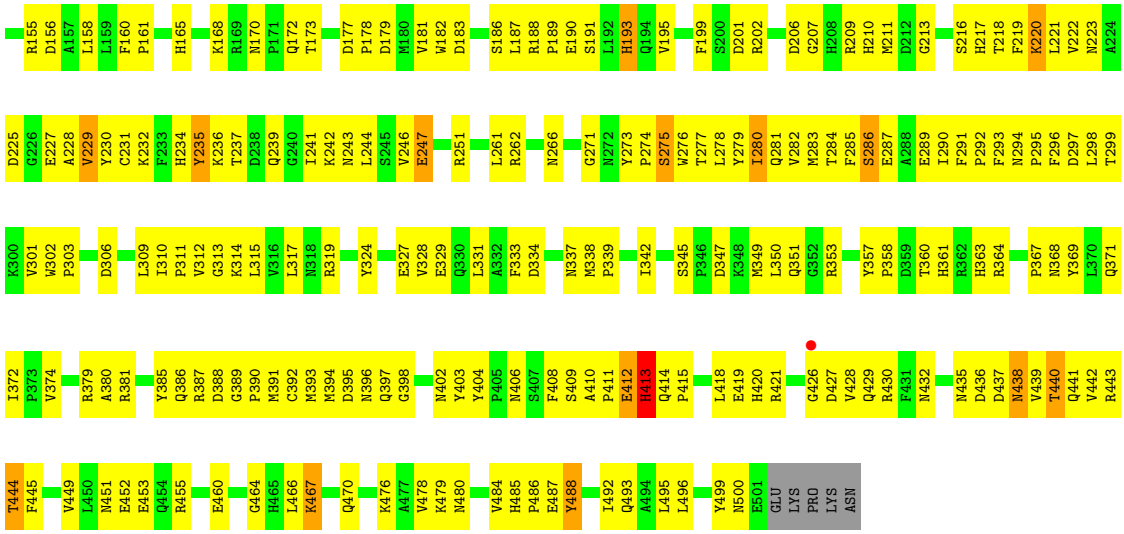




- Molecule 1: Catalase

Chain D:




R155 D156 A157 L158 L159 F160 P161 H165 K168 R169 N170 P171 Q172 T173 D177 P178 D179 M180 V181 W182 D183 S186 L187 R188 P189 E190 S191 L192 H193 Q194 V195 F199 S200 D201 R202 D206 G207 H208 R209 H210 M211 D212 G213 S216 H217 T218 F219 K220 L221 V222 N223 A224
D225 G226 E227 A228 V229 Y230 C231 K232 F233 H234 Y235 K236 T237 D238 Q239 G240 I241 K242 N243 L244 S245 V246 E247 R251 L261 R262 N266 G271 N272 Y273 P274 S275 W276 T277 L278 Y279 I280 Q281 V282 M283 T284 F285 S286 E287 A288 E289 I290 F291 P292 F293 N294 P295 F296 D297 L298 T299
K300 V301 W302 P303 D306 L309 I310 P311 V312 G313 K314 L315 V316 L317 N318 R319 Y324 E327 V328 E329 Q330 L331 A332 F333 D334 N337 M338 P339 I342 S345 P346 D347 K348 M349 L350 Q351 G352 R353 Y357 P358 D359 T360 H361 R362 H363 R364 P367 N368 Y369 L370 Q371
I372 P373 V374 R379 A380 R381 Y385 Q386 R387 D388 G389 P390 M391 C392 M393 M394 D395 N396 Q397 G398 N402 Y403 Y404 P405 N406 S407 F408 S409 A410 P411 E412 H413 Q414 P415 L418 E419 H420 R421 G426 D427 V428 Q429 R430 F431 N432 N435 D436 D437 N438 V439 T440 Q441 V442 R443
T444 F445 V449 L450 N451 E452 E453 Q454 R455 E460 G464 H465 L466 K467 Q470 K476 A477 V478 K479 N480 V484 H485 P486 E487 Y488 I492 Q493 A494 L495 L496 Y499 N500 E501 GLU LYS PRO LYS ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.53Å 139.67Å 225.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 48.76 – 2.79	Depositor EDS
% Data completeness (in resolution range)	89.9 (40.00-2.80) 89.3 (48.76-2.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.249 0.201 , 0.252	Depositor DCC
R_{free} test set	1822 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17173	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.56	5/4137 (0.1%)	1.38	52/5619 (0.9%)
1	B	0.97	4/4137 (0.1%)	1.47	28/5619 (0.5%)
1	C	0.66	8/4137 (0.2%)	1.49	33/5619 (0.6%)
1	D	0.60	1/4137 (0.0%)	0.81	6/5619 (0.1%)
All	All	0.72	18/16548 (0.1%)	1.32	119/22476 (0.5%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CD-NE	49.59	2.30	1.46
1	D	413	HIS	CA-CB	-20.44	1.08	1.53
1	C	202	ARG	NE-CZ	16.98	1.55	1.33
1	B	319	ARG	NE-CZ	16.07	1.53	1.33
1	C	414	GLN	CA-CB	-9.86	1.32	1.53
1	C	292	PRO	C-N	9.66	1.56	1.34
1	C	413	HIS	CB-CG	8.79	1.65	1.50
1	C	292	PRO	CA-C	-8.64	1.35	1.52
1	A	421	ARG	CD-NE	-8.52	1.31	1.46
1	B	374	VAL	CA-CB	7.16	1.69	1.54
1	A	229	VAL	CA-CB	-6.97	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CA-CB	-6.46	1.39	1.53
1	A	176	LYS	CD-CE	6.43	1.67	1.51
1	C	485	HIS	ND1-CE1	-6.43	1.18	1.34
1	C	454	GLN	CB-CG	-5.67	1.37	1.52
1	A	304	HIS	CA-CB	-5.66	1.41	1.53
1	A	280	ILE	CA-CB	5.61	1.67	1.54
1	C	485	HIS	CD2-NE2	-5.19	1.26	1.38

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	202	ARG	NE-CZ-NH2	-52.90	93.85	120.30
1	B	319	ARG	NE-CZ-NH1	-46.73	96.93	120.30
1	C	202	ARG	NE-CZ-NH1	43.98	142.29	120.30
1	B	319	ARG	CG-CD-NE	-41.22	25.24	111.80
1	B	395	ASP	N-CA-CB	-31.45	53.99	110.60
1	B	126	ARG	CD-NE-CZ	29.40	164.76	123.60
1	D	413	HIS	CA-CB-CG	25.62	157.15	113.60
1	C	483	ASP	N-CA-CB	23.86	153.55	110.60
1	B	319	ARG	CB-CG-CD	-23.60	50.24	111.60
1	A	54	VAL	CA-CB-CG2	-22.29	77.47	110.90
1	A	229	VAL	CA-CB-CG2	21.75	143.52	110.90
1	A	421	ARG	CG-CD-NE	21.37	156.68	111.80
1	C	453	GLU	CB-CG-CD	20.09	168.45	114.20
1	A	49	LEU	CB-CG-CD2	19.99	144.98	111.00
1	A	418	LEU	N-CA-CB	19.67	149.74	110.40
1	A	395	ASP	CA-CB-CG	19.24	155.73	113.40
1	A	421	ARG	CB-CG-CD	19.19	161.50	111.60
1	C	292	PRO	O-C-N	-19.01	92.29	122.70
1	A	395	ASP	N-CA-CB	18.71	144.28	110.60
1	C	501	GLU	CB-CA-C	18.66	147.72	110.40
1	B	487	GLU	CA-CB-CG	18.42	153.93	113.40
1	A	456	LYS	CG-CD-CE	18.24	166.62	111.90
1	B	487	GLU	CB-CG-CD	17.61	161.76	114.20
1	B	319	ARG	CA-CB-CG	17.61	152.15	113.40
1	D	453	GLU	CB-CG-CD	17.43	161.27	114.20
1	C	453	GLU	N-CA-CB	17.32	141.78	110.60
1	C	414	GLN	CA-CB-CG	16.88	150.54	113.40
1	A	456	LYS	CB-CG-CD	16.65	154.89	111.60
1	C	453	GLU	CA-CB-CG	16.14	148.91	113.40
1	C	292	PRO	N-CA-C	16.01	153.73	112.10
1	C	52	GLN	CB-CG-CD	15.59	152.12	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	374	VAL	CB-CA-C	-15.48	81.98	111.40
1	A	402	ASN	CA-CB-CG	15.46	147.42	113.40
1	A	476	LYS	CD-CE-NZ	15.41	147.15	111.70
1	D	97	LYS	CG-CD-CE	15.31	157.84	111.90
1	B	429	GLN	CA-CB-CG	15.24	146.93	113.40
1	A	118	GLU	N-CA-CB	-15.18	83.28	110.60
1	B	32	ASN	CB-CG-OD1	14.98	151.56	121.60
1	C	454	GLN	CB-CG-CD	14.93	150.43	111.60
1	C	454	GLN	N-CA-CB	-14.89	83.79	110.60
1	B	32	ASN	CB-CG-ND2	-14.44	82.04	116.70
1	A	501	GLU	CB-CA-C	14.41	139.22	110.40
1	B	412	GLU	CB-CG-CD	14.16	152.43	114.20
1	A	381	ARG	CG-CD-NE	13.98	141.15	111.80
1	A	435	ASN	CB-CA-C	13.84	138.09	110.40
1	C	289	GLU	CG-CD-OE2	-13.74	90.81	118.30
1	A	97	LYS	CG-CD-CE	13.60	152.71	111.90
1	A	421	ARG	CD-NE-CZ	13.54	142.56	123.60
1	B	478	VAL	CA-CB-CG1	-13.27	91.00	110.90
1	C	292	PRO	CA-C-O	13.26	152.02	120.20
1	D	453	GLU	CA-CB-CG	13.19	142.42	113.40
1	B	412	GLU	N-CA-CB	13.05	134.09	110.60
1	C	292	PRO	CB-CA-C	-12.52	80.69	112.00
1	B	319	ARG	NE-CZ-NH2	12.49	126.55	120.30
1	A	500	ASN	N-CA-CB	-12.41	88.27	110.60
1	A	435	ASN	CA-CB-CG	12.37	140.61	113.40
1	C	414	GLN	CB-CA-C	11.91	134.22	110.40
1	A	284	THR	CA-CB-CG2	-11.84	95.82	112.40
1	C	395	ASP	CA-CB-CG	-11.82	87.40	113.40
1	A	304	HIS	N-CA-CB	-11.74	89.47	110.60
1	C	289	GLU	CB-CA-C	11.50	133.39	110.40
1	B	374	VAL	N-CA-CB	11.23	136.20	111.50
1	D	394	MET	CB-CG-SD	10.98	145.34	112.40
1	A	421	ARG	CA-CB-CG	10.85	137.27	113.40
1	A	202	ARG	CD-NE-CZ	10.79	138.70	123.60
1	A	476	LYS	CG-CD-CE	10.78	144.25	111.90
1	C	289	GLU	CA-CB-CG	10.77	137.09	113.40
1	C	483	ASP	CB-CA-C	-10.76	88.88	110.40
1	B	412	GLU	CA-CB-CG	10.76	137.07	113.40
1	B	395	ASP	CA-CB-CG	10.70	136.93	113.40
1	A	418	LEU	CB-CA-C	-10.57	90.12	110.20
1	A	453	GLU	CB-CG-CD	10.46	142.45	114.20
1	A	456	LYS	CA-CB-CG	10.23	135.90	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	176	LYS	CD-CE-NZ	-10.21	88.22	111.70
1	A	490	SER	CA-CB-OG	10.13	138.55	111.20
1	C	231	CYS	CA-CB-SG	-10.12	95.79	114.00
1	A	280	ILE	CB-CA-C	-10.05	91.51	111.60
1	B	478	VAL	CA-CB-CG2	10.00	125.91	110.90
1	A	243	ASN	CB-CA-C	-9.89	90.62	110.40
1	A	304	HIS	CB-CA-C	9.76	129.91	110.40
1	C	501	GLU	CB-CG-CD	9.57	140.05	114.20
1	A	37	LYS	CG-CD-CE	9.54	140.53	111.90
1	A	284	THR	CA-CB-OG1	9.52	129.00	109.00
1	B	478	VAL	CB-CA-C	9.48	129.41	111.40
1	B	277	THR	CB-CA-C	9.41	137.00	111.60
1	B	416	SER	N-CA-CB	-9.40	96.39	110.50
1	C	501	GLU	N-CA-CB	-9.35	93.76	110.60
1	A	304	HIS	CA-CB-CG	9.07	129.02	113.60
1	B	478	VAL	N-CA-CB	-8.68	92.40	111.50
1	C	454	GLN	CB-CA-C	-8.52	93.36	110.40
1	A	501	GLU	N-CA-CB	-8.23	95.78	110.60
1	C	414	GLN	N-CA-CB	-8.03	96.15	110.60
1	B	319	ARG	CB-CA-C	-7.79	94.82	110.40
1	A	500	ASN	CA-CB-CG	7.77	130.50	113.40
1	A	453	GLU	CA-CB-CG	7.61	130.15	113.40
1	C	309	LEU	CB-CG-CD1	7.60	123.92	111.00
1	B	374	VAL	CA-CB-CG1	-7.59	99.52	110.90
1	C	309	LEU	CB-CG-CD2	-7.53	98.19	111.00
1	A	284	THR	CB-CA-C	-7.48	91.41	111.60
1	A	49	LEU	CB-CG-CD1	-7.47	98.30	111.00
1	C	478	VAL	CB-CA-C	7.33	125.32	111.40
1	B	374	VAL	CA-CB-CG2	-7.25	100.02	110.90
1	A	435	ASN	N-CA-CB	-7.16	97.71	110.60
1	A	280	ILE	CA-CB-CG1	7.15	124.58	111.00
1	A	280	ILE	CA-CB-CG2	-7.13	96.64	110.90
1	A	395	ASP	CB-CA-C	-6.79	96.81	110.40
1	C	292	PRO	C-N-CA	6.71	138.47	121.70
1	C	202	ARG	CD-NE-CZ	6.25	132.35	123.60
1	A	176	LYS	CG-CD-CE	6.19	130.46	111.90
1	A	342	ILE	CB-CA-C	-5.95	99.70	111.60
1	B	319	ARG	N-CA-CB	5.94	121.29	110.60
1	C	413	HIS	CB-CG-ND1	-5.62	109.14	123.20
1	A	229	VAL	CB-CA-C	-5.61	100.74	111.40
1	A	37	LYS	CD-CE-NZ	-5.54	98.96	111.70
1	A	54	VAL	CB-CA-C	5.47	121.80	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	ILE	N-CA-CB	5.47	123.39	110.80
1	A	500	ASN	CB-CA-C	5.46	121.33	110.40
1	D	20	ALA	N-CA-CB	-5.41	102.52	110.10
1	C	236	LYS	CG-CD-CE	5.21	127.52	111.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	395	ASP	CA
1	C	453	GLU	CA
1	C	501	GLU	CA

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4017	0	3840	292	0
1	B	4017	0	3840	394	0
1	C	4017	0	3839	323	2
1	D	4017	0	3839	315	0
2	A	43	0	30	36	0
2	B	43	0	30	28	0
2	C	43	0	30	18	0
2	D	43	0	30	29	0
3	A	229	0	0	22	0
3	B	236	0	0	28	2
3	C	236	0	0	21	2
3	D	232	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17173	0	15478	1161	3

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 37.

