



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:43 am BST

PDB ID : 1TH3
Title : Crystal structure of NADPH depleted bovine live catalase complexed with cyanide
Authors : Sugadev, R.; Balasundaresan, D.; Ponnuswamy, M.N.; Kumaran, D.; Swaminathan, S.; Sekar, K.
Deposited on : 2004-06-01
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

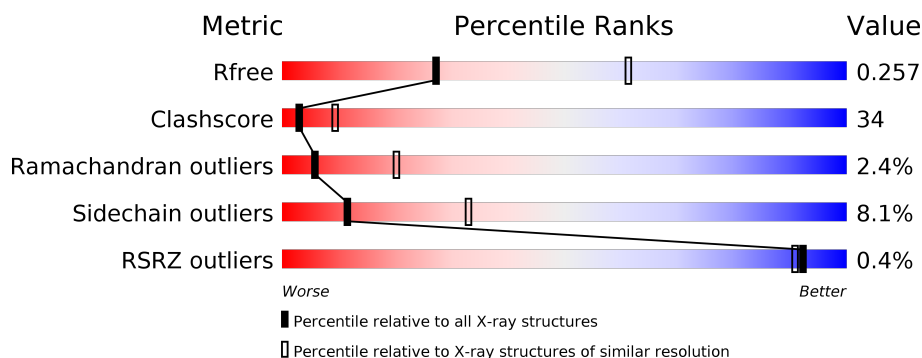
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 on 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	
1	B	506	
1	C	506	
1	D	506	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CYN	A	3000	-	-	X	-
3	HEM	B	2001	-	-	X	-
3	HEM	C	2002	-	-	X	-
3	HEM	D	2003	-	-	X	-

2 Entry composition [i](#)

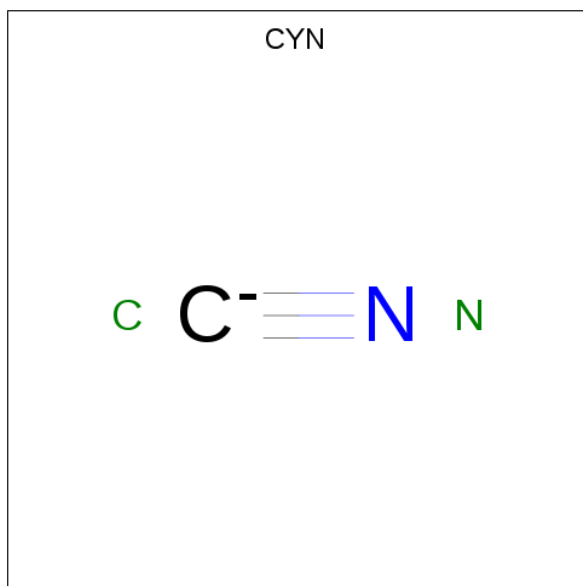
There are 4 unique types of molecules in this entry. The entry contains 16932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Catalase.

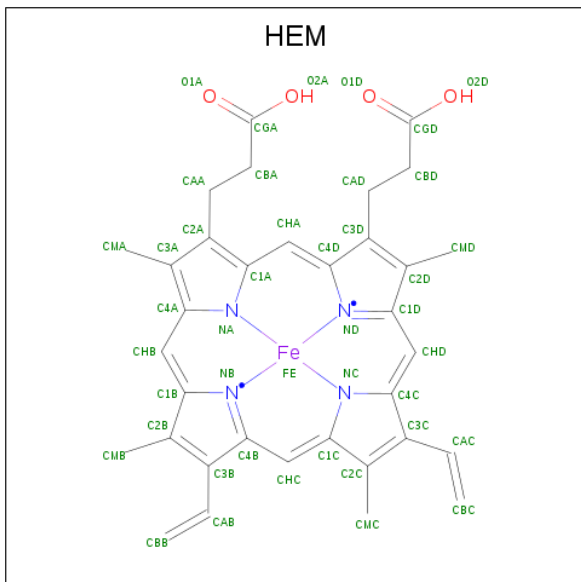
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	B	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	C	499	Total	C	N	O	S	1	0	0
			4017	2548	715	740	14			
1	D	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			

- Molecule 2 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

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



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

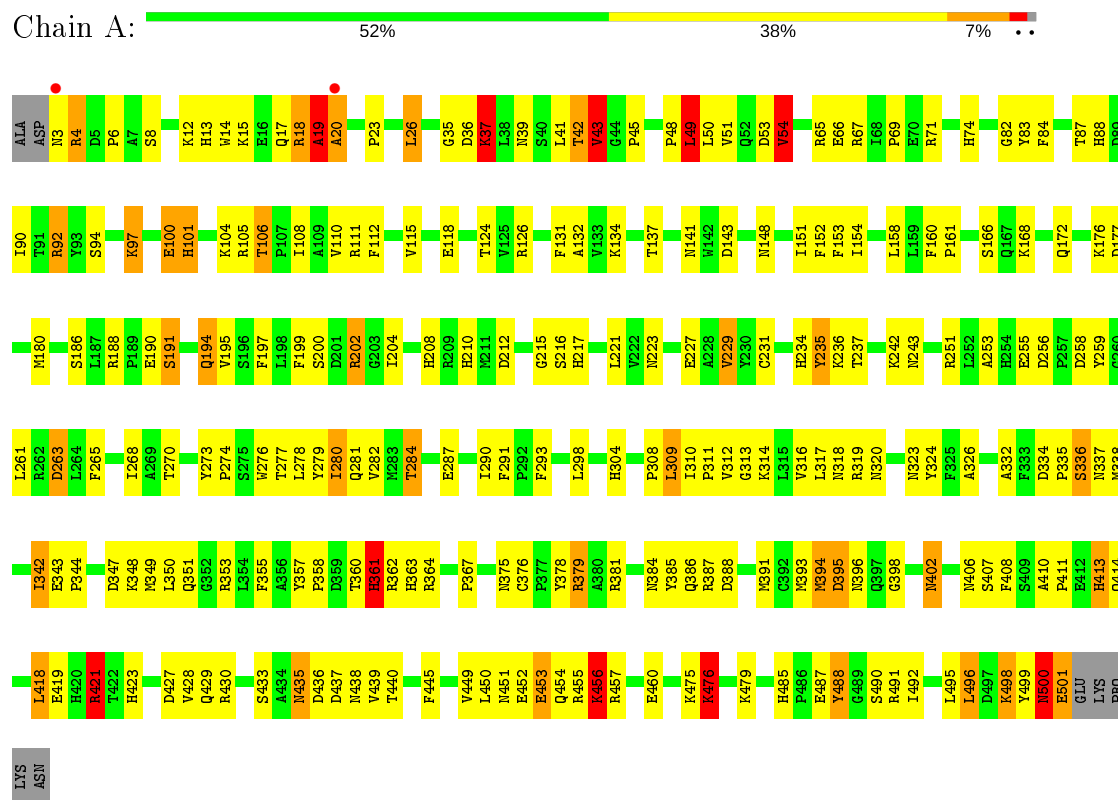
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total	O	0	0
			201	201		
4	B	195	Total	O	0	0
			195	195		
4	C	138	Total	O	0	0
			138	138		
4	D	154	Total	O	0	0
			154	154		

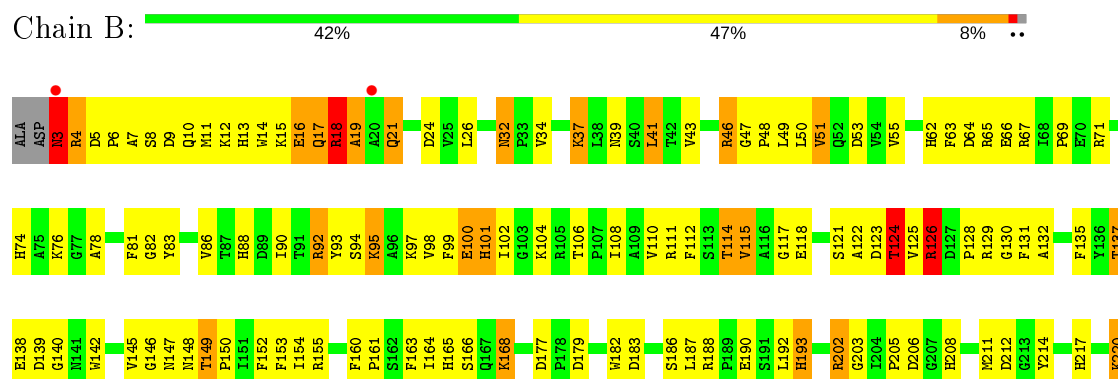
3 Residue-property plots

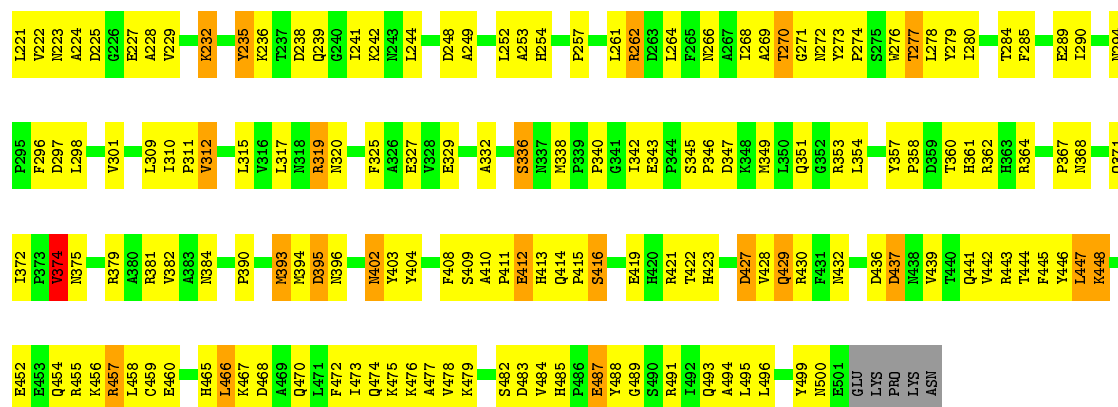
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

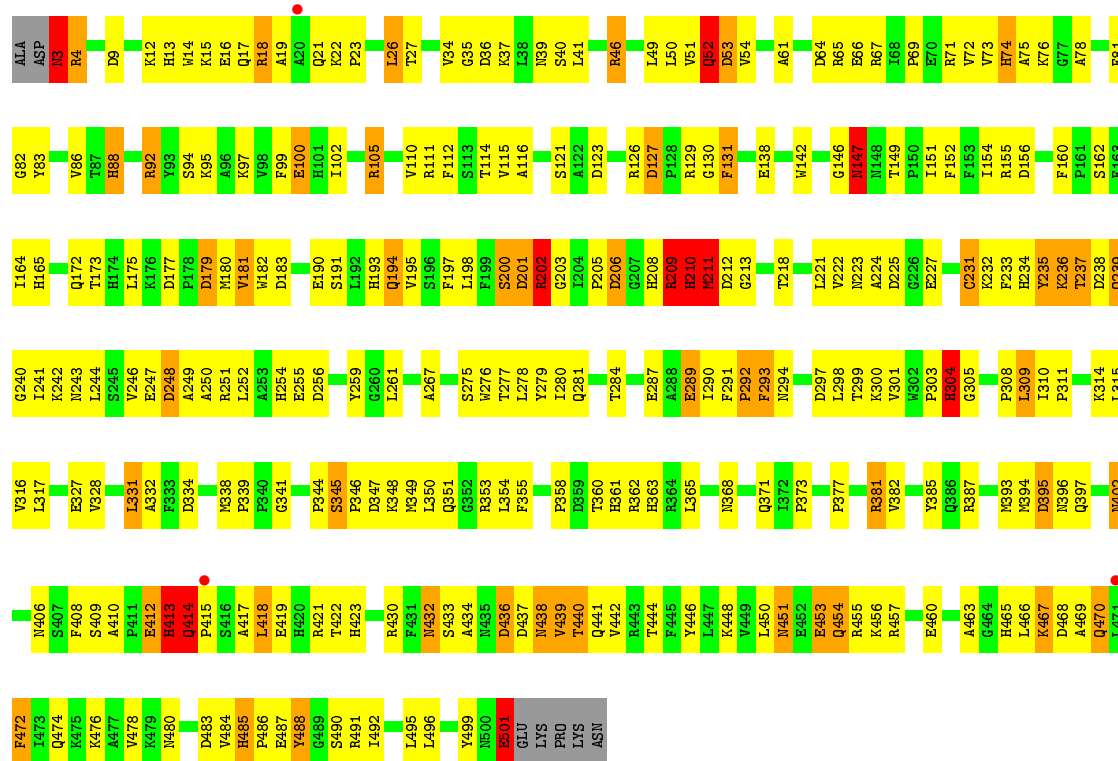


• Molecule 1: Catalase

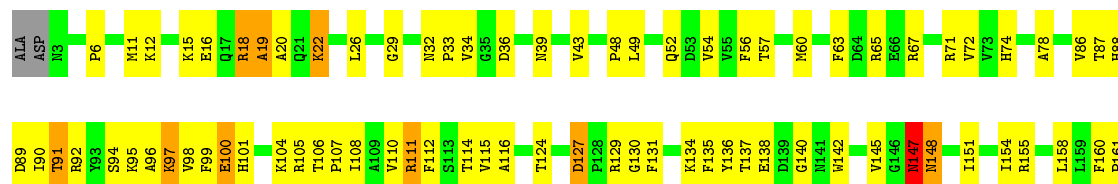




• Molecule 1: Catalase



• Molecule 1: Catalase



E501	S407	E329	Q239	L164
GLU	F408	E332	K242	H165
LYS	S409	A332	V246	K168
PRO	A410	F333	E247	R169
LYS	P411	D334	L261	N170
ASN	E412	P335	R262	F171
	H413	S336	D263	Q172
	L418	N337	N266	T173
	E419	P339	T270	H174
	H420	I342	G271	D177
	R421	E343	N272	F178
	T422	P346	Y273	D179
	H423	D347	P274	M180
	Q429	K348	S275	V181
	R430	N349	W276	W182
	F431	R353	T277	D183
	D437	Y357	Y279	L187
	N438	P358	I280	R188
	V439	H361	Q281	P189
	T440	R362	T284	E190
	Q441	N368	F285	S191
	V442	I371	S286	L192
	F445	I372	E287	H193
	V449	P373	A288	Q194
	L450	I374	E289	V195
	N451	N375	L290	D206
	E452	G376	F291	G207
	Q454	P377	P292	H208
	R455	Y378	F293	R209
	E460	R379	N294	D212
	L466	A380	P295	S216
	R467	R381	F296	H217
	L471	V382	D297	T218
	V478	A383	T299	F219
	K479	N384	K300	K220
	N480	D388	V301	L221
	V484	G389	W302	V222
	H485	P390	P303	N223
	P486	N391	H304	A224
	E487	C392	G305	G226
	Y488	N393	D306	E227
	I492	M394	Y307	A228
	Q493	Q397	P308	V229
	A494	I310	L309	Y230
	L495	P311	I310	C231
	Y499	V312	P311	K232
	N500	N402	V312	F233
		Y403	L317	H234
		P405	V322	Y235
			N323	K236
				T237
				D238

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.06Å 140.11Å 226.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.21 – 2.80 42.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	76.4 (39.21-2.80) 76.5 (42.27-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.261 0.199 , 0.257	Depositor DCC
R_{free} test set	1553 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16932	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: HEM, CYN

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	0.71	8/4137 (0.2%)	1.63	67/5619 (1.2%)
1	B	0.98	5/4137 (0.1%)	1.47	29/5619 (0.5%)
1	C	0.70	12/4137 (0.3%)	1.63	50/5619 (0.9%)
1	D	0.60	1/4137 (0.0%)	0.83	8/5619 (0.1%)
All	All	0.76	26/16548 (0.2%)	1.43	154/22476 (0.7%)

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	2	6
1	B	0	4
1	C	3	4
All	All	5	14

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CD-NE	48.75	2.29	1.46
1	D	413	HIS	CA-CB	-20.31	1.09	1.53
1	A	43	VAL	C-O	18.23	1.57	1.23
1	C	202	ARG	NE-CZ	16.64	1.54	1.33
1	B	319	ARG	NE-CZ	15.74	1.53	1.33
1	A	92	ARG	CG-CD	14.29	1.87	1.51
1	A	20	ALA	CA-C	-12.12	1.21	1.52
1	B	3	ASN	C-N	11.00	1.59	1.34
1	A	43	VAL	N-CA	10.14	1.66	1.46
1	C	292	PRO	C-N	9.22	1.55	1.34
1	C	413	HIS	CB-CG	8.62	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	ARG	CD-NE	-8.47	1.32	1.46
1	C	292	PRO	CA-C	-8.35	1.36	1.52
1	C	211	MET	N-CA	-7.18	1.31	1.46
1	C	9	ASP	CB-CG	7.13	1.66	1.51
1	B	374	VAL	CA-CB	7.10	1.69	1.54
1	A	229	VAL	CA-CB	-6.91	1.40	1.54
1	B	319	ARG	CA-CB	-6.44	1.39	1.53
1	A	176	LYS	CD-CE	6.39	1.67	1.51
1	C	485	HIS	ND1-CE1	-6.29	1.19	1.34
1	C	9	ASP	CA-CB	6.28	1.67	1.53
1	C	454	GLN	CB-CG	-5.66	1.37	1.52
1	A	280	ILE	CA-CB	5.59	1.67	1.54
1	C	210	HIS	CA-C	-5.16	1.39	1.52
1	C	414	GLN	CA-CB	5.03	1.65	1.53
1	C	210	HIS	C-N	-5.02	1.22	1.34

