



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:03 PM UTC

PDB ID : 1TH3 / pdb_00001th3
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

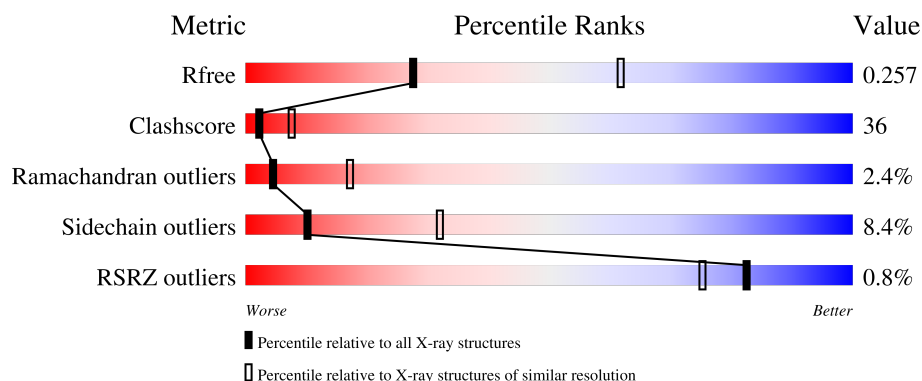
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

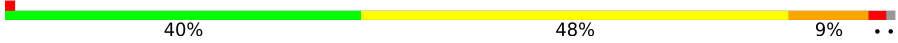
The reported resolution of this entry is 2.80 Å.

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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 criteria:

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](#)

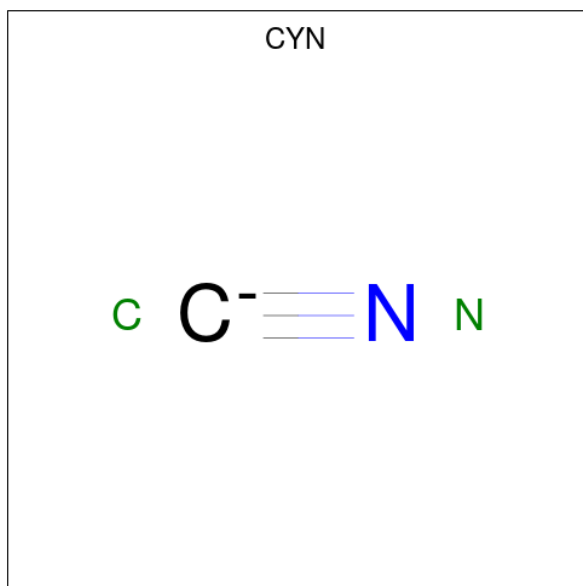
There are 4 unique types of molecules in this entry. The entry contains 16932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

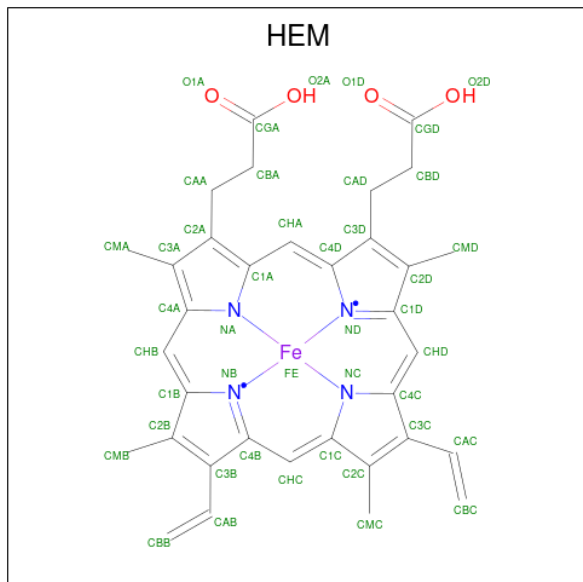
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	B	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	C	499	Total	C	N	O	S	1	0	0
			4017	2548	715	740	14			
1	D	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			

- Molecule 2 is CYANIDE ION (CCD ID: 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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

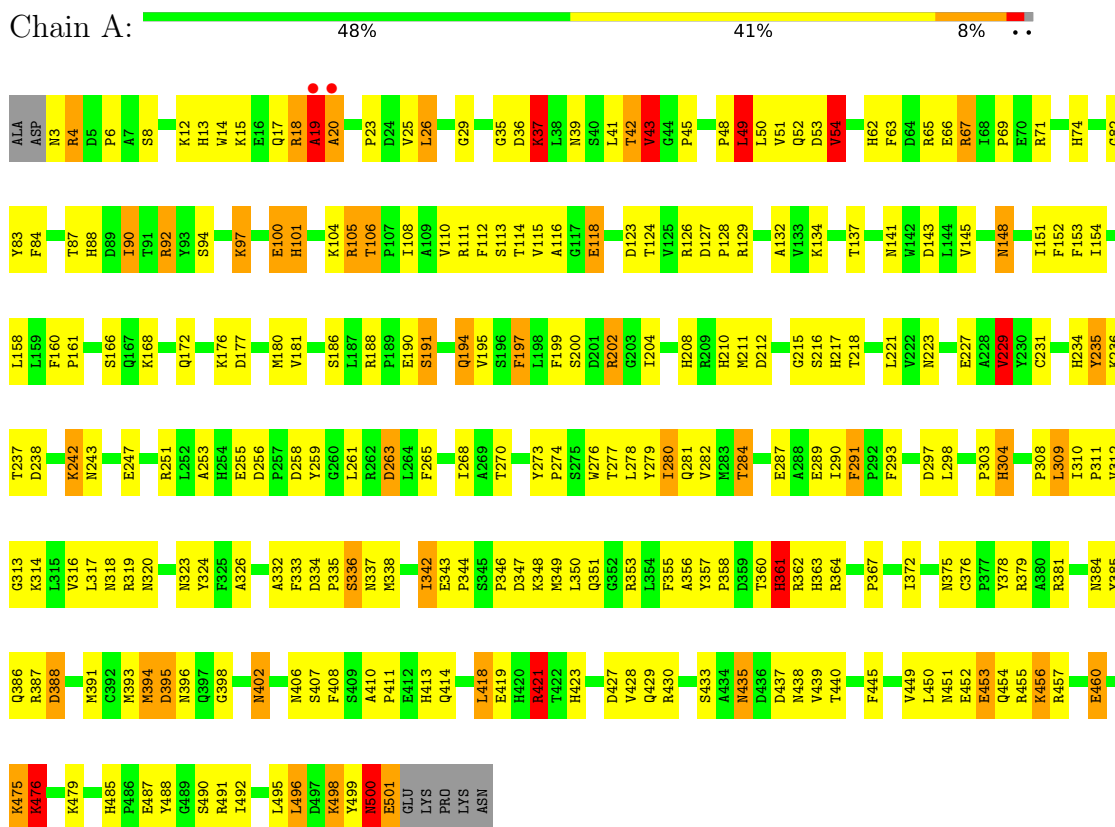
- Molecule 4 is water.

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

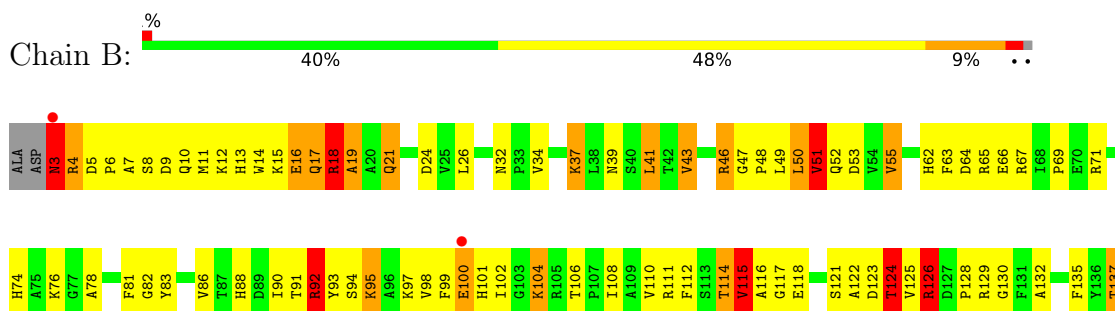
3 Residue-property plots

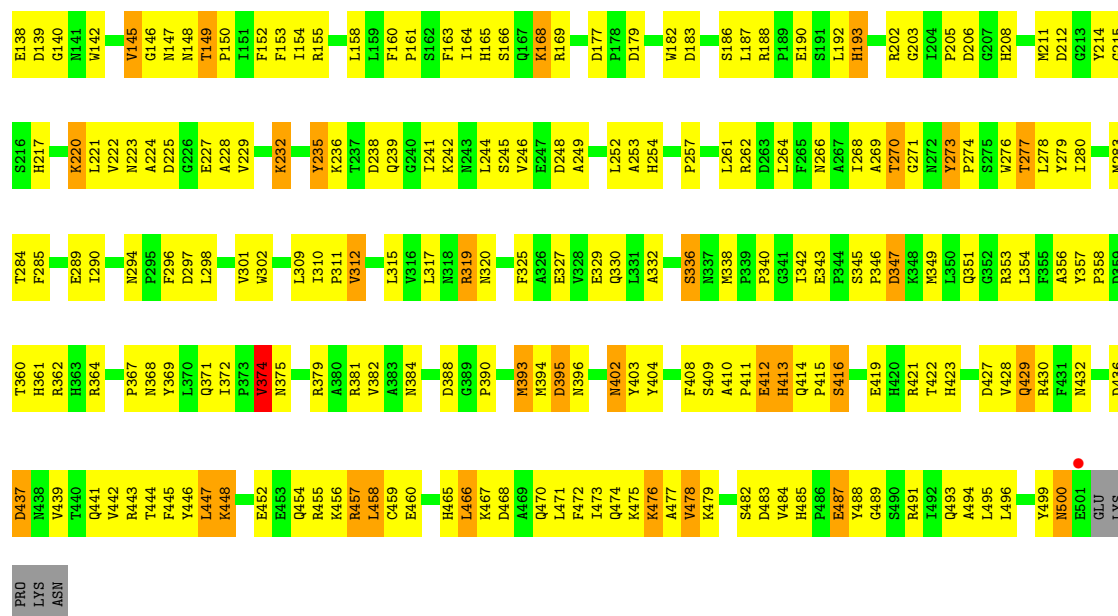
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Catalase