All (1161) 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:421:ARG:HD2	1:B:429:GLN:CG	1.19	1.58
1:B:353:ARG:HG3	2:B:2001:HEM:CBB	1.34	1.57
1:D:147:ASN:ND2	2:D:2003:HEM:CAC	1.74	1.50
1:B:353:ARG:CG	2:B:2001:HEM:HBB2	1.02	1.49
1:D:147:ASN:ND2	2:D:2003:HEM:HAC	1.27	1.44
1:A:421:ARG:CD	1:B:429:GLN:HG2	1.47	1.41
1:A:421:ARG:CG	1:B:429:GLN:HG3	1.59	1.31
1:B:147:ASN:ND2	2:B:2001:HEM:HAC	1.45	1.31
1:A:421:ARG:HD3	3:A:2187:HOH:O	1.28	1.29
1:A:395:ASP:OD1	1:C:327:GLU:OE2	1.54	1.26
1:B:353:ARG:CG	2:B:2001:HEM:CBB	1.95	1.25
1:A:421:ARG:CD	1:B:429:GLN:CG	2.09	1.22
1:A:160:PHE:CD1	2:A:2000:HEM:HAB	1.76	1.20
1:A:421:ARG:NH2	3:A:2157:HOH:O	1.72	1.19
1:D:147:ASN:CG	2:D:2003:HEM:HAC	1.61	1.19
1:A:421:ARG:CZ	3:A:2157:HOH:O	1.92	1.14
1:A:501:GLU:OE1	1:A:501:GLU:CA	1.94	1.13
1:B:485:HIS:HE1	1:B:487:GLU:HG3	1.05	1.12
1:A:37:LYS:HE2	1:A:59:GLU:OE2	1.45	1.12
1:B:485:HIS:CE1	1:B:487:GLU:HG3	1.85	1.11
1:D:147:ASN:ND2	2:D:2003:HEM:C3C	2.18	1.11
1:A:74:HIS:HD2	2:A:2000:HEM:C4D	1.70	1.10
1:A:421:ARG:HG3	1:B:429:GLN:HG3	1.18	1.09
1:C:421:ARG:NH1	3:C:2184:HOH:O	1.89	1.06
1:B:360:THR:HG21	3:B:2010:HOH:O	1.54	1.05
1:A:74:HIS:CD2	2:A:2000:HEM:C4D	2.46	1.04
1:A:421:ARG:NE	3:A:2157:HOH:O	1.88	1.03
1:B:147:ASN:ND2	2:B:2001:HEM:CAC	2.20	1.03
1:B:19:ALA:HB3	1:B:21:GLN:HE21	1.23	1.02
1:D:223:ASN:HD21	1:D:227:GLU:HB3	1.19	1.01
1:B:353:ARG:HG2	2:B:2001:HEM:HBB2	1.36	1.01
1:B:147:ASN:CG	2:B:2001:HEM:HAC	1.83	0.99
1:B:254:HIS:HB3	1:C:254:HIS:HB3	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:THR:CG2	3:B:2010:HOH:O	2.09	0.97
1:C:151:ILE:HG13	1:C:194:GLN:HG2	1.46	0.96
1:A:72:VAL:CG1	2:A:2000:HEM:HMA1	1.95	0.96
1:A:72:VAL:HG12	2:A:2000:HEM:HMA1	1.47	0.96
1:D:111:ARG:HD3	2:D:2003:HEM:O1D	1.64	0.96
1:D:189:PRO:HG3	1:D:480:ASN:ND2	1.79	0.96
1:A:501:GLU:OE1	1:A:501:GLU:HA	1.62	0.96
1:B:353:ARG:CD	2:B:2001:HEM:HBB2	1.96	0.96
1:A:421:ARG:HG2	1:B:429:GLN:HG3	1.48	0.95
1:C:190:GLU:HA	1:C:438:ASN:HB3	1.44	0.95
1:D:126:ARG:HE	1:D:199:PHE:HA	1.31	0.95
1:C:402:ASN:H	1:C:402:ASN:HD22	0.97	0.95
1:D:406:ASN:HD21	1:D:410:ALA:HB3	1.30	0.95
1:C:22:LYS:HE2	3:C:2077:HOH:O	1.67	0.95
1:B:71:ARG:HG3	1:B:71:ARG:HH11	1.31	0.94
1:A:421:ARG:HG3	1:B:429:GLN:CG	1.96	0.94
1:B:261:LEU:HD23	1:C:175:LEU:HD23	1.49	0.93
1:D:111:ARG:CD	2:D:2003:HEM:O1D	2.17	0.93
1:B:353:ARG:HG2	2:B:2001:HEM:C3B	2.04	0.92
1:D:357:TYR:CZ	2:D:2003:HEM:NA	2.38	0.91
1:B:62:HIS:HE1	1:D:368:ASN:HD21	1.12	0.91
1:A:74:HIS:CD2	2:A:2000:HEM:C3D	2.58	0.91
1:A:37:LYS:HE2	1:A:59:GLU:CD	1.91	0.90
1:D:444:THR:HG21	3:D:2174:HOH:O	1.70	0.90
1:B:238:ASP:OD1	1:B:277:THR:CG2	2.20	0.90
1:D:147:ASN:HD22	2:D:2003:HEM:CAC	1.74	0.90
1:A:296:PHE:CD1	1:A:346:PRO:HD2	2.07	0.89
1:B:125:VAL:HG23	3:B:2098:HOH:O	1.72	0.89
1:A:160:PHE:CD1	2:A:2000:HEM:CAB	2.56	0.89
1:B:353:ARG:HG2	2:B:2001:HEM:CBB	1.96	0.88
1:B:78:ALA:HB2	1:B:261:LEU:HD12	1.55	0.87
1:D:220:LYS:HE2	3:D:2168:HOH:O	1.75	0.86
1:B:112:PHE:HA	1:B:130:GLY:O	1.75	0.86
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.41	0.85
1:A:460:GLU:OE2	3:A:2222:HOH:O	1.95	0.85
1:B:444:THR:HG22	3:B:2211:HOH:O	1.75	0.85
1:C:402:ASN:HD22	1:C:402:ASN:N	1.75	0.85
1:C:353:ARG:HG3	2:C:2002:HEM:HBB2	1.57	0.84
1:A:487:GLU:O	1:A:491:ARG:HG3	1.77	0.84
1:C:24:ASP:OD2	3:C:2083:HOH:O	1.94	0.84
1:A:421:ARG:CD	1:B:429:GLN:HG3	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:HG2	1:B:202:ARG:HH11	1.43	0.84
1:C:281:GLN:HG2	1:C:309:LEU:HD12	1.60	0.83
1:B:208:HIS:O	1:B:211:MET:HG2	1.79	0.82
1:D:357:TYR:CZ	2:D:2003:HEM:C4A	2.67	0.82
1:B:39:ASN:OD1	3:B:2082:HOH:O	1.97	0.82
1:B:393:MET:CE	1:D:372:ILE:HA	2.10	0.82
1:A:145:VAL:O	2:A:2000:HEM:HBC2	1.79	0.82
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.44	0.82
1:D:363:HIS:HD2	3:D:2105:HOH:O	1.62	0.81
1:A:351:GLN:HE22	1:C:52:GLN:HE21	1.27	0.81
1:C:12:LYS:O	1:C:16:GLU:HG3	1.80	0.81
1:B:62:HIS:HE1	1:D:368:ASN:ND2	1.78	0.81
1:B:73:VAL:HG11	1:B:164:ILE:HD12	1.61	0.81
1:B:444:THR:O	1:B:448:LYS:HB3	1.79	0.81
1:C:474:GLN:HE22	1:C:496:LEU:HD12	1.45	0.81
1:C:402:ASN:H	1:C:402:ASN:ND2	1.79	0.81
1:B:124:THR:HG21	1:B:252:LEU:HB3	1.62	0.81
1:A:421:ARG:NE	1:B:429:GLN:HG2	1.96	0.80
1:D:191:SER:O	1:D:195:VAL:HG23	1.82	0.80
1:B:413:HIS:CD2	3:B:2213:HOH:O	2.34	0.80
1:D:279:TYR:HB2	1:D:309:LEU:HD23	1.64	0.80
1:D:223:ASN:ND2	1:D:227:GLU:HB3	1.97	0.79
1:A:97:LYS:NZ	3:A:2053:HOH:O	2.14	0.79
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.65	0.79
1:A:49:LEU:HD13	1:B:51:VAL:HG11	1.65	0.79
1:A:35:GLY:HA2	1:C:414:GLN:O	1.82	0.78
1:D:334:ASP:HB3	1:D:358:PRO:HG3	1.64	0.78
1:C:451:ASN:OD1	1:C:454:GLN:HG3	1.83	0.78
1:D:291:PHE:HE1	1:D:293:PHE:HB2	1.46	0.78
1:C:281:GLN:CG	1:C:309:LEU:HD12	2.14	0.78
1:D:189:PRO:HG3	1:D:480:ASN:HD22	1.44	0.78
1:B:62:HIS:CE1	1:D:368:ASN:HD21	2.01	0.77
1:A:414:GLN:O	1:C:35:GLY:HA2	1.84	0.77
1:B:406:ASN:ND2	1:B:410:ALA:HB3	1.99	0.77
1:B:357:TYR:CE1	2:B:2001:HEM:C1B	2.73	0.77
1:D:177:ASP:O	1:D:181:VAL:HG23	1.84	0.77
1:D:178:PRO:HD2	3:D:2085:HOH:O	1.83	0.77
1:B:182:TRP:HE1	1:B:465:HIS:HD1	0.79	0.77
1:A:351:GLN:HE22	1:C:52:GLN:NE2	1.83	0.77
1:D:189:PRO:HB2	1:D:438:ASN:HD22	1.48	0.77
1:A:160:PHE:CG	2:A:2000:HEM:HAB	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:CE1	1:A:346:PRO:HD2	2.20	0.76
1:C:347:ASP:HB3	1:C:350:LEU:HB3	1.68	0.76
1:C:251:ARG:HG3	1:C:252:LEU:N	1.99	0.75
1:C:50:LEU:HD22	1:D:48:PRO:HB2	1.66	0.75
1:A:37:LYS:CE	1:A:59:GLU:OE2	2.29	0.75
1:A:155:ARG:HH21	1:A:190:GLU:HB3	1.52	0.75
1:C:436:ASP:O	1:C:437:ASP:HB3	1.86	0.75
1:B:393:MET:HE3	1:D:372:ILE:HA	1.69	0.74
1:D:357:TYR:CE2	2:D:2003:HEM:NA	2.53	0.74
1:A:421:ARG:CG	1:B:429:GLN:CG	2.37	0.74
1:C:381:ARG:HH11	1:C:381:ARG:HB2	1.52	0.74
1:B:439:VAL:HG23	1:B:440:THR:H	1.53	0.73
1:B:382:VAL:HG13	1:B:382:VAL:O	1.87	0.73
1:B:238:ASP:OD1	1:B:277:THR:HG23	1.87	0.73
1:D:94:SER:HB2	1:D:221:LEU:HD22	1.70	0.73
1:A:74:HIS:N	3:A:2099:HOH:O	2.22	0.73
1:B:36:ASP:HB2	1:D:418:LEU:HD21	1.68	0.73
1:B:12:LYS:O	1:B:16:GLU:HG3	1.87	0.73
1:B:413:HIS:CE1	1:B:415:PRO:HD3	2.23	0.73
1:A:97:LYS:HE3	3:A:2118:HOH:O	1.89	0.73
1:B:148:ASN:HB3	1:B:211:MET:HE2	1.70	0.72
1:D:142:TRP:HA	1:D:337:ASN:O	1.89	0.72
1:B:223:ASN:HD21	1:B:227:GLU:HB2	1.54	0.72
1:C:223:ASN:HD21	1:C:227:GLU:HB2	1.54	0.72
1:D:190:GLU:HA	1:D:438:ASN:HB3	1.72	0.72
1:A:73:VAL:HA	3:A:2099:HOH:O	1.89	0.72
1:A:395:ASP:CG	1:C:327:GLU:OE2	2.27	0.72
1:B:294:ASN:ND2	1:C:46:ARG:HD2	2.05	0.72
1:D:207:GLY:HA3	3:D:2052:HOH:O	1.90	0.72
1:A:115:VAL:O	3:A:2099:HOH:O	2.07	0.72
1:B:485:HIS:HE1	1:B:487:GLU:CG	1.93	0.72
1:C:82:GLY:HA3	1:C:316:VAL:O	1.90	0.72
1:C:421:ARG:HE	1:D:429:GLN:NE2	1.87	0.72
1:C:353:ARG:NH2	2:C:2002:HEM:C4C	2.57	0.72
1:A:450:LEU:HA	1:A:454:GLN:NE2	2.05	0.71
1:D:357:TYR:CE1	2:D:2003:HEM:C1B	2.78	0.71
1:A:422:THR:O	1:B:428:VAL:HG22	1.90	0.71
1:B:19:ALA:CB	1:B:21:GLN:HE21	2.01	0.71
1:A:151:ILE:HG13	1:A:194:GLN:HG2	1.73	0.71
1:B:87:THR:HG23	1:B:313:GLY:HA2	1.73	0.71
1:D:291:PHE:CE1	1:D:293:PHE:HB2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASP:OD2	3:B:2216:HOH:O	2.08	0.71
1:A:74:HIS:O	1:A:111:ARG:NH2	2.24	0.71
1:D:406:ASN:ND2	1:D:410:ALA:HB3	2.04	0.71
1:D:347:ASP:HB3	1:D:350:LEU:HB3	1.73	0.71
1:C:336:SER:HB2	3:C:2168:HOH:O	1.90	0.70
1:B:124:THR:HG21	1:B:252:LEU:CB	2.21	0.70
1:D:234:HIS:O	1:D:278:LEU:HD12	1.91	0.70
1:A:160:PHE:CE2	2:A:2000:HEM:C2B	2.79	0.70
1:C:213:GLY:HA3	1:C:235:TYR:CE2	2.26	0.70
1:C:474:GLN:NE2	1:C:496:LEU:HD12	2.06	0.70
1:B:498:LYS:HD3	1:B:499:TYR:N	2.06	0.70
1:C:126:ARG:HD2	1:C:198:LEU:HG	1.72	0.70
1:D:90:ILE:HG21	1:D:312:VAL:HG22	1.72	0.70
1:A:106:THR:HG21	1:A:137:THR:HG22	1.73	0.70
1:B:25:VAL:O	1:B:27:THR:HG23	1.90	0.70
1:D:236:LYS:HE3	3:D:2064:HOH:O	1.90	0.70
1:C:413:HIS:C	1:C:413:HIS:ND1	2.44	0.70
1:B:183:ASP:O	1:B:187:LEU:HG	1.92	0.69
1:B:321:PRO:O	1:C:172:GLN:HG3	1.92	0.69
1:B:415:PRO:O	1:B:418:LEU:HD12	1.92	0.69
1:D:357:TYR:CE2	2:D:2003:HEM:C1A	2.80	0.69
1:B:5:ASP:OD2	1:B:7:ALA:HB3	1.92	0.69
1:C:177:ASP:O	1:C:181:VAL:HG23	1.91	0.69
1:D:218:THR:O	1:D:345:SER:HB3	1.92	0.69
1:B:454:GLN:HA	1:B:457:ARG:NH1	2.08	0.69
1:A:202:ARG:HG3	3:A:2077:HOH:O	1.91	0.69
1:B:353:ARG:HG2	2:B:2001:HEM:CAB	2.23	0.68
1:D:427:ASP:HB2	1:D:429:GLN:HE21	1.59	0.68
1:A:501:GLU:OE1	1:A:501:GLU:N	2.26	0.68
1:B:101:HIS:HA	3:B:2074:HOH:O	1.92	0.68
1:C:155:ARG:HH22	1:C:438:ASN:ND2	1.90	0.68
1:C:206:ASP:OD1	1:C:244:LEU:HD21	1.94	0.68
1:B:379:ARG:HD3	3:B:2180:HOH:O	1.94	0.68
1:D:291:PHE:HD1	1:D:293:PHE:H	1.40	0.68
1:B:23:PRO:HG3	1:D:412:GLU:OE1	1.94	0.68
1:C:451:ASN:O	1:C:454:GLN:HB2	1.94	0.68
1:A:98:VAL:HB	1:A:137:THR:HG21	1.76	0.68
1:A:160:PHE:CE2	2:A:2000:HEM:C1B	2.82	0.68
1:B:349:MET:O	2:B:2001:HEM:HBB1	1.94	0.68
1:A:72:VAL:HG11	2:A:2000:HEM:HMA1	1.76	0.67
1:A:235:TYR:HA	1:A:277:THR:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ARG:O	1:D:66:GLU:HG2	1.95	0.67
1:C:43:VAL:HG21	1:D:43:VAL:HG21	1.75	0.67
1:B:129:ARG:HB2	1:B:211:MET:HE1	1.76	0.67
1:C:492:ILE:HG22	1:C:496:LEU:CD2	2.24	0.67
1:C:460:GLU:HA	1:C:495:LEU:HD13	1.75	0.67
1:B:428:VAL:HG23	1:B:428:VAL:O	1.95	0.67
1:A:43:VAL:O	1:A:47:GLY:HA3	1.94	0.67
1:B:413:HIS:ND1	1:B:415:PRO:HD3	2.09	0.67
1:D:202:ARG:NH1	1:D:241:ILE:HG21	2.10	0.67
1:C:252:LEU:HA	1:C:255:GLU:HB2	1.77	0.66
1:C:179:ASP:O	1:C:183:ASP:HB2	1.94	0.66
1:A:160:PHE:CD2	2:A:2000:HEM:CMB	2.79	0.66
1:D:43:VAL:HG13	1:D:48:PRO:HD2	1.76	0.66
1:C:328:VAL:O	1:C:331:LEU:HB2	1.94	0.66
1:A:450:LEU:HA	1:A:454:GLN:HE22	1.60	0.66
1:B:95:LYS:HG3	1:B:222:VAL:O	1.96	0.65
1:B:467:LYS:HD3	1:B:499:TYR:CD1	2.31	0.65
1:C:291:PHE:CD1	1:C:292:PRO:HD2	2.30	0.65
1:D:235:TYR:HA	1:D:277:THR:O	1.96	0.65
1:A:351:GLN:NE2	1:C:52:GLN:HE21	1.93	0.65
1:C:239:GLN:HE22	1:C:275:SER:H	1.44	0.65
1:B:43:VAL:O	1:B:47:GLY:HA3	1.97	0.65
1:B:444:THR:HG23	3:B:2187:HOH:O	1.96	0.65
1:D:146:GLY:HA2	2:D:2003:HEM:CBC	2.26	0.65
1:B:97:LYS:HD3	1:B:138:GLU:HB2	1.78	0.65
1:A:44:GLY:N	3:A:2009:HOH:O	2.22	0.64
1:B:52:GLN:HB2	3:D:2011:HOH:O	1.97	0.64
1:B:336:SER:HB2	1:D:54:VAL:HG11	1.79	0.64
1:D:218:THR:OG1	1:D:232:LYS:HE3	1.97	0.64
1:B:439:VAL:HG23	1:B:440:THR:N	2.11	0.64
1:A:188:ARG:HB3	1:A:190:GLU:OE2	1.97	0.64
3:B:2113:HOH:O	1:C:424:PHE:HE1	1.80	0.64
1:A:43:VAL:CG1	1:A:48:PRO:HD2	2.27	0.64
1:A:231:CYS:SG	1:A:232:LYS:N	2.70	0.64
1:B:202:ARG:HG2	1:B:202:ARG:NH1	2.06	0.64
1:A:223:ASN:ND2	1:A:227:GLU:HB2	2.13	0.64
1:A:94:SER:HB2	1:A:221:LEU:HD22	1.80	0.64
1:D:223:ASN:HD21	1:D:227:GLU:CB	2.04	0.64
1:A:412:GLU:OE2	1:C:23:PRO:HG3	1.98	0.64
1:B:12:LYS:HD3	1:C:470:GLN:OE1	1.97	0.64
1:C:485:HIS:C	1:C:485:HIS:CD2	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASN:HD21	1:A:227:GLU:HB2	1.63	0.64
1:A:464:GLY:O	1:A:467:LYS:HG2	1.97	0.64
1:C:406:ASN:ND2	1:C:410:ALA:HB3	2.12	0.64
1:A:72:VAL:CG1	2:A:2000:HEM:CMA	2.72	0.63
1:B:163:PHE:HB2	1:B:184:PHE:CE2	2.32	0.63
1:C:147:ASN:ND2	2:C:2002:HEM:HAC	2.13	0.63
1:D:271:GLY:HA2	1:D:273:TYR:CE1	2.34	0.63
1:D:443:ARG:HG3	1:D:484:VAL:O	1.98	0.63
1:B:278:LEU:O	1:B:312:VAL:HG13	1.99	0.63
1:C:61:ALA:O	1:C:65:ARG:HG3	1.98	0.63
1:B:485:HIS:O	1:B:488:TYR:HB3	1.98	0.63
1:D:464:GLY:O	1:D:467:LYS:HE3	1.97	0.63
1:A:160:PHE:CZ	2:A:2000:HEM:C1B	2.87	0.63
1:A:232:LYS:HB2	1:A:281:GLN:HB2	1.81	0.63
1:B:303:PRO:HG3	3:B:2171:HOH:O	1.97	0.63
1:A:160:PHE:CE1	2:A:2000:HEM:C3B	2.86	0.63
1:C:165:HIS:HB3	1:D:402:ASN:OD1	1.99	0.63
1:A:74:HIS:HD2	2:A:2000:HEM:CHA	2.10	0.63
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.80	0.63
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.06	0.63
1:C:353:ARG:CG	2:C:2002:HEM:HBB2	2.29	0.63
1:B:43:VAL:CG1	1:B:48:PRO:HD2	2.29	0.62
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.64	0.62
1:A:412:GLU:CD	1:C:23:PRO:HG3	2.19	0.62
1:B:294:ASN:HD21	1:C:46:ARG:HD2	1.62	0.62
1:D:281:GLN:O	1:D:302:TRP:HZ3	1.82	0.62
1:B:261:LEU:HD23	1:C:175:LEU:CD2	2.26	0.62
1:A:97:LYS:HE2	1:A:138:GLU:HB3	1.80	0.62
1:D:26:LEU:HB3	1:D:34:VAL:HG22	1.81	0.62
1:D:279:TYR:CB	1:D:309:LEU:HD23	2.29	0.62
1:A:168:LYS:HE3	1:D:67:ARG:HH21	1.64	0.62
1:A:412:GLU:CD	1:C:23:PRO:CG	2.67	0.62
1:C:126:ARG:HG2	1:C:126:ARG:HH11	1.63	0.62
1:A:50:LEU:HD12	1:B:49:LEU:O	1.99	0.62
1:C:251:ARG:HG3	1:C:252:LEU:H	1.64	0.62
1:B:98:VAL:HG23	1:B:106:THR:OG1	2.00	0.62
1:B:101:HIS:HB2	3:B:2073:HOH:O	1.99	0.62
1:D:209:ARG:HG2	1:D:274:PRO:HB3	1.82	0.62
1:B:34:VAL:HG11	1:B:37:LYS:HB3	1.82	0.62
1:B:37:LYS:O	1:B:37:LYS:HG3	1.99	0.62
1:D:90:ILE:HD11	1:D:99:PHE:CG	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:HB2	1:C:396:ASN:HB2	1.82	0.61
1:C:394:MET:HG3	3:C:2061:HOH:O	2.00	0.61
1:D:187:LEU:O	1:D:188:ARG:HD2	2.00	0.61
1:B:250:ALA:O	1:B:253:ALA:HB3	2.00	0.61
1:B:256:ASP:OD2	1:B:259:TYR:HA	2.01	0.61
1:B:402:ASN:HD22	1:B:402:ASN:H	1.49	0.61
1:D:280:ILE:HD11	1:D:310:ILE:HB	1.82	0.61
1:B:239:GLN:NE2	1:B:275:SER:H	1.99	0.61
1:C:327:GLU:HA	1:C:374:VAL:HG11	1.83	0.61
1:A:14:TRP:O	1:A:17:GLN:HB3	2.00	0.61
1:B:239:GLN:HE22	1:B:275:SER:H	1.49	0.61
1:B:401:PRO:HB2	1:B:410:ALA:HB2	1.81	0.61
1:D:426:GLY:O	3:D:2209:HOH:O	2.16	0.61
1:B:205:PRO:HG3	1:B:211:MET:CE	2.31	0.61
1:D:221:LEU:HB2	1:D:229:VAL:HG23	1.82	0.61
1:B:41:LEU:O	1:B:49:LEU:HD23	2.01	0.61
1:B:479:LYS:HE2	1:B:483:ASP:OD2	2.00	0.61
1:C:236:LYS:HG3	1:C:279:TYR:HE2	1.66	0.61
1:A:37:LYS:NZ	1:A:59:GLU:OE1	2.34	0.60
1:A:412:GLU:OE1	1:C:23:PRO:HG2	2.01	0.60
1:B:64:ASP:HB3	1:C:360:THR:HB	1.82	0.60
1:D:112:PHE:HA	1:D:130:GLY:O	2.00	0.60
1:D:193:HIS:HA	1:D:442:VAL:HG22	1.83	0.60
1:D:126:ARG:NE	1:D:199:PHE:HA	2.11	0.60
1:A:160:PHE:CD2	2:A:2000:HEM:C2B	2.89	0.60
1:D:331:LEU:HD13	1:D:333:PHE:CZ	2.37	0.60
1:B:453:GLU:HB2	3:B:2192:HOH:O	2.02	0.60
1:C:171:PRO:HG3	1:D:402:ASN:HD22	1.66	0.60
1:C:492:ILE:HG22	1:C:496:LEU:HD21	1.82	0.60
1:C:413:HIS:CD2	3:C:2074:HOH:O	2.54	0.60
1:A:72:VAL:HG13	1:A:73:VAL:HG13	1.82	0.60
1:B:62:HIS:CE1	1:D:368:ASN:ND2	2.65	0.60
1:B:456:LYS:O	1:B:460:GLU:HG3	2.02	0.60
1:C:451:ASN:OD1	1:C:451:ASN:C	2.40	0.60
1:D:111:ARG:CG	2:D:2003:HEM:O1D	2.49	0.60
1:B:148:ASN:CB	1:B:211:MET:HE2	2.32	0.60
1:A:146:GLY:HA2	2:A:2000:HEM:CBC	2.31	0.59
1:B:382:VAL:O	1:B:382:VAL:CG1	2.50	0.59
1:D:111:ARG:HD3	2:D:2003:HEM:CGD	2.31	0.59
1:C:404:TYR:HE2	3:C:2074:HOH:O	1.83	0.59
1:B:331:LEU:HD13	1:B:333:PHE:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLY:HA3	1:B:235:TYR:CE2	2.38	0.59
1:D:146:GLY:HA2	2:D:2003:HEM:HBC1	1.84	0.59
1:D:170:ASN:HD22	1:D:173:THR:H	1.49	0.59
1:B:47:GLY:HA2	1:C:424:PHE:CE1	2.38	0.59
1:D:426:GLY:N	3:D:2209:HOH:O	2.35	0.59
1:C:357:TYR:CZ	2:C:2002:HEM:NA	2.69	0.59
1:D:43:VAL:CG1	1:D:48:PRO:HD2	2.32	0.59
1:B:72:VAL:HG23	3:B:2010:HOH:O	2.03	0.59
1:B:231:CYS:HA	1:B:281:GLN:O	2.03	0.59
1:C:3:ASN:C	1:C:4:ARG:HG3	2.22	0.59
1:C:377:PRO:HG2	1:C:382:VAL:CG2	2.32	0.59
1:A:160:PHE:CE1	2:A:2000:HEM:C4B	2.91	0.59
1:B:384:ASN:HB2	3:B:2118:HOH:O	2.03	0.59
1:D:294:ASN:HB3	1:D:297:ASP:HB2	1.85	0.59
1:C:94:SER:HB2	1:C:221:LEU:HD22	1.84	0.58
1:C:250:ALA:O	1:C:253:ALA:HB3	2.03	0.58
1:D:347:ASP:OD1	1:D:349:MET:HB2	2.03	0.58
1:C:145:VAL:HG12	1:C:353:ARG:HH22	1.68	0.58
1:C:247:GLU:HG3	1:C:248:ASP:N	2.17	0.58
1:D:387:ARG:HG2	1:D:387:ARG:HH11	1.68	0.58
1:A:332:ALA:HB1	1:A:361:HIS:CE1	2.37	0.58
1:B:69:PRO:HD3	1:C:69:PRO:HG3	1.85	0.58
1:B:353:ARG:CD	2:B:2001:HEM:CBB	2.66	0.58
1:B:439:VAL:O	1:B:442:VAL:HB	2.03	0.58
1:D:280:ILE:CD1	1:D:310:ILE:HB	2.34	0.58
1:A:296:PHE:CG	1:A:346:PRO:HD2	2.39	0.58
1:B:273:TYR:HB3	1:B:317:LEU:O	2.03	0.58
1:C:155:ARG:NH2	1:C:438:ASN:ND2	2.51	0.58
1:C:485:HIS:CD2	1:C:487:GLU:H	2.22	0.58
1:D:189:PRO:HG3	1:D:480:ASN:HD21	1.66	0.58
1:B:43:VAL:HG13	1:B:48:PRO:HD2	1.84	0.58
1:B:232:LYS:O	1:B:280:ILE:HA	2.03	0.58
1:B:349:MET:O	2:B:2001:HEM:CBB	2.51	0.58
1:A:37:LYS:O	1:D:158:LEU:HD13	2.04	0.58
1:A:281:GLN:HG3	1:A:309:LEU:HD13	1.84	0.58
1:A:351:GLN:NE2	1:C:52:GLN:NE2	2.50	0.58
1:C:418:LEU:HD11	3:D:2091:HOH:O	2.03	0.58
1:C:168:LYS:HD3	3:C:2119:HOH:O	2.04	0.57
1:D:338:MET:HE2	1:D:342:ILE:HG22	1.85	0.57
1:A:296:PHE:HB3	1:A:347:ASP:HA	1.85	0.57
1:B:419:GLU:CD	1:B:419:GLU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:HIS:HB3	1:C:242:LYS:H	1.68	0.57
1:C:487:GLU:O	1:C:491:ARG:HB2	2.03	0.57
1:C:298:LEU:CD2	1:C:349:MET:HG2	2.34	0.57
1:C:364:ARG:NE	2:C:2002:HEM:O1A	2.30	0.57
1:C:395:ASP:O	1:C:395:ASP:CG	2.42	0.57
1:C:148:ASN:HA	1:C:212:ASP:O	2.04	0.57
1:C:451:ASN:OD1	1:C:453:GLU:N	2.38	0.57
1:A:73:VAL:O	1:A:74:HIS:HB2	2.04	0.57
1:B:147:ASN:HD21	2:B:2001:HEM:CAC	2.15	0.57
1:B:268:ILE:HB	1:B:320:ASN:HD21	1.70	0.57
1:C:18:ARG:HH12	1:C:23:PRO:HA	1.69	0.57
1:D:221:LEU:O	1:D:228:ALA:HA	2.05	0.57
1:D:367:PRO:HG2	1:D:390:PRO:HG2	1.86	0.57
1:C:478:VAL:HG11	1:C:493:GLN:HB2	1.84	0.57
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.86	0.57
1:D:209:ARG:O	1:D:239:GLN:HB2	2.05	0.57
1:A:23:PRO:HB2	1:C:412:GLU:HG2	1.85	0.57
1:A:413:HIS:ND1	3:A:2229:HOH:O	1.88	0.57
1:C:445:PHE:HA	1:C:449:VAL:CG2	2.35	0.57
1:C:97:LYS:HD2	1:C:138:GLU:HB2	1.87	0.57
1:D:231:CYS:HA	1:D:281:GLN:O	2.04	0.57
1:B:447:LEU:HD21	1:B:485:HIS:CD2	2.39	0.57
1:D:357:TYR:O	1:D:360:THR:HG22	2.04	0.57
1:B:186:SER:OG	1:B:476:LYS:HB3	2.05	0.57
1:A:92:ARG:HH11	1:A:92:ARG:HB3	1.70	0.56