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	ARG	NE-CZ-NH2	-52.37	94.12	120.30
1	B	319	ARG	NE-CZ-NH1	-46.12	97.24	120.30
1	C	202	ARG	NE-CZ-NH1	43.99	142.29	120.30
1	B	319	ARG	CG-CD-NE	-41.07	25.55	111.80
1	A	19	ALA	O-C-N	-36.47	64.35	122.70
1	B	395	ASP	N-CA-CB	-31.42	54.04	110.60
1	B	126	ARG	CD-NE-CZ	29.09	164.32	123.60
1	A	304	HIS	CA-CB-CG	27.88	161.00	113.60
1	D	413	HIS	CA-CB-CG	24.99	156.08	113.60
1	C	483	ASP	N-CA-CB	23.74	153.33	110.60
1	B	319	ARG	CB-CG-CD	-23.52	50.45	111.60
1	A	304	HIS	CB-CA-C	23.17	156.73	110.40
1	A	54	VAL	CA-CB-CG2	-22.17	77.64	110.90
1	A	229	VAL	CA-CB-CG2	21.61	143.32	110.90
1	A	421	ARG	CG-CD-NE	21.26	156.45	111.80
1	C	453	GLU	CB-CG-CD	20.03	168.28	114.20
1	A	49	LEU	CB-CG-CD2	19.96	144.93	111.00
1	A	418	LEU	N-CA-CB	19.58	149.57	110.40
1	A	421	ARG	CB-CG-CD	19.15	161.40	111.60
1	C	414	GLN	CA-CB-CG	19.00	155.19	113.40
1	A	395	ASP	CA-CB-CG	18.84	154.84	113.40
1	C	501	GLU	CB-CA-C	18.65	147.70	110.40
1	C	292	PRO	O-C-N	-18.60	92.93	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ASP	N-CA-CB	18.43	143.77	110.60
1	B	487	GLU	CA-CB-CG	18.33	153.72	113.40
1	A	456	LYS	CG-CD-CE	18.19	166.47	111.90
1	B	487	GLU	CB-CG-CD	17.52	161.49	114.20
1	B	319	ARG	CA-CB-CG	17.51	151.93	113.40
1	D	453	GLU	CB-CG-CD	17.34	161.01	114.20
1	C	453	GLU	N-CA-CB	17.29	141.72	110.60
1	C	147	ASN	CB-CA-C	17.13	144.66	110.40
1	A	43	VAL	O-C-N	-16.82	94.61	123.20
1	C	9	ASP	CA-CB-CG	16.74	150.23	113.40
1	A	456	LYS	CB-CG-CD	16.61	154.78	111.60
1	A	361	HIS	N-CA-CB	-16.54	80.83	110.60
1	A	43	VAL	CA-C-N	16.39	148.99	116.20
1	C	453	GLU	CA-CB-CG	16.08	148.78	113.40
1	A	304	HIS	N-CA-CB	-16.01	81.79	110.60
1	C	292	PRO	N-CA-C	15.85	153.31	112.10
1	C	3	ASN	CB-CA-C	15.64	141.67	110.40
1	C	52	GLN	CB-CG-CD	15.59	152.13	111.60
1	B	374	VAL	CB-CA-C	-15.46	82.03	111.40
1	A	476	LYS	CD-CE-NZ	15.44	147.20	111.70
1	D	97	LYS	CG-CD-CE	15.32	157.88	111.90
1	B	429	GLN	CA-CB-CG	15.20	146.83	113.40
1	A	118	GLU	N-CA-CB	-15.14	83.35	110.60
1	A	402	ASN	CA-CB-CG	15.13	146.68	113.40
1	C	454	GLN	CB-CG-CD	14.91	150.36	111.60
1	B	32	ASN	CB-CG-OD1	14.89	151.38	121.60
1	C	454	GLN	N-CA-CB	-14.83	83.90	110.60
1	C	9	ASP	N-CA-CB	-14.46	84.58	110.60
1	A	501	GLU	CB-CA-C	14.38	139.17	110.40
1	B	32	ASN	CB-CG-ND2	-14.36	82.23	116.70
1	B	412	GLU	CB-CG-CD	14.10	152.27	114.20
1	A	381	ARG	CG-CD-NE	13.98	141.16	111.80
1	A	19	ALA	CA-C-N	13.92	147.82	117.20
1	A	435	ASN	CB-CA-C	13.69	137.78	110.40
1	C	289	GLU	CG-CD-OE2	-13.67	90.97	118.30
1	A	97	LYS	CG-CD-CE	13.63	152.81	111.90
1	A	421	ARG	CD-NE-CZ	13.58	142.61	123.60
1	B	478	VAL	CA-CB-CG1	-13.15	91.17	110.90
1	D	453	GLU	CA-CB-CG	13.13	142.29	113.40
1	B	319	ARG	NE-CZ-NH2	13.10	126.85	120.30
1	B	412	GLU	N-CA-CB	13.01	134.02	110.60
1	C	292	PRO	CA-C-O	12.83	150.99	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	ASP	CB-CG-OD1	12.44	129.50	118.30
1	A	500	ASN	N-CA-CB	-12.41	88.26	110.60
1	C	292	PRO	CB-CA-C	-12.27	81.33	112.00
1	A	435	ASN	CA-CB-CG	12.24	140.34	113.40
1	C	9	ASP	CB-CG-OD2	-11.91	107.58	118.30
1	B	3	ASN	O-C-N	-11.89	103.68	122.70
1	A	20	ALA	CB-CA-C	-11.80	92.39	110.10
1	C	210	HIS	O-C-N	11.79	141.57	122.70
1	A	284	THR	CA-CB-CG2	-11.79	95.90	112.40
1	C	395	ASP	CA-CB-CG	-11.73	87.58	113.40
1	C	289	GLU	CB-CA-C	11.48	133.36	110.40
1	C	147	ASN	CA-CB-CG	11.40	138.49	113.40
1	B	374	VAL	N-CA-CB	11.20	136.13	111.50
1	A	92	ARG	CG-CD-NE	-11.02	88.66	111.80
1	D	394	MET	CB-CG-SD	10.98	145.35	112.40
1	C	147	ASN	OD1-CG-ND2	-10.97	96.67	121.90
1	C	9	ASP	CB-CA-C	10.90	132.21	110.40
1	A	421	ARG	CA-CB-CG	10.86	137.28	113.40
1	A	476	LYS	CG-CD-CE	10.79	144.28	111.90
1	A	202	ARG	CD-NE-CZ	10.78	138.69	123.60
1	B	412	GLU	CA-CB-CG	10.75	137.05	113.40
1	C	483	ASP	CB-CA-C	-10.73	88.94	110.40
1	C	289	GLU	CA-CB-CG	10.71	136.97	113.40
1	B	395	ASP	CA-CB-CG	10.62	136.76	113.40
1	A	418	LEU	CB-CA-C	-10.56	90.14	110.20
1	A	453	GLU	CB-CG-CD	10.42	142.34	114.20
1	A	456	LYS	CA-CB-CG	10.25	135.95	113.40
1	A	176	LYS	CD-CE-NZ	-10.19	88.26	111.70
1	A	42	THR	C-N-CA	10.17	147.13	121.70
1	A	490	SER	CA-CB-OG	10.12	138.54	111.20
1	C	231	CYS	CA-CB-SG	-10.09	95.84	114.00
1	A	280	ILE	CB-CA-C	-10.01	91.59	111.60
1	B	478	VAL	CA-CB-CG2	9.94	125.80	110.90
1	A	243	ASN	CB-CA-C	-9.87	90.67	110.40
1	C	3	ASN	CA-C-N	-9.75	95.75	117.20
1	C	210	HIS	N-CA-CB	9.71	128.07	110.60
1	C	501	GLU	CB-CG-CD	9.57	140.04	114.20
1	A	37	LYS	CG-CD-CE	9.56	140.60	111.90
1	A	284	THR	CA-CB-OG1	9.49	128.93	109.00
1	C	414	GLN	CB-CA-C	9.42	129.24	110.40
1	B	416	SER	N-CA-CB	-9.41	96.38	110.50
1	B	478	VAL	CB-CA-C	9.40	129.26	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	THR	CB-CA-C	9.38	136.93	111.60
1	C	501	GLU	N-CA-CB	-9.27	93.91	110.60
1	C	3	ASN	CA-C-O	8.88	138.74	120.10
1	B	478	VAL	N-CA-CB	-8.67	92.43	111.50
1	C	454	GLN	CB-CA-C	-8.49	93.41	110.40
1	C	210	HIS	CA-C-N	-8.30	98.94	117.20
1	A	501	GLU	N-CA-CB	-8.25	95.75	110.60
1	D	147	ASN	CB-CA-C	7.82	126.05	110.40
1	B	319	ARG	CB-CA-C	-7.74	94.93	110.40
1	A	500	ASN	CA-CB-CG	7.70	130.34	113.40
1	C	309	LEU	CB-CG-CD1	7.59	123.90	111.00
1	A	453	GLU	CA-CB-CG	7.57	130.06	113.40
1	C	309	LEU	CB-CG-CD2	-7.54	98.18	111.00
1	B	374	VAL	CA-CB-CG1	-7.53	99.60	110.90
1	D	147	ASN	CA-CB-CG	7.52	129.95	113.40
1	A	49	LEU	CB-CG-CD1	-7.49	98.27	111.00
1	A	92	ARG	CB-CG-CD	-7.49	92.13	111.60
1	A	284	THR	CB-CA-C	-7.44	91.50	111.60
1	C	478	VAL	CB-CA-C	7.29	125.25	111.40
1	B	374	VAL	CA-CB-CG2	-7.16	100.17	110.90
1	A	280	ILE	CA-CB-CG2	-7.11	96.68	110.90
1	A	280	ILE	CA-CB-CG1	7.10	124.49	111.00
1	A	435	ASN	N-CA-CB	-7.06	97.89	110.60
1	C	292	PRO	C-N-CA	6.64	138.29	121.70
1	A	395	ASP	CB-CA-C	-6.55	97.31	110.40
1	C	74	HIS	CA-CB-CG	6.54	124.72	113.60
1	C	147	ASN	CB-CG-OD1	6.44	134.47	121.60
1	C	202	ARG	CD-NE-CZ	6.41	132.58	123.60
1	A	20	ALA	CA-C-N	-6.41	103.11	117.20
1	C	210	HIS	CB-CG-ND1	-6.32	107.39	123.20
1	A	361	HIS	CB-CA-C	6.28	122.97	110.40
1	A	176	LYS	CG-CD-CE	6.19	130.46	111.90
1	A	342	ILE	CB-CA-C	-5.94	99.72	111.60
1	B	319	ARG	N-CA-CB	5.93	121.27	110.60
1	A	20	ALA	CA-C-O	5.80	132.29	120.10
1	A	229	VAL	CB-CA-C	-5.68	100.61	111.40
1	A	43	VAL	CA-C-O	-5.64	108.26	120.10
1	C	413	HIS	CB-CG-ND1	-5.57	109.29	123.20
1	A	37	LYS	CD-CE-NZ	-5.56	98.92	111.70
1	A	342	ILE	N-CA-CB	5.47	123.37	110.80
1	A	500	ASN	CB-CA-C	5.45	121.30	110.40
1	A	54	VAL	CB-CA-C	5.44	121.73	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	HIS	CA-CB-CG	5.42	122.81	113.60
1	D	20	ALA	N-CA-CB	-5.39	102.55	110.10
1	C	236	LYS	CG-CD-CE	5.21	127.54	111.90
1	A	43	VAL	N-CA-C	-5.18	97.02	111.00
1	A	43	VAL	N-CA-CB	-5.11	100.27	111.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	43	VAL	CA
1	A	395	ASP	CA
1	C	147	ASN	CA
1	C	453	GLU	CA
1	C	501	GLU	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ALA	Mainchain,Peptide
1	A	42	THR	Peptide
1	A	421	ARG	Sidechain
1	A	43	VAL	Mainchain,Peptide
1	B	126	ARG	Sidechain
1	B	3	ASN	Mainchain,Peptide
1	B	319	ARG	Sidechain
1	C	147	ASN	Sidechain
1	C	210	HIS	Sidechain
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	3837	240	0
1	B	4017	0	3840	343	0
1	C	4017	0	3839	327	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4017	0	3839	270	0
2	A	2	0	0	6	0
2	D	2	0	0	0	0
3	A	43	0	30	16	0
3	B	43	0	30	25	0
3	C	43	0	30	26	0
3	D	43	0	30	21	0
4	A	201	0	0	33	0
4	B	195	0	0	33	0
4	C	138	0	0	16	0
4	D	154	0	0	20	0
All	All	16932	0	15475	1083	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (1083) 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:92:ARG:CD	1:A:92:ARG:CG	1.87	1.49
1:C:147:ASN:CG	3:C:2002:HEM:HAC	1.16	1.45
1:C:147:ASN:OD1	3:C:2002:HEM:CAC	1.63	1.42
1:C:147:ASN:ND2	3:C:2002:HEM:HAC	1.26	1.40
1:B:111:ARG:CD	3:B:2001:HEM:O1D	1.70	1.38
1:D:111:ARG:CD	3:D:2003:HEM:O2D	1.69	1.37
1:C:209:ARG:NH1	1:C:267:ALA:HB1	1.43	1.34
1:C:147:ASN:OD1	3:C:2002:HEM:C3C	1.81	1.33
1:A:351:GLN:HE22	1:C:52:GLN:NE2	1.34	1.25
1:B:384:ASN:HB2	4:B:2078:HOH:O	1.27	1.23
1:C:209:ARG:NH1	1:C:267:ALA:CB	1.99	1.23
1:D:52:GLN:HB2	4:D:3005:HOH:O	1.40	1.21
1:A:351:GLN:NE2	1:C:52:GLN:HE21	1.39	1.19
1:C:147:ASN:CG	3:C:2002:HEM:CAC	2.02	1.18
1:D:147:ASN:OD1	3:D:2003:HEM:CAC	1.90	1.18
1:A:298:LEU:HD21	3:A:2000:HEM:HBC1	1.19	1.16
1:C:147:ASN:OD1	3:C:2002:HEM:HAC	1.27	1.14
1:B:111:ARG:HD2	3:B:2001:HEM:O1D	1.40	1.14
1:B:39:ASN:OD1	4:B:2053:HOH:O	1.62	1.14
1:B:111:ARG:HD3	3:B:2001:HEM:O1D	1.33	1.12
1:B:3:ASN:O	1:B:4:ARG:O	1.70	1.09
1:D:111:ARG:HD3	3:D:2003:HEM:O2D	1.46	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3000:CYN:C	3:A:2000:HEM:NC	2.17	1.08
1:C:147:ASN:ND2	3:C:2002:HEM:CAC	2.14	1.07
1:B:396:ASN:ND2	4:B:2120:HOH:O	1.86	1.06
1:D:406:ASN:HD21	1:D:410:ALA:HB3	1.12	1.05
1:B:413:HIS:NE2	4:B:2134:HOH:O	1.86	1.05
1:A:298:LEU:CD2	3:A:2000:HEM:HBC1	1.87	1.03
1:C:209:ARG:CZ	1:C:267:ALA:HB2	1.87	1.03
1:B:413:HIS:CD2	4:B:2134:HOH:O	2.07	1.03
1:D:111:ARG:HD2	3:D:2003:HEM:O2D	1.55	1.01
1:C:190:GLU:HA	1:C:438:ASN:HB3	1.38	1.01
1:D:39:ASN:OD1	4:D:3021:HOH:O	1.78	1.01
1:C:394:MET:HE2	4:C:2137:HOH:O	1.62	1.00
1:A:413:HIS:ND1	4:A:3145:HOH:O	1.94	1.00
1:B:19:ALA:HB3	1:B:21:GLN:HE21	1.25	0.99
1:D:174:HIS:ND1	4:D:3042:HOH:O	1.92	0.99
1:B:78:ALA:HB2	1:B:261:LEU:HD12	1.41	0.98
1:A:298:LEU:HD21	3:A:2000:HEM:CBC	1.94	0.98
1:B:100:GLU:HB3	1:B:104:LYS:HG3	1.46	0.97
1:B:242:LYS:NZ	4:B:2095:HOH:O	1.89	0.95
1:B:112:PHE:HA	1:B:130:GLY:O	1.67	0.93
1:C:402:ASN:HD22	1:C:402:ASN:H	1.05	0.93
1:D:147:ASN:OD1	3:D:2003:HEM:HAC	1.66	0.93
1:A:92:ARG:CB	1:A:92:ARG:CD	2.45	0.93
1:C:208:HIS:O	1:C:209:ARG:HG2	1.69	0.92
1:A:223:ASN:HD21	1:A:227:GLU:HB2	1.34	0.92
1:D:223:ASN:HD21	1:D:227:GLU:HB3	1.36	0.90
1:A:92:ARG:NE	1:A:92:ARG:CG	2.35	0.89
1:A:324:TYR:OH	4:A:3179:HOH:O	1.89	0.89
1:A:429:GLN:NE2	1:B:421:ARG:HD2	1.87	0.88
1:D:90:ILE:HG21	1:D:312:VAL:HG22	1.56	0.88
1:D:406:ASN:ND2	1:D:410:ALA:HB3	1.87	0.88
1:A:351:GLN:NE2	1:C:52:GLN:NE2	2.09	0.88
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.39	0.88
1:C:209:ARG:NH1	1:C:267:ALA:HB2	1.85	0.87
1:C:394:MET:CE	4:C:2137:HOH:O	2.21	0.87
1:A:451:ASN:H	1:A:454:GLN:HE21	1.16	0.87
1:C:205:PRO:HG2	1:C:211:MET:HE2	1.57	0.87
1:D:291:PHE:HE1	1:D:293:PHE:HB2	1.39	0.86
1:B:129:ARG:HB2	1:B:211:MET:HE1	1.57	0.86
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.39	0.85
1:B:15:LYS:HD2	1:D:408:PHE:HA	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:ASP:HB3	4:C:2106:HOH:O	1.75	0.85
2:A:3000:CYN:C	3:A:2000:HEM:NB	2.40	0.84
1:C:74:HIS:CE1	3:C:2002:HEM:C1D	2.65	0.84
1:D:190:GLU:HA	1:D:438:ASN:HB3	1.58	0.84
1:C:209:ARG:HH11	1:C:267:ALA:HB1	1.42	0.83
1:C:151:ILE:HG13	1:C:194:GLN:HG2	1.60	0.83
3:B:2001:HEM:HBD2	4:B:2179:HOH:O	1.78	0.83
1:B:92:ARG:HD2	4:B:2163:HOH:O	1.78	0.83
1:C:129:ARG:CB	1:C:211:MET:HE1	2.09	0.83
1:A:223:ASN:ND2	1:A:227:GLU:HB2	1.92	0.83
1:C:212:ASP:OD1	1:C:236:LYS:HA	1.79	0.83
1:D:170:ASN:ND2	1:D:172:GLN:H	1.74	0.83
1:C:413:HIS:CD2	4:C:2037:HOH:O	2.31	0.82
1:B:92:ARG:CG	4:B:2163:HOH:O	2.26	0.82
1:A:36:ASP:OD2	1:A:39:ASN:HB2	1.80	0.81
2:A:3000:CYN:C	3:A:2000:HEM:FE	1.62	0.81
1:C:402:ASN:HD22	1:C:402:ASN:N	1.75	0.81
1:C:488:TYR:O	1:C:492:ILE:HG12	1.80	0.81
2:A:3000:CYN:C	3:A:2000:HEM:ND	2.43	0.81
1:C:177:ASP:O	1:C:181:VAL:HG23	1.80	0.81
1:C:209:ARG:CZ	1:C:267:ALA:CB	2.54	0.81
1:C:146:GLY:O	1:C:147:ASN:HB3	1.81	0.81
1:C:334:ASP:OD2	4:C:2085:HOH:O	1.99	0.80
1:A:451:ASN:H	1:A:454:GLN:NE2	1.79	0.80
1:B:124:THR:HG22	1:B:249:ALA:HA	1.63	0.80
1:B:202:ARG:HH21	1:B:241:ILE:HD13	1.46	0.80
1:A:391:MET:HE3	1:A:393:MET:HE1	1.64	0.80
1:B:444:THR:O	1:B:448:LYS:HB3	1.80	0.80
1:C:50:LEU:HD22	1:D:48:PRO:HB2	1.63	0.79
1:C:402:ASN:HD21	1:D:180:MET:HE1	1.46	0.79
1:B:361:HIS:CD2	3:B:2001:HEM:O1A	2.35	0.79
1:B:223:ASN:HD21	1:B:227:GLU:HB2	1.45	0.79
1:D:333:PHE:CE1	3:D:2003:HEM:O1D	2.35	0.79
2:A:3000:CYN:C	3:A:2000:HEM:NA	2.46	0.79
4:A:3093:HOH:O	1:C:22:LYS:HE2	1.83	0.79
1:A:357:TYR:O	1:A:361:HIS:HB2	1.84	0.78
1:D:136:TYR:O	1:D:379:ARG:HG3	1.84	0.78
1:B:100:GLU:CB	1:B:104:LYS:HG3	2.14	0.78
1:B:285:PHE:HD1	4:B:2172:HOH:O	1.67	0.78
1:B:372:ILE:HB	1:B:375:ASN:HD22	1.48	0.78
1:A:100:GLU:O	1:A:101:HIS:HB3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:LYS:HG2	4:A:3100:HOH:O	1.83	0.78
1:D:111:ARG:NE	3:D:2003:HEM:O2D	2.16	0.78
1:C:209:ARG:HH12	1:C:267:ALA:HB1	1.48	0.77
1:D:111:ARG:CD	3:D:2003:HEM:CGD	2.61	0.77
1:C:147:ASN:OD1	3:C:2002:HEM:C4C	2.38	0.77
1:B:101:HIS:O	1:B:104:LYS:HB2	1.85	0.77
1:B:443:ARG:HD3	4:B:2184:HOH:O	1.83	0.77
1:C:147:ASN:HD21	3:C:2002:HEM:HAC	1.45	0.77
1:D:111:ARG:HD2	3:D:2003:HEM:CGD	2.15	0.77
1:A:12:LYS:NZ	4:A:3157:HOH:O	2.17	0.76
1:D:170:ASN:HD22	1:D:172:GLN:H	1.32	0.76
1:C:147:ASN:CB	3:C:2002:HEM:HAC	2.16	0.76
1:C:123:ASP:OD1	4:C:2021:HOH:O	2.04	0.76
1:B:485:HIS:CE1	1:B:487:GLU:HG3	2.20	0.76
1:D:223:ASN:ND2	1:D:227:GLU:HB3	2.00	0.76
1:B:294:ASN:ND2	1:C:46:ARG:HD2	2.01	0.76
1:D:418:LEU:HD23	1:D:419:GLU:H	1.48	0.75
1:C:486:PRO:HD3	4:C:2140:HOH:O	1.86	0.75
1:A:177:ASP:HB3	1:A:180:MET:HB2	1.69	0.75
1:C:402:ASN:H	1:C:402:ASN:ND2	1.83	0.75
1:B:393:MET:CE	1:D:372:ILE:HA	2.15	0.75
1:B:129:ARG:CB	1:B:211:MET:HE1	2.17	0.75
1:A:284:THR:OG1	1:A:287:GLU:HG3	1.87	0.74
1:A:485:HIS:HD2	1:A:487:GLU:HB3	1.51	0.74
1:B:208:HIS:O	1:B:211:MET:HG2	1.86	0.74
1:B:447:LEU:HD21	1:B:485:HIS:HD2	1.52	0.74
1:C:450:LEU:HA	1:C:454:GLN:HE21	1.50	0.74
1:B:95:LYS:HB3	1:B:224:ALA:N	2.01	0.74
1:A:391:MET:CE	1:A:393:MET:HE1	2.18	0.74
1:C:402:ASN:HD21	1:D:180:MET:CE	2.00	0.74
1:C:147:ASN:N	3:C:2002:HEM:HBC1	2.02	0.74
1:B:268:ILE:HB	1:B:320:ASN:ND2	2.02	0.74
1:B:217:HIS:NE2	3:B:2001:HEM:CBC	2.51	0.73
1:B:205:PRO:HG3	1:B:211:MET:HE3	1.69	0.73
1:C:432:ASN:HD22	1:C:433:SER:N	1.85	0.73