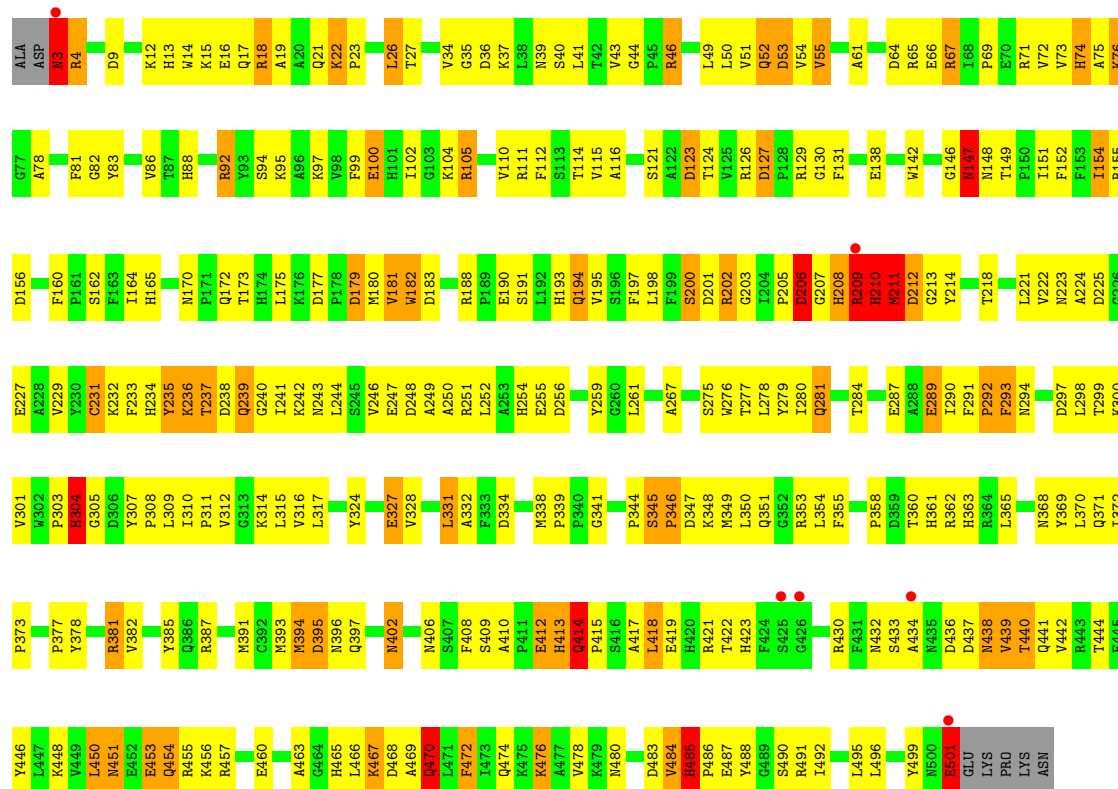
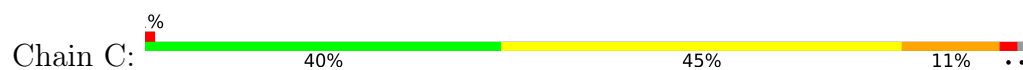


• Molecule 1: Catalase



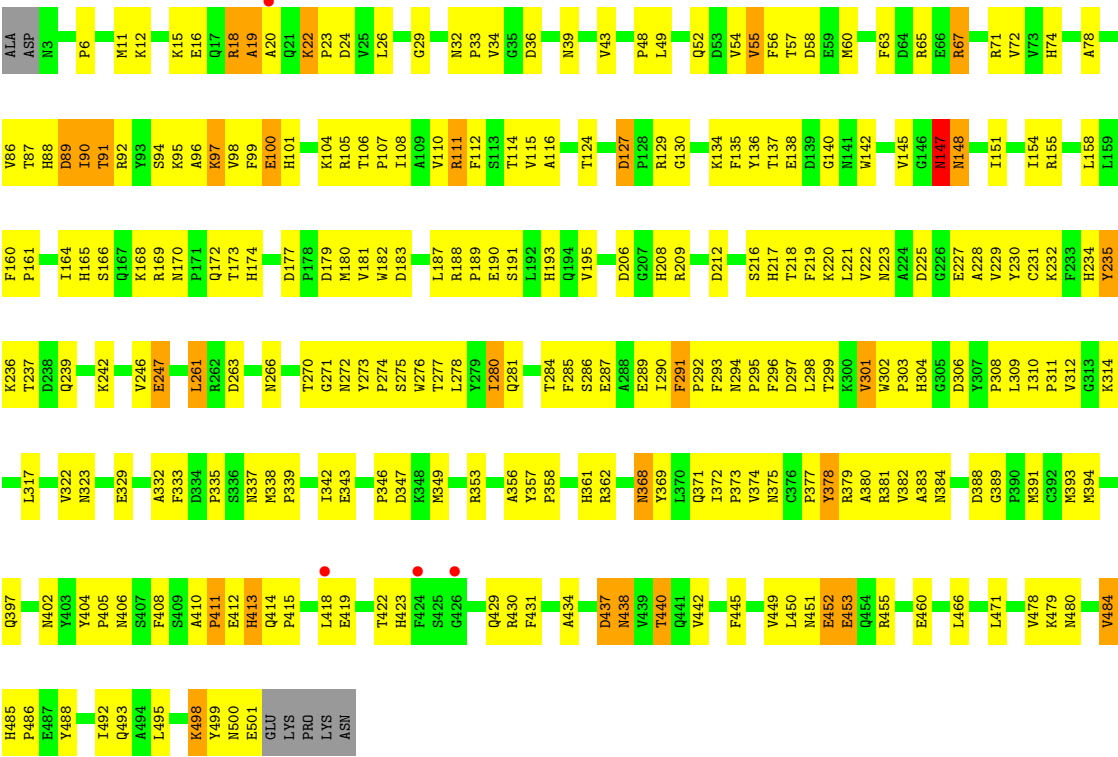


• Molecule 1: Catalase



• Molecule 1: Catalase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.06Å 140.11Å 226.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.21 – 2.80 39.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	76.4 (39.21-2.80) 76.5 (39.21-2.80)	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 0.196 , 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)	0.32 , 53.3	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	1.00	11/4137 (0.3%)	2.12	80/5619 (1.4%)
1	B	1.22	5/4137 (0.1%)	1.71	40/5619 (0.7%)
1	C	0.95	18/4137 (0.4%)	1.96	74/5619 (1.3%)
1	D	0.75	1/4137 (0.0%)	1.27	22/5619 (0.4%)
All	All	0.99	35/16548 (0.2%)	1.79	216/22476 (1.0%)

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CD-NE	59.34	2.29	1.46
1	A	43	VAL	C-O	28.50	1.57	1.24
1	D	413	HIS	CA-CB	-26.16	1.09	1.53
1	A	20	ALA	CA-C	-23.37	1.21	1.52
1	C	202	ARG	NE-CZ	19.66	1.54	1.33
1	B	319	ARG	NE-CZ	18.61	1.53	1.33
1	B	3	ASN	C-N	18.32	1.59	1.33
1	A	43	VAL	N-CA	16.23	1.66	1.46
1	C	292	PRO	C-N	15.48	1.55	1.33
1	A	229	VAL	CA-CB	-14.82	1.40	1.55
1	C	485	HIS	ND1-CE1	-13.53	1.19	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	292	PRO	CA-C	-12.49	1.36	1.52
1	A	92	ARG	CG-CD	11.74	1.87	1.52
1	C	413	HIS	CB-CG	11.01	1.65	1.50
1	C	211	MET	N-CA	-11.00	1.31	1.46
1	C	9	ASP	CA-CB	10.76	1.67	1.53
1	B	374	VAL	CA-CB	10.38	1.69	1.54
1	A	421	ARG	CD-NE	-10.14	1.32	1.46
1	C	485	HIS	CD2-NE2	-9.88	1.26	1.37
1	C	210	HIS	CA-C	-9.87	1.39	1.52
1	A	280	ILE	CA-CB	8.56	1.67	1.55
1	C	414	GLN	CA-CB	8.40	1.65	1.53
1	C	210	HIS	C-N	-7.99	1.22	1.33
1	A	19	ALA	C-N	-7.15	1.23	1.33
1	B	319	ARG	CA-CB	-7.00	1.39	1.53
1	C	212	ASP	N-CA	-6.51	1.38	1.45
1	A	25	VAL	CA-C	6.47	1.60	1.52
1	C	453	GLU	CA-CB	6.34	1.63	1.53
1	C	209	ARG	C-N	-6.27	1.25	1.33
1	C	485	HIS	CE1-NE2	6.04	1.38	1.32
1	A	49	LEU	CB-CG	-5.93	1.41	1.53
1	C	9	ASP	CB-CG	5.87	1.66	1.52
1	C	208	HIS	CB-CG	5.60	1.57	1.50
1	A	243	ASN	N-CA	5.34	1.52	1.45
1	C	454	GLN	CB-CG	-5.06	1.37	1.52