1:A:387:ARG:O	1:C:66:GLU:HG2	2.05	0.56
1:C:111:ARG:NE	2:C:2002:HEM:O1D	2.28	0.56
1:A:72:VAL:HG11	2:A:2000:HEM:CMA	2.34	0.56
1:B:220:LYS:HD3	1:B:228:ALA:HB1	1.87	0.56
1:D:88:HIS:CD2	1:D:311:PRO:HG2	2.40	0.56
1:D:110:VAL:HG21	1:D:317:LEU:HD21	1.88	0.56
1:D:478:VAL:HG21	1:D:493:GLN:OE1	2.05	0.56
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.87	0.56
1:A:155:ARG:NH1	1:A:297:ASP:OD2	2.38	0.56
1:B:129:ARG:CB	1:B:211:MET:HE1	2.34	0.56
1:A:23:PRO:CB	1:C:412:GLU:HG2	2.36	0.56
1:C:235:TYR:HA	1:C:277:THR:O	2.06	0.56
1:D:145:VAL:CG1	1:D:353:ARG:HH22	2.19	0.56
1:D:357:TYR:CZ	2:D:2003:HEM:CHB	2.86	0.56
1:B:25:VAL:CG1	1:D:414:GLN:HG3	2.36	0.56
1:B:129:ARG:HB2	1:B:211:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ASN:HA	1:C:46:ARG:HH12	1.68	0.56
1:B:429:GLN:OE1	1:B:431:PHE:CE1	2.59	0.56
1:C:381:ARG:HH11	1:C:381:ARG:CB	2.19	0.56
1:A:160:PHE:CD1	2:A:2000:HEM:C3B	2.93	0.56
1:A:450:LEU:HD23	1:A:454:GLN:NE2	2.21	0.56
1:B:408:PHE:O	1:B:409:SER:HB2	2.06	0.56
1:D:18:ARG:O	1:D:21:GLN:HB2	2.06	0.56
1:A:220:LYS:HD2	1:A:420:HIS:CD2	2.41	0.56
1:C:234:HIS:O	1:C:279:TYR:N	2.30	0.56
1:D:12:LYS:O	1:D:16:GLU:HG3	2.05	0.56
1:D:86:VAL:HG23	1:D:104:LYS:O	2.05	0.56
1:D:170:ASN:ND2	1:D:172:GLN:H	2.03	0.56
1:A:279:TYR:HB3	1:A:309:LEU:HB3	1.88	0.56
1:A:334:ASP:OD1	1:A:361:HIS:CE1	2.59	0.56
1:B:50:LEU:HD22	1:B:50:LEU:N	2.21	0.56
1:C:395:ASP:N	3:C:2214:HOH:O	2.31	0.56
1:D:15:LYS:O	1:D:18:ARG:HB3	2.06	0.56
1:A:239:GLN:NE2	1:A:275:SER:H	2.04	0.56
1:B:19:ALA:HB3	1:B:21:GLN:NE2	2.07	0.56
1:B:145:VAL:HG21	1:B:335:PRO:HD3	1.88	0.56
1:C:145:VAL:CG1	1:C:353:ARG:HH22	2.19	0.56
1:D:488:TYR:CE1	1:D:492:ILE:HD11	2.41	0.56
1:B:26:LEU:HD21	1:B:37:LYS:HD2	1.88	0.55
1:D:90:ILE:HD11	1:D:99:PHE:CD2	2.42	0.55
1:D:189:PRO:HD2	3:D:2144:HOH:O	2.06	0.55
1:B:340:PRO:HG3	1:B:417:ALA:HB1	1.89	0.55
1:A:343:GLU:HB3	1:A:344:PRO:HD2	1.89	0.55
1:C:480:ASN:O	1:C:484:VAL:HG23	2.06	0.55
1:B:218:THR:O	1:B:345:SER:HB3	2.07	0.55
1:C:152:PHE:HA	1:C:194:GLN:HG3	1.88	0.55
1:A:23:PRO:HB2	1:C:412:GLU:CG	2.37	0.55
1:C:456:LYS:O	1:C:460:GLU:HG3	2.06	0.55
1:B:115:VAL:HG21	1:B:128:PRO:HD2	1.89	0.55
1:B:456:LYS:HB2	1:B:491:ARG:HH22	1.72	0.55
1:C:234:HIS:HB2	1:C:279:TYR:HB2	1.89	0.55
1:A:296:PHE:CE1	1:A:346:PRO:CD	2.90	0.55
1:A:450:LEU:CD2	1:A:454:GLN:NE2	2.70	0.55
1:A:487:GLU:CD	1:A:491:ARG:HD2	2.28	0.55
1:C:369:TYR:C	1:C:371:GLN:H	2.09	0.55
1:A:388:ASP:OD1	1:A:388:ASP:N	2.36	0.55
1:B:14:TRP:CH2	1:B:18:ARG:HD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:PRO:HG3	1:B:211:MET:HE3	1.88	0.55
1:C:73:VAL:CG2	2:C:2002:HEM:C1A	2.89	0.55
1:D:95:LYS:HG2	1:D:222:VAL:O	2.07	0.55
1:B:413:HIS:ND1	1:B:413:HIS:C	2.59	0.54
1:A:101:HIS:HE1	3:A:2109:HOH:O	1.90	0.54
1:B:26:LEU:HD21	1:B:37:LYS:CD	2.37	0.54
1:D:436:ASP:O	1:D:437:ASP:HB3	2.06	0.54
1:B:148:ASN:HA	1:B:212:ASP:O	2.07	0.54
1:C:129:ARG:HB2	1:C:148:ASN:CG	2.27	0.54
1:C:453:GLU:OE1	1:C:456:LYS:HD3	2.07	0.54
1:D:331:LEU:HD13	1:D:333:PHE:HZ	1.72	0.54
1:A:431:PHE:CD1	1:D:45:PRO:HB3	2.42	0.54
1:A:453:GLU:HG2	1:A:457:ARG:HH12	1.71	0.54
1:B:49:LEU:HD23	1:B:50:LEU:H	1.71	0.54
1:B:466:LEU:HD22	1:B:474:GLN:HG2	1.90	0.54
1:D:60:MET:HE3	1:D:63:PHE:HB3	1.89	0.54
1:D:147:ASN:CB	2:D:2003:HEM:HAC	2.36	0.54
1:D:286:SER:O	1:D:289:GLU:HB3	2.08	0.54
1:B:64:ASP:HB3	1:C:360:THR:CB	2.37	0.54
1:B:238:ASP:OD1	1:B:277:THR:HG22	2.03	0.54
1:B:447:LEU:O	1:B:448:LYS:HB2	2.06	0.54
1:C:18:ARG:NH1	1:C:23:PRO:HA	2.22	0.54
1:B:142:TRP:HA	1:B:337:ASN:O	2.07	0.54
1:B:268:ILE:HB	1:B:320:ASN:ND2	2.23	0.54
1:C:46:ARG:CG	1:C:46:ARG:HH11	2.20	0.54
1:A:73:VAL:HG22	2:A:2000:HEM:C2A	2.43	0.54
1:C:427:ASP:HB3	1:C:429:GLN:OE1	2.08	0.54
1:B:152:PHE:CD1	2:B:2001:HEM:HMC1	2.43	0.54
1:B:235:TYR:HA	1:B:277:THR:O	2.08	0.54
1:B:294:ASN:HA	1:C:46:ARG:NH1	2.23	0.54
1:C:195:VAL:O	1:C:199:PHE:HD1	1.91	0.54
1:C:438:ASN:ND2	1:C:438:ASN:N	2.56	0.54
1:A:428:VAL:HG12	1:A:428:VAL:O	2.08	0.53
1:B:334:ASP:O	1:B:337:ASN:HB2	2.08	0.53
1:B:413:HIS:HD2	3:B:2213:HOH:O	1.78	0.53
1:A:136:TYR:HA	1:A:141:ASN:OD1	2.08	0.53
1:B:81:PHE:HZ	1:B:327:GLU:HB3	1.73	0.53
1:C:4:ARG:HD3	1:C:9:ASP:OD1	2.08	0.53
1:C:74:HIS:HA	1:C:114:THR:O	2.08	0.53
1:C:353:ARG:NH2	2:C:2002:HEM:CHD	2.72	0.53
1:D:220:LYS:NZ	1:D:420:HIS:HD2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HA	1:D:172:GLN:HE21	1.73	0.53
1:A:343:GLU:HB3	1:A:344:PRO:CD	2.38	0.53
1:B:49:LEU:CD2	1:B:50:LEU:N	2.71	0.53
1:B:73:VAL:CG1	1:B:164:ILE:HD12	2.35	0.53
1:A:88:HIS:CE1	1:A:311:PRO:HB2	2.43	0.53
1:A:396:ASN:HB2	1:C:326:ALA:HB2	1.90	0.53
1:B:439:VAL:O	1:B:442:VAL:N	2.41	0.53
1:C:157:ALA:HA	1:C:349:MET:HE3	1.90	0.53
1:C:459:CYS:HA	1:C:492:ILE:CD1	2.39	0.53
1:D:298:LEU:HD23	1:D:349:MET:HG3	1.91	0.53
1:C:486:PRO:O	1:C:490:SER:HB2	2.09	0.53
1:A:37:LYS:HE2	1:A:59:GLU:OE1	2.09	0.53
1:B:49:LEU:CD2	1:B:50:LEU:H	2.22	0.53
1:B:291:PHE:CD1	1:B:292:PRO:HD2	2.44	0.53
1:C:437:ASP:OD2	1:C:440:THR:HB	2.09	0.53
1:A:220:LYS:HD2	1:A:420:HIS:HD2	1.74	0.53
1:D:94:SER:HB2	1:D:221:LEU:HB3	1.89	0.53
1:B:6:PRO:HG2	1:B:266:ASN:OD1	2.09	0.52
1:B:396:ASN:O	1:B:397:GLN:HB2	2.09	0.52
1:C:413:HIS:ND1	1:C:413:HIS:O	2.41	0.52
1:B:17:GLN:C	1:B:19:ALA:H	2.11	0.52
1:B:39:ASN:O	1:C:430:ARG:HB3	2.08	0.52
1:B:353:ARG:HD2	2:B:2001:HEM:CBB	2.39	0.52
1:C:298:LEU:HD23	1:C:349:MET:HG2	1.90	0.52
1:C:472:PHE:HB3	3:C:2235:HOH:O	2.09	0.52
1:A:304:HIS:CE1	3:A:2088:HOH:O	2.62	0.52
1:B:38:LEU:HD22	1:C:159:LEU:HD11	1.90	0.52
1:B:49:LEU:HD22	1:B:50:LEU:N	2.24	0.52
1:D:232:LYS:O	1:D:280:ILE:HA	2.10	0.52
1:A:48:PRO:HB2	1:B:50:LEU:HD12	1.91	0.52
1:A:115:VAL:HG11	3:A:2113:HOH:O	2.10	0.52
1:C:450:LEU:HG	1:C:454:GLN:HB3	1.90	0.52
1:C:470:GLN:O	1:C:474:GLN:HG3	2.09	0.52
1:D:96:ALA:HB3	1:D:99:PHE:CD2	2.44	0.52
1:D:441:GLN:O	1:D:444:THR:HG23	2.10	0.52
1:A:427:ASP:HA	1:B:423:HIS:HA	1.91	0.52
1:B:66:GLU:HB3	1:D:388:ASP:HB2	1.91	0.52
1:B:357:TYR:CE1	2:B:2001:HEM:NB	2.78	0.52
1:C:209:ARG:HD2	1:C:274:PRO:HB3	1.90	0.52
1:D:148:ASN:C	1:D:148:ASN:HD22	2.12	0.52
1:A:213:GLY:HA3	1:A:235:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:TRP:HB2	1:C:339:PRO:CD	2.39	0.52
1:A:474:GLN:OE1	1:A:496:LEU:HG	2.10	0.52
1:A:132:ALA:HB1	1:A:333:PHE:CD2	2.44	0.52
1:B:155:ARG:HB3	1:B:299:THR:HG23	1.92	0.52
1:B:213:GLY:HA3	1:B:235:TYR:CD2	2.45	0.52
1:D:228:ALA:HB3	1:D:285:PHE:CZ	2.44	0.52
1:A:421:ARG:NE	3:A:2187:HOH:O	2.32	0.52
1:C:291:PHE:CD2	1:C:293:PHE:O	2.63	0.52
1:A:421:ARG:HD2	1:B:429:GLN:HG2	0.53	0.52
1:A:496:LEU:O	1:A:500:ASN:HB2	2.10	0.52
1:B:11:MET:CE	1:C:180:MET:HG2	2.40	0.52
1:B:496:LEU:O	1:B:500:ASN:N	2.41	0.52
1:C:394:MET:HB2	3:C:2061:HOH:O	2.10	0.52
1:A:323:ASN:CG	1:C:396:ASN:HB3	2.30	0.51
1:B:206:ASP:HA	1:B:244:LEU:HD11	1.93	0.51
1:A:248:ASP:HA	1:A:251:ARG:NH1	2.26	0.51
1:A:452:GLU:HA	1:A:455:ARG:HH11	1.76	0.51
1:D:140:GLY:H	1:D:380:ALA:HB2	1.75	0.51
1:B:186:SER:OG	1:B:476:LYS:HG2	2.10	0.51
1:D:97:LYS:HE3	3:D:2059:HOH:O	2.09	0.51
1:A:126:ARG:HA	1:A:203:GLY:O	2.10	0.51
1:B:235:TYR:N	1:B:235:TYR:CD1	2.78	0.51
1:A:190:GLU:HA	1:A:438:ASN:HB3	1.91	0.51
1:B:73:VAL:O	1:B:74:HIS:HB2	2.11	0.51
1:B:127:ASP:O	1:B:129:ARG:NH1	2.44	0.51
1:C:212:ASP:OD1	1:C:236:LYS:HA	2.10	0.51
1:D:219:PHE:O	1:D:230:TYR:HA	2.10	0.51
1:D:451:ASN:OD1	1:D:451:ASN:C	2.49	0.51
1:C:178:PRO:HA	1:C:181:VAL:CG2	2.41	0.51
1:C:190:GLU:HA	1:C:438:ASN:CB	2.29	0.51
1:D:160:PHE:CE2	2:D:2003:HEM:C2B	2.98	0.51
1:D:284:THR:OG1	1:D:287:GLU:HG3	2.11	0.51
1:A:21:GLN:NE2	3:A:2175:HOH:O	2.43	0.51
1:B:41:LEU:HD11	1:C:428:VAL:CG1	2.41	0.51
1:C:40:SER:HB3	1:C:49:LEU:CD1	2.41	0.51
1:C:273:TYR:HB3	1:C:317:LEU:O	2.10	0.51
1:D:357:TYR:CE1	2:D:2003:HEM:CHB	2.94	0.51
1:B:124:THR:HB	1:B:249:ALA:O	2.11	0.51
1:C:73:VAL:O	1:C:74:HIS:HB2	2.10	0.51
1:D:217:HIS:CG	1:D:350:LEU:HB2	2.45	0.51
1:B:367:PRO:HD2	1:B:390:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:CE	1:A:59:GLU:OE1	2.59	0.50
1:B:454:GLN:HB3	1:B:457:ARG:HH22	1.76	0.50
1:D:360:THR:HG21	2:D:2003:HEM:HMA3	1.93	0.50
1:A:367:PRO:HG3	1:C:65:ARG:HD3	1.94	0.50
1:A:294:ASN:HB3	1:A:297:ASP:HB2	1.93	0.50
1:A:296:PHE:HB3	1:A:347:ASP:CA	2.40	0.50
1:B:71:ARG:HE	2:B:2001:HEM:CGD	2.24	0.50
1:B:279:TYR:HA	1:B:310:ILE:O	2.11	0.50
1:B:353:ARG:HG3	2:B:2001:HEM:HBB2	0.50	0.50
1:C:485:HIS:HD2	1:C:486:PRO:N	2.08	0.50
1:A:248:ASP:HA	1:A:251:ARG:HH12	1.77	0.50
1:A:395:ASP:OD2	1:C:323:ASN:HB3	2.11	0.50
1:D:78:ALA:HB2	1:D:261:LEU:HG	1.92	0.50
1:A:346:PRO:O	1:A:347:ASP:C	2.50	0.50
1:B:110:VAL:CG2	1:B:317:LEU:HD21	2.42	0.50
1:B:238:ASP:OD2	1:B:275:SER:OG	2.24	0.50
1:B:348:LYS:HG3	3:B:2110:HOH:O	2.10	0.50
1:C:424:PHE:O	3:D:2209:HOH:O	2.18	0.50
1:D:290:ILE:O	1:D:291:PHE:C	2.49	0.50
1:D:293:PHE:O	1:D:295:PRO:HD3	2.11	0.50
1:D:485:HIS:ND1	1:D:487:GLU:HB3	2.26	0.50
1:A:100:GLU:O	1:A:101:HIS:HB3	2.12	0.50
1:B:110:VAL:HG21	1:B:317:LEU:HD21	1.94	0.50
1:B:193:HIS:NE2	1:B:441:GLN:HB3	2.27	0.50
1:D:285:PHE:HD1	3:D:2153:HOH:O	1.95	0.50
1:A:140:GLY:HA3	1:C:31:GLY:C	2.32	0.50
1:B:151:ILE:HD13	1:B:193:HIS:ND1	2.27	0.50
1:B:197:PHE:O	1:B:200:SER:HB3	2.12	0.50
1:B:408:PHE:CE2	1:D:11:MET:HE3	2.47	0.50
1:D:94:SER:CB	1:D:221:LEU:HD22	2.40	0.50
1:A:412:GLU:CD	1:C:23:PRO:HG2	2.32	0.50
1:B:94:SER:HB2	1:B:221:LEU:HB3	1.94	0.50
1:C:126:ARG:O	1:C:127:ASP:HB2	2.12	0.50
1:C:178:PRO:HA	1:C:181:VAL:HG23	1.93	0.50
1:D:460:GLU:HA	1:D:495:LEU:CD1	2.42	0.50
1:A:152:PHE:HA	1:A:194:GLN:HG3	1.93	0.50
1:A:168:LYS:HE3	1:D:67:ARG:NH2	2.27	0.50
1:C:266:ASN:HA	1:C:269:ALA:HB3	1.94	0.50
1:B:180:MET:HG3	1:C:11:MET:CE	2.42	0.49
1:B:274:PRO:HB2	1:B:276:TRP:CH2	2.47	0.49
1:B:217:HIS:ND1	1:B:298:LEU:HD13	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LYS:HB2	1:B:491:ARG:NH2	2.28	0.49
1:C:46:ARG:NH1	1:C:46:ARG:HG2	2.27	0.49
1:C:241:ILE:N	1:C:241:ILE:HD12	2.26	0.49
1:C:358:PRO:O	1:C:362:ARG:HG3	2.13	0.49
1:D:106:THR:O	1:D:108:ILE:HG23	2.12	0.49
1:A:477:ALA:HA	1:A:480:ASN:HD22	1.77	0.49
1:B:456:LYS:HG3	3:B:2194:HOH:O	2.12	0.49
1:D:97:LYS:HA	1:D:100:GLU:HG3	1.93	0.49
1:A:239:GLN:HE22	1:A:275:SER:H	1.58	0.49
1:B:74:HIS:O	1:B:111:ARG:NH2	2.45	0.49
1:B:487:GLU:O	1:B:491:ARG:HG3	2.13	0.49
1:C:445:PHE:HA	1:C:449:VAL:HG23	1.94	0.49
1:A:97:LYS:O	1:A:100:GLU:HB2	2.12	0.49
1:B:444:THR:O	1:B:448:LYS:CB	2.58	0.49
1:C:156:ASP:HB3	1:C:159:LEU:HD23	1.94	0.49
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.93	0.49
1:C:87:THR:C	1:C:88:HIS:ND1	2.66	0.49
1:C:281:GLN:CG	1:C:309:LEU:CD1	2.88	0.49
1:C:413:HIS:HD2	3:C:2074:HOH:O	1.91	0.49
1:B:160:PHE:N	1:B:161:PRO:HD2	2.28	0.49
1:B:478:VAL:O	1:B:479:LYS:C	2.50	0.49
1:C:156:ASP:OD2	1:C:348:LYS:HD3	2.13	0.49
1:C:108:ILE:HD13	1:C:315:LEU:HD22	1.94	0.49
1:C:423:HIS:HA	1:D:427:ASP:HA	1.95	0.49
1:A:51:VAL:HG12	1:B:51:VAL:HA	1.94	0.49
1:B:44:GLY:HA3	3:B:2083:HOH:O	2.12	0.49
1:C:73:VAL:HG23	2:C:2002:HEM:C1A	2.48	0.49
1:D:439:VAL:HG23	1:D:440:THR:N	2.28	0.49
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.48	0.49
1:B:70:GLU:HG2	3:B:2054:HOH:O	2.13	0.49
1:B:360:THR:HG23	1:C:64:ASP:O	2.13	0.49
1:D:19:ALA:C	1:D:21:GLN:H	2.16	0.49
1:A:33:PRO:HB2	1:C:414:GLN:NE2	2.28	0.48
1:A:160:PHE:CG	2:A:2000:HEM:CAB	2.89	0.48
1:A:487:GLU:OE2	1:A:491:ARG:HD2	2.12	0.48
1:B:14:TRP:O	1:B:17:GLN:HG2	2.13	0.48
1:B:98:VAL:HG13	1:B:99:PHE:CD1	2.48	0.48
1:D:209:ARG:HD2	3:D:2015:HOH:O	2.12	0.48
1:D:223:ASN:OD1	1:D:225:ASP:N	2.42	0.48
1:A:457:ARG:O	1:A:461:ASN:ND2	2.46	0.48
1:C:162:SER:HB3	1:D:404:TYR:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:PRO:HG2	1:C:382:VAL:HG23	1.94	0.48
1:A:71:ARG:NH1	1:A:111:ARG:NH1	2.61	0.48
1:B:217:HIS:CD2	1:B:353:ARG:HH11	2.30	0.48
1:D:88:HIS:O	1:D:102:ILE:HG12	2.13	0.48
1:A:461:ASN:ND2	3:A:2125:HOH:O	2.44	0.48
1:B:125:VAL:HG22	1:B:126:ARG:N	2.29	0.48
1:B:147:ASN:ND2	2:B:2001:HEM:C3C	2.78	0.48
1:C:14:TRP:O	1:C:18:ARG:HB2	2.13	0.48
1:C:290:ILE:O	1:C:291:PHE:C	2.51	0.48
1:C:414:GLN:HA	1:C:415:PRO:HD2	1.83	0.48
1:D:74:HIS:CD2	2:D:2003:HEM:C4D	3.02	0.48
1:D:217:HIS:CE1	1:D:298:LEU:HD22	2.49	0.48
1:B:402:ASN:HD22	1:B:402:ASN:N	2.09	0.48
1:C:349:MET:HE3	2:C:2002:HEM:HBB1	1.95	0.48
1:D:35:GLY:O	1:D:36:ASP:HB2	2.14	0.48
1:D:218:THR:O	1:D:345:SER:CB	2.60	0.48
1:A:73:VAL:CA	3:A:2099:HOH:O	2.54	0.48
1:D:353:ARG:CG	2:D:2003:HEM:HBB2	2.43	0.48
1:B:466:LEU:HD11	1:B:477:ALA:CB	2.43	0.48
1:C:22:LYS:HD3	1:C:23:PRO:HD2	1.95	0.48
1:C:72:VAL:HG13	1:C:73:VAL:HG13	1.95	0.48
1:D:145:VAL:HG12	1:D:353:ARG:HH22	1.79	0.48
1:A:265:PHE:CE2	1:D:173:THR:HG22	2.48	0.48
1:B:269:ALA:C	1:B:271:GLY:H	2.17	0.48
1:C:112:PHE:HB3	1:C:208:HIS:ND1	2.29	0.48
1:A:81:PHE:HZ	1:A:327:GLU:HB3	1.79	0.48
1:C:151:ILE:CG2	1:C:301:VAL:CG1	2.92	0.48
1:D:213:GLY:HA3	1:D:235:TYR:CE2	2.48	0.48
1:D:228:ALA:C	1:D:229:VAL:HG22	2.33	0.48
1:A:430:ARG:HE	1:B:419:GLU:CD	2.17	0.48
1:B:23:PRO:HG2	1:D:412:GLU:HB2	1.95	0.48
1:B:78:ALA:O	1:B:111:ARG:HG2	2.14	0.48
1:C:206:ASP:HA	1:C:244:LEU:HG	1.95	0.48
1:A:14:TRP:CZ3	1:A:18:ARG:HD2	2.48	0.47
1:B:252:LEU:HD12	1:B:252:LEU:HA	1.64	0.47
1:B:403:TYR:CD1	1:B:403:TYR:N	2.82	0.47
1:C:97:LYS:HB2	1:C:97:LYS:HZ3	1.79	0.47
1:C:213:GLY:HA3	1:C:235:TYR:CD2	2.49	0.47
1:C:215:GLY:HA3	1:C:233:PHE:HB2	1.96	0.47
1:A:12:LYS:HG3	1:D:470:GLN:HE22	1.79	0.47
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:O	1:B:228:ALA:HA	2.14	0.47
1:A:160:PHE:CZ	2:A:2000:HEM:C4B	3.02	0.47
1:A:347:ASP:HB3	1:A:350:LEU:HB3	1.96	0.47
1:A:450:LEU:HD22	1:A:454:GLN:HB3	1.95	0.47
1:D:148:ASN:C	1:D:148:ASN:ND2	2.68	0.47
1:B:206:ASP:HA	1:B:244:LEU:CD1	2.45	0.47
1:B:368:ASN:O	1:B:371:GLN:HB2	2.14	0.47
1:C:357:TYR:CE2	2:C:2002:HEM:C1A	3.03	0.47
1:D:247:GLU:O	1:D:251:ARG:HB2	2.15	0.47
1:A:37:LYS:C	1:D:158:LEU:HD13	2.34	0.47
1:A:421:ARG:HG2	1:B:429:GLN:CG	2.27	0.47
1:B:198:LEU:O	1:B:203:GLY:HA3	2.14	0.47
1:D:415:PRO:HB3	3:D:2188:HOH:O	2.15	0.47
1:B:78:ALA:O	1:B:111:ARG:CG	2.62	0.47
1:B:152:PHE:CD1	2:B:2001:HEM:CMC	2.96	0.47
1:B:357:TYR:HE1	2:B:2001:HEM:C1B	2.27	0.47
1:D:22:LYS:HD3	1:D:23:PRO:HD2	1.96	0.47
1:D:93:TYR:CE1	1:D:282:VAL:HG11	2.49	0.47
1:A:51:VAL:HG13	1:B:49:LEU:O	2.14	0.47
1:A:108:ILE:HA	1:A:134:LYS:O	2.14	0.47
1:A:159:LEU:HA	3:B:2005:HOH:O	2.14	0.47
1:A:323:ASN:ND2	1:C:396:ASN:HB3	2.29	0.47
1:A:393:MET:SD	1:C:393:MET:HG3	2.55	0.47
1:A:396:ASN:HB3	1:C:323:ASN:CG	2.34	0.47
1:A:396:ASN:HB3	1:C:323:ASN:ND2	2.29	0.47
1:C:410:ALA:HB1	1:C:411:PRO:HD2	1.96	0.47
1:D:357:TYR:HE2	2:D:2003:HEM:C1A	2.32	0.47
1:A:143:ASP:HB2	1:A:334:ASP:O	2.15	0.47
1:B:43:VAL:O	1:B:43:VAL:HG22	2.14	0.47
1:B:273:TYR:HA	1:B:274:PRO:HD3	1.78	0.47
1:B:396:ASN:ND2	3:B:2181:HOH:O	2.47	0.47
1:C:171:PRO:HG3	1:D:402:ASN:ND2	2.29	0.47
1:D:209:ARG:HB3	1:D:239:GLN:HG2	1.96	0.47
1:A:51:VAL:HG11	1:B:49:LEU:HD13	1.96	0.47
1:B:5:ASP:HB2	1:B:6:PRO:HD2	1.97	0.47
1:B:25:VAL:HG11	1:D:414:GLN:HG3	1.97	0.47
1:B:65:ARG:HD3	1:D:367:PRO:HB3	1.97	0.47
1:B:73:VAL:HG11	1:B:164:ILE:CD1	2.41	0.47
1:B:164:ILE:O	1:B:164:ILE:HG22	2.15	0.47
1:D:88:HIS:C	1:D:102:ILE:HG12	2.35	0.47
1:D:126:ARG:HH21	1:D:199:PHE:C	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:VAL:HG23	1:B:284:THR:HA	1.97	0.47
1:B:298:LEU:HD23	1:B:349:MET:HE2	1.97	0.47
1:B:310:ILE:HD12	1:B:310:ILE:N	2.30	0.47
1:C:22:LYS:HD3	1:C:23:PRO:CD	2.45	0.47
1:D:381:ARG:HH11	1:D:381:ARG:HG2	1.80	0.47
1:A:181:VAL:HA	3:A:2121:HOH:O	2.14	0.46
1:B:71:ARG:NH1	1:B:71:ARG:CG	2.75	0.46
1:D:353:ARG:HG2	2:D:2003:HEM:HBB2	1.97	0.46
1:B:205:PRO:HG3	1:B:211:MET:HE1	1.96	0.46
3:B:2002:HOH:O	1:D:52:GLN:HB2	2.15	0.46
1:C:493:GLN:HA	1:C:496:LEU:HD23	1.98	0.46
1:D:141:ASN:O	1:D:337:ASN:HB3	2.16	0.46
1:B:262:ARG:HB3	1:C:175:LEU:HD11	1.96	0.46
1:B:370:LEU:HD13	1:D:29:GLY:C	2.35	0.46
1:B:451:ASN:O	1:B:454:GLN:HG2	2.16	0.46
1:C:434:ALA:C	1:C:435:ASN:HD22	2.18	0.46
1:D:186:SER:OG	1:D:476:LYS:HD2	2.15	0.46
1:A:28:THR:HG23	1:A:32:ASN:O	2.15	0.46
1:A:49:LEU:HB2	1:D:351:GLN:HB3	1.97	0.46
1:A:139:ASP:HB3	1:A:340:PRO:HD2	1.98	0.46
1:B:301:VAL:HG22	1:B:441:GLN:OE1	2.16	0.46
1:C:78:ALA:HB2	1:C:261:LEU:HD22	1.96	0.46
1:C:81:PHE:N	1:C:81:PHE:CD1	2.83	0.46
1:C:115:VAL:HG12	1:C:116:ALA:N	2.30	0.46
1:D:283:MET:HE2	1:D:291:PHE:HD2	1.79	0.46
1:A:353:ARG:NH2	2:A:2000:HEM:C4C	2.84	0.46
1:B:274:PRO:HB2	1:B:276:TRP:CZ3	2.50	0.46
1:C:87:THR:OG1	1:C:313:GLY:HA2	2.15	0.46
1:C:395:ASP:CB	3:C:2214:HOH:O	2.63	0.46
1:D:279:TYR:HA	1:D:310:ILE:O	2.15	0.46
1:D:364:ARG:NE	2:D:2003:HEM:O1A	2.39	0.46
1:A:334:ASP:OD1	1:A:361:HIS:ND1	2.49	0.46
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.97	0.46
1:D:357:TYR:CE2	2:D:2003:HEM:C4A	3.03	0.46
1:B:323:ASN:HB2	1:D:398:GLY:HA2	1.98	0.46
1:D:71:ARG:HB2	1:D:75:ALA:HA	1.96	0.46
1:A:130:GLY:HA2	1:A:147:ASN:OD1	2.15	0.46
1:B:168:LYS:HE3	1:C:67:ARG:HH21	1.80	0.46
1:B:191:SER:O	1:B:192:LEU:C	2.53	0.46
1:C:369:TYR:C	1:C:371:GLN:N	2.69	0.46
1:D:86:VAL:HB	1:D:103:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ASP:O	1:D:187:LEU:HG	2.15	0.46
1:B:32:ASN:HA	1:D:139:ASP:O	2.16	0.46
1:B:41:LEU:HD22	1:B:41:LEU:HA	1.84	0.46
1:B:223:ASN:C	1:B:225:ASP:H	2.19	0.46
1:C:246:VAL:HG21	1:C:461:ASN:HD21	1.81	0.46
1:C:349:MET:CE	2:C:2002:HEM:HBB1	2.46	0.46
1:D:142:TRP:HB2	1:D:339:PRO:HD3	1.98	0.46