1:A:186:SER:HB2	1:A:476:LYS:HG2	1.69	0.73
1:D:111:ARG:HH11	1:D:111:ARG:HG3	1.54	0.73
1:B:92:ARG:CD	4:B:2163:HOH:O	2.36	0.72
1:A:51:VAL:HG21	1:B:49:LEU:HD23	1.71	0.72
1:D:115:VAL:HB	1:D:127:ASP:OD2	1.88	0.72
1:B:479:LYS:O	1:B:482:SER:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:HB3	1:D:388:ASP:HB2	1.70	0.72
1:D:97:LYS:HA	1:D:100:GLU:HG3	1.70	0.72
1:D:183:ASP:O	1:D:187:LEU:HG	1.88	0.72
1:B:428:VAL:O	1:B:428:VAL:HG23	1.89	0.72
1:C:78:ALA:HB2	1:C:261:LEU:HD22	1.70	0.72
1:B:183:ASP:O	1:B:187:LEU:HG	1.90	0.71
1:D:220:LYS:HD2	1:D:343:GLU:HB2	1.73	0.71
1:C:209:ARG:O	1:C:210:HIS:CG	2.44	0.71
1:C:88:HIS:CD2	1:C:311:PRO:HB2	2.25	0.71
1:B:360:THR:OG1	1:C:64:ASP:HB3	1.91	0.71
1:C:421:ARG:HD3	4:D:3049:HOH:O	1.89	0.71
1:A:188:ARG:O	1:A:191:SER:OG	2.09	0.71
1:B:95:LYS:HG3	1:B:222:VAL:O	1.91	0.70
1:B:124:THR:CG2	1:B:249:ALA:HA	2.21	0.70
1:B:268:ILE:HB	1:B:320:ASN:HD21	1.57	0.70
1:C:74:HIS:O	1:C:111:ARG:NH2	2.25	0.70
1:C:239:GLN:HE22	1:C:275:SER:H	1.38	0.70
1:C:492:ILE:HG22	1:C:496:LEU:HD23	1.73	0.70
1:A:487:GLU:O	1:A:491:ARG:HG3	1.91	0.70
1:C:197:PHE:O	1:C:200:SER:HB3	1.91	0.70
1:C:487:GLU:HA	1:C:490:SER:HB3	1.73	0.69
1:D:362:ARG:NH1	4:D:3111:HOH:O	2.25	0.69
1:B:320:ASN:OD1	4:B:2055:HOH:O	2.10	0.69
1:B:26:LEU:HD12	1:D:384:ASN:HA	1.73	0.69
1:B:34:VAL:HG11	1:B:37:LYS:HB3	1.72	0.69
1:B:476:LYS:NZ	4:B:2168:HOH:O	2.20	0.69
1:B:447:LEU:HD21	1:B:485:HIS:CD2	2.28	0.68
1:D:286:SER:O	1:D:289:GLU:HB3	1.93	0.68
1:C:205:PRO:HG2	1:C:211:MET:CE	2.22	0.68
1:B:254:HIS:HB3	1:C:254:HIS:HB3	1.75	0.68
1:A:453:GLU:HG2	1:A:457:ARG:HH12	1.59	0.68
1:C:308:PRO:O	1:C:310:ILE:HD12	1.94	0.68
1:D:147:ASN:OD1	3:D:2003:HEM:C3C	2.47	0.68
1:C:129:ARG:HB2	1:C:211:MET:HE1	1.75	0.68
1:A:74:HIS:NE2	1:A:115:VAL:HG22	2.09	0.68
1:D:291:PHE:HD1	1:D:293:PHE:H	1.39	0.68
1:C:154:ILE:HG13	1:C:349:MET:HE1	1.75	0.68
1:D:148:ASN:HD22	1:D:148:ASN:H	1.40	0.68
1:D:333:PHE:CD1	3:D:2003:HEM:O1D	2.47	0.68
1:B:368:ASN:O	1:B:371:GLN:HB2	1.94	0.67
1:A:376:CYS:SG	4:A:3184:HOH:O	2.50	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:GLY:HA3	1:C:316:VAL:O	1.93	0.67
1:C:92:ARG:HD3	1:C:92:ARG:H	1.59	0.67
1:A:485:HIS:CD2	1:A:487:GLU:HB3	2.29	0.67
1:B:182:TRP:NE1	1:B:465:HIS:ND1	2.40	0.67
1:C:248:ASP:HA	1:C:251:ARG:NH1	2.09	0.67
1:A:215:GLY:O	1:A:216:SER:HB2	1.94	0.67
1:B:413:HIS:ND1	1:B:413:HIS:O	2.28	0.67
1:B:496:LEU:O	1:B:500:ASN:HB2	1.95	0.67
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.60	0.67
1:B:217:HIS:CD2	3:B:2001:HEM:CBC	2.78	0.67
1:D:71:ARG:HG3	1:D:71:ARG:HH11	1.58	0.67
1:D:12:LYS:O	1:D:16:GLU:HG3	1.94	0.67
1:C:191:SER:O	1:C:195:VAL:HG23	1.95	0.66
1:B:393:MET:HE2	1:D:373:PRO:HD3	1.77	0.66
1:C:162:SER:HB3	1:D:404:TYR:H	1.60	0.66
1:A:332:ALA:HB1	1:A:361:HIS:CE1	2.30	0.66
1:C:460:GLU:HA	1:C:495:LEU:HD13	1.76	0.66
1:A:43:VAL:HG12	1:A:50:LEU:HD21	1.77	0.66
1:B:422:THR:HG22	1:B:423:HIS:H	1.59	0.66
1:C:115:VAL:HG12	1:C:116:ALA:N	2.10	0.66
1:D:291:PHE:CE1	1:D:293:PHE:HB2	2.26	0.66
1:B:69:PRO:HD3	1:C:69:PRO:HG3	1.77	0.66
1:B:97:LYS:HD3	1:B:138:GLU:HB2	1.77	0.66
1:C:210:HIS:CD2	1:C:242:LYS:HB3	2.31	0.66
3:B:2001:HEM:CBD	4:B:2179:HOH:O	2.41	0.66
1:C:74:HIS:CE1	3:C:2002:HEM:C2D	2.84	0.66
1:C:160:PHE:CE1	1:C:164:ILE:HD11	2.31	0.66
1:D:418:LEU:HD23	1:D:419:GLU:N	2.11	0.66
1:B:106:THR:HG23	1:B:379:ARG:NH2	2.10	0.65
1:B:5:ASP:OD2	1:B:7:ALA:HB3	1.95	0.65
1:C:208:HIS:O	1:C:209:ARG:CG	2.44	0.65
1:A:49:LEU:HD13	1:B:51:VAL:HG11	1.79	0.65
1:B:466:LEU:HD22	1:B:474:GLN:HG2	1.78	0.65
1:C:193:HIS:HA	1:C:442:VAL:HG22	1.79	0.65
1:D:6:PRO:HD2	1:D:266:ASN:OD1	1.96	0.65
3:A:2000:HEM:O2D	4:A:3016:HOH:O	2.15	0.65
1:B:457:ARG:HH11	1:B:457:ARG:HB2	1.61	0.65
1:C:287:GLU:HA	1:C:290:ILE:HG12	1.77	0.65
1:D:333:PHE:HE1	3:D:2003:HEM:O1D	1.79	0.65
1:A:210:HIS:HB3	1:A:242:LYS:H	1.62	0.65
1:B:338:MET:HE2	1:B:342:ILE:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:HIS:CD2	1:C:309:LEU:HD13	2.32	0.65
1:C:450:LEU:HG	1:C:454:GLN:HB3	1.79	0.65
1:C:231:CYS:HA	1:C:281:GLN:O	1.97	0.65
1:B:135:PHE:HB2	1:B:142:TRP:HB3	1.79	0.64
1:D:111:ARG:HD3	3:D:2003:HEM:CGD	2.27	0.64
1:A:108:ILE:HA	1:A:134:LYS:O	1.97	0.64
1:B:124:THR:HG21	1:B:252:LEU:HB2	1.79	0.64
1:B:217:HIS:CD2	1:B:353:ARG:HH11	2.16	0.64
1:B:5:ASP:HB2	1:B:6:PRO:HD2	1.79	0.64
1:D:148:ASN:N	1:D:148:ASN:HD22	1.95	0.64
1:B:19:ALA:CB	1:B:21:GLN:HE21	2.06	0.64
1:B:457:ARG:NH1	1:B:457:ARG:HB2	2.11	0.64
1:C:200:SER:OG	1:C:201:ASP:N	2.30	0.64
1:D:294:ASN:HB3	1:D:297:ASP:HB2	1.80	0.64
1:D:26:LEU:O	1:D:34:VAL:HG22	1.97	0.64
1:A:217:HIS:NE2	3:A:2000:HEM:CBC	2.61	0.64
1:B:238:ASP:OD1	1:B:277:THR:HG22	1.98	0.64
1:A:309:LEU:N	1:A:309:LEU:HD22	2.13	0.63
1:A:358:PRO:O	1:A:362:ARG:HG3	1.98	0.63
1:D:232:LYS:O	1:D:280:ILE:HA	1.98	0.63
1:C:238:ASP:OD2	1:C:314:LYS:HE3	1.98	0.63
1:C:492:ILE:HG22	1:C:496:LEU:CD2	2.27	0.63
1:A:353:ARG:NH2	1:A:357:TYR:OH	2.32	0.63
1:B:261:LEU:HD23	1:C:175:LEU:HD23	1.81	0.63
1:C:129:ARG:HG2	1:C:211:MET:HE3	1.80	0.63
1:C:436:ASP:O	1:C:437:ASP:HB3	1.97	0.63
1:C:209:ARG:HH12	1:C:267:ALA:CB	2.06	0.63
1:C:453:GLU:HB3	1:C:457:ARG:HH12	1.63	0.63
1:D:310:ILE:HD12	1:D:310:ILE:N	2.14	0.63
1:A:309:LEU:H	1:A:309:LEU:HD22	1.63	0.63
1:A:3:ASN:N	4:A:3165:HOH:O	2.32	0.62
1:D:235:TYR:HA	1:D:277:THR:O	1.99	0.62
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.64	0.62
1:A:455:ARG:CZ	4:A:3196:HOH:O	2.46	0.62
1:D:189:PRO:HG3	1:D:480:ASN:ND2	2.14	0.62
1:D:154:ILE:HG13	1:D:349:MET:CE	2.29	0.62
1:A:74:HIS:O	1:A:111:ARG:NH2	2.33	0.62
1:C:112:PHE:HA	1:C:130:GLY:O	2.00	0.62
1:D:246:VAL:HG22	4:D:3141:HOH:O	1.98	0.62
1:B:206:ASP:OD1	1:B:244:LEU:HD21	1.99	0.62
1:C:179:ASP:O	1:C:183:ASP:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LYS:HB2	4:B:2040:HOH:O	1.98	0.62
1:A:456:LYS:HD3	1:A:460:GLU:OE2	2.00	0.61
1:D:148:ASN:ND2	1:D:148:ASN:H	1.98	0.61
1:D:239:GLN:HE22	1:D:275:SER:H	1.47	0.61
1:A:26:LEU:HD22	1:C:385:TYR:HE2	1.65	0.61
1:B:419:GLU:HB2	4:B:2022:HOH:O	1.99	0.61
1:C:487:GLU:CG	1:C:491:ARG:HD2	2.31	0.61
1:D:135:PHE:HB2	1:D:142:TRP:HB3	1.81	0.61
1:A:172:GLN:HE21	1:D:322:VAL:HA	1.65	0.61
1:B:97:LYS:HD2	1:B:139:ASP:CG	2.20	0.61
1:D:338:MET:HE2	1:D:342:ILE:HG22	1.82	0.61
1:D:460:GLU:HA	1:D:495:LEU:HD13	1.83	0.61
1:A:92:ARG:CD	1:A:92:ARG:HB3	2.29	0.61
1:C:298:LEU:CD2	1:C:349:MET:HG2	2.31	0.61
1:D:142:TRP:HA	1:D:337:ASN:O	2.01	0.61
1:A:332:ALA:HB1	1:A:361:HIS:NE2	2.15	0.61
1:A:50:LEU:HD12	1:B:48:PRO:HB2	1.83	0.61
1:C:328:VAL:O	1:C:331:LEU:HB2	2.01	0.61
1:C:154:ILE:CG1	1:C:349:MET:HE1	2.31	0.61
1:A:496:LEU:O	1:A:500:ASN:HB2	2.01	0.61
1:C:129:ARG:HG2	1:C:211:MET:CE	2.31	0.61
1:A:336:SER:OG	4:A:3181:HOH:O	2.16	0.60
1:B:160:PHE:N	1:B:161:PRO:HD2	2.16	0.60
1:C:154:ILE:HG13	1:C:349:MET:CE	2.30	0.60
1:C:205:PRO:CG	1:C:211:MET:HE2	2.30	0.60
1:B:222:VAL:HG22	1:B:228:ALA:HB2	1.83	0.60
1:B:223:ASN:ND2	1:B:227:GLU:HB2	2.14	0.60
1:C:193:HIS:CA	1:C:442:VAL:HG22	2.31	0.60
1:D:52:GLN:N	4:D:3005:HOH:O	2.23	0.60
1:D:90:ILE:HD11	1:D:99:PHE:CG	2.36	0.60
1:B:76:LYS:HE3	1:B:121:SER:O	2.01	0.60
1:C:350:LEU:O	1:C:353:ARG:N	2.34	0.60
1:D:231:CYS:HA	1:D:281:GLN:O	2.01	0.60
1:B:94:SER:HB2	1:B:221:LEU:HD22	1.82	0.60
1:B:393:MET:HE2	1:D:372:ILE:HA	1.83	0.60
1:A:421:ARG:CG	1:B:429:GLN:HG2	2.32	0.60
1:B:485:HIS:HE1	1:B:487:GLU:HG3	1.64	0.60
1:C:18:ARG:O	1:C:21:GLN:HB2	2.01	0.60
1:B:152:PHE:HB3	1:B:298:LEU:HD23	1.82	0.60
1:B:454:GLN:HA	1:B:457:ARG:NH1	2.17	0.60
4:B:2002:HOH:O	1:D:29:GLY:HA3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.37	0.59
1:B:145:VAL:HG23	4:B:2061:HOH:O	2.01	0.59
1:B:63:PHE:O	1:B:66:GLU:HG3	2.02	0.59
1:D:221:LEU:O	1:D:228:ALA:HA	2.02	0.59
1:B:90:ILE:O	1:B:93:TYR:HB2	2.02	0.59
1:C:251:ARG:HG3	1:C:252:LEU:N	2.17	0.59
1:D:145:VAL:HG12	3:D:2003:HEM:CMD	2.32	0.59
1:B:12:LYS:O	1:B:16:GLU:HG3	2.01	0.59
1:B:447:LEU:CD2	1:B:485:HIS:CD2	2.85	0.59
1:D:94:SER:HB2	1:D:221:LEU:HD22	1.84	0.59
1:D:338:MET:CE	1:D:342:ILE:HG22	2.32	0.59
1:D:293:PHE:HZ	1:D:440:THR:HG21	1.68	0.59
1:B:97:LYS:HD2	1:B:139:ASP:OD2	2.00	0.59
1:B:217:HIS:NE2	3:B:2001:HEM:HBC1	2.16	0.59
1:B:88:HIS:CE1	1:B:311:PRO:HB2	2.37	0.59
1:B:4:ARG:HD2	1:B:8:SER:HB3	1.82	0.59
1:C:351:GLN:O	1:C:354:LEU:HB2	2.02	0.59
1:B:111:ARG:CD	3:B:2001:HEM:CGD	2.74	0.59
1:B:393:MET:HE1	1:D:372:ILE:HA	1.82	0.59
1:C:298:LEU:HD22	1:C:349:MET:HG2	1.84	0.59
1:B:294:ASN:HA	1:C:46:ARG:HH12	1.66	0.59
1:B:50:LEU:N	1:B:50:LEU:HD22	2.18	0.59
1:C:3:ASN:C	1:C:4:ARG:HG3	2.23	0.59
1:D:151:ILE:HD13	1:D:193:HIS:CD2	2.37	0.59
1:B:64:ASP:HB3	1:C:360:THR:HB	1.83	0.59
1:B:147:ASN:OD1	3:B:2001:HEM:C3C	2.56	0.59
1:C:438:ASN:ND2	1:C:438:ASN:N	2.49	0.59
1:A:4:ARG:HH22	1:D:179:ASP:CG	2.06	0.59
1:B:110:VAL:HA	1:B:132:ALA:O	2.03	0.59
1:B:248:ASP:O	1:B:252:LEU:HD13	2.02	0.59
1:B:147:ASN:OD1	3:B:2001:HEM:CMC	2.51	0.58
1:C:486:PRO:O	1:C:490:SER:HB2	2.03	0.58
1:A:17:GLN:HA	4:A:3158:HOH:O	2.02	0.58
1:C:173:THR:O	1:C:175:LEU:HG	2.04	0.58
1:A:94:SER:HB2	1:A:221:LEU:HD22	1.86	0.58
1:B:273:TYR:HB3	1:B:317:LEU:O	2.04	0.58
1:C:414:GLN:HE22	1:C:417:ALA:HB2	1.67	0.58
1:D:106:THR:HG21	1:D:137:THR:HG22	1.85	0.58
1:A:67:ARG:HH21	1:D:168:LYS:HE3	1.67	0.58
1:B:422:THR:HG22	1:B:423:HIS:N	2.18	0.58
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:HG12	1:B:102:ILE:HD13	1.85	0.58
1:C:130:GLY:HA2	1:C:147:ASN:HB2	1.85	0.58
1:C:94:SER:HB2	1:C:221:LEU:HD22	1.85	0.58
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.85	0.58
1:B:413:HIS:O	1:B:415:PRO:HD3	2.04	0.58
1:C:76:LYS:HE3	1:C:121:SER:O	2.02	0.58
1:D:111:ARG:HG3	1:D:111:ARG:NH1	2.18	0.58
1:B:456:LYS:O	1:B:460:GLU:HG3	2.03	0.58
1:B:64:ASP:HB3	1:C:360:THR:CB	2.33	0.58
1:C:74:HIS:NE2	3:C:2002:HEM:C1D	2.72	0.58
1:C:234:HIS:HB2	1:C:279:TYR:HB2	1.85	0.58
1:C:432:ASN:ND2	1:C:434:ALA:H	2.02	0.58
1:D:112:PHE:HA	1:D:130:GLY:O	2.04	0.57
1:A:18:ARG:NE	4:A:3200:HOH:O	2.37	0.57
1:A:358:PRO:HD3	4:A:3181:HOH:O	2.05	0.57
1:B:338:MET:CE	1:B:342:ILE:HG22	2.33	0.57
1:D:160:PHE:CZ	1:D:164:ILE:HD11	2.39	0.57
1:B:358:PRO:HB2	1:B:362:ARG:NH1	2.19	0.57
1:C:418:LEU:HD11	4:D:3037:HOH:O	2.04	0.57
1:A:253:ALA:HA	4:A:3021:HOH:O	2.04	0.57
1:C:415:PRO:O	1:C:418:LEU:HB2	2.05	0.57
1:C:492:ILE:O	1:C:496:LEU:HD23	2.04	0.57
1:A:84:PHE:O	1:A:105:ARG:HA	2.05	0.57
1:C:75:ALA:N	4:C:2022:HOH:O	2.37	0.57
1:B:140:GLY:HA3	1:D:32:ASN:HD22	1.68	0.57
1:B:358:PRO:HB2	1:B:362:ARG:HH12	1.70	0.57
1:A:51:VAL:HG12	1:B:51:VAL:HA	1.86	0.57
1:C:110:VAL:HG21	1:C:317:LEU:HD11	1.85	0.57
1:D:145:VAL:HB	1:D:353:ARG:HH22	1.69	0.57
1:B:336:SER:HB3	1:D:54:VAL:HG11	1.85	0.57
1:B:361:HIS:HD2	3:B:2001:HEM:O1A	1.86	0.57
1:B:393:MET:SD	1:D:393:MET:HG3	2.45	0.57
1:C:347:ASP:HB3	1:C:350:LEU:CB	2.35	0.57
1:A:319:ARG:NH2	4:A:3028:HOH:O	2.36	0.57
1:B:382:VAL:O	1:B:382:VAL:HG13	2.05	0.57
1:C:126:ARG:HE	1:C:203:GLY:HA3	1.70	0.57
1:A:151:ILE:HG13	1:A:194:GLN:HG2	1.87	0.57
1:A:53:ASP:CG	1:D:430:ARG:HH22	2.08	0.57
1:B:479:LYS:HE2	1:B:483:ASP:OD2	2.05	0.57
1:D:78:ALA:HB2	1:D:261:LEU:HG	1.86	0.57
1:A:309:LEU:CD2	1:A:309:LEU:H	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:GLY:C	3:C:2002:HEM:HBC1	2.26	0.56
1:C:485:HIS:CE1	1:C:487:GLU:H	2.23	0.56
1:C:190:GLU:HA	1:C:438:ASN:CB	2.24	0.56
1:A:217:HIS:CE1	3:A:2000:HEM:CBC	2.88	0.56
1:B:186:SER:OG	1:B:476:LYS:HG2	2.06	0.56
1:C:251:ARG:O	1:C:255:GLU:HG3	2.05	0.56
1:C:347:ASP:HB3	1:C:350:LEU:HB3	1.87	0.56
1:D:108:ILE:HA	1:D:134:LYS:O	2.05	0.56
1:B:111:ARG:HD2	3:B:2001:HEM:CGD	2.29	0.56
1:B:106:THR:HG23	1:B:379:ARG:HH21	1.67	0.56
1:C:146:GLY:C	3:C:2002:HEM:CBC	2.73	0.56
1:C:437:ASP:C	1:C:438:ASN:HD22	2.09	0.56
1:B:62:HIS:HE1	1:D:368:ASN:ND2	2.02	0.56
1:B:278:LEU:O	1:B:312:VAL:HG13	2.05	0.56
1:B:17:GLN:C	1:B:19:ALA:H	2.09	0.56
1:C:147:ASN:HD21	3:C:2002:HEM:CAC	2.05	0.56
1:B:62:HIS:HE1	1:D:368:ASN:HD21	1.54	0.56
1:A:394:MET:HG3	4:A:3187:HOH:O	2.05	0.56
1:C:438:ASN:N	1:C:438:ASN:HD22	2.03	0.56
1:A:124:THR:HA	4:A:3171:HOH:O	2.04	0.56
1:B:202:ARG:HH21	1:B:241:ILE:CD1	2.16	0.56
1:C:234:HIS:O	1:C:279:TYR:N	2.32	0.56
1:A:277:THR:OG1	1:A:314:LYS:NZ	2.39	0.56
1:A:298:LEU:CD2	3:A:2000:HEM:CBC	2.67	0.56
1:B:6:PRO:HG2	1:B:266:ASN:OD1	2.06	0.56
1:A:355:PHE:CZ	1:D:57:THR:HG23	2.41	0.55
1:B:349:MET:SD	3:B:2001:HEM:HBB1	2.46	0.55
1:A:430:ARG:NE	1:B:419:GLU:OE1	2.39	0.55
1:C:14:TRP:O	1:C:18:ARG:HB2	2.06	0.55
1:D:95:LYS:HG2	1:D:222:VAL:O	2.06	0.55
1:B:332:ALA:HB1	1:B:361:HIS:CE1	2.41	0.55
1:B:269:ALA:C	1:B:271:GLY:H	2.09	0.55
1:D:187:LEU:O	1:D:188:ARG:HD2	2.06	0.55
1:C:74:HIS:CE1	3:C:2002:HEM:CHD	2.90	0.55
1:C:377:PRO:HG2	1:C:382:VAL:CG2	2.36	0.55
1:C:74:HIS:CD2	3:C:2002:HEM:C4D	2.95	0.55
1:A:13:HIS:O	1:A:17:GLN:HB2	2.07	0.55
1:C:61:ALA:O	1:C:65:ARG:HG3	2.07	0.55
1:D:43:VAL:CG1	1:D:48:PRO:HD2	2.37	0.55
1:C:451:ASN:O	1:C:454:GLN:HB2	2.06	0.55
1:D:110:VAL:HG21	1:D:317:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:LEU:CD2	1:D:349:MET:HG3	2.37	0.55
1:D:140:GLY:H	1:D:380:ALA:HB2	1.71	0.55
1:D:499:TYR:C	1:D:501:GLU:H	2.09	0.55
1:A:166:SER:HA	1:A:180:MET:HE2	1.89	0.55
1:B:220:LYS:HD3	1:B:228:ALA:HB1	1.89	0.55
1:D:145:VAL:HG12	3:D:2003:HEM:C2D	2.42	0.55
1:A:451:ASN:N	1:A:454:GLN:HE21	1.96	0.55
1:B:235:TYR:CD1	1:B:235:TYR:N	2.74	0.55
1:C:485:HIS:ND1	1:C:485:HIS:C	2.60	0.55
1:A:323:ASN:HD21	1:C:396:ASN:HD22	1.53	0.55
1:C:112:PHE:CG	1:C:208:HIS:HB3	2.42	0.55
1:C:247:GLU:HG3	1:C:248:ASP:N	2.22	0.55
1:C:413:HIS:C	1:C:413:HIS:ND1	2.60	0.55
1:B:221:LEU:O	1:B:228:ALA:HA	2.07	0.54
1:B:277:THR:HG21	4:B:2026:HOH:O	2.07	0.54
1:A:408:PHE:HA	1:C:15:LYS:HD2	1.89	0.54
1:D:332:ALA:HB1	1:D:361:HIS:CE1	2.41	0.54
1:B:26:LEU:CD1	1:D:384:ASN:HA	2.37	0.54
1:A:71:ARG:HG3	4:A:3007:HOH:O	2.06	0.54
1:B:24:ASP:O	1:D:411:PRO:HA	2.07	0.54
1:B:232:LYS:O	1:B:280:ILE:HA	2.07	0.54