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	HIS	CA-CB-CG	47.20	161.00	113.80
1	A	19	ALA	O-C-N	-43.79	64.35	122.59
1	D	413	HIS	CA-CB-CG	42.28	156.08	113.80
1	A	395	ASP	CA-CB-CG	42.24	154.84	112.60
1	B	319	ARG	CG-CD-NE	-39.30	25.55	112.00
1	C	9	ASP	CA-CB-CG	37.63	150.23	112.60
1	B	395	ASP	N-CA-CB	-36.87	54.04	110.44
1	A	402	ASN	CA-CB-CG	34.08	146.68	112.60
1	C	453	GLU	CB-CG-CD	32.75	168.28	112.60
1	C	292	PRO	N-CA-C	31.17	153.31	114.35
1	B	487	GLU	CB-CG-CD	28.76	161.49	112.60
1	B	126	ARG	CD-NE-CZ	28.52	164.32	124.40
1	D	453	GLU	CB-CG-CD	28.48	161.01	112.60
1	C	202	ARG	NE-CZ-NH2	-27.87	94.12	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	ASN	CA-CB-CG	27.74	140.34	112.60
1	A	304	HIS	CB-CA-C	27.70	156.73	110.74
1	B	319	ARG	CB-CG-CD	-26.45	50.45	111.30
1	C	292	PRO	CA-C-O	26.24	150.99	118.98
1	C	147	ASN	OD1-CG-ND2	-25.93	96.67	122.60
1	C	147	ASN	CA-CB-CG	25.89	138.49	112.60
1	A	418	LEU	N-CA-CB	25.84	149.57	110.29
1	C	483	ASP	N-CA-CB	25.55	153.33	110.41
1	C	395	ASP	CA-CB-CG	-25.02	87.58	112.60
1	B	319	ARG	NE-CZ-NH1	-24.26	97.24	121.50
1	B	395	ASP	CA-CB-CG	24.16	136.76	112.60
1	A	456	LYS	CG-CD-CE	23.99	166.47	111.30
1	B	412	GLU	CB-CG-CD	23.34	152.27	112.60
1	C	52	GLN	CB-CG-CD	23.25	152.13	112.60
1	B	32	ASN	CB-CG-ND2	-22.78	82.23	116.40
1	A	395	ASP	N-CA-CB	22.75	143.77	110.56
1	A	43	VAL	O-C-N	-22.36	94.61	122.57
1	C	454	GLN	CB-CG-CD	22.21	150.36	112.60
1	C	453	GLU	N-CA-CB	21.89	141.72	109.98
1	A	421	ARG	CB-CG-CD	21.78	161.40	111.30
1	C	292	PRO	CB-CA-C	-20.96	81.33	110.88
1	C	202	ARG	NE-CZ-NH1	20.80	142.29	121.50
1	C	414	GLN	CA-CB-CG	20.55	155.19	114.10
1	D	97	LYS	CG-CD-CE	20.25	157.88	111.30
1	A	421	ARG	CG-CD-NE	20.20	156.45	112.00
1	A	361	HIS	N-CA-CB	-19.93	80.83	110.12
1	B	487	GLU	CA-CB-CG	19.81	153.72	114.10
1	C	501	GLU	CB-CA-C	19.79	147.70	110.10
1	B	374	VAL	CB-CA-C	-19.44	82.03	112.16
1	A	229	VAL	CA-CB-CG2	19.36	143.32	110.40
1	A	54	VAL	CA-CB-CG2	-19.27	77.64	110.40
1	B	319	ARG	CA-CB-CG	18.91	151.93	114.10
1	A	456	LYS	CB-CG-CD	18.91	154.78	111.30
1	A	118	GLU	N-CA-CB	-18.82	83.35	110.45
1	C	9	ASP	N-CA-CB	-18.36	84.58	110.65
1	A	97	LYS	CG-CD-CE	18.05	152.81	111.30
1	C	292	PRO	O-C-N	-17.94	92.93	122.36
1	C	454	GLN	N-CA-CB	-17.84	83.90	110.12
1	A	500	ASN	CA-CB-CG	17.74	130.34	112.60
1	A	453	GLU	CB-CG-CD	17.50	142.34	112.60
1	D	147	ASN	CA-CB-CG	17.35	129.95	112.60
1	C	453	GLU	CA-CB-CG	17.34	148.78	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	414	GLN	CB-CA-C	17.18	129.24	110.17
1	A	304	HIS	N-CA-CB	-17.17	81.79	109.78
1	A	435	ASN	CB-CA-C	16.62	137.78	111.02
1	C	3	ASN	CB-CA-C	16.62	141.67	110.10
1	B	277	THR	CB-CA-C	16.51	136.93	110.19
1	B	429	GLN	CA-CB-CG	16.36	146.83	114.10
1	B	478	VAL	N-CA-CB	-16.29	92.43	110.51
1	C	501	GLU	CB-CG-CD	16.14	140.04	112.60
1	A	501	GLU	CB-CA-C	15.30	139.17	110.10
1	B	32	ASN	CB-CG-OD1	15.29	151.38	120.80
1	C	147	ASN	CB-CA-C	15.24	144.66	110.67
1	B	412	GLU	N-CA-CB	15.05	134.02	110.85
1	B	374	VAL	N-CA-CB	14.90	136.13	110.65
1	C	289	GLU	CB-CA-C	14.46	133.36	110.95
1	A	476	LYS	CG-CD-CE	14.34	144.28	111.30
1	C	210	HIS	O-C-N	14.27	141.57	122.59
1	D	453	GLU	CA-CB-CG	14.09	142.29	114.10
1	A	42	THR	CA-C-N	13.98	147.13	121.97
1	A	42	THR	C-N-CA	13.98	147.13	121.97
1	C	9	ASP	CB-CA-C	13.75	132.21	111.17
1	A	490	SER	CA-CB-OG	13.72	138.54	111.10
1	B	478	VAL	CB-CA-C	13.57	129.26	111.88
1	A	381	ARG	CG-CD-NE	13.25	141.16	112.00
1	A	500	ASN	N-CA-CB	-13.15	88.26	110.49
1	A	421	ARG	CD-NE-CZ	13.01	142.61	124.40
1	A	284	THR	CA-CB-OG1	12.88	128.93	109.60
1	A	37	LYS	CG-CD-CE	12.74	140.60	111.30
1	B	3	ASN	O-C-N	-12.08	103.68	123.00
1	C	289	GLU	CG-CD-OE2	-11.93	90.97	118.40
1	A	421	ARG	CA-CB-CG	11.59	137.28	114.10
1	B	412	GLU	CA-CB-CG	11.47	137.05	114.10
1	C	289	GLU	CA-CB-CG	11.44	136.97	114.10
1	A	49	LEU	CB-CG-CD2	11.41	144.93	110.70
1	B	478	VAL	CA-CB-CG1	-11.31	91.17	110.40
1	A	476	LYS	CD-CE-NZ	11.03	147.20	111.90
1	A	456	LYS	CA-CB-CG	10.92	135.95	114.10
1	C	74	HIS	CA-CB-CG	10.92	124.72	113.80
1	A	280	ILE	CB-CA-C	-10.88	91.59	111.18
1	D	394	MET	CB-CG-SD	10.88	145.35	112.70
1	A	92	ARG	CG-CD-NE	-10.61	88.66	112.00
1	C	3	ASN	CA-C-O	10.55	138.74	120.80
1	C	483	ASP	CB-CA-C	-10.55	88.94	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	LEU	CB-CA-C	-10.50	90.14	109.46
1	C	454	GLN	CB-CA-C	-10.47	93.41	110.79
1	A	243	ASN	CB-CA-C	-10.41	90.67	110.24
1	C	210	HIS	N-CA-CB	10.40	128.07	110.49
1	A	202	ARG	CD-NE-CZ	10.20	138.69	124.40
1	C	210	HIS	CB-CG-ND1	-10.20	107.39	122.70
1	A	43	VAL	CA-C-O	-10.02	108.26	120.78
1	D	356	ALA	N-CA-C	9.76	121.52	111.07
1	C	501	GLU	N-CA-CB	-9.76	93.91	110.50
1	A	356	ALA	N-CA-C	9.74	121.90	111.28
1	A	145	VAL	N-CA-C	9.22	116.08	106.21
1	C	292	PRO	CA-C-N	9.21	138.29	122.81
1	C	292	PRO	C-N-CA	9.21	138.29	122.81
1	A	284	THR	CB-CA-C	-9.17	91.50	109.76
1	B	478	VAL	CA-CB-CG2	9.06	125.80	110.40
1	A	20	ALA	CB-CA-C	-9.06	92.39	110.42
1	C	210	HIS	CA-CB-CG	9.01	122.81	113.80
1	C	413	HIS	CB-CG-CD2	8.96	142.84	131.20
1	C	413	HIS	CB-CG-ND1	-8.94	109.29	122.70
1	A	501	GLU	N-CA-CB	-8.68	95.75	110.50
1	B	416	SER	N-CA-CB	-8.66	96.38	110.42
1	A	284	THR	CA-CB-CG2	-8.59	95.90	110.50
1	B	319	ARG	NE-CZ-NH2	8.50	126.85	119.20
1	A	92	ARG	CB-CG-CD	-8.34	92.13	111.30
1	A	176	LYS	CG-CD-CE	8.33	130.46	111.30
1	A	280	ILE	CA-CB-CG1	8.29	124.49	110.40
1	A	20	ALA	CA-C-O	8.23	132.29	120.51
1	A	435	ASN	N-CA-CB	-8.15	97.89	110.92
1	A	280	ILE	CA-CB-CG2	-8.13	96.68	110.50
1	C	231	CYS	CA-CB-SG	-8.07	95.84	114.40
1	A	229	VAL	CB-CA-C	-8.05	100.61	111.80
1	C	478	VAL	CB-CA-C	8.02	125.25	112.26
1	C	55	VAL	N-CA-C	-8.02	102.44	110.62
1	A	453	GLU	CA-CB-CG	7.98	130.06	114.10
1	A	395	ASP	CB-CA-C	-7.84	97.31	110.56
1	D	89	ASP	CA-CB-CG	7.51	120.11	112.60
1	A	176	LYS	CD-CE-NZ	-7.39	88.26	111.90
1	A	342	ILE	N-CA-CB	7.36	123.37	111.23
1	A	361	HIS	CB-CA-C	7.33	122.97	110.79
1	C	394	MET	CB-CA-C	-7.29	108.17	116.63
1	D	484	VAL	N-CA-C	-7.29	103.36	110.72
1	C	210	HIS	CB-CG-CD2	7.26	140.64	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ASP	N-CA-C	7.22	119.15	111.28
1	B	319	ARG	CB-CA-C	-7.12	94.93	109.38
1	C	372	ILE	N-CA-C	-7.11	102.52	108.63
1	C	236	LYS	CG-CD-CE	7.06	127.54	111.30
1	A	342	ILE	CB-CA-C	-7.05	99.72	111.29
1	B	215	GLY	N-CA-C	-7.05	106.09	115.32
1	B	388	ASP	N-CA-C	7.03	118.41	108.00
1	B	55	VAL	N-CA-C	-7.00	103.64	110.72
1	C	289	GLU	CB-CG-CD	6.99	124.48	112.60
1	C	147	ASN	CB-CG-OD1	6.84	134.47	120.80
1	A	116	ALA	N-CA-C	6.65	119.51	111.40
1	D	55	VAL	N-CA-C	-6.65	104.00	110.72
1	A	43	VAL	N-CA-CB	-6.65	100.27	111.23
1	A	333	PHE	CA-CB-CG	6.63	120.43	113.80
1	B	32	ASN	CA-CB-CG	-6.60	106.00	112.60
1	C	484	VAL	N-CA-C	-6.58	105.33	111.45
1	A	388	ASP	N-CA-C	6.56	117.71	108.00
1	D	169	ARG	N-CA-C	6.46	120.05	110.48
1	B	374	VAL	CA-CB-CG1	-6.35	99.60	110.40
1	C	188	ARG	CA-C-N	6.34	125.91	119.19
1	C	188	ARG	C-N-CA	6.34	125.91	119.19
1	A	67	ARG	N-CA-C	6.18	119.58	109.76
1	A	114	THR	N-CA-C	-6.16	100.56	109.31
1	B	356	ALA	N-CA-C	6.15	117.98	111.28
1	B	273	TYR	N-CA-C	6.12	117.10	109.57
1	B	374	VAL	CA-CB-CG2	-6.02	100.17	110.40
1	D	90	ILE	N-CA-C	-6.00	106.89	113.43
1	A	43	VAL	N-CA-C	-5.92	97.02	109.34
1	C	485	HIS	CA-C-N	5.87	127.17	119.84
1	C	485	HIS	C-N-CA	5.87	127.17	119.84
1	C	202	ARG	CD-NE-CZ	5.84	132.58	124.40
1	C	483	ASP	N-CA-C	-5.84	106.12	113.18
1	B	92	ARG	N-CA-C	-5.83	106.25	113.19
1	A	291	PHE	CA-C-N	5.82	125.49	119.56
1	A	291	PHE	C-N-CA	5.82	125.49	119.56
1	C	324	TYR	N-CA-C	5.78	117.26	111.07
1	D	434	ALA	N-CA-C	5.77	117.57	111.28
1	D	147	ASN	N-CA-CB	5.75	119.54	110.39
1	C	124	THR	N-CA-C	5.73	118.53	108.56
1	D	67	ARG	N-CA-C	5.72	119.24	110.20
1	A	372	ILE	N-CA-C	-5.70	102.74	108.96
1	C	307	TYR	CA-C-N	5.69	125.45	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	TYR	C-N-CA	5.69	125.45	119.76
1	C	44	GLY	CA-C-N	5.68	126.06	119.47
1	C	44	GLY	C-N-CA	5.68	126.06	119.47
1	B	319	ARG	N-CA-CB	5.67	121.27	111.13
1	C	209	ARG	O-C-N	-5.60	115.14	122.59
1	B	116	ALA	N-CA-C	5.58	117.36	111.28
1	D	273	TYR	N-CA-C	5.57	116.42	109.57
1	A	289	GLU	CB-CG-CD	-5.51	103.24	112.60
1	D	20	ALA	N-CA-CB	-5.49	102.55	110.56
1	B	169	ARG	N-CA-C	5.47	118.62	110.52
1	A	500	ASN	CB-CA-C	5.47	121.30	110.42
1	C	378	TYR	N-CA-C	5.43	119.01	112.38
1	D	147	ASN	CB-CA-C	5.42	126.05	113.15
1	A	113	SER	N-CA-C	5.42	116.68	108.07
1	A	90	ILE	N-CA-C	-5.41	106.14	111.77
1	C	312	VAL	N-CA-C	5.34	115.84	111.62
1	C	207	GLY	O-C-N	5.33	129.24	122.85
1	A	238	ASP	N-CA-C	-5.32	106.83	113.38
1	C	67	ARG	N-CA-C	5.31	118.59	110.20
1	C	206	ASP	CA-C-N	-5.31	115.95	122.75
1	C	206	ASP	C-N-CA	-5.31	115.95	122.75
1	A	197	PHE	N-CA-C	-5.30	105.42	111.14
1	D	18	ARG	N-CA-C	-5.29	104.92	111.33
1	A	218	THR	N-CA-C	-5.27	101.94	110.32
1	C	281	GLN	N-CA-C	-5.26	100.66	109.24
1	C	327	GLU	N-CA-C	5.18	119.88	113.50
1	A	181	VAL	N-CA-C	5.17	115.39	110.42
1	D	498	LYS	N-CA-C	-5.12	105.34	111.03
1	C	182	TRP	N-CA-C	5.12	116.55	111.07
1	A	123	ASP	N-CA-C	5.06	116.88	111.36
1	B	51	VAL	N-CA-C	-5.04	104.63	111.89
1	D	291	PHE	CA-C-N	5.04	124.65	119.56
1	D	291	PHE	C-N-CA	5.04	124.65	119.56
1	B	413	HIS	CA-CB-CG	-5.03	108.77	113.80