1:D:179:ASP:O	1:D:183:ASP:HB2	2.16	0.46
1:D:202:ARG:NH1	3:D:2156:HOH:O	2.49	0.46
1:D:369:TYR:C	1:D:371:GLN:H	2.18	0.46
1:A:421:ARG:CZ	1:B:429:GLN:HG2	2.45	0.46
1:B:25:VAL:HG13	1:D:414:GLN:HG3	1.97	0.46
3:B:2045:HOH:O	1:C:70:GLU:HG2	2.16	0.46
1:C:76:LYS:NZ	1:C:121:SER:O	2.50	0.46
1:C:157:ALA:HA	1:C:349:MET:CE	2.46	0.46
1:C:177:ASP:OD1	1:C:179:ASP:HB2	2.16	0.46
1:A:81:PHE:CZ	1:A:327:GLU:HB3	2.52	0.45
1:A:87:THR:OG1	1:A:313:GLY:HA2	2.16	0.45
1:A:451:ASN:H	1:A:454:GLN:NE2	2.14	0.45
1:B:393:MET:SD	1:D:393:MET:HG3	2.56	0.45
1:C:499:TYR:C	1:C:501:GLU:H	2.19	0.45
1:D:235:TYR:N	1:D:235:TYR:CD1	2.84	0.45
1:D:286:SER:O	1:D:290:ILE:HG13	2.15	0.45
1:D:452:GLU:OE1	1:D:455:ARG:NE	2.45	0.45
1:A:296:PHE:CE2	1:A:346:PRO:HG2	2.50	0.45
1:B:10:GLN:HE21	1:C:172:GLN:NE2	2.14	0.45
1:C:280:ILE:HG13	1:C:280:ILE:O	2.16	0.45
1:C:430:ARG:NE	1:D:419:GLU:OE1	2.47	0.45
1:A:179:ASP:OD2	1:A:470:GLN:HG3	2.16	0.45
1:A:403:TYR:CE1	1:B:180:MET:HG2	2.51	0.45
1:B:14:TRP:HZ3	1:D:408:PHE:O	1.97	0.45
1:B:83:TYR:CA	1:B:108:ILE:HG12	2.47	0.45
1:B:98:VAL:O	3:B:2011:HOH:O	2.21	0.45
1:B:456:LYS:NZ	1:B:460:GLU:OE2	2.50	0.45
1:C:472:PHE:CD1	1:C:472:PHE:C	2.89	0.45
1:D:301:VAL:O	1:D:303:PRO:HD3	2.16	0.45
1:A:139:ASP:O	1:C:32:ASN:HA	2.16	0.45
1:B:36:ASP:HB3	1:C:430:ARG:CD	2.46	0.45
1:C:22:LYS:CE	3:C:2077:HOH:O	2.45	0.45
1:C:49:LEU:HD23	1:D:51:VAL:HG21	1.99	0.45
1:A:160:PHE:CZ	2:A:2000:HEM:C2B	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASP:O	1:B:12:LYS:HB3	2.17	0.45
1:B:241:ILE:HG22	1:B:242:LYS:N	2.32	0.45
1:B:479:LYS:O	1:B:482:SER:HB2	2.17	0.45
1:A:309:LEU:N	1:A:309:LEU:HD22	2.31	0.45
1:A:450:LEU:CA	1:A:454:GLN:NE2	2.79	0.45
1:B:95:LYS:HB3	1:B:224:ALA:N	2.31	0.45
1:B:116:ALA:O	1:B:168:LYS:NZ	2.49	0.45
1:B:139:ASP:O	1:D:32:ASN:HA	2.17	0.45
1:B:141:ASN:OD1	1:B:377:PRO:HB3	2.17	0.45
1:C:291:PHE:HD1	1:C:307:TYR:OH	1.99	0.45
1:C:303:PRO:HD2	1:C:307:TYR:HD2	1.82	0.45
1:D:351:GLN:OE1	3:D:2011:HOH:O	2.21	0.45
1:D:437:ASP:OD2	1:D:440:THR:HB	2.17	0.45
1:A:421:ARG:CZ	1:B:429:GLN:HE21	2.29	0.45
1:C:129:ARG:HB2	1:C:148:ASN:ND2	2.32	0.45
1:C:459:CYS:HA	1:C:492:ILE:HD13	1.99	0.45
1:D:188:ARG:HB3	1:D:190:GLU:OE1	2.16	0.45
1:A:155:ARG:NH2	1:A:190:GLU:HB3	2.25	0.45
1:B:85:GLU:HA	1:B:104:LYS:O	2.17	0.45
1:B:472:PHE:CD2	1:B:472:PHE:C	2.89	0.45
1:C:74:HIS:CD2	2:C:2002:HEM:C4D	3.05	0.45
1:D:81:PHE:HZ	1:D:327:GLU:HB3	1.82	0.45
1:D:106:THR:HG21	1:D:137:THR:HG22	1.99	0.45
1:D:367:PRO:HG2	1:D:390:PRO:CG	2.46	0.45
1:D:391:MET:HB3	1:D:391:MET:HE2	1.80	0.45
1:A:97:LYS:HD3	1:A:138:GLU:HB2	1.99	0.45
1:D:239:GLN:NE2	1:D:275:SER:H	2.15	0.45
1:D:285:PHE:N	1:D:285:PHE:CD1	2.85	0.44
1:D:442:VAL:HG12	1:D:484:VAL:HG11	1.99	0.44
1:B:76:LYS:HE3	1:B:121:SER:O	2.18	0.44
1:B:439:VAL:O	1:B:440:THR:C	2.56	0.44
1:B:485:HIS:O	1:B:488:TYR:CB	2.63	0.44
3:B:2017:HOH:O	1:D:386:GLN:HG2	2.16	0.44
1:C:485:HIS:CD2	1:C:486:PRO:N	2.85	0.44
1:D:87:THR:H	1:D:313:GLY:HA2	1.81	0.44
1:A:155:ARG:NH2	1:A:438:ASN:OD1	2.49	0.44
1:B:50:LEU:C	1:B:52:GLN:N	2.69	0.44
1:B:422:THR:HG22	1:B:423:HIS:N	2.32	0.44
1:B:470:GLN:O	1:B:473:ILE:HB	2.17	0.44
1:A:74:HIS:HA	1:A:114:THR:O	2.17	0.44
1:A:500:ASN:O	1:A:501:GLU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ARG:O	1:C:381:ARG:HG3	2.17	0.44
1:D:89:ASP:HB2	1:D:102:ILE:HD11	2.00	0.44
1:A:43:VAL:O	1:A:43:VAL:HG22	2.17	0.44
1:B:65:ARG:O	1:D:389:GLY:HA2	2.18	0.44
1:B:107:PRO:HG2	1:B:136:TYR:HB2	1.99	0.44
1:B:418:LEU:HG	1:D:35:GLY:HA3	2.00	0.44
1:B:452:GLU:OE2	1:B:491:ARG:NH1	2.50	0.44
1:B:469:ALA:HB1	1:B:473:ILE:HG21	2.00	0.44
1:C:26:LEU:HD21	1:C:37:LYS:HD3	2.00	0.44
1:C:89:ASP:HA	3:C:2108:HOH:O	2.18	0.44
1:C:492:ILE:O	1:C:495:LEU:HB2	2.18	0.44
1:D:206:ASP:HA	1:D:244:LEU:HG	1.99	0.44
1:D:357:TYR:O	1:D:361:HIS:ND1	2.50	0.44
1:A:33:PRO:CB	1:C:414:GLN:NE2	2.81	0.44
1:A:175:LEU:HD11	1:D:262:ARG:HB2	1.99	0.44
1:A:293:PHE:HZ	1:A:440:THR:HG21	1.82	0.44
1:B:114:THR:HB	1:B:115:VAL:H	1.66	0.44
1:B:120:GLY:CA	1:C:118:GLU:HB2	2.47	0.44
1:B:279:TYR:HB3	1:B:309:LEU:HB3	1.99	0.44
1:C:334:ASP:OD1	1:C:361:HIS:ND1	2.51	0.44
1:D:71:ARG:NH2	1:D:329:GLU:O	2.51	0.44
1:D:142:TRP:CE2	1:D:342:ILE:HD13	2.53	0.44
1:D:213:GLY:HA3	1:D:235:TYR:CD2	2.52	0.44
1:A:88:HIS:CD2	1:A:311:PRO:HG2	2.52	0.44
1:A:218:THR:OG1	1:A:232:LYS:HE2	2.16	0.44
1:A:498:LYS:O	1:A:499:TYR:C	2.56	0.44
1:C:450:LEU:HD12	1:C:450:LEU:HA	1.84	0.44
1:D:43:VAL:O	1:D:47:GLY:HA3	2.17	0.44
1:D:135:PHE:HB2	1:D:142:TRP:HB3	2.00	0.44
1:A:188:ARG:HB3	1:A:190:GLU:CD	2.38	0.44
1:B:15:LYS:HD2	1:D:408:PHE:HA	1.98	0.44
1:B:62:HIS:HD2	3:B:2004:HOH:O	1.99	0.44
1:C:346:PRO:O	1:C:347:ASP:C	2.56	0.44
1:C:369:TYR:O	1:C:371:GLN:N	2.51	0.44
1:D:381:ARG:HG2	1:D:381:ARG:NH1	2.33	0.44
1:A:273:TYR:HA	1:A:274:PRO:HD3	1.87	0.44
1:B:430:ARG:HG2	1:C:41:LEU:HD13	1.99	0.44
1:C:83:TYR:CD1	1:C:105:ARG:HD3	2.53	0.44
1:C:459:CYS:HA	1:C:492:ILE:HD11	2.00	0.44
1:D:86:VAL:O	1:D:103:GLY:N	2.49	0.44
1:D:86:VAL:HG12	1:D:88:HIS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ILE:HD13	1:D:280:ILE:H	1.83	0.44
1:D:291:PHE:HD1	1:D:293:PHE:N	2.13	0.44
1:D:369:TYR:C	1:D:371:GLN:N	2.71	0.44
1:A:291:PHE:HD2	1:A:293:PHE:O	2.01	0.43
1:C:126:ARG:HH11	1:C:126:ARG:CG	2.30	0.43
1:C:247:GLU:CG	1:C:248:ASP:N	2.81	0.43
1:C:308:PRO:O	1:C:310:ILE:HD12	2.18	0.43
1:C:434:ALA:C	1:C:435:ASN:ND2	2.72	0.43
1:A:51:VAL:HG12	1:B:51:VAL:N	2.33	0.43
1:B:36:ASP:CB	1:D:418:LEU:HD21	2.43	0.43
1:B:92:ARG:H	1:B:92:ARG:HG3	1.61	0.43
1:B:439:VAL:CG2	1:B:440:THR:H	2.28	0.43
1:B:466:LEU:HD21	1:B:474:GLN:HA	1.99	0.43
1:A:281:GLN:CG	1:A:309:LEU:HD13	2.46	0.43
1:B:281:GLN:O	1:B:302:TRP:HZ3	2.01	0.43
1:B:408:PHE:O	1:D:14:TRP:HZ3	2.01	0.43
1:C:439:VAL:O	1:C:440:THR:C	2.55	0.43
1:D:4:ARG:HB2	1:D:8:SER:OG	2.18	0.43
1:D:188:ARG:HB3	1:D:190:GLU:CD	2.38	0.43
1:D:427:ASP:HB2	1:D:429:GLN:NE2	2.29	0.43
1:D:488:TYR:HE1	1:D:492:ILE:HD11	1.84	0.43
1:A:85:GLU:OE1	1:A:105:ARG:HD3	2.17	0.43
1:A:112:PHE:HA	1:A:130:GLY:O	2.17	0.43
1:B:428:VAL:O	1:B:428:VAL:CG2	2.65	0.43
1:C:492:ILE:HG22	1:C:496:LEU:HD23	1.99	0.43
1:D:160:PHE:CG	2:D:2003:HEM:HAB	2.53	0.43
1:A:442:VAL:HG11	1:A:484:VAL:HG21	2.00	0.43
1:C:467:LYS:HE2	1:C:468:ASP:CG	2.39	0.43
1:D:74:HIS:HA	1:D:114:THR:O	2.19	0.43
1:D:189:PRO:C	1:D:191:SER:N	2.72	0.43
1:D:232:LYS:HB2	1:D:281:GLN:HB2	2.01	0.43
1:A:50:LEU:C	1:A:52:GLN:N	2.67	0.43
1:A:370:LEU:HD13	1:C:29:GLY:C	2.39	0.43
1:B:175:LEU:HD21	1:C:261:LEU:HB3	2.00	0.43
1:B:356:ALA:HB3	2:B:2001:HEM:HMB3	1.99	0.43
1:C:97:LYS:O	1:C:100:GLU:HB2	2.18	0.43
1:A:51:VAL:HG12	1:B:51:VAL:CA	2.48	0.43
1:A:452:GLU:HG2	1:A:455:ARG:NH1	2.34	0.43
1:B:37:LYS:HE3	1:B:59:GLU:OE1	2.18	0.43
1:B:96:ALA:C	1:B:98:VAL:H	2.22	0.43
1:B:182:TRP:NE1	1:B:465:HIS:ND1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:HB3	1:C:175:LEU:CD1	2.48	0.43
1:B:414:GLN:HB2	1:D:25:VAL:HG13	2.01	0.43
1:C:43:VAL:O	1:C:43:VAL:HG13	2.19	0.43
1:D:239:GLN:HE22	1:D:275:SER:H	1.65	0.43
1:A:440:THR:HG22	1:A:441:GLN:N	2.32	0.43
1:B:388:ASP:O	1:D:62:HIS:HE1	2.02	0.43
1:B:470:GLN:NE2	1:C:12:LYS:HD2	2.34	0.43
1:C:142:TRP:HB2	1:C:339:PRO:HD3	2.01	0.43
1:D:368:ASN:O	1:D:371:GLN:HB2	2.18	0.43
1:A:177:ASP:OD1	1:A:179:ASP:HB2	2.19	0.43
1:B:55:VAL:HG21	1:C:430:ARG:NH2	2.34	0.43
1:B:86:VAL:CG1	1:B:88:HIS:O	2.67	0.43
1:B:291:PHE:CG	1:B:292:PRO:HD2	2.54	0.43
1:C:111:ARG:HG3	1:C:328:VAL:HG13	2.01	0.43
1:D:136:TYR:O	1:D:379:ARG:HG3	2.19	0.43
1:A:353:ARG:NH2	2:A:2000:HEM:CHD	2.82	0.43
1:A:381:ARG:HH11	1:A:381:ARG:HD3	1.71	0.43
1:B:17:GLN:HE21	1:B:17:GLN:HB3	1.65	0.43
1:B:190:GLU:HA	1:B:438:ASN:HB3	2.01	0.43
1:B:385:TYR:CE2	1:B:404:TYR:HB2	2.54	0.43
1:C:177:ASP:HB3	1:C:180:MET:CE	2.48	0.43
1:C:184:PHE:O	1:C:188:ARG:HB2	2.19	0.43
1:D:276:TRP:HB2	1:D:315:LEU:HB2	2.01	0.43
1:A:349:MET:HE3	2:A:2000:HEM:CBB	2.49	0.42
1:B:353:ARG:CG	2:B:2001:HEM:CAB	2.76	0.42
1:B:442:VAL:HG12	1:B:484:VAL:HG11	2.01	0.42
1:C:338:MET:CE	1:C:344:PRO:HD3	2.49	0.42
1:C:460:GLU:HA	1:C:495:LEU:CD1	2.44	0.42
1:D:440:THR:HG22	1:D:441:GLN:N	2.34	0.42
1:D:485:HIS:CE1	1:D:486:PRO:HG2	2.54	0.42
1:A:148:ASN:HD22	1:A:148:ASN:H	1.67	0.42
1:A:148:ASN:HD22	1:A:148:ASN:N	2.16	0.42
1:A:395:ASP:OD2	1:C:323:ASN:CB	2.68	0.42
1:A:485:HIS:HD2	1:A:487:GLU:CB	2.32	0.42
1:B:238:ASP:OD2	1:B:277:THR:HG22	2.20	0.42
1:B:331:LEU:HD13	1:B:333:PHE:CZ	2.54	0.42
1:B:384:ASN:HB2	1:B:385:TYR:H	1.67	0.42
1:C:186:SER:HB3	1:C:476:LYS:HB3	2.01	0.42
1:C:293:PHE:CD1	1:C:293:PHE:N	2.87	0.42
1:C:351:GLN:O	1:C:354:LEU:HB2	2.19	0.42
1:D:97:LYS:CA	1:D:100:GLU:HG3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:PHE:O	1:B:100:GLU:C	2.57	0.42
1:B:131:PHE:N	1:B:146:GLY:O	2.39	0.42
1:B:238:ASP:HB2	1:B:275:SER:OG	2.19	0.42
1:B:404:TYR:OH	1:B:413:HIS:CD2	2.73	0.42
1:B:485:HIS:CE1	1:B:487:GLU:CG	2.78	0.42
1:C:112:PHE:HA	1:C:130:GLY:O	2.19	0.42
1:C:210:HIS:HB3	1:C:242:LYS:N	2.34	0.42
1:C:247:GLU:O	1:C:250:ALA:HB3	2.19	0.42
1:C:483:ASP:HB3	3:C:2044:HOH:O	2.19	0.42
1:A:62:HIS:HE1	1:C:387:ARG:O	2.03	0.42
1:A:85:GLU:O	1:A:313:GLY:HA3	2.20	0.42
1:A:155:ARG:NH2	1:A:190:GLU:CB	2.82	0.42
1:C:231:CYS:HA	1:C:302:TRP:CZ3	2.54	0.42
1:B:90:ILE:O	1:B:93:TYR:HB2	2.20	0.42
1:B:338:MET:HE2	1:B:342:ILE:HG22	2.02	0.42
1:C:199:PHE:CG	1:C:462:ILE:HG12	2.55	0.42
1:C:235:TYR:CD1	1:C:235:TYR:N	2.87	0.42
1:C:493:GLN:O	1:C:496:LEU:HB2	2.19	0.42
1:D:211:MET:O	1:D:237:THR:HB	2.20	0.42
1:A:160:PHE:CD2	2:A:2000:HEM:HMB2	2.53	0.42
1:A:160:PHE:CZ	2:A:2000:HEM:C3B	3.08	0.42
1:B:467:LYS:HD3	1:B:499:TYR:CE1	2.54	0.42
1:C:126:ARG:HE	1:C:203:GLY:HA3	1.84	0.42
1:C:236:LYS:HG3	1:C:279:TYR:CE2	2.51	0.42
1:C:357:TYR:CE2	2:C:2002:HEM:NA	2.86	0.42
1:D:296:PHE:HB3	1:D:347:ASP:HA	2.02	0.42
1:A:39:ASN:CG	1:D:432:ASN:HA	2.40	0.42
1:A:275:SER:HA	1:A:315:LEU:O	2.20	0.42
1:A:340:PRO:HG2	1:C:33:PRO:HG2	2.00	0.42
1:B:202:ARG:HH21	1:B:241:ILE:HD13	1.85	0.42
1:C:18:ARG:HG3	3:C:2092:HOH:O	2.19	0.42
1:D:246:VAL:HG23	1:D:247:GLU:OE1	2.20	0.42
1:A:209:ARG:HB2	3:A:2030:HOH:O	2.19	0.42
1:A:209:ARG:NH2	1:A:263:ASP:OD2	2.41	0.42
1:A:357:TYR:HB2	1:A:358:PRO:HD3	2.02	0.42
1:B:294:ASN:CG	1:C:46:ARG:NH1	2.73	0.42
1:C:279:TYR:HA	1:C:310:ILE:O	2.18	0.42
1:C:335:PRO:HD2	1:C:357:TYR:HB2	2.01	0.42
1:D:110:VAL:CG2	1:D:317:LEU:HD21	2.48	0.42
1:D:291:PHE:HA	1:D:292:PRO:HD3	1.83	0.42
1:A:235:TYR:CD1	1:A:235:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:TYR:CE1	1:C:282:VAL:HG11	2.54	0.42
1:A:387:ARG:HB3	1:A:388:ASP:OD1	2.19	0.42
1:A:391:MET:HE3	1:A:393:MET:HE3	2.02	0.42
1:B:65:ARG:HD3	1:D:367:PRO:HG3	2.01	0.42
1:B:88:HIS:HB2	1:B:311:PRO:O	2.20	0.42
1:B:208:HIS:HD2	1:B:264:LEU:HD22	1.85	0.42
1:A:188:ARG:HD3	1:B:405:PRO:CD	2.50	0.41
1:B:65:ARG:CD	1:D:367:PRO:HB3	2.50	0.41
1:B:252:LEU:HG	1:B:259:TYR:CD1	2.55	0.41
1:B:275:SER:HA	1:B:315:LEU:O	2.20	0.41
1:C:43:VAL:CG1	1:C:48:PRO:HD2	2.50	0.41
1:C:151:ILE:CG1	1:C:194:GLN:HG2	2.33	0.41
1:D:231:CYS:HA	1:D:302:TRP:HZ3	1.85	0.41
1:A:146:GLY:HA2	2:A:2000:HEM:HBC2	2.02	0.41
1:A:349:MET:CE	2:A:2000:HEM:CBB	2.98	0.41
1:A:419:GLU:OE2	1:B:430:ARG:NH1	2.53	0.41
1:B:73:VAL:HG23	2:B:2001:HEM:C1A	2.56	0.41
1:B:472:PHE:CZ	1:B:473:ILE:HG13	2.56	0.41
1:C:50:LEU:HD23	1:D:50:LEU:CD2	2.51	0.41
1:C:72:VAL:HG12	2:C:2002:HEM:HMA1	2.01	0.41
1:C:98:VAL:HG13	1:C:99:PHE:CD1	2.55	0.41
1:D:97:LYS:HA	1:D:100:GLU:CG	2.50	0.41
1:A:11:MET:CE	1:D:179:ASP:HB3	2.51	0.41
1:B:100:GLU:HB3	1:B:101:HIS:H	1.54	0.41
1:C:231:CYS:HA	1:C:281:GLN:O	2.20	0.41
1:D:26:LEU:HD13	1:D:34:VAL:HG21	2.01	0.41
1:D:73:VAL:O	1:D:74:HIS:HB2	2.20	0.41
1:D:476:LYS:O	1:D:480:ASN:OD1	2.37	0.41
1:A:234:HIS:O	1:A:278:LEU:HD12	2.20	0.41
1:A:234:HIS:O	1:A:279:TYR:N	2.42	0.41
1:C:99:PHE:O	1:C:100:GLU:C	2.58	0.41
1:C:395:ASP:HB3	3:C:2214:HOH:O	2.20	0.41
1:D:142:TRP:HB2	1:D:339:PRO:CD	2.51	0.41
1:A:41:LEU:HD12	1:D:430:ARG:HG3	2.02	0.41
1:A:129:ARG:H	1:A:148:ASN:ND2	2.18	0.41
1:A:209:ARG:HG2	1:A:274:PRO:HB3	2.02	0.41
1:B:236:LYS:O	1:B:276:TRP:HA	2.20	0.41
1:B:238:ASP:CG	1:B:277:THR:HG22	2.41	0.41
1:B:262:ARG:O	1:B:263:ASP:C	2.58	0.41
1:B:369:TYR:C	1:B:371:GLN:N	2.73	0.41
1:C:169:ARG:HD3	1:C:174:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:PHE:CD1	2:D:2003:HEM:HAB	2.55	0.41
1:D:182:TRP:CD2	1:D:466:LEU:HD13	2.55	0.41
1:D:210:HIS:CD2	1:D:242:LYS:HB2	2.56	0.41
1:D:327:GLU:O	1:D:374:VAL:HG21	2.20	0.41
1:A:66:GLU:HG2	1:C:387:ARG:O	2.20	0.41
1:A:83:TYR:CD1	1:A:83:TYR:C	2.94	0.41
1:B:36:ASP:HB3	1:C:430:ARG:HD3	2.02	0.41
1:B:83:TYR:HA	1:B:108:ILE:HG12	2.02	0.41
1:B:97:LYS:O	1:B:104:LYS:NZ	2.53	0.41
1:B:120:GLY:N	1:C:118:GLU:HB2	2.36	0.41
1:C:22:LYS:CD	3:C:2077:HOH:O	2.67	0.41
1:C:49:LEU:CD2	1:D:51:VAL:HG21	2.50	0.41
1:C:151:ILE:CG2	1:C:301:VAL:HG13	2.51	0.41
1:D:6:PRO:HD2	1:D:266:ASN:OD1	2.21	0.41
1:B:106:THR:HG21	1:B:137:THR:HG22	2.02	0.41
1:B:454:GLN:HA	1:B:457:ARG:HH12	1.83	0.41
1:C:202:ARG:HG3	3:C:2131:HOH:O	2.19	0.41
1:C:234:HIS:CD2	1:C:309:LEU:HD11	2.55	0.41
1:C:251:ARG:O	1:C:252:LEU:C	2.58	0.41
1:D:26:LEU:HB3	1:D:34:VAL:CG2	2.48	0.41
1:D:237:THR:HA	1:D:276:TRP:CD1	2.55	0.41
1:A:82:GLY:HA3	1:A:316:VAL:O	2.21	0.41
1:A:177:ASP:HB3	1:A:180:MET:CG	2.51	0.41
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.91	0.41
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.74	0.41
1:A:358:PRO:O	1:A:361:HIS:HB2	2.20	0.41
1:A:391:MET:CE	1:A:393:MET:HE3	2.50	0.41
1:B:25:VAL:HG13	1:D:414:GLN:CG	2.51	0.41
1:B:201:ASP:HB3	1:B:243:ASN:ND2	2.36	0.41
1:B:323:ASN:CG	1:D:396:ASN:HB3	2.40	0.41
1:B:430:ARG:HB3	1:C:39:ASN:O	2.21	0.41
1:B:467:LYS:HG3	1:B:468:ASP:N	2.35	0.41
1:C:472:PHE:CZ	1:C:473:ILE:HG13	2.55	0.41
1:D:155:ARG:NH1	1:D:299:THR:HG21	2.35	0.41
1:D:201:ASP:O	1:D:243:ASN:HB3	2.20	0.41
1:D:467:LYS:HE2	1:D:499:TYR:CE1	2.56	0.41
1:A:108:ILE:HD13	1:A:315:LEU:HD22	2.03	0.41
1:A:349:MET:SD	2:A:2000:HEM:HBB1	2.60	0.41
1:A:433:SER:HA	1:A:436:ASP:OD1	2.21	0.41
1:B:112:PHE:O	1:B:113:SER:HB3	2.21	0.41
1:B:223:ASN:ND2	1:B:227:GLU:HB2	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:TYR:CD2	1:B:404:TYR:HB2	2.56	0.41
1:B:429:GLN:C	1:C:41:LEU:HD12	2.41	0.41
1:B:439:VAL:CG2	1:B:440:THR:N	2.81	0.41
1:C:229:VAL:HG11	3:C:2115:HOH:O	2.20	0.41
1:C:237:THR:OG1	1:C:239:GLN:HG2	2.21	0.41
1:D:74:HIS:CE1	1:D:115:VAL:HG22	2.56	0.41
1:D:124:THR:HG22	1:D:244:LEU:HD12	2.03	0.41
1:D:427:ASP:O	1:D:429:GLN:HG2	2.20	0.41
1:D:460:GLU:CG	1:D:495:LEU:HD11	2.50	0.41
1:B:65:ARG:HA	1:C:363:HIS:CD2	2.56	0.41
1:B:145:VAL:HG22	1:B:333:PHE:HB3	2.01	0.41
1:C:110:VAL:CG1	1:C:111:ARG:N	2.83	0.41
1:C:485:HIS:HA	1:C:486:PRO:HD2	1.65	0.41
1:D:142:TRP:HB2	1:D:339:PRO:CG	2.51	0.41
1:D:155:ARG:NH1	1:D:299:THR:CG2	2.84	0.41
1:D:324:TYR:CE1	1:D:328:VAL:HG11	2.56	0.41
1:D:445:PHE:O	1:D:449:VAL:HB	2.20	0.41
1:A:172:GLN:OE1	1:D:10:GLN:NE2	2.46	0.40
1:A:410:ALA:HB1	1:A:411:PRO:HD2	2.02	0.40
1:C:73:VAL:CG2	2:C:2002:HEM:C2A	3.04	0.40
1:C:228:ALA:C	1:C:229:VAL:CG1	2.89	0.40
1:C:364:ARG:HE	2:C:2002:HEM:CGA	2.27	0.40
1:C:402:ASN:HB2	1:D:165:HIS:HD1	1.86	0.40
1:C:451:ASN:CG	1:C:454:GLN:HG3	2.40	0.40
1:D:385:TYR:HA	1:D:387:ARG:HH12	1.86	0.40
1:A:25:VAL:HG11	1:A:33:PRO:HB3	2.02	0.40
1:A:155:ARG:HH21	1:A:190:GLU:CB	2.27	0.40
1:A:216:SER:HB3	1:A:298:LEU:HD11	2.03	0.40
1:B:110:VAL:HG12	1:B:111:ARG:N	2.36	0.40
1:B:353:ARG:HD2	2:B:2001:HEM:HHC	2.03	0.40
1:D:189:PRO:CG	1:D:480:ASN:HD22	2.23	0.40
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.87	0.40
1:A:92:ARG:HH11	1:A:92:ARG:CB	2.33	0.40
1:A:242:LYS:HD3	1:A:243:ASN:N	2.36	0.40
1:B:126:ARG:HE	1:B:199:PHE:HA	1.87	0.40
1:B:414:GLN:HA	1:B:415:PRO:HD2	1.92	0.40
1:D:116:ALA:O	1:D:168:LYS:NZ	2.45	0.40
1:D:124:THR:HG22	1:D:244:LEU:CD1	2.51	0.40
1:D:209:ARG:HG2	1:D:274:PRO:CB	2.49	0.40
1:A:160:PHE:CE2	2:A:2000:HEM:CHB	3.05	0.40
1:A:295:PRO:HD3	1:D:46:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:HD21	2:A:2000:HEM:CMC	2.51	0.40
1:B:49:LEU:HB2	1:C:351:GLN:HB3	2.02	0.40
1:B:155:ARG:HA	1:B:349:MET:HG3	2.03	0.40
1:D:115:VAL:HB	1:D:127:ASP:OD2	2.21	0.40
1:D:156:ASP:OD1	1:D:158:LEU:HB2	2.22	0.40
1:D:189:PRO:C	1:D:191:SER:H	2.24	0.40
1:D:338:MET:CE	1:D:342:ILE:HG22	2.51	0.40
1:A:159:LEU:HD21	1:A:188:ARG:NE	2.37	0.40
1:A:232:LYS:HG3	1:A:302:TRP:CD2	2.57	0.40
1:A:377:PRO:HB3	1:C:30:GLY:O	2.21	0.40
1:A:485:HIS:HD2	1:A:487:GLU:HB3	1.87	0.40
1:B:112:PHE:CG	1:B:208:HIS:HB3	2.57	0.40
1:B:382:VAL:HA	1:D:27:THR:OG1	2.21	0.40
1:B:442:VAL:O	1:B:445:PHE:HB3	2.21	0.40
1:B:466:LEU:HD11	1:B:477:ALA:HB1	2.04	0.40
1:C:291:PHE:CE2	1:C:293:PHE:O	2.75	0.40
1:D:16:GLU:HG3	1:D:16:GLU:H	1.66	0.40
1:D:26:LEU:O	1:D:34:VAL:HG22	2.22	0.40
1:D:395:ASP:O	1:D:396:ASN:CB	2.70	0.40
1:D:427:ASP:O	1:D:428:VAL:C	2.57	0.40
1:D:496:LEU:O	1:D:500:ASN:N	2.48	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2109:HOH:O	3:C:2220:HOH:O[3_655]	2.15	0.05
1:C:85:GLU:OE2	3:C:2084:HOH:O[3_645]	2.15	0.05
1:C:102:ILE:O	3:B:2221:HOH:O[3_645]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/506 (98%)	452 (91%)	42 (8%)	3 (1%)	25	56
1	B	497/506 (98%)	419 (84%)	70 (14%)	8 (2%)	9	31
1	C	497/506 (98%)	434 (87%)	55 (11%)	8 (2%)	9	31
1	D	497/506 (98%)	435 (88%)	55 (11%)	7 (1%)	11	34
All	All	1988/2024 (98%)	1740 (88%)	222 (11%)	26 (1%)	12	36