1:A:251:ARG:O	1:A:255:GLU:HG3	2.07	0.54
1:A:67:ARG:CZ	1:D:72:VAL:HG23	2.38	0.54
1:B:353:ARG:NH1	3:B:2001:HEM:HBC2	2.22	0.54
1:A:190:GLU:HA	1:A:438:ASN:HB3	1.88	0.54
1:B:168:LYS:NZ	1:C:67:ARG:HH21	2.04	0.54
1:B:367:PRO:HG2	1:B:390:PRO:CG	2.38	0.54
1:A:387:ARG:O	1:C:66:GLU:HG2	2.07	0.54
1:D:18:ARG:O	1:D:19:ALA:HB3	2.08	0.54
1:A:106:THR:HG23	1:A:379:ARG:NH2	2.22	0.54
1:A:414:GLN:O	1:C:35:GLY:HA2	2.07	0.54
1:A:4:ARG:HB2	1:A:8:SER:HB2	1.89	0.54
1:D:381:ARG:HG2	1:D:381:ARG:HH11	1.73	0.54
1:B:279:TYR:HB3	1:B:309:LEU:HB3	1.89	0.54
1:B:37:LYS:O	1:B:37:LYS:HG3	2.08	0.54
1:A:367:PRO:HG3	1:C:65:ARG:HD3	1.90	0.53
1:B:202:ARG:NH2	1:B:241:ILE:HD13	2.19	0.53
1:A:23:PRO:HB2	1:C:412:GLU:CG	2.38	0.53
1:B:442:VAL:HG12	1:B:484:VAL:HG11	1.89	0.53
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.16	0.53
1:C:126:ARG:HD2	1:C:198:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:GLN:O	1:C:54:VAL:HG13	2.08	0.53
1:B:148:ASN:HB3	1:B:211:MET:HE2	1.89	0.53
1:A:499:TYR:O	1:A:501:GLU:N	2.35	0.53
1:C:328:VAL:HA	1:C:331:LEU:HD12	1.90	0.53
1:A:65:ARG:HG3	1:A:65:ARG:HH11	1.74	0.53
1:B:261:LEU:HD23	1:C:175:LEU:CD2	2.37	0.53
1:A:353:ARG:HG3	3:A:2000:HEM:HBB2	1.90	0.53
1:B:452:GLU:N	1:B:455:ARG:NH2	2.57	0.53
1:C:160:PHE:CZ	1:C:164:ILE:HD11	2.44	0.53
1:A:39:ASN:C	1:D:158:LEU:HD12	2.29	0.53
1:B:154:ILE:O	1:B:349:MET:HE2	2.08	0.53
1:B:41:LEU:HB2	1:B:53:ASP:HB2	1.91	0.53
1:C:252:LEU:HA	1:C:255:GLU:HB2	1.90	0.53
1:C:297:ASP:OD1	1:C:299:THR:N	2.41	0.53
1:D:191:SER:O	1:D:195:VAL:HG23	2.08	0.53
1:A:166:SER:HA	1:A:180:MET:CE	2.38	0.53
1:A:479:LYS:O	1:A:479:LYS:HD2	2.08	0.53
1:B:345:SER:HB2	1:B:346:PRO:HD2	1.91	0.53
1:D:298:LEU:HD23	1:D:349:MET:HG3	1.91	0.53
1:A:101:HIS:CE1	1:A:104:LYS:HB2	2.44	0.53
1:A:450:LEU:HA	1:A:454:GLN:NE2	2.23	0.53
1:B:69:PRO:O	1:B:364:ARG:HG3	2.08	0.53
1:C:147:ASN:CB	3:C:2002:HEM:CAC	2.80	0.53
1:A:195:VAL:O	1:A:199:PHE:HD1	1.92	0.53
1:A:353:ARG:CG	3:A:2000:HEM:HBB2	2.39	0.53
1:B:206:ASP:OD2	1:B:242:LYS:HD2	2.10	0.53
1:C:13:HIS:O	1:C:17:GLN:HG2	2.09	0.53
1:C:235:TYR:HA	1:C:277:THR:O	2.09	0.53
1:D:378:TYR:CE1	1:D:379:ARG:HG2	2.45	0.53
1:B:439:VAL:O	1:B:442:VAL:HB	2.08	0.52
1:C:246:VAL:O	1:C:250:ALA:HB2	2.09	0.52
1:C:279:TYR:HA	1:C:310:ILE:O	2.08	0.52
1:D:33:PRO:HG3	4:D:3045:HOH:O	2.08	0.52
1:B:65:ARG:HA	1:C:363:HIS:CD2	2.45	0.52
1:D:378:TYR:CD1	1:D:379:ARG:HG2	2.44	0.52
1:B:360:THR:HG21	4:B:2003:HOH:O	2.09	0.52
1:A:308:PRO:HD2	4:A:3013:HOH:O	2.09	0.52
1:B:83:TYR:CA	1:B:108:ILE:HG12	2.38	0.52
1:C:177:ASP:OD1	1:C:179:ASP:HB2	2.09	0.52
1:D:293:PHE:O	1:D:295:PRO:HD3	2.10	0.52
1:C:421:ARG:HD2	1:D:429:GLN:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ILE:CD1	1:D:310:ILE:HB	2.40	0.52
1:C:332:ALA:HB1	1:C:361:HIS:CE1	2.45	0.52
1:C:413:HIS:CE1	4:C:2018:HOH:O	2.62	0.52
1:C:442:VAL:HG12	1:C:484:VAL:HG11	1.91	0.52
1:D:309:LEU:HD12	1:D:309:LEU:N	2.24	0.52
1:A:343:GLU:HB3	1:A:344:PRO:HD2	1.91	0.52
1:B:26:LEU:HD21	1:B:37:LYS:CD	2.40	0.52
1:C:160:PHE:CD1	3:C:2002:HEM:HAB	2.45	0.52
1:C:213:GLY:HA3	1:C:235:TYR:CE2	2.45	0.52
1:C:131:PHE:CD1	1:C:235:TYR:HE2	2.27	0.52
1:D:154:ILE:HG13	1:D:349:MET:HE1	1.90	0.52
1:A:393:MET:SD	1:C:393:MET:HG3	2.50	0.52
1:B:115:VAL:HG21	1:B:128:PRO:HD2	1.91	0.52
1:C:381:ARG:HG3	1:C:381:ARG:O	2.09	0.52
1:D:193:HIS:HE1	4:D:3028:HOH:O	1.93	0.52
1:A:235:TYR:HA	1:A:277:THR:O	2.10	0.52
1:A:487:GLU:CD	1:A:491:ARG:HD2	2.29	0.52
1:B:491:ARG:O	1:B:495:LEU:HD23	2.10	0.52
1:C:303:PRO:C	1:C:305:GLY:N	2.62	0.52
1:D:22:LYS:HE3	1:D:22:LYS:HA	1.90	0.52
1:D:67:ARG:N	4:D:3004:HOH:O	2.21	0.52
1:D:155:ARG:NH1	1:D:299:THR:OG1	2.42	0.52
1:A:343:GLU:HB3	1:A:344:PRO:CD	2.40	0.51
1:B:81:PHE:CD1	1:B:81:PHE:N	2.77	0.51
1:B:205:PRO:HG3	1:B:211:MET:CE	2.39	0.51
1:B:252:LEU:N	1:B:252:LEU:HD12	2.25	0.51
1:D:290:ILE:O	1:D:291:PHE:C	2.48	0.51
1:B:78:ALA:HB2	1:B:261:LEU:CD1	2.29	0.51
1:D:223:ASN:HD21	1:D:227:GLU:CB	2.16	0.51
1:D:437:ASP:OD2	1:D:440:THR:HB	2.10	0.51
1:A:168:LYS:HD3	4:A:3162:HOH:O	2.09	0.51
1:A:358:PRO:HB2	1:A:362:ARG:NH1	2.25	0.51
1:A:492:ILE:O	1:A:496:LEU:HD13	2.11	0.51
1:B:43:VAL:O	1:B:47:GLY:HA3	2.11	0.51
1:C:218:THR:O	1:C:345:SER:HB3	2.10	0.51
1:C:303:PRO:C	1:C:305:GLY:H	2.14	0.51
1:D:335:PRO:CD	1:D:357:TYR:CG	2.93	0.51
1:B:34:VAL:HG13	1:B:55:VAL:HG11	1.92	0.51
1:A:323:ASN:ND2	1:C:396:ASN:HD22	2.09	0.51
1:A:23:PRO:HB2	1:C:412:GLU:HG2	1.91	0.51
1:A:290:ILE:C	1:A:290:ILE:HD12	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:GLU:OE1	1:A:501:GLU:CA	2.59	0.51
1:A:50:LEU:HD13	1:B:50:LEU:HD13	1.92	0.51
1:B:88:HIS:HB2	1:B:312:VAL:HA	1.93	0.51
1:B:428:VAL:O	1:B:428:VAL:CG2	2.57	0.51
1:B:92:ARG:HG3	4:B:2163:HOH:O	2.04	0.51
1:C:234:HIS:O	1:C:278:LEU:HD12	2.11	0.51
1:C:395:ASP:CB	4:C:2106:HOH:O	2.47	0.51
1:A:347:ASP:HB3	1:A:350:LEU:HB3	1.92	0.51
1:B:148:ASN:CB	1:B:211:MET:HE2	2.41	0.51
1:B:217:HIS:CD2	3:B:2001:HEM:HBC2	2.45	0.51
1:C:22:LYS:HD3	1:C:23:PRO:CD	2.41	0.51
1:D:221:LEU:HB2	1:D:229:VAL:CG2	2.41	0.51
1:D:301:VAL:O	1:D:303:PRO:HD3	2.11	0.51
1:A:4:ARG:HD3	1:A:8:SER:HB3	1.93	0.51
1:B:43:VAL:CG1	1:B:48:PRO:HD2	2.41	0.51
1:C:97:LYS:HD2	1:C:138:GLU:HB2	1.92	0.51
1:D:445:PHE:HA	1:D:449:VAL:CG2	2.41	0.51
1:A:498:LYS:O	1:A:499:TYR:C	2.49	0.50
1:D:206:ASP:OD2	1:D:242:LYS:HE3	2.11	0.50
1:A:45:PRO:HD3	1:D:431:PHE:CZ	2.46	0.50
1:A:326:ALA:HB2	1:C:396:ASN:HB2	1.93	0.50
1:A:485:HIS:HB3	1:A:488:TYR:HB2	1.94	0.50
1:B:74:HIS:ND1	1:B:114:THR:O	2.44	0.50
1:B:395:ASP:HA	4:B:2080:HOH:O	2.10	0.50
1:A:48:PRO:HB2	1:B:50:LEU:HD12	1.93	0.50
1:A:143:ASP:HB2	1:A:334:ASP:O	2.12	0.50
1:C:182:TRP:O	1:C:183:ASP:C	2.49	0.50
1:D:71:ARG:HG3	1:D:71:ARG:NH1	2.24	0.50
1:B:83:TYR:HA	1:B:108:ILE:HG12	1.93	0.50
1:B:81:PHE:HZ	1:B:327:GLU:HB3	1.75	0.50
1:D:19:ALA:O	4:D:3145:HOH:O	2.19	0.50
1:A:71:ARG:NH1	4:A:3007:HOH:O	2.32	0.50
1:D:234:HIS:O	1:D:278:LEU:HD12	2.11	0.50
1:D:71:ARG:NH2	1:D:329:GLU:O	2.43	0.50
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.92	0.50
1:A:433:SER:HB3	4:A:3030:HOH:O	2.10	0.50
1:B:360:THR:OG1	1:C:64:ASP:CB	2.60	0.50
1:B:98:VAL:HG13	1:B:99:PHE:CD1	2.46	0.50
1:B:4:ARG:NH2	1:C:470:GLN:HG3	2.26	0.50
1:C:472:PHE:C	1:C:472:PHE:CD1	2.85	0.50
1:B:374:VAL:CG2	4:B:2178:HOH:O	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLY:HA2	1:C:414:GLN:O	2.11	0.50
1:A:423:HIS:HA	1:B:427:ASP:HA	1.93	0.50
1:B:135:PHE:O	1:B:137:THR:HG23	2.11	0.50
1:C:338:MET:HE3	1:C:344:PRO:HD3	1.94	0.50
1:C:418:LEU:HD23	1:C:419:GLU:H	1.76	0.50
1:D:193:HIS:CE1	4:D:3028:HOH:O	2.64	0.50
1:A:355:PHE:CE2	1:D:57:THR:HG23	2.46	0.50
1:B:160:PHE:CE1	1:B:164:ILE:HD11	2.47	0.50
1:A:87:THR:HG23	1:A:313:GLY:HA2	1.93	0.49
1:A:82:GLY:HA3	1:A:316:VAL:O	2.12	0.49
1:C:126:ARG:O	1:C:127:ASP:HB2	2.12	0.49
1:C:165:HIS:HB3	1:D:402:ASN:OD1	2.13	0.49
1:C:223:ASN:C	1:C:225:ASP:H	2.15	0.49
1:A:258:ASP:HB3	1:A:261:LEU:HD12	1.92	0.49
1:C:353:ARG:HG3	3:C:2002:HEM:HBB2	1.94	0.49
1:C:303:PRO:O	1:C:305:GLY:N	2.45	0.49
1:C:451:ASN:ND2	1:C:453:GLU:H	2.10	0.49
1:D:170:ASN:HD22	1:D:173:THR:H	1.58	0.49
1:D:270:THR:O	1:D:272:ASN:N	2.45	0.49
1:D:285:PHE:HD1	1:D:285:PHE:H	1.58	0.49
1:A:384:ASN:HA	1:C:26:LEU:HD13	1.94	0.49
1:B:360:THR:CG2	4:B:2003:HOH:O	2.61	0.49
1:C:290:ILE:O	1:C:291:PHE:C	2.49	0.49
1:A:66:GLU:HG2	1:C:387:ARG:O	2.13	0.49
1:D:129:ARG:O	1:D:147:ASN:HB3	2.12	0.49
1:D:142:TRP:CZ2	1:D:342:ILE:HD13	2.48	0.49
1:D:189:PRO:HG3	1:D:480:ASN:HD21	1.77	0.49
1:B:367:PRO:HD2	4:B:2005:HOH:O	2.13	0.49
1:D:372:ILE:HB	1:D:375:ASN:HD22	1.76	0.49
1:A:291:PHE:HD2	1:A:293:PHE:O	1.96	0.49
1:B:90:ILE:O	1:B:93:TYR:N	2.41	0.49
1:B:11:MET:CE	1:C:180:MET:HG2	2.43	0.49
1:B:294:ASN:HA	1:C:46:ARG:NH1	2.27	0.49
1:C:83:TYR:CD1	1:C:105:ARG:HD3	2.47	0.49
1:B:163:PHE:O	1:B:166:SER:HB3	2.13	0.49
1:D:222:VAL:HG22	1:D:228:ALA:HB2	1.95	0.49
1:D:281:GLN:O	1:D:302:TRP:HZ3	1.95	0.49
1:A:212:ASP:OD1	1:A:236:LYS:HA	2.13	0.49
1:A:460:GLU:HA	1:A:495:LEU:HD13	1.95	0.49
1:C:338:MET:CE	1:C:344:PRO:HD3	2.43	0.49
1:C:474:GLN:NE2	1:C:496:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ALA:O	1:D:168:LYS:NZ	2.45	0.49
1:A:14:TRP:CZ3	1:A:18:ARG:HD2	2.48	0.49
1:A:231:CYS:HB2	1:A:281:GLN:O	2.12	0.49
1:B:71:ARG:HH11	1:B:71:ARG:CG	2.15	0.49
1:B:168:LYS:HZ1	1:C:67:ARG:HH21	1.61	0.49
1:D:148:ASN:N	1:D:148:ASN:ND2	2.60	0.49
1:A:395:ASP:OD1	1:C:327:GLU:OE2	2.31	0.49
1:B:125:VAL:HG22	1:B:126:ARG:N	2.27	0.49
1:B:327:GLU:OE2	4:B:2082:HOH:O	2.20	0.49
1:C:86:VAL:HG12	1:C:102:ILE:HA	1.94	0.49
1:C:142:TRP:HB2	1:C:339:PRO:CD	2.43	0.49
1:C:439:VAL:O	1:C:440:THR:C	2.50	0.49
1:D:193:HIS:HA	1:D:442:VAL:HG22	1.95	0.49
1:A:67:ARG:NH2	1:D:72:VAL:HG23	2.28	0.49
1:B:117:GLY:O	4:B:2160:HOH:O	2.20	0.48
1:C:22:LYS:HD3	1:C:23:PRO:HD2	1.94	0.48
1:C:74:HIS:HA	1:C:114:THR:O	2.13	0.48
1:D:72:VAL:O	1:D:168:LYS:HE3	2.13	0.48
1:C:78:ALA:HB2	1:C:261:LEU:CD2	2.40	0.48
1:D:306:ASP:O	1:D:308:PRO:HD3	2.13	0.48
1:B:10:GLN:HE21	1:C:172:GLN:NE2	2.12	0.48
1:A:126:ARG:HA	1:A:204:ILE:HG12	1.93	0.48
1:B:53:ASP:OD2	1:C:430:ARG:NH1	2.41	0.48
1:C:350:LEU:O	1:C:351:GLN:C	2.51	0.48
1:D:239:GLN:NE2	1:D:275:SER:H	2.10	0.48
1:D:142:TRP:CE2	1:D:342:ILE:HD13	2.48	0.48
1:D:471:LEU:HG	4:D:3023:HOH:O	2.14	0.48
1:A:335:PRO:HD2	4:A:3181:HOH:O	2.13	0.48
1:A:348:LYS:NZ	4:D:3021:HOH:O	2.47	0.48
1:A:349:MET:O	1:A:353:ARG:HG3	2.12	0.48
1:A:43:VAL:CG1	1:A:50:LEU:HD21	2.43	0.48
1:B:155:ARG:HD3	1:B:297:ASP:OD1	2.13	0.48
1:C:485:HIS:CE1	1:C:487:GLU:HB3	2.49	0.48
1:D:74:HIS:CE1	1:D:115:VAL:HG22	2.49	0.48
1:A:256:ASP:OD2	1:A:259:TYR:HA	2.14	0.48
1:B:14:TRP:CH2	1:B:18:ARG:HD2	2.49	0.48
1:B:266:ASN:O	1:B:270:THR:HG23	2.13	0.48
1:B:4:ARG:HH21	1:C:470:GLN:H	1.61	0.48
1:D:88:HIS:CD2	1:D:311:PRO:HG2	2.48	0.48
1:A:501:GLU:HA	1:A:501:GLU:OE1	2.14	0.48
1:C:18:ARG:HH12	1:C:23:PRO:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ILE:HG13	1:C:291:PHE:N	2.29	0.48
1:D:43:VAL:HG13	1:D:48:PRO:HD2	1.95	0.48
1:C:18:ARG:NH1	1:C:23:PRO:HA	2.28	0.48
1:D:378:TYR:CD1	1:D:378:TYR:C	2.88	0.48
1:A:45:PRO:HD3	1:D:431:PHE:CE2	2.49	0.48
1:D:155:ARG:NH2	1:D:438:ASN:OD1	2.47	0.48
1:D:89:ASP:OD1	1:D:91:THR:OG1	2.32	0.48
1:A:263:ASP:C	1:A:263:ASP:OD1	2.52	0.48
1:A:54:VAL:HG22	1:A:54:VAL:H	1.62	0.48
1:A:71:ARG:HG3	1:A:71:ARG:NH1	2.25	0.48
1:B:154:ILE:HG13	1:B:349:MET:HE1	1.96	0.48
1:C:111:ARG:HB3	3:C:2002:HEM:O1D	2.12	0.48
1:C:365:LEU:HD22	4:C:2125:HOH:O	2.14	0.48
1:C:41:LEU:HB3	1:C:53:ASP:HB2	1.96	0.48
1:C:51:VAL:HG21	1:D:49:LEU:HD23	1.95	0.48
1:B:118:GLU:OE1	1:B:118:GLU:N	2.47	0.47
1:C:26:LEU:HD12	1:C:27:THR:N	2.30	0.47
1:C:377:PRO:HG2	1:C:382:VAL:HG23	1.95	0.47
1:D:97:LYS:CA	1:D:100:GLU:HG3	2.42	0.47
1:D:177:ASP:O	1:D:181:VAL:HG23	2.14	0.47
1:D:219:PHE:O	1:D:230:TYR:HA	2.13	0.47
1:D:110:VAL:CG2	1:D:317:LEU:HD21	2.44	0.47
1:D:357:TYR:CE2	3:D:2003:HEM:CHA	2.97	0.47
1:A:279:TYR:HA	1:A:310:ILE:O	2.13	0.47
1:B:146:GLY:HA3	1:B:214:TYR:O	2.14	0.47
1:C:223:ASN:HD21	1:C:227:GLU:HB2	1.80	0.47
1:D:488:TYR:CE1	1:D:492:ILE:HD11	2.49	0.47
1:A:112:PHE:CG	1:A:208:HIS:HB3	2.49	0.47
1:A:53:ASP:OD2	1:D:430:ARG:NH1	2.44	0.47
1:A:97:LYS:O	1:A:100:GLU:HB2	2.14	0.47
1:D:99:PHE:O	1:D:100:GLU:C	2.53	0.47
1:D:381:ARG:HG2	1:D:381:ARG:NH1	2.30	0.47
1:D:90:ILE:HD13	1:D:312:VAL:HG13	1.96	0.47
1:B:65:ARG:O	1:D:389:GLY:HA2	2.15	0.47
1:D:52:GLN:CB	4:D:3005:HOH:O	2.21	0.47
1:C:211:MET:HG2	1:C:212:ASP:N	2.29	0.47
1:C:396:ASN:O	1:C:397:GLN:HB2	2.15	0.47
1:B:329:GLU:OE1	1:B:329:GLU:HA	2.14	0.47
1:C:142:TRP:HB2	1:C:339:PRO:HD3	1.96	0.47
1:C:394:MET:HB3	4:C:2089:HOH:O	2.15	0.47
1:D:335:PRO:HD3	1:D:357:TYR:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ILE:O	1:D:92:ARG:N	2.47	0.47
1:A:23:PRO:CB	1:C:412:GLU:HG2	2.45	0.47
1:A:358:PRO:HB2	1:A:362:ARG:HH12	1.80	0.47
1:B:446:TYR:CE1	1:B:455:ARG:HG2	2.49	0.47
1:D:86:VAL:HG23	1:D:104:LYS:O	2.14	0.47
1:A:15:LYS:NZ	4:A:3112:HOH:O	2.44	0.47
1:A:500:ASN:O	1:A:501:GLU:O	2.33	0.47
1:B:274:PRO:HB2	1:B:276:TRP:CZ3	2.50	0.47
1:A:43:VAL:HG21	1:B:43:VAL:HG21	1.97	0.47
1:B:71:ARG:HG2	3:B:2001:HEM:O2A	2.14	0.47
3:C:2002:HEM:HHC	3:C:2002:HEM:HMC1	1.48	0.47
1:C:476:LYS:HB3	1:C:476:LYS:NZ	2.30	0.47
1:B:16:GLU:O	1:B:18:ARG:N	2.48	0.47
1:B:404:TYR:OH	1:B:413:HIS:CD2	2.67	0.47
1:B:4:ARG:NH2	1:C:179:ASP:OD2	2.48	0.47
1:C:256:ASP:OD2	1:C:259:TYR:HA	2.15	0.47
1:C:72:VAL:HG13	1:C:73:VAL:HG22	1.96	0.47
1:A:455:ARG:NE	4:A:3196:HOH:O	2.48	0.47
1:A:487:GLU:OE1	1:A:491:ARG:HD2	2.15	0.47
1:D:145:VAL:HG12	3:D:2003:HEM:HMD2	1.96	0.47
1:B:310:ILE:HD12	1:B:310:ILE:N	2.31	0.46
1:C:368:ASN:O	1:C:371:GLN:HB2	2.14	0.46
1:A:152:PHE:HA	1:A:194:GLN:HG3	1.97	0.46
1:B:123:ASP:O	1:B:125:VAL:N	2.48	0.46
1:C:74:HIS:NE2	3:C:2002:HEM:ND	2.63	0.46
1:C:209:ARG:O	1:C:210:HIS:ND1	2.47	0.46
1:C:432:ASN:HD22	1:C:432:ASN:C	2.15	0.46
1:A:234:HIS:O	1:A:278:LEU:HD12	2.15	0.46
1:A:237:THR:HA	1:A:276:TRP:CD1	2.50	0.46
1:A:43:VAL:HG12	1:A:50:LEU:CD2	2.44	0.46
1:B:160:PHE:CD1	3:B:2001:HEM:HAB	2.50	0.46
1:D:26:LEU:HB3	1:D:34:VAL:CG2	2.45	0.46
1:B:229:VAL:HG23	1:B:284:THR:HA	1.98	0.46
1:B:217:HIS:CD2	1:B:353:ARG:NH1	2.82	0.46
1:C:52:GLN:O	1:C:54:VAL:N	2.49	0.46
1:D:154:ILE:HG13	1:D:349:MET:HE2	1.97	0.46
1:D:223:ASN:OD1	1:D:225:ASP:N	2.48	0.46
1:D:450:LEU:O	1:D:455:ARG:NH1	2.45	0.46
1:A:37:LYS:NZ	1:A:37:LYS:O	2.41	0.46
1:B:152:PHE:HB3	1:B:298:LEU:CD2	2.44	0.46
1:B:212:ASP:OD1	1:B:236:LYS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:HIS:HA	4:D:3042:HOH:O	2.16	0.46
1:D:460:GLU:HA	1:D:495:LEU:CD1	2.45	0.46
1:B:188:ARG:NE	1:B:190:GLU:OE2	2.44	0.46
1:B:472:PHE:CZ	1:B:473:ILE:HG13	2.51	0.46
1:B:9:ASP:O	1:B:12:LYS:HB3	2.15	0.46
1:C:129:ARG:HB3	1:C:211:MET:HE1	1.94	0.46
1:D:323:ASN:ND2	4:D:3007:HOH:O	2.48	0.46
1:D:90:ILE:HD11	1:D:99:PHE:CD1	2.50	0.46