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

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Mol	Chain	Res	Type	Atom
1	C	501	GLU	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ALA	Peptide,Mainchain
1	A	42	THR	Peptide
1	A	421	ARG	Sidechain
1	A	43	VAL	Peptide,Mainchain
1	B	126	ARG	Sidechain
1	B	3	ASN	Peptide,Mainchain
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	3838	259	0
1	B	4017	0	3840	361	0
1	C	4017	0	3839	347	0
1	D	4017	0	3839	281	0
2	A	2	0	0	6	0
2	D	2	0	0	0	0
3	A	43	0	30	17	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	32	0
4	B	195	0	0	33	0
4	C	138	0	0	16	0
4	D	154	0	0	19	0
All	All	16932	0	15476	1147	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 36.

All (1147) 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:C:147:ASN:CG	3:C:2002:HEM:HAC	1.16	1.50
1:A:92:ARG:CD	1:A:92:ARG:CG	1.87	1.49
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:C:147:ASN:CG	3:C:2002:HEM:CAC	2.02	1.21
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: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
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:C:129:ARG:HG2	1:C:211:MET:HE1	1.38	1.04
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:B:78:ALA:HB2	1:B:261:LEU:HD12	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:338:MET:HE2	1:B:342:ILE:HG22	1.48	0.94
1:B:112:PHE:HA	1:B:130:GLY:O	1.67	0.93
1:C:402:ASN:H	1:C:402:ASN:HD22	1.05	0.93
1:D:147:ASN:OD1	3:D:2003:HEM:HAC	1.66	0.93
1:A:92:ARG:CD	1:A:92:ARG:CB	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:391:MET:HE3	1:A:393:MET:CE	2.01	0.90
1:A:92:ARG:CG	1:A:92:ARG:NE	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:393:MET:HE2	1:D:372:ILE:HA	1.55	0.88
1:B:71:ARG:HG3	1:B:71:ARG:HH11	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:D:291:PHE:HE1	1:D:293:PHE:HB2	1.39	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
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
1:A:391:MET:HE3	1:A:393:MET:HE1	1.59	0.83
1:B:92:ARG:HD2	4:B:2163:HOH:O	1.78	0.83
3:B:2001:HEM:HBD2	4:B:2179:HOH:O	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:402:ASN:HD21	1:D:180:MET:HE3	1.43	0.81
1:A:166:SER:HA	1:A:180:MET:HE2	1.63	0.80
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: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:129:ARG:CG	1:C:211:MET:HE1	2.12	0.79
1:B:223:ASN:HD21	1:B:227:GLU:HB2	1.45	0.79
1:B:361:HIS:CD2	3:B:2001:HEM:O1A	2.35	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:D:338:MET:HE2	1:D:342:ILE:HG22	1.64	0.78
1:A:100:GLU:O	1:A:101:HIS:HB3	1.84	0.78
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:B:129:ARG:HB2	1:B:211:MET:HE1	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:HG3	1:D:111:ARG:HH11	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:66:GLU:HB3	1:D:388:ASP:HB2	1.70	0.72
1:B:479:LYS:O	1:B:482:SER:HB2	1.89	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:HG23	1:B:428:VAL:O	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:88:HIS:CD2	1:C:311:PRO:HB2	2.25	0.71
1:C:209:ARG:O	1:C:210:HIS:CG	2.44	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:D:391:MET:HE3	1:D:393:MET:HE3	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:60:MET:HE1	1:D:63:PHE:HD2	1.57	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:205:PRO:HG2	1:C:211:MET:CE	2.22	0.69
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: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:B:129:ARG:CB	1:B:211:MET:HE1	2.23	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:D:148:ASN:H	1:D:148:ASN:HD22	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
1:B:148:ASN:HB3	1:B:211:MET:HE2	1.76	0.67
1:C:82:GLY:HA3	1:C:316:VAL:O	1.93	0.67
1:C:92:ARG:H	1:C:92:ARG:HD3	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:O	1:B:413:HIS:ND1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:LYS:HD2	1:B:139:ASP:CG	2.20	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:5:ASP:OD2	1:B:7:ALA:HB3	1.95	0.65
1:B:106:THR:HG23	1:B:379:ARG:NH2	2.10	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: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:HD22	1:D:148:ASN:N	1.95	0.64
1:C:3:ASN:C	1:C:4:ARG:HG3	2.23	0.64
1:B:19:ALA:CB	1:B:21:GLN:HE21	2.06	0.64
1:B:457:ARG:HB2	1:B:457:ARG:NH1	2.11	0.64
1:C:200:SER:OG	1:C:201:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LEU:O	1:D:34:VAL:HG22	1.97	0.64
1:D:294:ASN:HB3	1:D:297:ASP:HB2	1.80	0.64
1:D:338:MET:HE1	1:D:343:GLU:C	2.23	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:A:4:ARG:HH22	1:D:179:ASP:CG	2.06	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: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:HD22	1:A:309:LEU:H	1.63	0.63
1:D:60:MET:HE1	1:D:63:PHE:CD2	2.34	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:C:436:ASP:O	1:C:437:ASP:HB3	1.97	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
1:B:97:LYS:HB2	4:B:2040:HOH:O	1.98	0.62
1:A:53:ASP:CG	1:D:430:ARG:HH22	2.08	0.62
1:A:456:LYS:HD3	1:A:460:GLU:OE2	2.00	0.61
1:D:148:ASN:H	1:D:148:ASN:ND2	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:146:GLY:C	3:C:2002:HEM:HBC1	2.26	0.61
1:C:437:ASP:C	1:C:438:ASN:HD22	2.09	0.61
1:C:487:GLU:CG	1:C:491:ARG:HD2	2.31	0.61
1:A:172:GLN:HE21	1:D:322:VAL:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:MET:HE3	1:A:393:MET:HE3	1.81	0.61
1:D:135:PHE:HB2	1:D:142:TRP:HB3	1.81	0.61
1:B:17:GLN:C	1:B:19:ALA:H	2.09	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:A:208:HIS:HA	1:A:211:MET:HE2	1.82	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:50:LEU:HD12	1:B:48:PRO:HB2	1.83	0.61
1:A:332:ALA:HB1	1:A:361:HIS:NE2	2.15	0.61
1:C:146:GLY:C	3:C:2002:HEM:CBC	2.73	0.61
1:C:328:VAL:O	1:C:331:LEU:HB2	2.01	0.61
1:A:496:LEU:O	1:A:500:ASN:HB2	2.01	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: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:C:391:MET:HE3	1:C:393:MET:HE1	1.83	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: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:205:PRO:HG3	1:B:211:MET:HE3	1.84	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
1:C:148:ASN:ND2	1:C:211:MET:HE2	2.17	0.60
1:D:499:TYR:C	1:D:501:GLU:H	2.09	0.60
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.37	0.59
1:B:63:PHE:O	1:B:66:GLU:HG3	2.02	0.59
1:B:145:VAL:HG23	4:B:2061:HOH:O	2.01	0.59
1:D:221:LEU:O	1:D:228:ALA:HA	2.02	0.59
1:A:391:MET:CE	1:A:393:MET:HE1	2.32	0.59
1:B:90:ILE:O	1:B:93:TYR:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:MET:HE1	1:D:372:ILE:HG12	1.83	0.59
1:C:251:ARG:HG3	1:C:252:LEU:N	2.17	0.59
1:C:485:HIS:ND1	1:C:485:HIS:C	2.60	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:269:ALA:C	1:B:271:GLY:H	2.09	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:293:PHE:HZ	1:D:440:THR:HG21	1.68	0.59
1:B:88:HIS:CE1	1:B:311:PRO:HB2	2.37	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:C:413:HIS:C	1:C:413:HIS:ND1	2.60	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:294:ASN:HA	1:C:46:ARG:HH12	1.66	0.59
1:C:298:LEU:HD22	1:C:349:MET:HG2	1.84	0.59
1:B:50:LEU:HD22	1:B:50:LEU:N	2.18	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:B:148:ASN:CB	1:B:211:MET:HE2	2.32	0.59
1:C:438:ASN:N	1:C:438:ASN:ND2	2.49	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:402:ASN:ND2	1:D:180:MET:HE3	2.17	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:86:VAL:HG12	1:B:102:ILE:HD13	1.85	0.58
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.85	0.58
1:C:94:SER:HB2	1:C:221:LEU:HD22	1.85	0.58
1:C:130:GLY:HA2	1:C:147:ASN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:64:ASP:HB3	1:C:360:THR:CB	2.33	0.58
1:B:456:LYS:O	1:B:460:GLU:HG3	2.03	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:A:39:ASN:C	1:D:158:LEU:HD12	2.29	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: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:D:154:ILE:HG13	1:D:349:MET:HE2	1.86	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:D:391:MET:HE3	1:D:393:MET:CE	2.34	0.57
1:A:84:PHE:O	1:A:105:ARG:HA	2.05	0.57
1:B:140:GLY:HA3	1:D:32:ASN:HD22	1.68	0.57
1:C:75:ALA:N	4:C:2022:HOH:O	2.37	0.57
1:A:51:VAL:HG12	1:B:51:VAL:HA	1.86	0.57
1:B:336:SER:HB3	1:D:54:VAL:HG11	1.85	0.57
1:B:358:PRO:HB2	1:B:362:ARG:HH12	1.70	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: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:HG13	1:B:382:VAL:O	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: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:H	1:A:309:LEU:CD2	2.17	0.56
1:C:485:HIS:CE1	1:C:487:GLU:H	2.23	0.56
1:A:217:HIS:CE1	3:A:2000:HEM:CBC	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLU:CD	1:A:491:ARG:HD2	2.29	0.56
1:B:186:SER:OG	1:B:476:LYS:HG2	2.06	0.56
1:C:190:GLU:HA	1:C:438:ASN:CB	2.24	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:62:HIS:HE1	1:D:368:ASN:ND2	2.02	0.56
1:B:106:THR:HG23	1:B:379:ARG:HH21	1.67	0.56
1:B:111:ARG:HD2	3:B:2001:HEM:CGD	2.29	0.56
1:B:278:LEU:O	1:B:312:VAL:HG13	2.05	0.56
1:D:290:ILE:O	1:D:291:PHE:C	2.48	0.56
1:B:62:HIS:HE1	1:D:368:ASN:HD21	1.54	0.56
1:C:147:ASN:HD21	3:C:2002:HEM:CAC	2.05	0.56
1:D:338:MET:CE	1:D:342:ILE:HG22	2.32	0.56
1:C:303:PRO:C	1:C:305:GLY:H	2.14	0.56
1:A:394:MET:HG3	4:A:3187:HOH:O	2.05	0.56
1:C:438:ASN:HD22	1:C:438:ASN:N	2.03	0.56
1:A:124:THR:HA	4:A:3171:HOH:O	2.04	0.56
1:A:290:ILE:HD12	1:A:290:ILE:C	2.31	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:A:430:ARG:NE	1:B:419:GLU:OE1	2.39	0.55
1:B:349:MET:SD	3:B:2001:HEM:HBB1	2.46	0.55
1:C:14:TRP:O	1:C:18:ARG:HB2	2.06	0.55
1:C:129:ARG:CB	1:C:211:MET:HE1	2.35	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:D:187:LEU:O	1:D:188:ARG:HD2	2.06	0.55
1:A:498:LYS:O	1:A:499:TYR:C	2.49	0.55
1:B:154:ILE:O	1:B:349:MET:HE2	2.06	0.55
1:C:74:HIS:CE1	3:C:2002:HEM:CHD	2.90	0.55
1:C:74:HIS:CD2	3:C:2002:HEM:C4D	2.95	0.55