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	B	100	GLU
1	B	124	THR
1	D	36	ASP
1	A	440	THR
1	B	121	SER
1	B	440	THR
1	B	448	LYS
1	D	413	HIS
1	A	100	GLU
1	B	437	ASP
1	B	446	TYR
1	C	485	HIS
1	D	411	PRO
1	C	100	GLU
1	C	440	THR
1	D	91	THR
1	B	192	LEU
1	C	370	LEU
1	D	24	ASP
1	D	440	THR
1	C	121	SER
1	C	347	ASP
1	D	216	SER
1	C	181	VAL
1	C	127	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/437 (99%)	396 (92%)	35 (8%)	11	33
1	B	431/437 (99%)	380 (88%)	51 (12%)	5	16
1	C	431/437 (99%)	387 (90%)	44 (10%)	7	22
1	D	431/437 (99%)	399 (93%)	32 (7%)	13	37
All	All	1724/1748 (99%)	1562 (91%)	162 (9%)	8	26

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	ARG
1	A	18	ARG
1	A	37	LYS
1	A	41	LEU
1	A	43	VAL
1	A	49	LEU
1	A	50	LEU
1	A	51	VAL
1	A	54	VAL
1	A	92	ARG
1	A	118	GLU
1	A	131	PHE
1	A	148	ASN
1	A	149	THR
1	A	194	GLN
1	A	229	VAL
1	A	231	CYS
1	A	235	TYR
1	A	263	ASP
1	A	306	ASP
1	A	336	SER
1	A	374	VAL
1	A	379	ARG
1	A	388	ASP
1	A	402	ASN
1	A	407	SER
1	A	413	HIS
1	A	421	ARG
1	A	435	ASN