1:A:439:VAL:O	1:A:440:THR:C	2.54	0.46
1:B:122:ALA:HB2	1:B:257:PRO:HB3	1.97	0.46
1:B:46:ARG:NH1	1:C:294:ASN:HB2	2.31	0.46
1:D:190:GLU:HA	1:D:438:ASN:CB	2.38	0.46
1:D:235:TYR:CD1	1:D:235:TYR:N	2.83	0.46
1:D:485:HIS:CE1	1:D:486:PRO:HG2	2.51	0.46
1:A:298:LEU:HD22	3:A:2000:HEM:HBC1	1.91	0.46
1:A:141:ASN:O	1:A:337:ASN:HB3	2.15	0.46
1:D:368:ASN:O	1:D:371:GLN:HB2	2.15	0.46
1:A:391:MET:CE	1:A:393:MET:CE	2.92	0.46
1:B:129:ARG:HB2	1:B:148:ASN:ND2	2.31	0.46
1:B:43:VAL:HG13	1:B:48:PRO:HD2	1.98	0.46
1:C:291:PHE:CD2	1:C:293:PHE:O	2.69	0.46
1:C:414:GLN:HA	1:C:415:PRO:HD2	1.82	0.46
1:D:209:ARG:HG2	1:D:274:PRO:HB3	1.97	0.46
1:D:442:VAL:HG12	1:D:484:VAL:HG11	1.98	0.46
1:A:110:VAL:HA	1:A:132:ALA:O	2.16	0.46
1:A:126:ARG:CA	1:A:204:ILE:HG12	2.46	0.46
1:A:452:GLU:O	1:A:453:GLU:C	2.54	0.46
1:B:26:LEU:HA	1:D:383:ALA:O	2.16	0.46
1:B:332:ALA:HB1	1:B:361:HIS:ND1	2.31	0.46
1:C:40:SER:HB3	1:C:49:LEU:CD1	2.46	0.46
1:A:421:ARG:CD	1:B:429:GLN:HG2	2.46	0.45
1:B:41:LEU:O	1:B:50:LEU:HD23	2.15	0.45
1:D:246:VAL:HG23	1:D:247:GLU:OE1	2.16	0.45
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.81	0.45
1:A:153:PHE:CD1	1:A:194:GLN:HB3	2.52	0.45
1:A:451:ASN:N	1:A:454:GLN:NE2	2.56	0.45
1:B:403:TYR:CD1	1:B:403:TYR:N	2.85	0.45
1:B:78:ALA:O	1:B:111:ARG:HA	2.15	0.45
1:C:130:GLY:HA2	1:C:147:ASN:CB	2.46	0.45
1:D:145:VAL:CG1	3:D:2003:HEM:C2D	2.99	0.45
1:D:284:THR:OG1	1:D:287:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LYS:HA	1:C:441:GLN:OE1	2.16	0.45
1:D:182:TRP:CD2	1:D:466:LEU:HD13	2.51	0.45
1:B:13:HIS:O	1:B:17:GLN:HG2	2.17	0.45
1:B:140:GLY:HA3	1:D:32:ASN:ND2	2.30	0.45
1:D:60:MET:HE3	1:D:63:PHE:HB3	1.98	0.45
1:A:90:ILE:HD13	1:A:312:VAL:HG22	1.97	0.45
1:B:239:GLN:N	1:B:239:GLN:CD	2.70	0.45
1:B:41:LEU:CB	1:B:53:ASP:HB2	2.47	0.45
1:B:474:GLN:O	1:B:477:ALA:HB3	2.17	0.45
1:D:26:LEU:HB3	1:D:34:VAL:HG22	1.99	0.45
1:B:154:ILE:HG13	1:B:349:MET:CE	2.47	0.45
1:C:308:PRO:O	1:C:310:ILE:CD1	2.64	0.45
1:C:467:LYS:HD3	1:C:499:TYR:CD1	2.51	0.45
1:A:74:HIS:HE1	4:A:3009:HOH:O	2.00	0.45
1:B:86:VAL:CG1	1:B:102:ILE:HD13	2.45	0.45
1:C:151:ILE:CG2	1:C:301:VAL:HG13	2.47	0.45
1:A:428:VAL:O	4:A:3193:HOH:O	2.20	0.45
1:A:445:PHE:HA	1:A:449:VAL:CG2	2.46	0.45
1:A:455:ARG:HD2	4:A:3196:HOH:O	2.16	0.45
1:B:476:LYS:HB2	1:B:476:LYS:HE3	1.63	0.45
1:C:395:ASP:C	1:C:395:ASP:OD2	2.46	0.45
1:D:339:PRO:HD2	1:D:342:ILE:HD12	1.98	0.45
1:C:395:ASP:CG	1:C:395:ASP:O	2.55	0.45
1:A:154:ILE:HG13	1:A:349:MET:CE	2.47	0.45
1:A:378:TYR:CD1	1:A:378:TYR:C	2.91	0.45
1:B:374:VAL:HG23	4:B:2178:HOH:O	2.17	0.45
1:B:41:LEU:HB2	1:B:53:ASP:OD2	2.17	0.45
1:C:126:ARG:HH11	1:C:126:ARG:HG2	1.82	0.45
1:C:152:PHE:HB3	1:C:298:LEU:CD2	2.47	0.45
4:A:3200:HOH:O	1:C:409:SER:HB3	2.17	0.45
1:D:90:ILE:HD11	1:D:99:PHE:CD2	2.52	0.45
1:A:338:MET:HB3	1:A:342:ILE:O	2.17	0.44
1:B:99:PHE:O	1:B:100:GLU:C	2.55	0.44
1:C:275:SER:HA	1:C:315:LEU:O	2.17	0.44
1:C:362:ARG:NH1	4:C:2008:HOH:O	2.50	0.44
1:D:151:ILE:HD13	1:D:193:HIS:CG	2.52	0.44
1:A:418:LEU:HB3	1:A:419:GLU:H	1.55	0.44
1:B:192:LEU:HD13	1:B:484:VAL:CG2	2.47	0.44
1:B:467:LYS:HG3	1:B:468:ASP:N	2.32	0.44
1:C:99:PHE:O	1:C:100:GLU:C	2.55	0.44
1:D:11:MET:O	1:D:12:LYS:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ILE:O	1:D:280:ILE:HD13	2.17	0.44
1:D:378:TYR:HD1	1:D:378:TYR:C	2.21	0.44
1:A:18:ARG:CD	4:A:3200:HOH:O	2.65	0.44
1:A:229:VAL:HG11	1:A:282:VAL:CG1	2.46	0.44
1:A:384:ASN:OD1	1:A:386:GLN:HB2	2.16	0.44
1:B:455:ARG:HG3	1:B:455:ARG:HH11	1.82	0.44
1:B:467:LYS:HD3	1:B:499:TYR:CD1	2.53	0.44
1:C:247:GLU:O	1:C:250:ALA:HB3	2.17	0.44
1:C:297:ASP:OD1	1:C:300:LYS:HG2	2.17	0.44
1:A:363:HIS:CD2	1:D:65:ARG:HA	2.52	0.44
1:B:129:ARG:H	1:B:148:ASN:CG	2.21	0.44
1:B:81:PHE:CZ	1:B:327:GLU:HB3	2.53	0.44
1:D:304:HIS:CD2	1:D:309:LEU:HD11	2.52	0.44
1:D:96:ALA:C	1:D:98:VAL:H	2.21	0.44
1:B:122:ALA:HB1	1:B:257:PRO:HA	1.99	0.44
1:B:374:VAL:HG22	4:B:2178:HOH:O	2.18	0.44
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.98	0.44
1:C:237:THR:HA	1:C:276:TRP:CD1	2.52	0.44
1:C:92:ARG:HH11	1:C:92:ARG:HG3	1.82	0.44
1:D:15:LYS:O	1:D:18:ARG:HB3	2.18	0.44
1:D:404:TYR:CD1	1:D:405:PRO:HA	2.52	0.44
1:B:285:PHE:O	1:B:289:GLU:HG3	2.18	0.44
1:B:456:LYS:HB2	1:B:491:ARG:HH22	1.83	0.44
1:C:155:ARG:NH2	1:C:438:ASN:ND2	2.65	0.44
1:C:485:HIS:HA	1:C:486:PRO:HD2	1.66	0.44
1:D:107:PRO:HG2	1:D:136:TYR:HB2	1.99	0.44
1:D:112:PHE:CD1	1:D:208:HIS:HB3	2.52	0.44
1:A:6:PRO:HG2	1:A:270:THR:CG2	2.48	0.44
1:B:361:HIS:NE2	3:B:2001:HEM:O1A	2.49	0.44
1:D:285:PHE:N	1:D:285:PHE:CD1	2.86	0.44
1:D:296:PHE:HB3	1:D:347:ASP:HA	1.99	0.44
1:A:485:HIS:HD2	1:A:487:GLU:CB	2.26	0.44
1:C:155:ARG:HH22	1:C:438:ASN:ND2	2.15	0.44
1:C:293:PHE:CD1	1:C:293:PHE:N	2.85	0.44
1:D:451:ASN:OD1	1:D:451:ASN:C	2.56	0.44
1:D:60:MET:CE	1:D:63:PHE:HD2	2.31	0.44
1:A:229:VAL:HG11	1:A:282:VAL:HG13	1.99	0.44
1:B:100:GLU:HB3	1:B:101:HIS:H	1.62	0.44
1:B:315:LEU:HD23	1:B:315:LEU:HA	1.89	0.44
1:B:454:GLN:HA	1:B:457:ARG:HH12	1.82	0.44
1:C:129:ARG:CG	1:C:211:MET:HE1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:TYR:CD1	1:C:311:PRO:HA	2.53	0.44
1:A:450:LEU:HD22	1:A:454:GLN:HB3	1.99	0.43
1:B:163:PHE:O	1:B:166:SER:N	2.51	0.43
1:A:427:ASP:HA	1:B:423:HIS:HA	2.00	0.43
1:B:71:ARG:HG3	4:B:2159:HOH:O	2.18	0.43
1:C:241:ILE:H	1:C:241:ILE:HD12	1.83	0.43
1:C:402:ASN:OD1	1:D:165:HIS:HB3	2.18	0.43
1:D:221:LEU:HB2	1:D:229:VAL:HG23	1.98	0.43
1:D:220:LYS:HA	1:D:229:VAL:O	2.18	0.43
1:A:88:HIS:CD2	1:A:311:PRO:HG2	2.53	0.43
1:B:262:ARG:HG3	1:B:266:ASN:ND2	2.32	0.43
1:C:406:ASN:ND2	1:C:410:ALA:HB3	2.19	0.43
1:A:455:ARG:CD	4:A:3196:HOH:O	2.67	0.43
1:B:273:TYR:HA	1:B:274:PRO:HD3	1.79	0.43
1:B:351:GLN:O	1:B:354:LEU:HB2	2.18	0.43
1:C:451:ASN:OD1	1:C:454:GLN:HG3	2.19	0.43
1:A:273:TYR:HA	1:A:274:PRO:HD3	1.87	0.43
1:B:139:ASP:HB3	1:B:340:PRO:HD2	2.01	0.43
1:C:234:HIS:O	1:C:278:LEU:HA	2.18	0.43
1:C:421:ARG:HD2	1:D:429:GLN:HB2	2.00	0.43
1:A:410:ALA:HB1	1:A:411:PRO:HD2	2.00	0.43
1:A:485:HIS:CD2	1:A:487:GLU:CB	2.98	0.43
1:C:456:LYS:O	1:C:460:GLU:HG3	2.18	0.43
1:D:101:HIS:CD2	4:D:3063:HOH:O	2.72	0.43
1:D:237:THR:HA	1:D:276:TRP:CD1	2.54	0.43
1:B:160:PHE:N	1:B:161:PRO:CD	2.82	0.43
1:C:12:LYS:HG2	1:C:16:GLU:OE2	2.17	0.43
1:C:182:TRP:CD2	1:C:466:LEU:HD13	2.53	0.43
1:C:244:LEU:HB3	1:C:249:ALA:HB2	2.00	0.43
1:C:152:PHE:HB3	1:C:298:LEU:HD23	2.01	0.43
1:A:391:MET:HE2	1:A:393:MET:CE	2.49	0.43
1:B:357:TYR:CZ	3:B:2001:HEM:NA	2.86	0.43
1:B:446:TYR:CE2	1:B:488:TYR:HB2	2.54	0.43
1:C:156:ASP:OD2	1:C:348:LYS:HD3	2.18	0.43
1:C:81:PHE:CD1	1:C:81:PHE:N	2.86	0.43
1:D:212:ASP:OD1	1:D:236:LYS:HA	2.19	0.43
1:B:82:GLY:HA3	1:B:317:LEU:HA	2.01	0.43
1:B:296:PHE:CE1	1:B:346:PRO:HD2	2.54	0.43
1:C:232:LYS:O	1:C:280:ILE:HA	2.18	0.43
1:D:170:ASN:ND2	1:D:173:THR:H	2.16	0.43
1:D:377:PRO:HG2	1:D:382:VAL:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLN:HG3	1:B:21:GLN:H	1.54	0.43
1:B:353:ARG:NH1	3:B:2001:HEM:CBC	2.82	0.43
1:B:487:GLU:O	1:B:491:ARG:HG3	2.19	0.43
1:C:281:GLN:CG	1:C:309:LEU:HD12	2.49	0.43
1:C:381:ARG:HB2	1:C:381:ARG:HH11	1.84	0.43
1:B:90:ILE:HD13	1:B:312:VAL:HB	2.00	0.43
1:C:279:TYR:HD1	1:C:311:PRO:HA	1.84	0.43
1:C:402:ASN:N	1:C:402:ASN:ND2	2.46	0.43
1:B:41:LEU:HD23	1:C:430:ARG:CZ	2.49	0.43
1:C:469:ALA:O	1:C:470:GLN:C	2.58	0.43
1:D:160:PHE:CE1	1:D:164:ILE:HD11	2.54	0.42
1:D:160:PHE:HB3	1:D:161:PRO:HD3	2.01	0.42
1:D:357:TYR:HB2	1:D:358:PRO:HD3	1.99	0.42
1:A:83:TYR:CD1	1:A:105:ARG:HD2	2.53	0.42
1:A:309:LEU:N	1:A:309:LEU:CD2	2.78	0.42
1:A:388:ASP:H	1:A:396:ASN:HD21	1.67	0.42
1:B:18:ARG:O	1:B:19:ALA:C	2.57	0.42
1:B:430:ARG:HD3	1:C:36:ASP:HB3	2.00	0.42
1:C:355:PHE:O	1:C:358:PRO:HD2	2.19	0.42
1:D:137:THR:O	1:D:379:ARG:HB2	2.19	0.42
1:D:220:LYS:O	1:D:221:LEU:HD23	2.19	0.42
1:D:43:VAL:HG13	1:D:43:VAL:O	2.19	0.42
2:A:3000:CYN:N	3:A:2000:HEM:NC	2.62	0.42
1:B:149:THR:OG1	1:B:150:PRO:HD2	2.19	0.42
1:B:145:VAL:HB	1:B:353:ARG:NH2	2.35	0.42
1:B:4:ARG:HD2	1:B:8:SER:CB	2.49	0.42
1:D:422:THR:HG22	1:D:423:HIS:N	2.33	0.42
1:A:82:GLY:HA3	1:A:317:LEU:HA	2.00	0.42
1:B:188:ARG:NH2	1:B:190:GLU:OE2	2.47	0.42
1:B:452:GLU:OE2	1:B:491:ARG:NH1	2.45	0.42
1:C:131:PHE:CE1	1:C:235:TYR:HE2	2.37	0.42
1:D:391:MET:HB3	1:D:391:MET:HE3	1.86	0.42
1:A:332:ALA:CB	1:A:361:HIS:NE2	2.82	0.42
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.49	0.42
1:B:223:ASN:C	1:B:225:ASP:H	2.21	0.42
1:D:160:PHE:CE2	1:D:164:ILE:HG13	2.55	0.42
1:B:264:LEU:HG	4:B:2055:HOH:O	2.19	0.42
1:D:106:THR:O	1:D:108:ILE:HG23	2.20	0.42
1:D:145:VAL:HB	1:D:353:ARG:NH2	2.35	0.42
1:A:197:PHE:O	1:A:200:SER:OG	2.27	0.42
1:B:217:HIS:CE1	3:B:2001:HEM:HBC1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:PHE:CE1	1:D:437:ASP:OD2	2.73	0.42
1:A:268:ILE:HB	1:A:320:ASN:HD21	1.85	0.42
1:B:393:MET:HE2	1:D:373:PRO:CD	2.48	0.42
1:B:402:ASN:HD22	1:B:402:ASN:C	2.23	0.42
1:B:66:GLU:HA	1:D:389:GLY:N	2.35	0.42
1:C:210:HIS:HD2	1:C:242:LYS:HB3	1.82	0.42
1:C:444:THR:HG22	1:C:444:THR:O	2.19	0.42
1:D:129:ARG:O	1:D:147:ASN:HA	2.20	0.42
1:A:273:TYR:CD1	1:A:318:ASN:HA	2.55	0.42
1:A:357:TYR:O	1:A:360:THR:HG22	2.20	0.42
1:A:284:THR:OG1	1:A:287:GLU:CG	2.64	0.42
1:A:41:LEU:HB3	1:A:53:ASP:HB2	2.01	0.42
1:C:95:LYS:HG2	1:C:222:VAL:O	2.19	0.42
1:C:22:LYS:HD3	1:C:23:PRO:N	2.35	0.42
1:C:422:THR:HG22	1:C:423:HIS:N	2.35	0.42
1:C:182:TRP:NE1	1:C:465:HIS:ND1	2.64	0.42
1:D:154:ILE:HB	4:D:3132:HOH:O	2.19	0.42
1:A:172:GLN:NE2	1:D:322:VAL:HA	2.30	0.42
1:B:71:ARG:CG	1:B:71:ARG:NH1	2.77	0.41
1:D:87:THR:C	1:D:88:HIS:ND1	2.73	0.41
1:A:439:VAL:HG23	1:A:440:THR:N	2.36	0.41
1:A:455:ARG:NH1	4:A:3196:HOH:O	2.52	0.41
1:B:472:PHE:C	1:B:472:PHE:CD2	2.94	0.41
1:A:50:LEU:CD1	1:B:48:PRO:HB2	2.50	0.41
1:B:74:HIS:CD2	3:B:2001:HEM:C4D	3.08	0.41
1:C:414:GLN:NE2	1:C:417:ALA:HB2	2.33	0.41
1:C:480:ASN:O	1:C:484:VAL:HG23	2.20	0.41
1:A:430:ARG:HE	1:B:419:GLU:CD	2.23	0.41
1:C:223:ASN:O	1:C:225:ASP:N	2.53	0.41
1:C:467:LYS:HE2	1:C:468:ASP:OD2	2.20	0.41
1:D:189:PRO:HB2	1:D:438:ASN:HD22	1.85	0.41
1:D:71:ARG:HH22	1:D:329:GLU:C	2.22	0.41
1:A:158:LEU:HD21	1:D:56:PHE:HA	2.03	0.41
1:A:15:LYS:HD2	1:C:408:PHE:HA	2.03	0.41
1:A:452:GLU:HA	1:A:455:ARG:HH11	1.85	0.41
1:B:432:ASN:HA	1:C:39:ASN:OD1	2.20	0.41
1:B:470:GLN:OE1	1:B:472:PHE:HE1	2.03	0.41
1:B:475:LYS:O	1:B:476:LYS:C	2.57	0.41
1:B:493:GLN:O	1:B:494:ALA:C	2.59	0.41
1:C:209:ARG:NH2	1:C:267:ALA:HB2	2.29	0.41
1:C:332:ALA:HB1	1:C:361:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:TYR:C	1:C:501:GLU:H	2.23	0.41
1:D:298:LEU:HD21	3:D:2003:HEM:HMC3	2.03	0.41
1:A:452:GLU:N	1:A:455:ARG:NH1	2.69	0.41
1:B:26:LEU:HD21	1:B:37:LYS:HD2	2.01	0.41
1:B:487:GLU:C	1:B:489:GLY:H	2.23	0.41
1:B:92:ARG:H	1:B:92:ARG:HG3	1.62	0.41
1:D:94:SER:HB2	1:D:221:LEU:HB3	2.01	0.41
1:D:209:ARG:O	1:D:239:GLN:HB2	2.20	0.41
1:B:193:HIS:HA	1:B:442:VAL:HG22	2.01	0.41
1:C:395:ASP:OD2	1:C:395:ASP:O	2.39	0.41
1:B:165:HIS:NE2	1:C:66:GLU:OE2	2.37	0.41
3:B:2001:HEM:CGD	4:B:2179:HOH:O	2.68	0.41
1:D:179:ASP:O	1:D:183:ASP:HB2	2.20	0.41
1:D:217:HIS:CD2	1:D:353:ARG:HH11	2.39	0.41
1:A:69:PRO:O	1:A:364:ARG:HG3	2.21	0.41
1:A:385:TYR:OH	1:A:410:ALA:HB3	2.21	0.41
1:B:43:VAL:HG22	1:B:43:VAL:O	2.21	0.41
1:B:177:ASP:C	1:B:177:ASP:OD1	2.59	0.41
1:B:332:ALA:N	1:B:375:ASN:OD1	2.54	0.41
1:A:421:ARG:NH2	1:B:429:GLN:NE2	2.69	0.41
1:D:114:THR:HB	1:D:115:VAL:H	1.74	0.41
1:D:291:PHE:HA	1:D:292:PRO:HD3	1.83	0.41
1:D:346:PRO:O	1:D:347:ASP:C	2.58	0.41
1:A:242:LYS:HD3	1:A:242:LYS:C	2.41	0.41
1:A:453:GLU:OE2	1:A:457:ARG:NH1	2.54	0.41
1:B:408:PHE:O	1:B:409:SER:HB2	2.20	0.41
1:B:442:VAL:O	1:B:445:PHE:HB3	2.20	0.41
1:C:115:VAL:HB	1:C:127:ASP:OD1	2.20	0.41
1:C:131:PHE:C	1:C:131:PHE:CD1	2.94	0.41
1:C:281:GLN:HG2	1:C:309:LEU:HD12	2.03	0.41
1:C:221:LEU:HA	1:C:341:GLY:O	2.20	0.41
1:D:147:ASN:OD1	3:D:2003:HEM:C4C	2.74	0.41
1:B:153:PHE:N	1:B:153:PHE:CD1	2.88	0.41
1:B:19:ALA:HB3	1:B:21:GLN:NE2	2.09	0.41
1:B:357:TYR:HB2	1:B:358:PRO:HD3	2.02	0.41
1:B:414:GLN:HA	1:B:415:PRO:HD2	1.89	0.41
1:B:301:VAL:HG22	1:B:441:GLN:OE1	2.21	0.41
1:B:442:VAL:HG12	1:B:484:VAL:CG1	2.51	0.41
1:C:202:ARG:HA	1:C:243:ASN:OD1	2.20	0.41
1:C:284:THR:HA	4:C:2136:HOH:O	2.20	0.41
1:C:487:GLU:HG2	1:C:491:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LYS:HE3	1:B:343:GLU:OE1	2.21	0.40
1:B:252:LEU:O	1:B:253:ALA:C	2.59	0.40
1:B:50:LEU:N	1:B:50:LEU:CD2	2.83	0.40
1:C:448:LYS:HD2	4:C:2115:HOH:O	2.22	0.40
1:B:139:ASP:O	1:D:32:ASN:HA	2.21	0.40
1:D:347:ASP:OD1	1:D:349:MET:HB2	2.20	0.40
1:D:500:ASN:O	1:D:501:GLU:C	2.60	0.40
1:A:413:HIS:O	1:A:413:HIS:HD2	2.04	0.40
1:B:252:LEU:CD1	1:B:252:LEU:N	2.84	0.40
1:B:220:LYS:N	1:B:343:GLU:O	2.52	0.40
1:B:371:GLN:OE1	1:B:393:MET:N	2.54	0.40
1:B:447:LEU:O	1:B:447:LEU:HD12	2.21	0.40
4:A:3145:HOH:O	1:C:37:LYS:N	2.08	0.40
1:D:145:VAL:CG1	3:D:2003:HEM:CMD	2.98	0.40
1:D:280:ILE:HD13	1:D:310:ILE:HB	2.03	0.40
1:D:452:GLU:HA	1:D:452:GLU:OE1	2.22	0.40
1:A:265:PHE:CE2	1:D:173:THR:HG22	2.56	0.40
1:A:395:ASP:OD2	1:A:398:GLY:HA2	2.21	0.40
1:B:83:TYR:N	1:B:108:ILE:HG12	2.36	0.40
1:B:296:PHE:CD2	1:B:346:PRO:HG2	2.56	0.40
1:B:458:LEU:HG	1:B:459:CYS:N	2.35	0.40
1:C:71:ARG:NE	3:C:2002:HEM:O2D	2.50	0.40
1:A:323:ASN:CG	1:C:396:ASN:HB3	2.42	0.40
1:B:177:ASP:OD1	1:B:179:ASP:HB2	2.21	0.40
1:B:436:ASP:O	1:B:437:ASP:O	2.39	0.40
1:C:233:PHE:N	4:C:2020:HOH:O	2.54	0.40
1:D:218:THR:HG23	1:D:302:TRP:CZ2	2.56	0.40
1:D:335:PRO:HD2	1:D:357:TYR:CG	2.56	0.40
1:D:478:VAL:HG21	1:D:493:GLN:OE1	2.22	0.40
1:A:280:ILE:HG12	1:A:310:ILE:HB	2.03	0.40
1:A:332:ALA:N	1:A:375:ASN:OD1	2.53	0.40
1:B:444:THR:O	1:B:448:LYS:CB	2.61	0.40
1:B:10:GLN:NE2	1:C:172:GLN:HE21	2.19	0.40
1:C:446:TYR:CE2	1:C:455:ARG:HD3	2.57	0.40
1:C:463:ALA:O	1:C:467:LYS:HB3	2.21	0.40
1:D:170:ASN:HD22	1:D:172:GLN:N	2.09	0.40