1:C:377:PRO:HG2	1:C:382:VAL:CG2	2.36	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:182:TRP:O	1:C:183:ASP:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:140:GLY:H	1:D:380:ALA:HB2	1.71	0.55
1:D:298:LEU:CD2	1:D:349:MET:HG3	2.37	0.55
1:B:220:LYS:HD3	1:B:228:ALA:HB1	1.89	0.55
1:C:223:ASN:C	1:C:225:ASP:H	2.15	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:N	1:B:235:TYR:CD1	2.74	0.55
1:A:323:ASN:HD21	1:C:396:ASN:HD22	1.53	0.55
1:C:472:PHE:C	1:C:472:PHE:CD1	2.85	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:A:408:PHE:HA	1:C:15:LYS:HD2	1.89	0.54
1:B:26:LEU:CD1	1:D:384:ASN:HA	2.37	0.54
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:C:205:PRO:HG2	1:C:211:MET:HE3	1.88	0.54
1:C:391:MET:HE3	1:C:393:MET:CE	2.38	0.54
1:D:332:ALA:HB1	1:D:361:HIS:CE1	2.41	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:67:ARG:CZ	1:D:72:VAL:HG23	2.38	0.54
1:A:251:ARG:O	1:A:255:GLU:HG3	2.07	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:A:387:ARG:O	1:C:66:GLU:HG2	2.07	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:C:290:ILE:O	1:C:291:PHE:C	2.49	0.54
1:D:18:ARG:O	1:D:19:ALA:HB3	2.08	0.54
1:A:4:ARG:HB2	1:A:8:SER:HB2	1.89	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:D:381:ARG:HH11	1:D:381:ARG:HG2	1.73	0.54
1:B:37:LYS:O	1:B:37:LYS:HG3	2.08	0.54
1:B:279:TYR:HB3	1:B:309:LEU:HB3	1.89	0.54
1:D:60:MET:O	1:D:60:MET:HE3	2.08	0.54
1:A:23:PRO:HB2	1:C:412:GLU:CG	2.38	0.53
1:A:367:PRO:HG3	1:C:65:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:NH2	1:B:241:ILE:HD13	2.19	0.53
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.16	0.53
1:B:442:VAL:HG12	1:B:484:VAL:HG11	1.89	0.53
1:C:52:GLN:O	1:C:54:VAL:HG13	2.08	0.53
1:C:126:ARG:HD2	1:C:198:LEU:HG	1.89	0.53
1:C:439:VAL:O	1:C:440:THR:C	2.50	0.53
1:A:499:TYR:O	1:A:501:GLU:N	2.35	0.53
1:C:154:ILE:HG13	1:C:349:MET:HE1	1.89	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: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:C:350:LEU:O	1:C:351:GLN:C	2.51	0.53
1:D:191:SER:O	1:D:195:VAL:HG23	2.08	0.53
1:A:479:LYS:HD2	1:A:479:LYS:O	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:C:205:PRO:HG2	1:C:211:MET:HE2	1.90	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:D:378:TYR:CD1	1:D:378:TYR:C	2.88	0.52
1:A:263:ASP:C	1:A:263:ASP:OD1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASN:O	1:B:4:ARG:C	2.50	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:B:205:PRO:HG3	1:B:211:MET:CE	2.39	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
1:D:280:ILE:CD1	1:D:310:ILE:HB	2.40	0.52
1:C:303:PRO:C	1:C:305:GLY:N	2.62	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:99:PHE:O	1:D:100:GLU:C	2.53	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:131:PHE:CD1	1:C:235:TYR:HE2	2.27	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: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:O	1:C:381:ARG:HG3	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:B:491:ARG:O	1:B:495:LEU:HD23	2.10	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:252:LEU:HD12	1:B:252:LEU:N	2.25	0.51
1:B:78:ALA:HB2	1:B:261:LEU:CD1	2.29	0.51
1:C:154:ILE:CG1	1:C:349:MET:HE1	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:PRO:CD	1:D:357:TYR:CG	2.93	0.51
1:A:323:ASN:ND2	1:C:396:ASN:HD22	2.09	0.51
1:B:34:VAL:HG13	1:B:55:VAL:HG11	1.92	0.51
1:A:23:PRO:HB2	1:C:412:GLU:HG2	1.91	0.51
1:A:50:LEU:HD13	1:B:50:LEU:HD13	1.92	0.51
1:A:501:GLU:OE1	1:A:501:GLU:CA	2.59	0.51
1:B:88:HIS:HB2	1:B:312:VAL:HA	1.93	0.51
1:B:92:ARG:HG3	4:B:2163:HOH:O	2.04	0.51
1:B:428:VAL:O	1:B:428:VAL:CG2	2.57	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: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:C:395:ASP:C	1:C:395:ASP:OD2	2.46	0.51
1:D:445:PHE:HA	1:D:449:VAL:CG2	2.41	0.51
1:A:439:VAL:O	1:A:440:THR:C	2.54	0.51
1:A:45:PRO:HD3	1:D:431:PHE:CZ	2.46	0.50
1:D:206:ASP:OD2	1:D:242:LYS:HE3	2.11	0.50
1:A:48:PRO:HB2	1:B:50:LEU:HD12	1.93	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:143:ASP:HB2	1:A:334:ASP:O	2.12	0.50
1:A:452:GLU:O	1:A:453:GLU:C	2.54	0.50
1:D:71:ARG:HG3	1:D:71:ARG:NH1	2.24	0.50
1:A:166:SER:HA	1:A:180:MET:CE	2.38	0.50
1:B:81:PHE:HZ	1:B:327:GLU:HB3	1.75	0.50
1:B:83:TYR:HA	1:B:108:ILE:HG12	1.93	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:71:ARG:NH2	1:D:329:GLU:O	2.43	0.50
1:D:234:HIS:O	1:D:278:LEU:HD12	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ARG:NH2	1:C:470:GLN:HG3	2.26	0.50
1:B:98:VAL:HG13	1:B:99:PHE:CD1	2.46	0.50
1:B:360:THR:OG1	1:C:64:ASP:CB	2.60	0.50
1:A:35:GLY:HA2	1:C:414:GLN:O	2.11	0.50
1:B:374:VAL:CG2	4:B:2178:HOH:O	2.58	0.50
1:C:432:ASN:HD22	1:C:432:ASN:C	2.15	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:B:239:GLN:N	1:B:239:GLN:CD	2.70	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:82:GLY:HA3	1:A:316:VAL:O	2.12	0.49
1:A:87:THR:HG23	1:A:313:GLY:HA2	1.93	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:A:258:ASP:HB3	1:A:261:LEU:HD12	1.92	0.49
1:C:303:PRO:O	1:C:305:GLY:N	2.45	0.49
1:C:353:ARG:HG3	3:C:2002:HEM:HBB2	1.94	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:66:GLU:HG2	1:C:387:ARG:O	2.13	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:395:ASP:O	1:C:395:ASP:CG	2.55	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:A:378:TYR:CD1	1:A:378:TYR:C	2.91	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:11:MET:CE	1:C:180:MET:HG2	2.43	0.49
1:B:90:ILE:O	1:B:93:TYR:N	2.41	0.49
1:B:99:PHE:O	1:B:100:GLU:C	2.55	0.49
1:B:294:ASN:HA	1:C:46:ARG:NH1	2.27	0.49
1:D:378:TYR:C	1:D:378:TYR:HD1	2.21	0.49
1:C:83:TYR:CD1	1:C:105:ARG:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PHE:O	1:C:100:GLU:C	2.55	0.49
1:D:11:MET:O	1:D:12:LYS:C	2.55	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:B:129:ARG:H	1:B:148:ASN:CG	2.21	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
1:D:96:ALA:C	1:D:98:VAL:H	2.21	0.49
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:A:67:ARG:NH2	1:D:72:VAL:HG23	2.28	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:D:193:HIS:HA	1:D:442:VAL:HG22	1.95	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:C:148:ASN:HD22	1:C:211:MET:HE2	1.79	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:D:142:TRP:CE2	1:D:342:ILE:HD13	2.48	0.48
1:D:239:GLN:NE2	1:D:275:SER:H	2.10	0.48
1:D:471:LEU:HG	4:D:3023:HOH:O	2.14	0.48
1:A:43:VAL:CG1	1:A:50:LEU:HD21	2.43	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:B:155:ARG:HD3	1:B:297:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4:ARG:HH21	1:C:470:GLN:H	1.61	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:D:88:HIS:CD2	1:D:311:PRO:HG2	2.48	0.48
1:A:501:GLU:OE1	1:A:501:GLU:HA	2.14	0.48
1:C:18:ARG:HH12	1:C:23:PRO:HA	1.79	0.48
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:A:45:PRO:HD3	1:D:431:PHE:CE2	2.49	0.48
1:C:18:ARG:NH1	1:C:23:PRO:HA	2.28	0.48
1:D:89:ASP:OD1	1:D:91:THR:OG1	2.32	0.48
1:D:155:ARG:NH2	1:D:438:ASN:OD1	2.47	0.48
1:A:54:VAL:H	1:A:54:VAL:HG22	1.62	0.48
1:A:71:ARG:HG3	1:A:71:ARG:NH1	2.25	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: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:D:451:ASN:OD1	1:D:451:ASN:C	2.56	0.48
1:B:118:GLU:OE1	1:B:118:GLU:N	2.47	0.47
1:B:223:ASN:C	1:B:225:ASP:H	2.21	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:110:VAL:CG2	1:D:317:LEU:HD21	2.44	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: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:C:469:ALA:O	1:C:470:GLN:C	2.58	0.47
1:D:488:TYR:CE1	1:D:492:ILE:HD11	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:A:112:PHE:CG	1:A:208:HIS:HB3	2.49	0.47
1:B:18:ARG:O	1:B:19:ALA:C	2.57	0.47
1:D:381:ARG:HG2	1:D:381:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:90:ILE:HD13	1:D:312:VAL:HG13	1.96	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: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: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:86:VAL:HG23	1:D:104:LYS:O	2.14	0.47
1:D:90:ILE:O	1:D:92:ARG:N	2.47	0.47
1:D:335:PRO:HD3	1:D:357:TYR:CG	2.50	0.47
1:A:43:VAL:HG21	1:B:43:VAL:HG21	1.97	0.47
1:A:500:ASN:O	1:A:501:GLU:O	2.33	0.47
1:B:71:ARG:HG2	3:B:2001:HEM:O2A	2.14	0.47
1:B:274:PRO:HB2	1:B:276:TRP:CZ3	2.50	0.47
1:C:476:LYS:NZ	1:C:476:LYS:HB3	2.30	0.47
1:A:217:HIS:HE2	3:A:2000:HEM:CBC	2.28	0.47
1:B:4:ARG:NH2	1:C:179:ASP:OD2	2.48	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:C:72:VAL:HG13	1:C:73:VAL:HG22	1.96	0.47
1:C:256:ASP:OD2	1:C:259:TYR:HA	2.15	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:B:402:ASN:C	1:B:402:ASN:HD22	2.23	0.46
1:B:487:GLU:C	1:B:489:GLY:H	2.23	0.46
1:C:368:ASN:O	1:C:371:GLN:HB2	2.14	0.46
1:A:37:LYS:O	1:A:37:LYS:NZ	2.41	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:B:329:GLU:OE1	1:B:329:GLU:HA	2.14	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:A:43:VAL:HG12	1:A:50:LEU:CD2	2.44	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:B:160:PHE:CD1	3:B:2001:HEM:HAB	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LEU:HB3	1:D:34:VAL:CG2	2.45	0.46
1:D:87:THR:C	1:D:88:HIS:ND1	2.73	0.46
1:A:430:ARG:HE	1:B:419:GLU:CD	2.23	0.46
1:B:217:HIS:CD2	1:B:353:ARG:NH1	2.82	0.46
1:B:229:VAL:HG23	1:B:284:THR:HA	1.98	0.46
1:B:472:PHE:C	1:B:472:PHE:CD2	2.94	0.46
1:C:52:GLN:O	1:C:54:VAL:N	2.49	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: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
1:D:71:ARG:HH22	1:D:329:GLU:C	2.22	0.46
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:9:ASP:O	1:B:12:LYS:HB3	2.15	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:475:LYS:O	1:B:476:LYS:C	2.57	0.46
1:B:493:GLN:O	1:B:494:ALA:C	2.59	0.46
1:C:499:TYR:C	1:C:501:GLU:H	2.23	0.46
1:D:90:ILE:HD11	1:D:99:PHE:CD1	2.50	0.46
1:D:323:ASN:ND2	4:D:3007:HOH:O	2.48	0.46
1:B:46:ARG:NH1	1:C:294:ASN:HB2	2.31	0.46
1:B:122:ALA:HB2	1:B:257:PRO:HB3	1.97	0.46
1:D:190:GLU:HA	1:D:438:ASN:CB	2.38	0.46
1:D:235:TYR:N	1:D:235:TYR:CD1	2.83	0.46
1:D:485:HIS:CE1	1:D:486:PRO:HG2	2.51	0.46
1:A:141:ASN:O	1:A:337:ASN:HB3	2.15	0.46