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Mol	Chain	Res	Type
1	A	436	ASP
1	A	438	ASN
1	A	488	TYR
1	A	495	LEU
1	A	501	GLU
1	B	18	ARG
1	B	21	GLN
1	B	32	ASN
1	B	37	LYS
1	B	41	LEU
1	B	43	VAL
1	B	46	ARG
1	B	49	LEU
1	B	67	ARG
1	B	73	VAL
1	B	85	GLU
1	B	92	ARG
1	B	94	SER
1	B	95	LYS
1	B	101	HIS
1	B	114	THR
1	B	121	SER
1	B	124	THR
1	B	126	ARG
1	B	127	ASP
1	B	131	PHE
1	B	149	THR
1	B	162	SER
1	B	200	SER
1	B	202	ARG
1	B	220	LYS
1	B	232	LYS
1	B	235	TYR
1	B	252	LEU
1	B	272	ASN
1	B	277	THR
1	B	290	ILE
1	B	319	ARG
1	B	330	GLN
1	B	374	VAL
1	B	381	ARG
1	B	393	MET

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Mol	Chain	Res	Type
1	B	394	MET
1	B	402	ASN
1	B	412	GLU
1	B	416	SER
1	B	427	ASP
1	B	447	LEU
1	B	457	ARG
1	B	466	LEU
1	B	472	PHE
1	B	476	LYS
1	B	488	TYR
1	B	498	LYS
1	B	499	TYR
1	B	501	GLU
1	C	3	ASN
1	C	4	ARG
1	C	18	ARG
1	C	26	LEU
1	C	34	VAL
1	C	46	ARG
1	C	52	GLN
1	C	65	ARG
1	C	92	ARG
1	C	97	LYS
1	C	105	ARG
1	C	131	PHE
1	C	149	THR
1	C	194	GLN
1	C	200	SER
1	C	229	VAL
1	C	235	TYR
1	C	239	GLN
1	C	245	SER
1	C	248	ASP
1	C	286	SER
1	C	289	GLU
1	C	293	PHE
1	C	336	SER
1	C	345	SER
1	C	381	ARG
1	C	402	ASN
1	C	413	HIS