There are no symmetry-related clashes.

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%)	450 (90%)	39 (8%)	8 (2%)	9	31
1	B	497/506 (98%)	425 (86%)	58 (12%)	14 (3%)	5	17
1	C	497/506 (98%)	427 (86%)	54 (11%)	16 (3%)	4	13
1	D	497/506 (98%)	438 (88%)	50 (10%)	9 (2%)	8	28
All	All	1988/2024 (98%)	1740 (88%)	201 (10%)	47 (2%)	6	20

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	100	GLU
1	B	4	ARG
1	B	100	GLU
1	B	124	THR
1	B	437	ASP
1	C	206	ASP
1	C	209	ARG
1	D	100	GLU
1	D	413	HIS
1	A	19	ALA
1	A	20	ALA
1	B	17	GLN
1	B	448	LYS
1	C	19	ALA
1	C	53	ASP
1	C	100	GLU
1	C	211	MET
1	C	224	ALA
1	C	240	GLY
1	D	91	THR
1	D	271	GLY

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Mol	Chain	Res	Type
1	A	101	HIS
1	A	437	ASP
1	A	500	ASN
1	B	19	ALA
1	C	440	THR
1	C	470	GLN
1	D	19	ALA
1	D	411	PRO
1	B	16	GLU
1	D	437	ASP
1	A	498	LYS
1	B	18	ARG
1	B	270	THR
1	B	325	PHE
1	C	346	PRO
1	D	36	ASP
1	D	216	SER
1	B	347	ASP
1	C	304	HIS
1	C	373	PRO
1	B	203	GLY
1	B	115	VAL
1	C	127	ASP
1	C	181	VAL
1	C	439	VAL