1:A:298:LEU:HD22	3:A:2000:HEM:HBC1	1.91	0.46
1:D:368:ASN:O	1:D:371:GLN:HB2	2.15	0.46
1:B:17:GLN:C	1:B:19:ALA:N	2.74	0.46
1:B:43:VAL:HG13	1:B:48:PRO:HD2	1.98	0.46
1:B:129:ARG:HB2	1:B:148:ASN:ND2	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:SER:HB3	1:C:49:LEU:CD1	2.46	0.46
1:D:346:PRO:O	1:D:347:ASP:C	2.58	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:B:393:MET:HE3	1:B:393:MET:HA	1.98	0.45
1:C:131:PHE:CD1	1:C:131:PHE:C	2.94	0.45
1:D:246:VAL:HG23	1:D:247:GLU:OE1	2.16	0.45
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.81	0.45
1:A:153:PHE:CD1	1:A:194:GLN:HB3	2.52	0.45
1:A:242:LYS:HD3	1:A:242:LYS:C	2.41	0.45
1:A:451:ASN:N	1:A:454:GLN:NE2	2.56	0.45
1:B:78:ALA:O	1:B:111:ARG:HA	2.15	0.45
1:B:177:ASP:C	1:B:177:ASP:OD1	2.59	0.45
1:B:403:TYR:CD1	1:B:403:TYR:N	2.85	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
1:B:252:LEU:O	1:B:253:ALA:C	2.59	0.45
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:A:180:MET:HE3	1:B:402:ASN:HD21	1.81	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:500:ASN:O	1:D:501:GLU:C	2.60	0.45
1:A:90:ILE:HD13	1:A:312:VAL:HG22	1.97	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:A:323:ASN:CG	1:C:396:ASN:HB3	2.42	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:D:339:PRO:HD2	1:D:342:ILE:HD12	1.98	0.45
1:A:154:ILE:HG13	1:A:349:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3200:HOH:O	1:C:409:SER:HB3	2.17	0.45
1:B:41:LEU:HB2	1:B:53:ASP:OD2	2.17	0.45
1:B:374:VAL:HG23	4:B:2178:HOH:O	2.17	0.45
1:C:126:ARG:HG2	1:C:126:ARG:HH11	1.82	0.45
1:C:152:PHE:HB3	1:C:298:LEU:CD2	2.47	0.45
1:D:90:ILE:HD11	1:D:99:PHE:CD2	2.52	0.45
1:A:129:ARG:HB2	1:A:148:ASN:CG	2.42	0.44
1:A:338:MET:HB3	1:A:342:ILE:O	2.17	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:D:280:ILE:HD13	1:D:280:ILE:O	2.17	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:A:419:GLU:H	1:A:419:GLU:CD	2.25	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:131:PHE:C	1:C:131:PHE:HD1	2.25	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: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:A:53:ASP:OD1	1:A:53:ASP:C	2.60	0.44
1:A:62:HIS:O	1:A:63:PHE:C	2.60	0.44
1:B:122:ALA:HB1	1:B:257:PRO:HA	1.99	0.44
1:B:188:ARG:HB3	1:B:190:GLU:CD	2.43	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:92:ARG:HG3	1:C:92:ARG:HH11	1.82	0.44
1:C:237:THR:HA	1:C:276:TRP:CD1	2.52	0.44
1:C:488:TYR:CD1	1:C:488:TYR:C	2.95	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:345:SER:C	1:B:347:ASP:H	2.25	0.44
1:B:456:LYS:HB2	1:B:491:ARG:HH22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:MET:HE3	1:B:302:TRP:CE2	2.53	0.44
1:B:361:HIS:NE2	3:B:2001:HEM:O1A	2.49	0.44
1:B:413:HIS:HD1	1:B:413:HIS:C	2.22	0.44
1:B:487:GLU:C	1:B:489:GLY:N	2.74	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:129:ARG:CB	1:C:211:MET:CE	2.96	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: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:223:ASN:C	1:C:225:ASP:N	2.75	0.44
1:C:279:TYR:CD1	1:C:311:PRO:HA	2.53	0.44
1:D:369:TYR:C	1:D:371:GLN:H	2.26	0.44
1:A:427:ASP:HA	1:B:423:HIS:HA	2.00	0.43
1:A:450:LEU:HD22	1:A:454:GLN:HB3	1.99	0.43
1:B:71:ARG:HG3	4:B:2159:HOH:O	2.18	0.43
1:B:163:PHE:O	1:B:166:SER:N	2.51	0.43
1:B:269:ALA:C	1:B:271:GLY:N	2.75	0.43
1:C:241:ILE:HD12	1:C:241:ILE:H	1.83	0.43
1:C:402:ASN:OD1	1:D:165:HIS:HB3	2.18	0.43
1:D:220:LYS:HA	1:D:229:VAL:O	2.18	0.43
1:D:221:LEU:HB2	1:D:229:VAL:HG23	1.98	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:D:499:TYR:C	1:D:501:GLU:N	2.75	0.43
1:A:50:LEU:C	1:A:52:GLN:N	2.73	0.43
1:A:148:ASN:C	1:A:148:ASN:HD22	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:ASP:HB3	1:C:180:MET:HE2	2.01	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:B:338:MET:CE	1:B:342:ILE:HG22	2.33	0.43
1:B:478:VAL:O	1:B:479:LYS:C	2.59	0.43
1:C:12:LYS:HG2	1:C:16:GLU:OE2	2.17	0.43
1:C:152:PHE:HB3	1:C:298:LEU:HD23	2.01	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:A:127:ASP:C	1:A:128:PRO:O	2.58	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:81:PHE:N	1:C:81:PHE:CD1	2.86	0.43
1:C:156:ASP:OD2	1:C:348:LYS:HD3	2.18	0.43
1:D:188:ARG:HB3	1:D:190:GLU:CD	2.43	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
1:A:419:GLU:CD	1:B:430:ARG:HH11	2.27	0.43
1:B:21:GLN:H	1:B:21:GLN:HG3	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:HH11	1:C:381:ARG:HB2	1.84	0.43
1:B:41:LEU:HD23	1:C:430:ARG:CZ	2.49	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:C:488:TYR:C	1:C:488:TYR:HD1	2.27	0.43
1:A:303:PRO:O	1:A:304:HIS:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:HD13	1:C:37:LYS:C	2.43	0.42
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:393:MET:HE2	1:D:373:PRO:HD3	1.99	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:43:VAL:HG13	1:D:43:VAL:O	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
2:A:3000:CYN:N	3:A:2000:HEM:NC	2.62	0.42
1:B:4:ARG:HD2	1:B:8:SER:CB	2.49	0.42
1:B:145:VAL:HB	1:B:353:ARG:NH2	2.35	0.42
1:B:149:THR:OG1	1:B:150:PRO:HD2	2.19	0.42
1:C:170:ASN:HA	1:C:180:MET:HE1	2.01	0.42
1:D:23:PRO:O	1:D:24:ASP:C	2.61	0.42
1:D:270:THR:C	1:D:272:ASN:N	2.77	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: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: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:C:391:MET:O	1:C:393:MET:HE2	2.20	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:A:338:MET:HE1	1:A:344:PRO:HB3	2.02	0.42
1:B:217:HIS:CE1	3:B:2001:HEM:HBC1	2.55	0.42
1:C:50:LEU:C	1:C:52:GLN:N	2.75	0.42
1:D:96:ALA:C	1:D:98:VAL:N	2.78	0.42
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:66:GLU:HA	1:D:389:GLY:N	2.35	0.42
1:B:475:LYS:C	1:B:477:ALA:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:HIS:HD2	1:C:242:LYS:HB3	1.82	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:41:LEU:HB3	1:A:53:ASP:HB2	2.01	0.42
1:A:172:GLN:NE2	1:D:322:VAL:HA	2.30	0.42
1:A:284:THR:OG1	1:A:287:GLU:CG	2.64	0.42
1:B:369:TYR:C	1:B:371:GLN:N	2.77	0.42
1:C:22:LYS:HD3	1:C:23:PRO:N	2.35	0.42
1:C:95:LYS:HG2	1:C:222:VAL:O	2.19	0.42
1:C:182:TRP:NE1	1:C:465:HIS:ND1	2.64	0.42
1:C:422:THR:HG22	1:C:423:HIS:N	2.35	0.42
1:D:154:ILE:HB	4:D:3132:HOH:O	2.19	0.42
1:A:29:GLY:C	1:C:370:LEU:HD13	2.45	0.41
1:A:251:ARG:HG2	1:A:255:GLU:CD	2.45	0.41
1:B:71:ARG:NH1	1:B:71:ARG:CG	2.77	0.41
1:D:166:SER:HA	1:D:180:MET:HE2	2.02	0.41
1:A:50:LEU:CD1	1:B:48:PRO:HB2	2.50	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:74:HIS:CD2	3:B:2001:HEM:C4D	3.08	0.41
1:C:346:PRO:O	1:C:347:ASP:C	2.63	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:D:57:THR:O	1:D:58:ASP:C	2.60	0.41
1:B:91:THR:C	1:B:93:TYR:H	2.26	0.41
1:C:223:ASN:O	1:C:225:ASP:N	2.53	0.41
1:C:444:THR:O	1:C:444:THR:HG22	2.19	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:A:15:LYS:HD2	1:C:408:PHE:HA	2.03	0.41
1:A:158:LEU:HD21	1:D:56: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:C:209:ARG:NH2	1:C:267:ALA:HB2	2.29	0.41
1:C:214:TYR:HD1	1:C:234:HIS:HD1	1.68	0.41
1:C:332:ALA:HB1	1:C:361:HIS:ND1	2.35	0.41
1:D:298:LEU:HD21	3:D:2003:HEM:HMC3	2.03	0.41
1:D:369:TYR:C	1:D:371:GLN:N	2.77	0.41
1:A:148:ASN:C	1:A:148:ASN:ND2	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:92:ARG:HG3	1:B:92:ARG:H	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:165:HIS:NE2	1:C:66:GLU:OE2	2.37	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
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:O	1:B:43:VAL:HG22	2.21	0.41
1:A:421:ARG:NH2	1:B:429:GLN:NE2	2.69	0.41
1:A:453:GLU:OE2	1:A:457:ARG:NH1	2.54	0.41
1:B:245:SER:O	1:B:246:VAL:C	2.64	0.41
1:B:332:ALA:N	1:B:375:ASN:OD1	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:83:TYR:CD1	1:C:83:TYR:C	2.98	0.41
1:C:115:VAL:HB	1:C:127:ASP:OD1	2.20	0.41
1:C:221:LEU:HA	1:C:341:GLY:O	2.20	0.41
1:C:281:GLN:HG2	1:C:309:LEU:HD12	2.03	0.41
1:C:369:TYR:C	1:C:371:GLN:H	2.28	0.41
1:C:432:ASN:ND2	1:C:432:ASN:C	2.78	0.41
1:D:114:THR:HB	1:D:115:VAL:H	1.74	0.41
1:D:147:ASN:OD1	3:D:2003:HEM:C4C	2.74	0.41
1:D:291:PHE:HA	1:D:292:PRO:HD3	1.83	0.41
1:B:19:ALA:HB3	1:B:21:GLN:NE2	2.09	0.41
1:B:153:PHE:CD1	1:B:153:PHE:N	2.88	0.41
1:B:301:VAL:HG22	1:B:441:GLN:OE1	2.21	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: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
3:C:2002:HEM:HHC	3:C:2002:HEM:HMC2	1.55	0.41
1:D:338:MET:HE1	1:D:343:GLU:O	2.21	0.41
1:B:50:LEU:N	1:B:50:LEU:CD2	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ASP:O	1:D:32:ASN:HA	2.21	0.40
1:B:220:LYS:HE3	1:B:343:GLU:OE1	2.21	0.40
1:C:448:LYS:HD2	4:C:2115:HOH:O	2.22	0.40
1:C:467:LYS:HE2	1:C:468:ASP:CG	2.46	0.40
1:D:347:ASP:OD1	1:D:349:MET:HB2	2.20	0.40
1:A:197:PHE:CD1	1:A:197:PHE:C	3.00	0.40
1:A:413:HIS:HD2	1:A:413:HIS:O	2.04	0.40
4:A:3145:HOH:O	1:C:37:LYS:N	2.08	0.40
1:B:50:LEU:C	1:B:52:GLN:N	2.77	0.40
1:B:220:LYS:N	1:B:343:GLU:O	2.52	0.40
1:B:252:LEU:N	1:B:252:LEU:CD1	2.84	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
1:C:154:ILE:HD12	1:C:349:MET:HE1	2.03	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:346:PRO:O	1:A:347:ASP:C	2.64	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:B:154:ILE:HG13	1:B:349:MET:HE1	2.03	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:414:GLN:O	1:D:415:PRO:C	2.64	0.40
1:D:478:VAL:HG21	1:D:493:GLN:OE1	2.22	0.40
1:A:83:TYR:CD1	1:A:83:TYR:C	2.98	0.40
1:A:280:ILE:HG12	1:A:310:ILE:HB	2.03	0.40
1:A:297:ASP:C	1:A:297:ASP:OD1	2.65	0.40
1:A:332:ALA:N	1:A:375:ASN:OD1	2.53	0.40
1:B:10:GLN:NE2	1:C:172:GLN:HE21	2.19	0.40
1:B:16:GLU:O	1:B:17:GLN:C	2.64	0.40
1:B:444:THR:O	1:B:448:LYS:CB	2.61	0.40
1:C:251:ARG:C	1:C:255:GLU:HG3	2.46	0.40
1:C:446:TYR:CE2	1:C:455:ARG:HD3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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%)	450 (90%)	39 (8%)	8 (2%)	7	27
1	B	497/506 (98%)	425 (86%)	58 (12%)	14 (3%)	4	14
1	C	497/506 (98%)	427 (86%)	54 (11%)	16 (3%)	3	11
1	D	497/506 (98%)	438 (88%)	50 (10%)	9 (2%)	6	23
All	All	1988/2024 (98%)	1740 (88%)	201 (10%)	47 (2%)	4	17