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Mol	Chain	Res	Type
1	C	414	GLN
1	C	418	LEU
1	C	421	ARG
1	C	427	ASP
1	C	436	ASP
1	C	438	ASN
1	C	450	LEU
1	C	451	ASN
1	C	453	GLU
1	C	454	GLN
1	C	467	LYS
1	C	470	GLN
1	C	471	LEU
1	C	472	PHE
1	C	488	TYR
1	C	501	GLU
1	D	18	ARG
1	D	22	LYS
1	D	26	LEU
1	D	60	MET
1	D	105	ARG
1	D	127	ASP
1	D	131	PHE
1	D	148	ASN
1	D	193	HIS
1	D	220	LYS
1	D	229	VAL
1	D	235	TYR
1	D	247	GLU
1	D	275	SER
1	D	280	ILE
1	D	286	SER
1	D	306	ASP
1	D	314	LYS
1	D	319	ARG
1	D	392	CYS
1	D	397	GLN
1	D	403	TYR
1	D	409	SER
1	D	412	GLU
1	D	413	HIS
1	D	421	ARG

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Mol	Chain	Res	Type
1	D	435	ASN
1	D	438	ASN
1	D	444	THR
1	D	467	LYS
1	D	479	LYS
1	D	488	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	21	GLN
1	A	74	HIS
1	A	148	ASN
1	A	254	HIS
1	A	304	HIS
1	A	320	ASN
1	A	337	ASN
1	A	420	HIS
1	A	429	GLN
1	A	454	GLN
1	A	480	ASN
1	A	485	HIS
1	B	17	GLN
1	B	21	GLN
1	B	32	ASN
1	B	62	HIS
1	B	208	HIS
1	B	239	GLN
1	B	243	ASN
1	B	272	ASN
1	B	337	ASN
1	B	396	ASN
1	B	402	ASN
1	B	413	HIS
1	B	435	ASN
1	B	461	ASN
1	B	485	HIS
1	C	17	GLN
1	C	21	GLN
1	C	32	ASN
1	C	52	GLN

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Mol	Chain	Res	Type
1	C	172	GLN
1	C	210	HIS
1	C	239	GLN
1	C	272	ASN
1	C	337	ASN
1	C	402	ASN
1	C	414	GLN
1	C	423	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	485	HIS
1	C	493	GLN
1	D	21	GLN
1	D	32	ASN
1	D	52	GLN
1	D	74	HIS
1	D	147	ASN
1	D	148	ASN
1	D	170	ASN
1	D	193	HIS
1	D	254	HIS
1	D	304	HIS
1	D	337	ASN
1	D	363	HIS
1	D	368	ASN
1	D	386	GLN
1	D	420	HIS
1	D	429	GLN
1	D	438	ASN
1	D	470	GLN
1	D	480	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	41,50,50	2.29	8 (19%)	45,82,82	1.00	2 (4%)
2	HEM	C	2002	1	41,50,50	1.50	7 (17%)	45,82,82	1.00	2 (4%)
2	HEM	B	2001	1	41,50,50	1.70	7 (17%)	45,82,82	0.98	2 (4%)
2	HEM	A	2000	1	41,50,50	1.62	6 (14%)	45,82,82	0.99	2 (4%)

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	-	3/12/54/54	-
2	HEM	C	2002	1	-	3/12/54/54	-
2	HEM	B	2001	1	-	3/12/54/54	-
2	HEM	A	2000	1	-	3/12/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2003	HEM	FE-ND	10.94	2.51	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	HEM	C4A-CHB	6.22	1.58	1.41
2	A	2000	HEM	CMC-C2C	-5.40	1.38	1.51
2	B	2001	HEM	C3C-CAC	-4.16	1.39	1.47
2	A	2000	HEM	C3C-CAC	-4.16	1.39	1.47
2	D	2003	HEM	C3C-CAC	-4.15	1.39	1.47
2	C	2002	HEM	C3C-CAC	-4.15	1.39	1.47
2	D	2003	HEM	FE-NB	-3.91	1.77	1.96
2	C	2002	HEM	FE-ND	3.26	2.13	1.96
2	B	2001	HEM	CAB-C3B	-3.19	1.38	1.47
2	D	2003	HEM	CAB-C3B	-3.17	1.38	1.47
2	C	2002	HEM	CAB-C3B	-3.16	1.38	1.47
2	A	2000	HEM	CAB-C3B	-3.11	1.39	1.47
2	A	2000	HEM	CHA-C4D	2.65	1.41	1.35
2	C	2002	HEM	CHA-C4D	2.64	1.41	1.35
2	D	2003	HEM	CHA-C4D	2.64	1.41	1.35
2	B	2001	HEM	CHA-C4D	2.64	1.41	1.35
2	D	2003	HEM	CBB-CAB	2.50	1.42	1.30
2	C	2002	HEM	CBB-CAB	2.50	1.42	1.30
2	A	2000	HEM	CBB-CAB	2.49	1.42	1.30
2	B	2001	HEM	CBB-CAB	2.49	1.42	1.30
2	C	2002	HEM	CBC-CAC	2.46	1.45	1.29
2	B	2001	HEM	CBC-CAC	2.44	1.45	1.29
2	D	2003	HEM	CBC-CAC	2.44	1.45	1.29
2	D	2003	HEM	C3C-C2C	-2.37	1.37	1.40
2	C	2002	HEM	C3C-C2C	-2.36	1.37	1.40
2	A	2000	HEM	C3C-C2C	-2.33	1.37	1.40
2	B	2001	HEM	C3C-C2C	-2.26	1.37	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	HEM	CBA-CAA-C2A	-2.68	108.05	112.62
2	C	2002	HEM	CBA-CAA-C2A	-2.66	108.08	112.62
2	D	2003	HEM	CBA-CAA-C2A	-2.65	108.10	112.62
2	A	2000	HEM	CBA-CAA-C2A	-2.63	108.13	112.62
2	C	2002	HEM	CMB-C2B-C1B	2.52	128.88	125.04
2	D	2003	HEM	CMB-C2B-C1B	2.52	128.88	125.04
2	B	2001	HEM	CMB-C2B-C1B	2.51	128.87	125.04
2	A	2000	HEM	CMB-C2B-C1B	2.48	128.82	125.04

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	HEM	C2B-C3B-CAB-CBB
2	A	2000	HEM	C4B-C3B-CAB-CBB
2	B	2001	HEM	C2B-C3B-CAB-CBB
2	B	2001	HEM	C4B-C3B-CAB-CBB
2	C	2002	HEM	C2B-C3B-CAB-CBB
2	C	2002	HEM	C4B-C3B-CAB-CBB
2	D	2003	HEM	C2B-C3B-CAB-CBB
2	D	2003	HEM	C4B-C3B-CAB-CBB
2	C	2002	HEM	CAA-CBA-CGA-O2A
2	A	2000	HEM	CAA-CBA-CGA-O2A
2	B	2001	HEM	CAA-CBA-CGA-O2A
2	D	2003	HEM	CAA-CBA-CGA-O2A

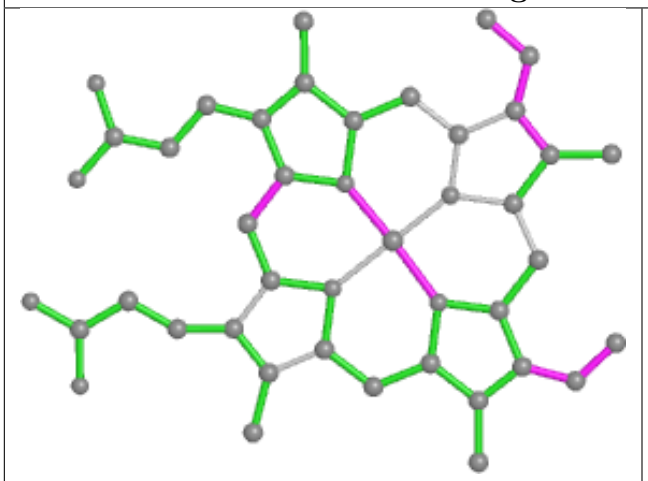
There are no ring outliers.

4 monomers are involved in 111 short contacts:

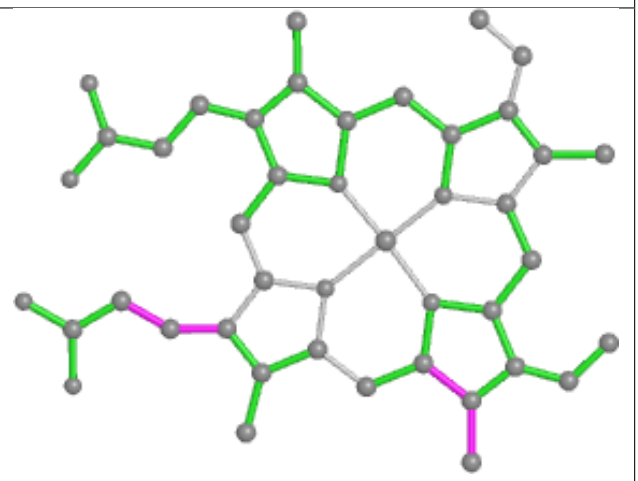
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2003	HEM	29	0
2	C	2002	HEM	18	0
2	B	2001	HEM	28	0
2	A	2000	HEM	36	0