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%)	400 (93%)	31 (7%)	14	38
1	B	431/437 (99%)	392 (91%)	39 (9%)	9	28
1	C	431/437 (99%)	388 (90%)	43 (10%)	7	22
1	D	431/437 (99%)	404 (94%)	27 (6%)	18	46
All	All	1724/1748 (99%)	1584 (92%)	140 (8%)	11	33

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	18	ARG
1	A	26	LEU
1	A	37	LYS
1	A	43	VAL
1	A	49	LEU
1	A	54	VAL
1	A	106	THR
1	A	131	PHE
1	A	137	THR
1	A	148	ASN
1	A	191	SER
1	A	194	GLN
1	A	202	ARG
1	A	235	TYR
1	A	263	ASP
1	A	309	LEU
1	A	336	SER
1	A	361	HIS
1	A	379	ARG
1	A	394	MET
1	A	402	ASN
1	A	407	SER
1	A	413	HIS
1	A	421	ARG
1	A	435	ASN
1	A	436	ASP
1	A	456	LYS
1	A	476	LYS
1	A	488	TYR
1	A	496	LEU
1	B	18	ARG
1	B	21	GLN
1	B	32	ASN
1	B	37	LYS
1	B	41	LEU
1	B	46	ARG
1	B	51	VAL
1	B	67	ARG
1	B	92	ARG
1	B	95	LYS
1	B	101	HIS

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Mol	Chain	Res	Type
1	B	114	THR
1	B	124	THR
1	B	126	ARG
1	B	131	PHE
1	B	137	THR
1	B	149	THR
1	B	168	LYS
1	B	193	HIS
1	B	202	ARG
1	B	220	LYS
1	B	232	LYS
1	B	235	TYR
1	B	262	ARG
1	B	272	ASN
1	B	290	ILE
1	B	312	VAL
1	B	336	SER
1	B	374	VAL
1	B	381	ARG
1	B	393	MET
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	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	88	HIS
1	C	92	ARG
1	C	105	ARG
1	C	131	PHE
1	C	147	ASN
1	C	149	THR
1	C	179	ASP

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Mol	Chain	Res	Type
1	C	194	GLN
1	C	200	SER
1	C	201	ASP
1	C	202	ARG
1	C	206	ASP
1	C	209	ARG
1	C	210	HIS
1	C	235	TYR
1	C	237	THR
1	C	239	GLN
1	C	248	ASP
1	C	293	PHE
1	C	304	HIS
1	C	331	LEU
1	C	345	SER
1	C	381	ARG
1	C	402	ASN
1	C	412	GLU
1	C	413	HIS
1	C	414	GLN
1	C	418	LEU
1	C	432	ASN
1	C	436	ASP
1	C	438	ASN
1	C	451	ASN
1	C	467	LYS
1	C	472	PHE
1	C	488	TYR
1	C	501	GLU
1	D	18	ARG
1	D	22	LYS
1	D	105	ARG
1	D	111	ARG
1	D	124	THR
1	D	127	ASP
1	D	131	PHE
1	D	138	GLU
1	D	147	ASN
1	D	148	ASN
1	D	193	HIS
1	D	235	TYR
1	D	247	GLU

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Mol	Chain	Res	Type
1	D	261	LEU
1	D	263	ASP
1	D	280	ILE
1	D	301	VAL
1	D	368	ASN
1	D	378	TYR
1	D	397	GLN
1	D	412	GLU
1	D	413	HIS
1	D	421	ARG
1	D	438	ASN
1	D	467	LYS
1	D	479	LYS
1	D	488	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	148	ASN
1	A	167	GLN
1	A	254	HIS
1	A	320	ASN
1	A	337	ASN
1	A	423	HIS
1	A	429	GLN
1	A	454	GLN
1	A	470	GLN
1	A	485	HIS
1	B	17	GLN
1	B	21	GLN
1	B	32	ASN
1	B	62	HIS
1	B	272	ASN
1	B	320	ASN
1	B	337	ASN
1	B	361	HIS
1	B	363	HIS
1	B	402	ASN
1	B	414	GLN
1	B	429	GLN
1	B	435	ASN

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Mol	Chain	Res	Type
1	B	461	ASN
1	C	17	GLN
1	C	52	GLN
1	C	167	GLN
1	C	172	GLN
1	C	239	GLN
1	C	272	ASN
1	C	337	ASN
1	C	402	ASN
1	C	414	GLN
1	C	432	ASN
1	C	435	ASN
1	C	438	ASN
1	C	454	GLN
1	C	461	ASN
1	C	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	193	HIS
1	D	239	GLN
1	D	337	ASN
1	D	368	ASN
1	D	413	HIS
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 carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	B	2001	1	27,50,50	12.24	9 (33%)	17,82,82	14.50	6 (35%)
2	CYN	D	3001	3	0,1,1	0.00	-	-		
3	HEM	A	2000	1	27,50,50	11.72	7 (25%)	17,82,82	12.89	2 (11%)
2	CYN	A	3000	-	0,1,1	0.00	-	-		
3	HEM	D	2003	1,2	27,50,50	1.79	6 (22%)	17,82,82	11.21	6 (35%)
3	HEM	C	2002	1	27,50,50	1.70	5 (18%)	17,82,82	2.84	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	2001	1	-	3/6/54/54	-
3	HEM	A	2000	1	-	0/6/54/54	-
3	HEM	D	2003	1,2	-	3/6/54/54	-
3	HEM	C	2002	1	-	0/6/54/54	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	HEM	CMC-C2C	46.72	2.62	1.51
3	B	2001	HEM	CMC-C2C	46.53	2.62	1.51
3	B	2001	HEM	C3C-CAC	42.28	2.34	1.47
3	A	2000	HEM	C3C-CAC	38.07	2.25	1.47
3	B	2001	HEM	C3B-CAB	-4.51	1.38	1.47
3	C	2002	HEM	C3B-CAB	-4.49	1.38	1.47
3	D	2003	HEM	C3B-CAB	-4.46	1.38	1.47
3	A	2000	HEM	C3B-CAB	-4.38	1.39	1.47
3	A	2000	HEM	C3B-C2B	-3.85	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2003	HEM	C3B-C2B	-3.84	1.35	1.40
3	C	2002	HEM	C3B-C2B	-3.78	1.35	1.40
3	B	2001	HEM	C3B-C2B	-3.74	1.35	1.40
3	A	2000	HEM	CBC-CAC	3.48	1.52	1.29
3	C	2002	HEM	CBC-CAC	3.45	1.52	1.29
3	D	2003	HEM	CBC-CAC	3.41	1.51	1.29
3	B	2001	HEM	CBC-CAC	3.27	1.51	1.29
3	A	2000	HEM	C3C-C2C	-3.13	1.36	1.40
3	B	2001	HEM	C3C-C2C	-3.06	1.36	1.40
3	B	2001	HEM	C4B-CHC	-2.86	1.33	1.41
3	C	2002	HEM	C3C-C2C	-2.48	1.36	1.40
3	D	2003	HEM	C3C-C2C	-2.43	1.37	1.40
3	B	2001	HEM	CAA-C2A	2.41	1.55	1.52
3	D	2003	HEM	C3C-CAC	2.26	1.52	1.47
3	C	2002	HEM	CBB-CAB	2.03	1.42	1.29
3	D	2003	HEM	CBB-CAB	2.02	1.42	1.29
3	B	2001	HEM	CBB-CAB	2.01	1.42	1.29
3	A	2000	HEM	CBB-CAB	2.01	1.42	1.29

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	HEM	CMC-C2C-C3C	-53.03	25.47	124.68
3	B	2001	HEM	CMC-C2C-C3C	-52.48	26.48	124.68
3	D	2003	HEM	CAA-CBA-CGA	34.43	170.43	112.67
3	D	2003	HEM	CBA-CAA-C2A	24.00	156.75	112.49
3	B	2001	HEM	CBD-CAD-C3D	16.51	142.90	112.48
3	B	2001	HEM	CAA-CBA-CGA	16.44	140.25	112.67
3	D	2003	HEM	CBD-CAD-C3D	15.41	140.87	112.48
3	B	2001	HEM	CAD-CBD-CGD	15.35	138.42	112.67
3	C	2002	HEM	CMC-C2C-C3C	11.19	145.62	124.68
3	D	2003	HEM	CAD-CBD-CGD	10.59	130.43	112.67
3	B	2001	HEM	CBA-CAA-C2A	-4.47	104.23	112.49
3	B	2001	HEM	CAA-C2A-C3A	4.04	138.85	127.25
3	D	2003	HEM	CAD-C3D-C2D	-3.62	116.86	127.25
3	D	2003	HEM	CAA-C2A-C3A	2.50	134.42	127.25
3	C	2002	HEM	CBA-CAA-C2A	-2.37	108.11	112.49
3	A	2000	HEM	CBA-CAA-C2A	-2.36	108.13	112.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	HEM	C2D-C3D-CAD-CBD
3	B	2001	HEM	C4D-C3D-CAD-CBD
3	D	2003	HEM	C2A-CAA-CBA-CGA
3	D	2003	HEM	C2D-C3D-CAD-CBD
3	D	2003	HEM	C4D-C3D-CAD-CBD
3	B	2001	HEM	C2A-CAA-CBA-CGA

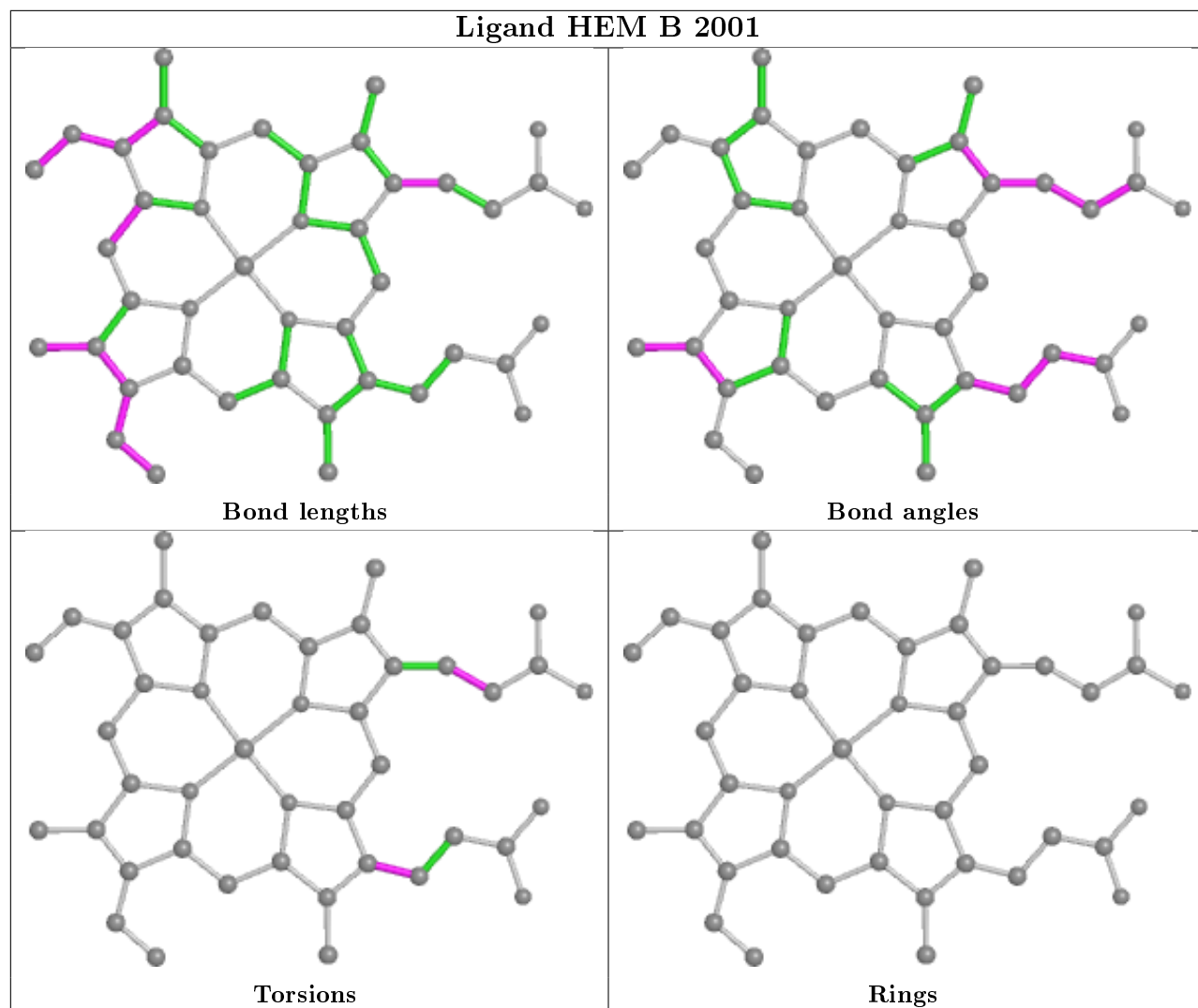
There are no ring outliers.