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

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Mol	Chain	Res	Type
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
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%)	399 (93%)	32 (7%)	13	37
1	B	431/437 (99%)	389 (90%)	42 (10%)	8	25
1	C	431/437 (99%)	387 (90%)	44 (10%)	7	23
1	D	431/437 (99%)	404 (94%)	27 (6%)	16	45
All	All	1724/1748 (99%)	1579 (92%)	145 (8%)	10	32

All (145) 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	105	ARG
1	A	106	THR
1	A	118	GLU
1	A	137	THR
1	A	148	ASN
1	A	191	SER
1	A	194	GLN
1	A	202	ARG
1	A	229	VAL
1	A	235	TYR
1	A	242	LYS
1	A	247	GLU
1	A	263	ASP
1	A	309	LEU
1	A	336	SER
1	A	361	HIS
1	A	394	MET
1	A	402	ASN
1	A	407	SER
1	A	421	ARG
1	A	435	ASN
1	A	460	GLU
1	A	475	LYS
1	A	476	LYS
1	A	496	LEU
1	B	18	ARG

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Mol	Chain	Res	Type
1	B	21	GLN
1	B	37	LYS
1	B	41	LEU
1	B	43	VAL
1	B	46	ARG
1	B	50	LEU
1	B	51	VAL
1	B	67	ARG
1	B	92	ARG
1	B	95	LYS
1	B	104	LYS
1	B	114	THR
1	B	115	VAL
1	B	124	THR
1	B	126	ARG
1	B	137	THR
1	B	145	VAL
1	B	149	THR
1	B	168	LYS
1	B	193	HIS
1	B	220	LYS
1	B	232	LYS
1	B	235	TYR
1	B	290	ILE
1	B	312	VAL
1	B	330	GLN
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	447	LEU
1	B	457	ARG
1	B	458	LEU
1	B	466	LEU
1	B	471	LEU
1	B	476	LYS
1	B	500	ASN
1	C	3	ASN

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Mol	Chain	Res	Type
1	C	4	ARG
1	C	18	ARG
1	C	22	LYS
1	C	26	LEU
1	C	34	VAL
1	C	43	VAL
1	C	46	ARG
1	C	55	VAL
1	C	76	LYS
1	C	92	ARG
1	C	104	LYS
1	C	105	ARG
1	C	147	ASN
1	C	149	THR
1	C	154	ILE
1	C	179	ASP
1	C	194	GLN
1	C	200	SER
1	C	206	ASP
1	C	209	ARG
1	C	210	HIS
1	C	229	VAL
1	C	235	TYR
1	C	237	THR
1	C	239	GLN
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	414	GLN
1	C	418	LEU
1	C	438	ASN
1	C	450	LEU
1	C	451	ASN
1	C	467	LYS
1	C	470	GLN
1	C	472	PHE
1	C	476	LYS
1	C	485	HIS

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Mol	Chain	Res	Type
1	C	501	GLU
1	D	22	LYS
1	D	55	VAL
1	D	105	ARG
1	D	111	ARG
1	D	124	THR
1	D	127	ASP
1	D	138	GLU
1	D	147	ASN
1	D	148	ASN
1	D	235	TYR
1	D	247	GLU
1	D	261	LEU
1	D	263	ASP
1	D	280	ILE
1	D	301	VAL
1	D	314	LYS
1	D	368	ASN
1	D	374	VAL
1	D	378	TYR
1	D	397	GLN
1	D	412	GLU
1	D	438	ASN
1	D	440	THR
1	D	452	GLU
1	D	453	GLU
1	D	479	LYS
1	D	498	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	32	ASN
1	A	148	ASN
1	A	167	GLN
1	A	243	ASN
1	A	254	HIS
1	A	320	ASN
1	A	337	ASN
1	A	429	GLN
1	A	432	ASN