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

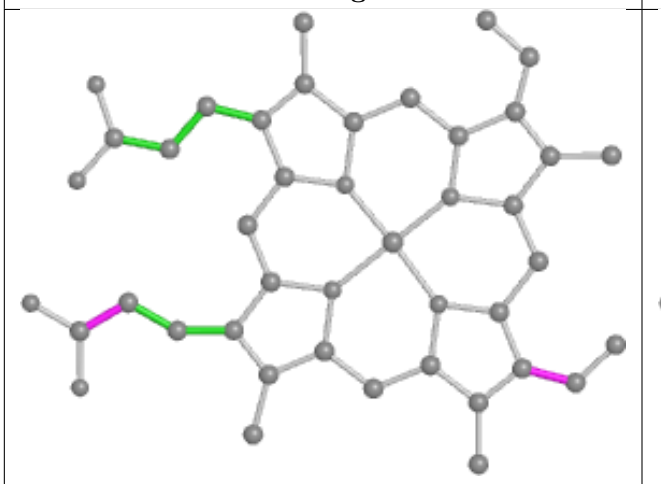
Ligand HEM D 2003



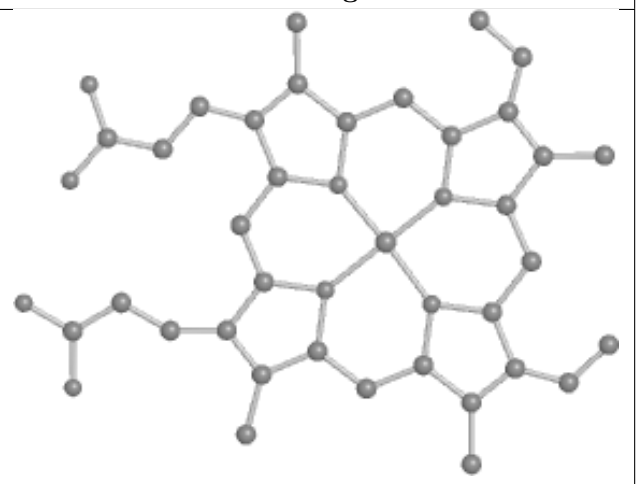
Bond lengths



Bond angles

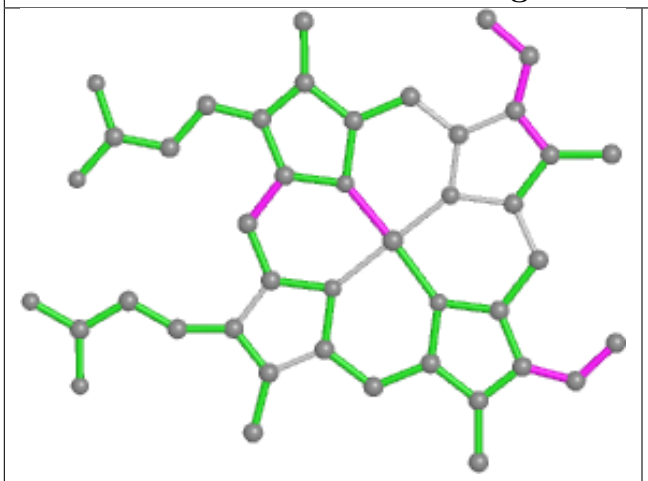


Torsions

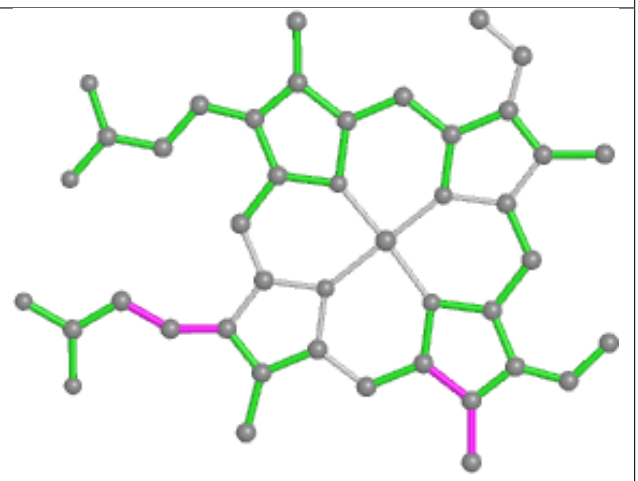


Rings

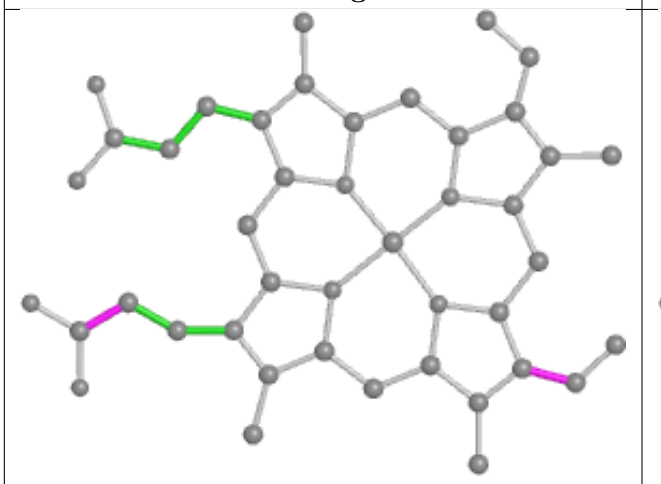
Ligand HEM C 2002



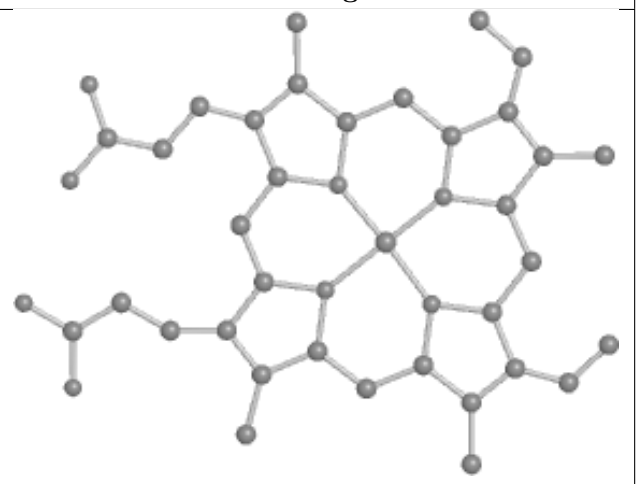
Bond lengths



Bond angles

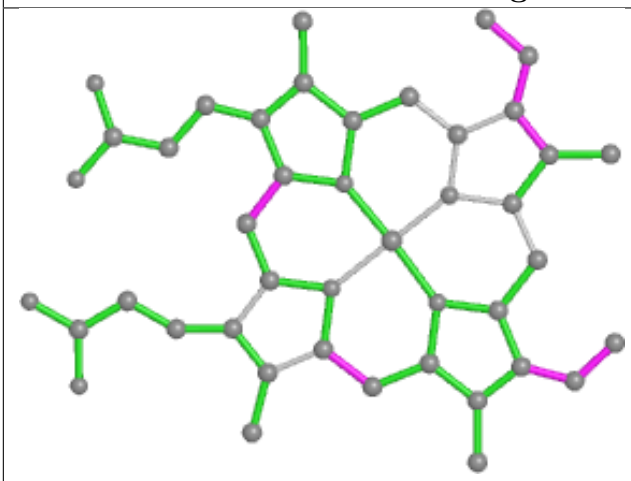


Torsions

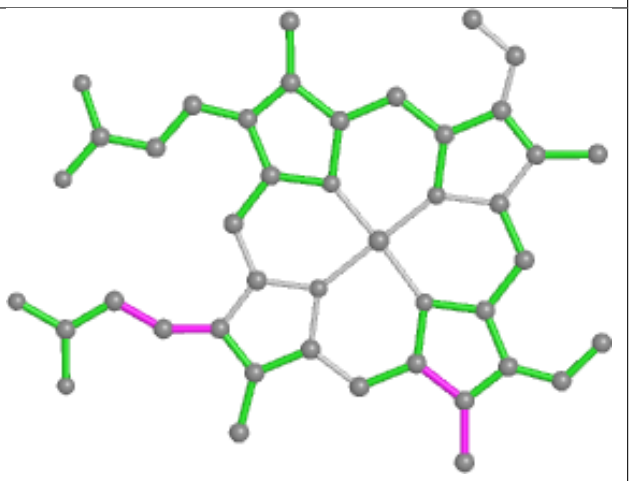


Rings

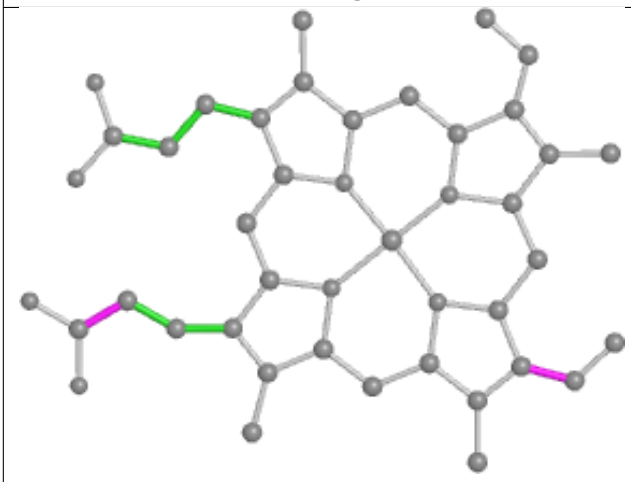
Ligand HEM B 2001



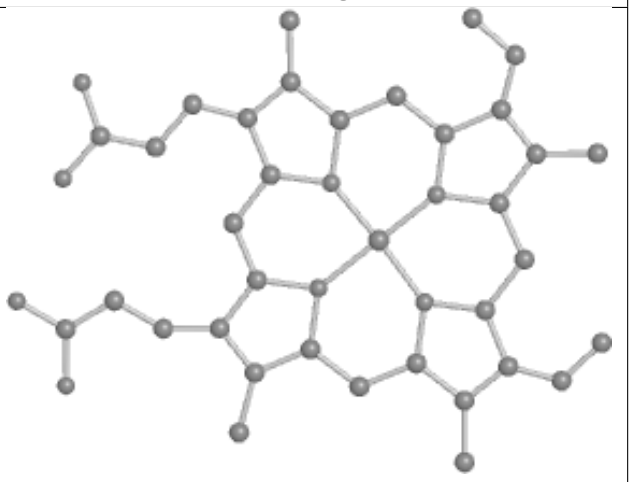
Bond lengths



Bond angles

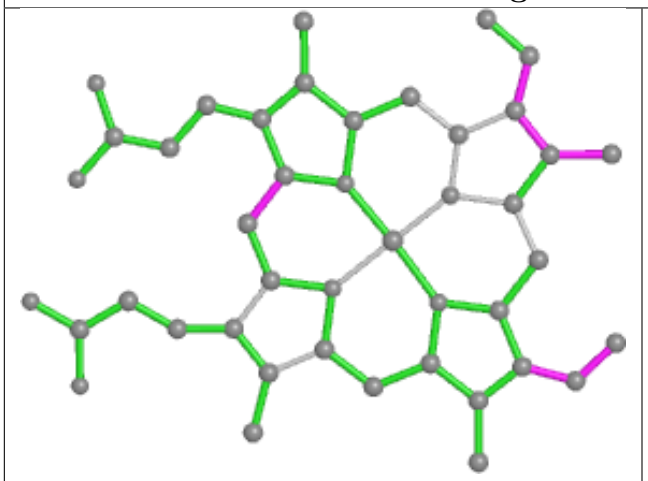


Torsions

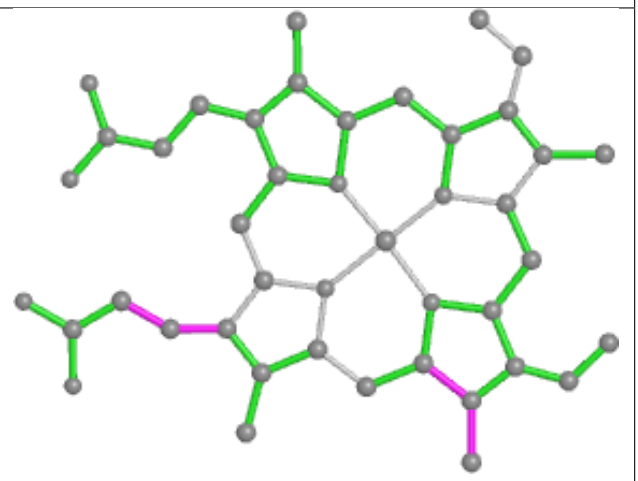


Rings

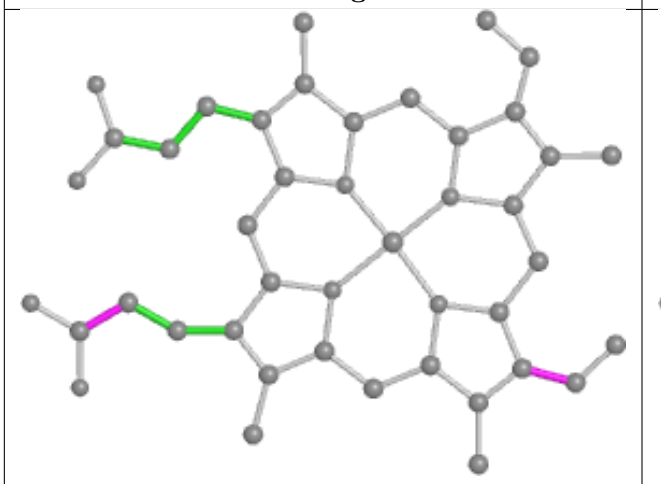
Ligand HEM A 2000



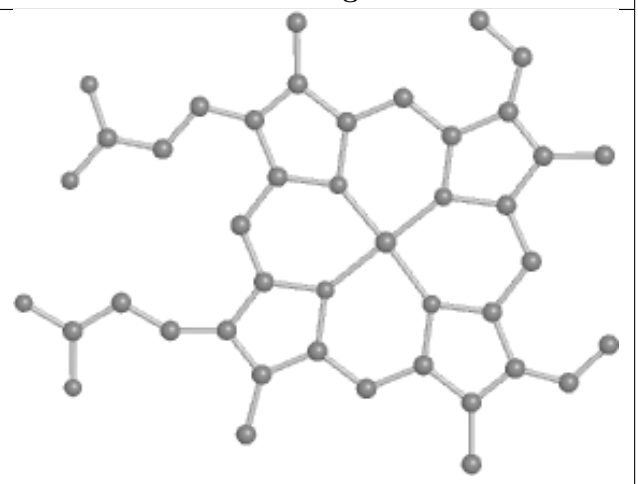
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.49	3 (0%) 89 86	8, 24, 48, 89	0
1	B	499/506 (98%)	-0.33	6 (1%) 79 73	10, 31, 56, 88	0
1	C	499/506 (98%)	-0.44	0 100 100	6, 27, 56, 81	1 (0%)
1	D	499/506 (98%)	-0.35	3 (0%) 89 86	10, 30, 60, 87	0
All	All	1996/2024 (98%)	-0.40	12 (0%) 89 86	6, 28, 55, 89	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	ALA	5.4
1	B	20	ALA	3.9
1	A	3	ASN	3.4
1	B	19	ALA	2.7
1	A	19	ALA	2.6
1	B	3	ASN	2.4
1	B	270	THR	2.3
1	B	421	ARG	2.3
1	D	20	ALA	2.3
1	B	21	GLN	2.2
1	D	426	GLY	2.1
1	D	3	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

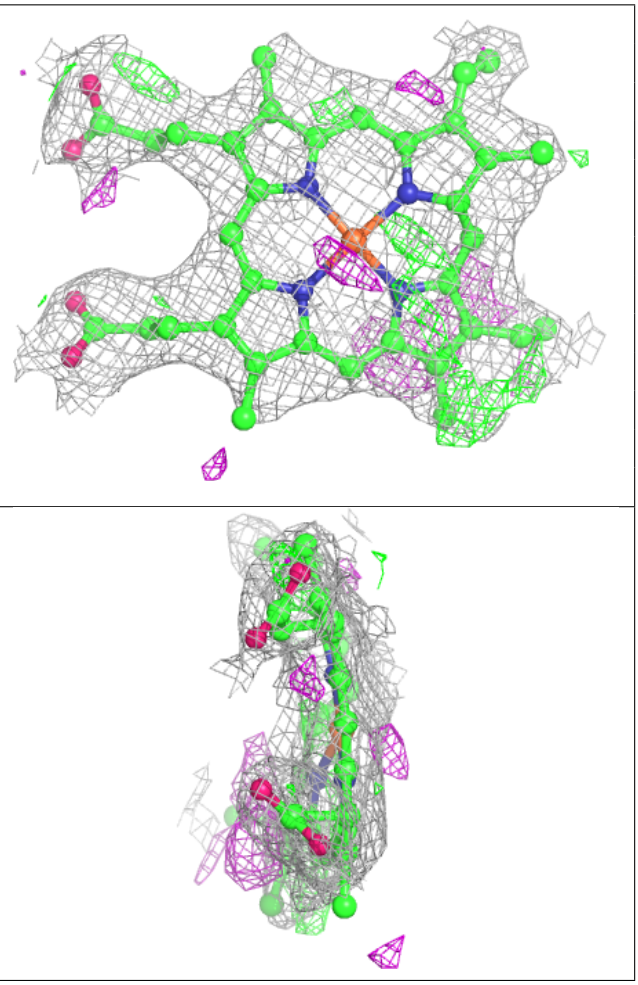
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	2001	43/43	0.92	0.25	16,35,50,71	0
2	HEM	D	2003	43/43	0.93	0.22	17,33,49,60	0
2	HEM	A	2000	43/43	0.95	0.19	4,30,44,49	0
2	HEM	C	2002	43/43	0.96	0.16	15,31,42,91	0

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

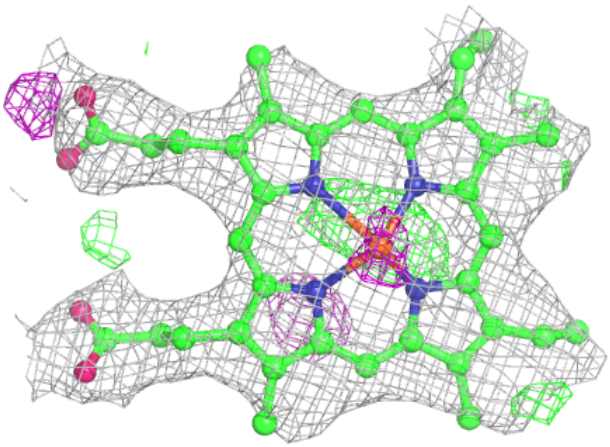
Electron density around HEM B 2001:

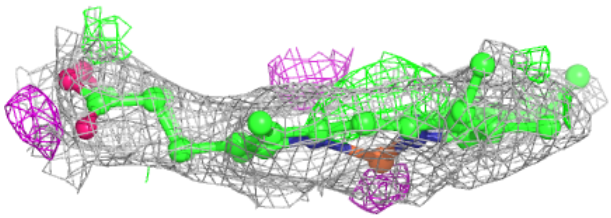
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

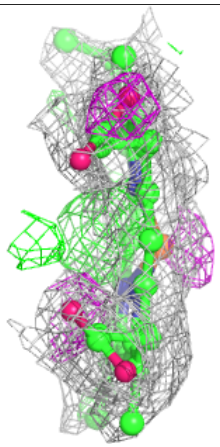


Electron density around HEM D 2003:

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

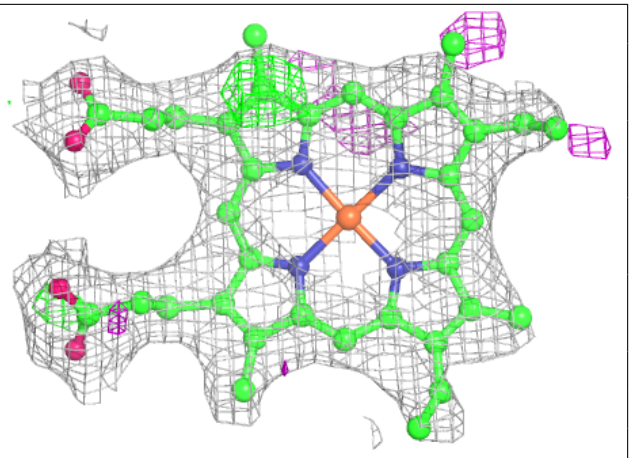


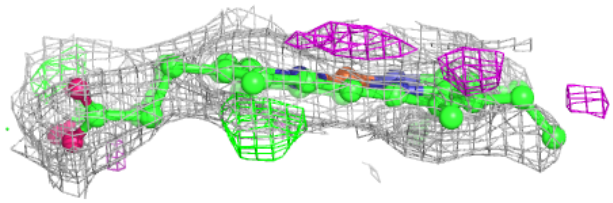


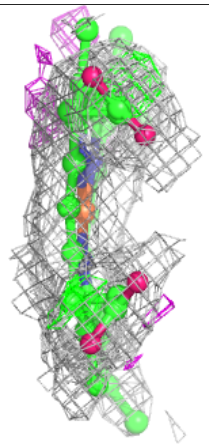


Electron density around HEM A 2000:

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

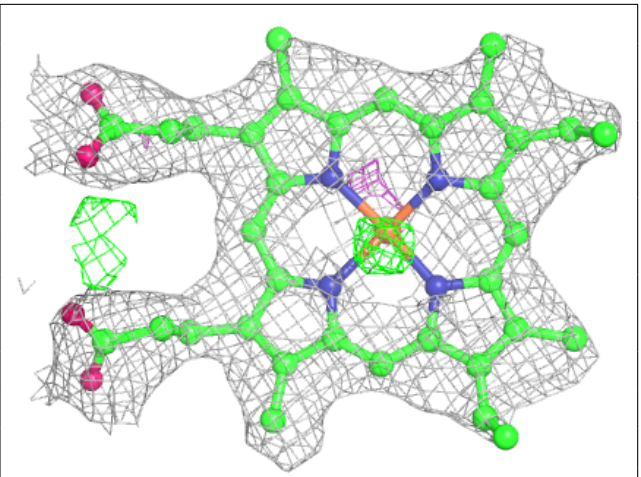


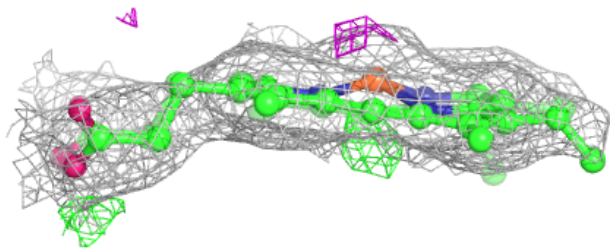


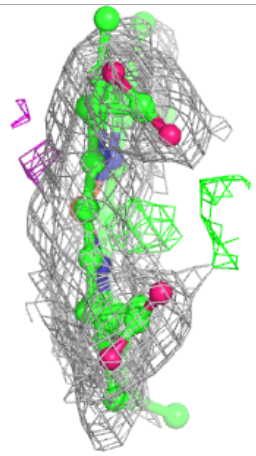


Electron density around HEM C 2002:

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







6.5 Other polymers (i)

There are no such residues in this entry.