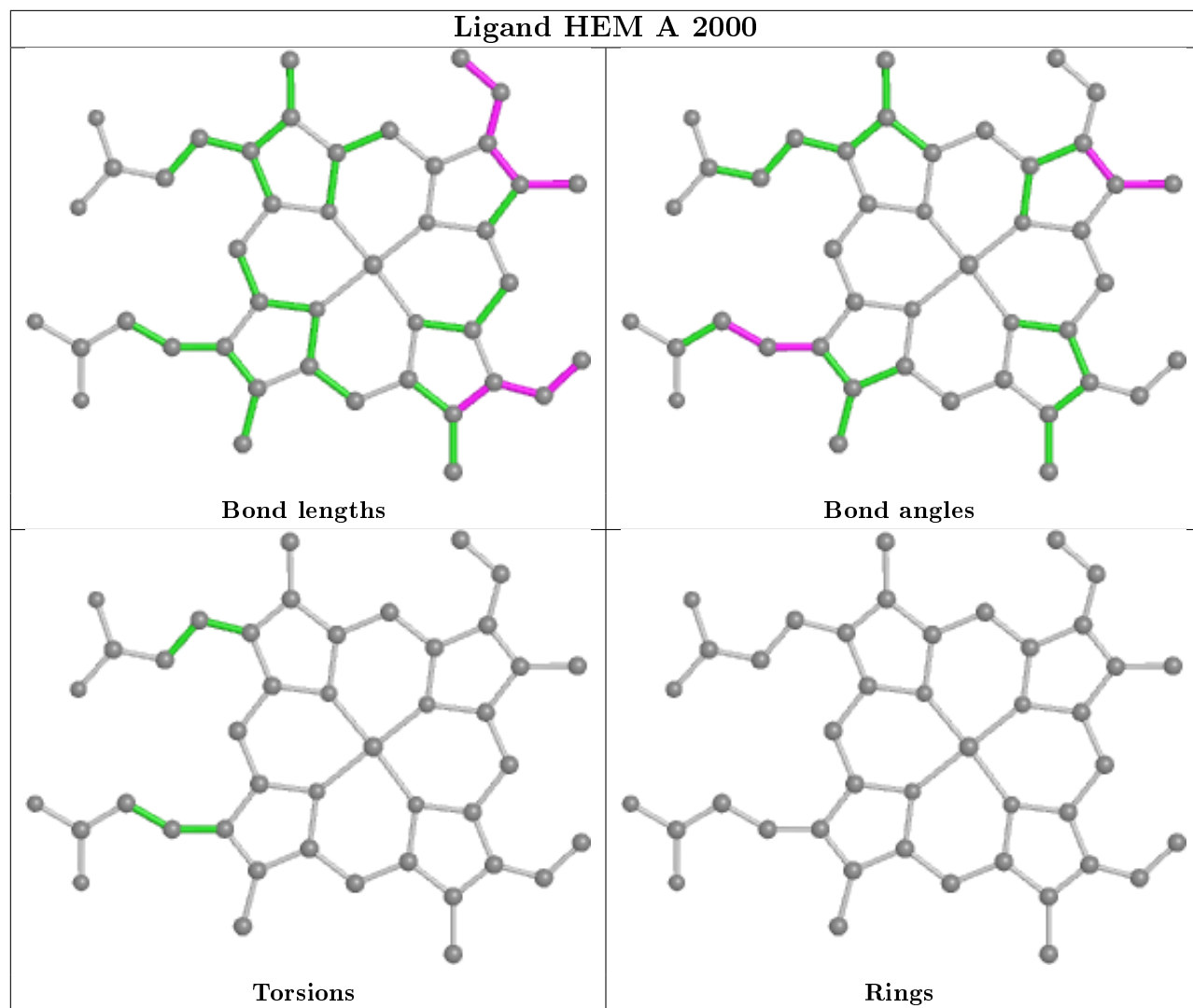
5 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	HEM	25	0
3	A	2000	HEM	16	0
2	A	3000	CYN	6	0
3	D	2003	HEM	21	0
3	C	2002	HEM	26	0

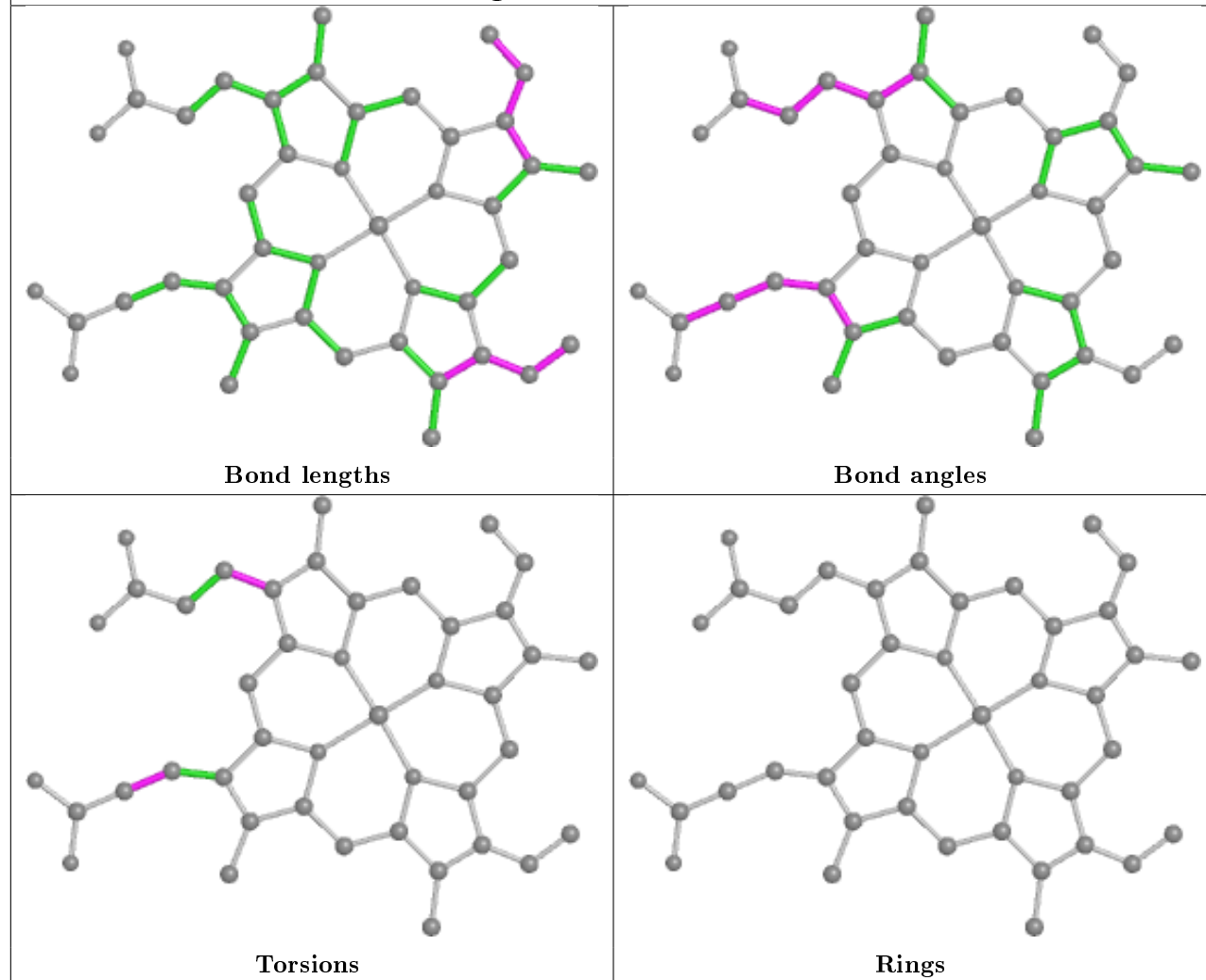
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

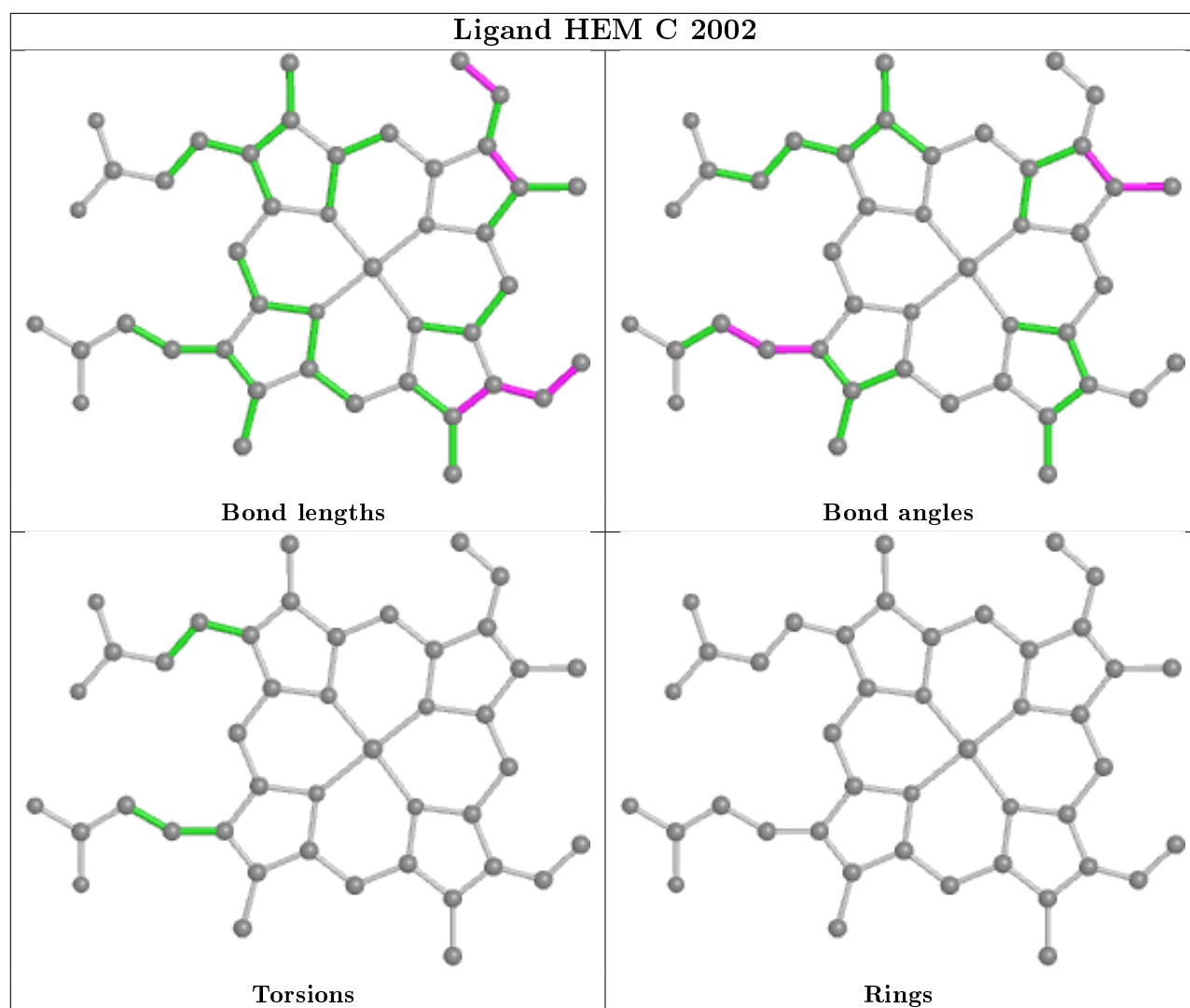
Ligand HEM B 2001





Ligand HEM D 2003





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%)	-0.62	2 (0%) 92 91	9, 29, 55, 85	0
1	B	499/506 (98%)	-0.50	2 (0%) 92 91	12, 37, 64, 97	0
1	C	499/506 (98%)	-0.49	3 (0%) 89 86	12, 33, 65, 90	1 (0%)
1	D	499/506 (98%)	-0.49	0 100 100	10, 35, 69, 89	0
All	All	1996/2024 (98%)	-0.52	7 (0%) 92 91	9, 34, 64, 97	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	2.8
1	A	3	ASN	2.6
1	C	20	ALA	2.6
1	A	20	ALA	2.4
1	C	471	LEU	2.3
1	B	20	ALA	2.2
1	C	415	PRO	2.2

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

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

6.3 Carbohydrates ⓘ

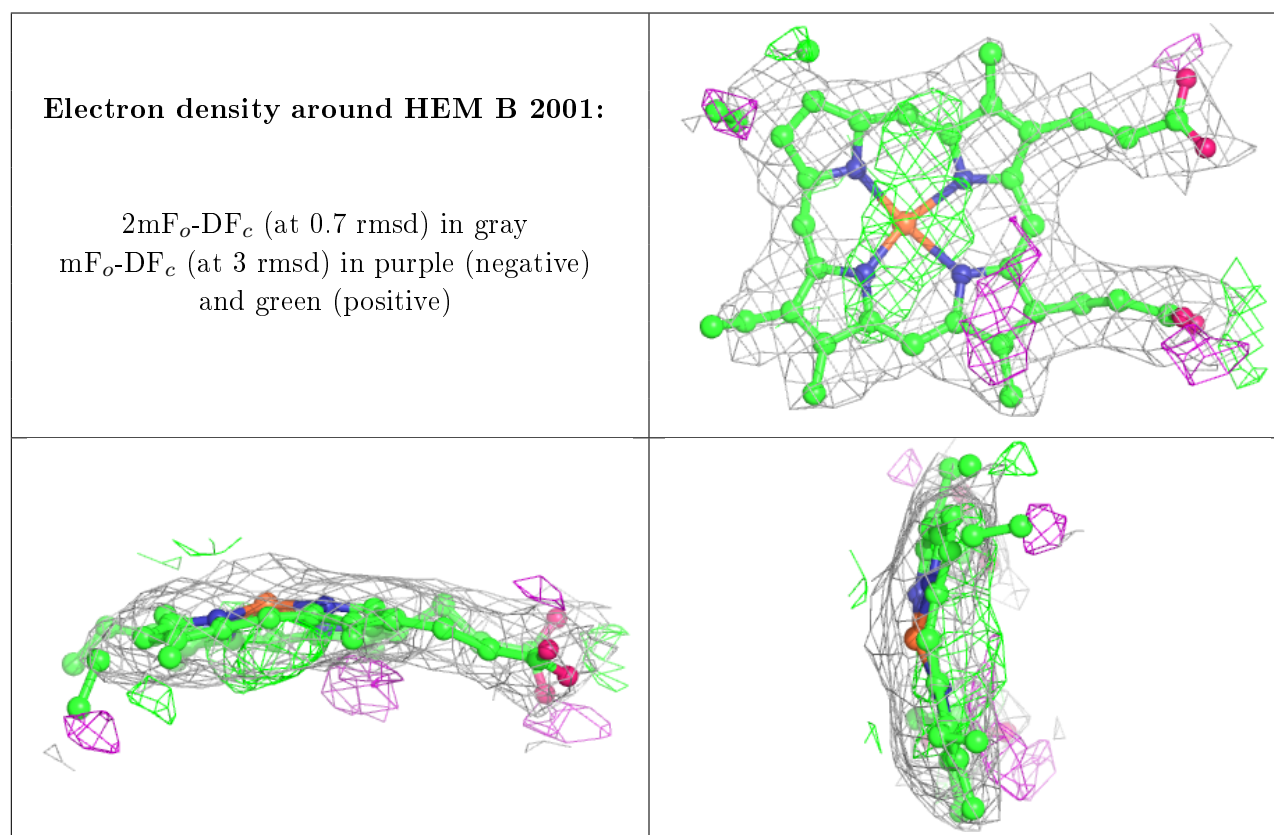
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

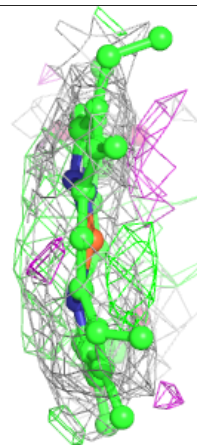
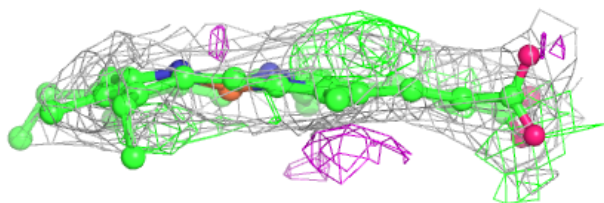
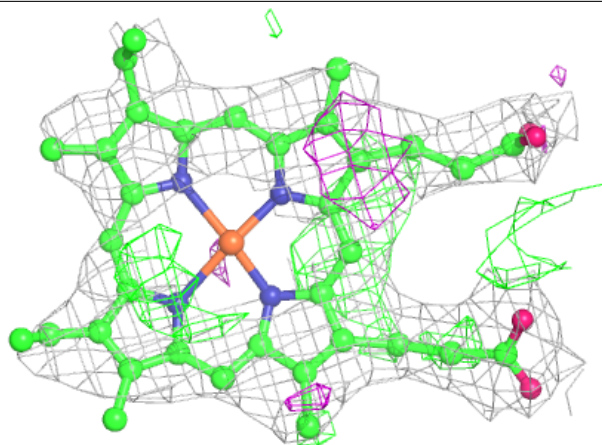
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HEM	B	2001	43/43	0.92	0.25	20,37,58,100	0
3	HEM	D	2003	43/43	0.93	0.27	21,48,68,78	0
3	HEM	C	2002	43/43	0.94	0.21	22,37,54,101	0
3	HEM	A	2000	43/43	0.97	0.18	7,26,38,101	0
2	CYN	D	3001	2/2	0.99	0.12	57,57,57,63	0
2	CYN	A	3000	2/2	1.00	0.17	41,41,41,48	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.



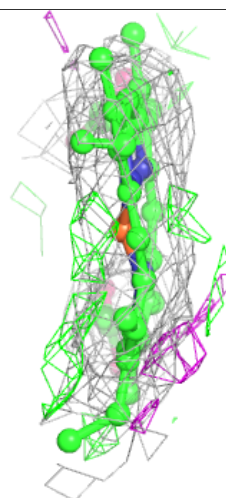
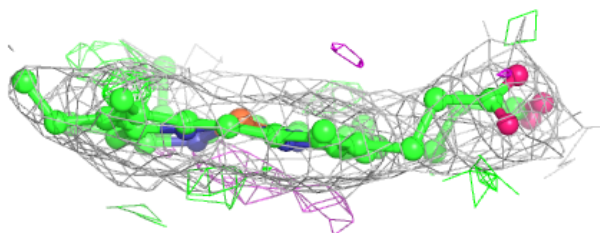
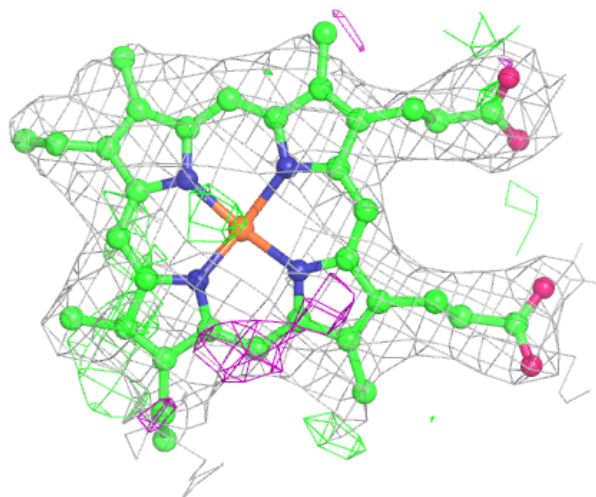
Electron density around HEM D 2003:

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



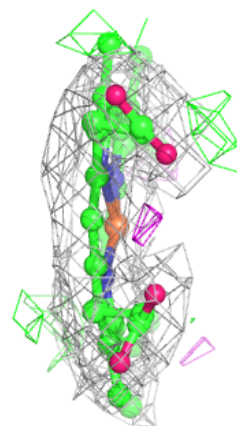
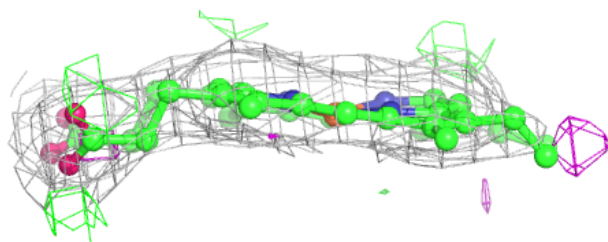
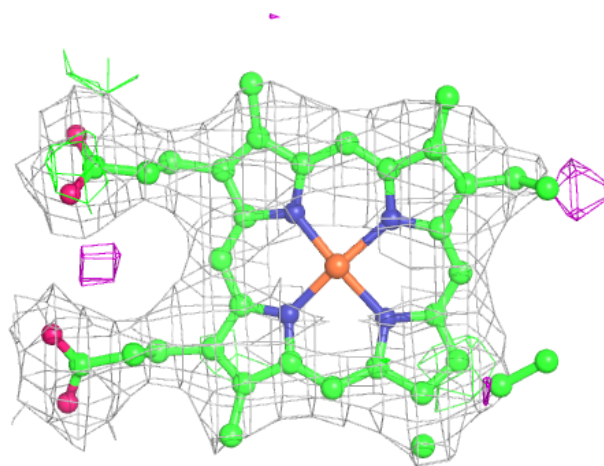
Electron density around HEM C 2002:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.