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Mol	Chain	Res	Type
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	167	GLN
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
1	B	461	ASN
1	B	470	GLN
1	C	17	GLN
1	C	21	GLN
1	C	32	ASN
1	C	52	GLN
1	C	101	HIS
1	C	147	ASN
1	C	172	GLN
1	C	239	GLN
1	C	337	ASN
1	C	402	ASN
1	C	414	GLN
1	C	420	HIS
1	C	432	ASN
1	C	435	ASN
1	C	438	ASN
1	C	454	GLN
1	C	461	ASN
1	C	474	GLN
1	C	480	ASN
1	C	500	ASN
1	D	32	ASN
1	D	39	ASN
1	D	52	GLN

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Mol	Chain	Res	Type
1	D	148	ASN
1	D	167	GLN
1	D	170	ASN
1	D	193	HIS
1	D	239	GLN
1	D	243	ASN
1	D	337	ASN
1	D	368	ASN
1	D	413	HIS
1	D	470	GLN
1	D	480	ASN
1	D	500	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	50,50,50	9.28	10 (20%)	67,82,82	8.38	24 (35%)
2	CYN	A	3000	-	1,1,1	0.40	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	2000	1	50,50,50	8.87	7 (14%)	67,82,82	6.37	7 (10%)
3	HEM	D	2003	1,2	50,50,50	2.32	11 (22%)	67,82,82	4.92	20 (29%)
2	CYN	D	3001	3	1,1,1	0.45	0	-		
3	HEM	C	2002	1	50,50,50	1.53	6 (12%)	67,82,82	1.90	4 (5%)

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	C	2002	1	-	7/14/54/54	-
3	HEM	A	2000	1	-	5/14/54/54	-
3	HEM	D	2003	1,2	-	11/14/54/54	-
3	HEM	B	2001	1	-	7/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	HEM	CMC-C2C	54.68	2.62	1.50
3	B	2001	HEM	CMC-C2C	54.46	2.62	1.50
3	B	2001	HEM	CAC-C3C	32.65	2.34	1.47
3	A	2000	HEM	CAC-C3C	29.41	2.25	1.47
3	B	2001	HEM	FE-NA	10.45	2.29	1.95
3	D	2003	HEM	FE-NB	10.04	2.25	1.94
3	D	2003	HEM	FE-NC	7.70	2.20	1.95
3	C	2002	HEM	FE-NA	6.31	2.16	1.95
3	B	2001	HEM	CHA-C4D	5.99	1.50	1.38
3	B	2001	HEM	FE-ND	5.42	2.11	1.94
3	B	2001	HEM	FE-NC	5.40	2.13	1.95
3	A	2000	HEM	CBC-CAC	4.58	1.52	1.30
3	C	2002	HEM	CBC-CAC	4.54	1.52	1.30
3	D	2003	HEM	CBC-CAC	4.48	1.51	1.30
3	B	2001	HEM	CBC-CAC	4.28	1.51	1.30
3	D	2003	HEM	CHD-C4C	3.26	1.44	1.38
3	B	2001	HEM	CAB-C3B	-3.24	1.38	1.47
3	C	2002	HEM	CAB-C3B	-3.22	1.38	1.47
3	D	2003	HEM	CAB-C3B	-3.20	1.38	1.47
3	D	2003	HEM	CHA-C1A	3.16	1.46	1.39
3	A	2000	HEM	CAB-C3B	-3.14	1.39	1.47
3	A	2000	HEM	FE-NC	3.01	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	HEM	CHC-C4B	-2.70	1.33	1.39
3	A	2000	HEM	FE-NB	2.62	2.03	1.94
3	C	2002	HEM	CBB-CAB	2.56	1.42	1.30
3	D	2003	HEM	CBB-CAB	2.54	1.42	1.30
3	B	2001	HEM	CBB-CAB	2.54	1.42	1.30
3	A	2000	HEM	CBB-CAB	2.53	1.42	1.30
3	D	2003	HEM	CHC-C4B	2.44	1.44	1.39
3	D	2003	HEM	FE-NA	-2.40	1.87	1.95
3	C	2002	HEM	FE-NB	2.32	2.02	1.94
3	C	2002	HEM	FE-ND	2.30	2.02	1.94
3	D	2003	HEM	CHB-C1B	2.23	1.43	1.38
3	D	2003	HEM	CHC-C1C	2.01	1.42	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	HEM	CMC-C2C-C3C	-42.55	25.47	128.43
3	B	2001	HEM	CMC-C2C-C3C	-42.13	26.48	128.43
3	B	2001	HEM	CAC-C3C-C2C	-27.79	38.09	128.43
3	A	2000	HEM	CAC-C3C-C2C	-26.94	40.83	128.43
3	B	2001	HEM	CHD-C4C-NC	-22.62	99.82	124.45
3	D	2003	HEM	CAA-CBA-CGA	21.40	170.43	113.67
3	B	2001	HEM	CHC-C1C-NC	-17.07	105.86	124.45
3	D	2003	HEM	CBA-CAA-C2A	15.99	156.75	112.53
3	D	2003	HEM	CHD-C4C-NC	-14.62	108.54	124.45
3	B	2001	HEM	CHD-C4C-C3C	14.38	149.46	125.21
3	C	2002	HEM	CMC-C2C-C1C	-11.63	104.25	124.73
3	B	2001	HEM	CAA-C2A-C1A	-11.15	103.15	124.94
3	B	2001	HEM	CBD-CAD-C3D	10.98	142.90	112.53
3	D	2003	HEM	CHB-C4A-NA	10.71	143.28	123.86
3	B	2001	HEM	C1C-CHC-C4B	10.54	148.43	126.02
3	D	2003	HEM	CBD-CAD-C3D	10.25	140.87	112.53
3	B	2001	HEM	CAA-CBA-CGA	10.02	140.25	113.67
3	B	2001	HEM	CHC-C4B-NB	-9.80	113.88	124.42
3	B	2001	HEM	C4C-CHD-C1D	9.51	146.23	126.02
3	B	2001	HEM	CAD-CBD-CGD	9.33	138.42	113.67
3	B	2001	HEM	CHA-C4D-ND	-9.05	113.17	124.37
3	D	2003	HEM	C4A-CHB-C1B	-8.84	105.47	126.25
3	B	2001	HEM	CHC-C1C-C2C	8.55	143.26	125.49
3	D	2003	HEM	CHB-C4A-C3A	-8.37	103.12	127.43
3	A	2000	HEM	CAC-C3C-C4C	8.23	144.47	124.82
3	B	2001	HEM	CAC-C3C-C4C	7.80	143.44	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2003	HEM	CHD-C4C-C3C	7.49	137.84	125.21
3	C	2002	HEM	CMC-C2C-C3C	7.10	145.62	128.43
3	D	2003	HEM	CAD-C3D-C4D	6.84	136.62	124.70
3	D	2003	HEM	CAD-CBD-CGD	6.32	130.43	113.67
3	B	2001	HEM	CHD-C1D-ND	6.28	131.18	124.42
3	A	2000	HEM	CBC-CAC-C3C	6.14	158.18	127.53
3	D	2003	HEM	CAD-C3D-C2D	-5.88	116.86	127.87
3	B	2001	HEM	CAA-C2A-C3A	5.25	138.85	127.07
3	B	2001	HEM	CHC-C4B-C3B	5.04	135.14	125.07
3	B	2001	HEM	CMC-C2C-C1C	4.87	133.30	124.73
3	D	2003	HEM	C1C-CHC-C4B	4.82	136.26	126.02
3	B	2001	HEM	CHD-C1D-C2D	-4.74	117.54	125.03
3	A	2000	HEM	CMC-C2C-C1C	4.63	132.89	124.73
3	D	2003	HEM	CHA-C1A-C2A	-4.45	115.56	125.30
3	D	2003	HEM	CAA-C2A-C1A	-4.40	116.34	124.94
3	D	2003	HEM	CAA-C2A-C3A	3.28	134.42	127.07
3	D	2003	HEM	C4C-CHD-C1D	3.17	132.76	126.02
3	D	2003	HEM	C1A-CHA-C4D	-3.14	118.85	126.25
3	B	2001	HEM	CBA-CAA-C2A	-3.00	104.23	112.53
3	B	2001	HEM	CHA-C4D-C3D	2.84	130.46	125.23
3	C	2002	HEM	CMB-C2B-C1B	2.49	128.93	125.03
3	B	2001	HEM	CMB-C2B-C1B	2.45	128.86	125.03
3	D	2003	HEM	CMB-C2B-C1B	2.45	128.86	125.03
3	A	2000	HEM	CMB-C2B-C1B	2.42	128.82	125.03
3	D	2003	HEM	CHB-C1B-NB	-2.39	121.41	124.37
3	D	2003	HEM	CHA-C1A-NA	2.09	127.65	123.86
3	A	2000	HEM	CHC-C1C-C2C	-2.06	121.19	125.49
3	C	2002	HEM	CHC-C1C-C2C	-2.03	121.26	125.49
3	B	2001	HEM	C3B-C4B-NB	2.02	110.92	109.47

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2000	HEM	C2B-C3B-CAB-CBB
3	A	2000	HEM	C4B-C3B-CAB-CBB
3	B	2001	HEM	C2B-C3B-CAB-CBB
3	C	2002	HEM	C2B-C3B-CAB-CBB
3	C	2002	HEM	C4B-C3B-CAB-CBB
3	C	2002	HEM	C2C-C3C-CAC-CBC
3	C	2002	HEM	C4C-C3C-CAC-CBC
3	D	2003	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	D	2003	HEM	C2C-C3C-CAC-CBC
3	D	2003	HEM	C4C-C3C-CAC-CBC
3	D	2003	HEM	C2D-C3D-CAD-CBD
3	D	2003	HEM	C4D-C3D-CAD-CBD
3	B	2001	HEM	C4D-C3D-CAD-CBD
3	D	2003	HEM	C2A-CAA-CBA-CGA
3	B	2001	HEM	C2D-C3D-CAD-CBD
3	B	2001	HEM	C4B-C3B-CAB-CBB
3	B	2001	HEM	C4C-C3C-CAC-CBC
3	D	2003	HEM	C4B-C3B-CAB-CBB
3	B	2001	HEM	C2A-CAA-CBA-CGA
3	A	2000	HEM	C4C-C3C-CAC-CBC
3	C	2002	HEM	C2D-C3D-CAD-CBD
3	D	2003	HEM	CAD-CBD-CGD-O2D
3	D	2003	HEM	CAA-CBA-CGA-O2A
3	D	2003	HEM	CAD-CBD-CGD-O1D
3	D	2003	HEM	CAA-CBA-CGA-O1A
3	A	2000	HEM	CAD-CBD-CGD-O2D
3	A	2000	HEM	CAD-CBD-CGD-O1D
3	C	2002	HEM	CAD-CBD-CGD-O1D
3	C	2002	HEM	CAD-CBD-CGD-O2D
3	B	2001	HEM	CAA-CBA-CGA-O2A

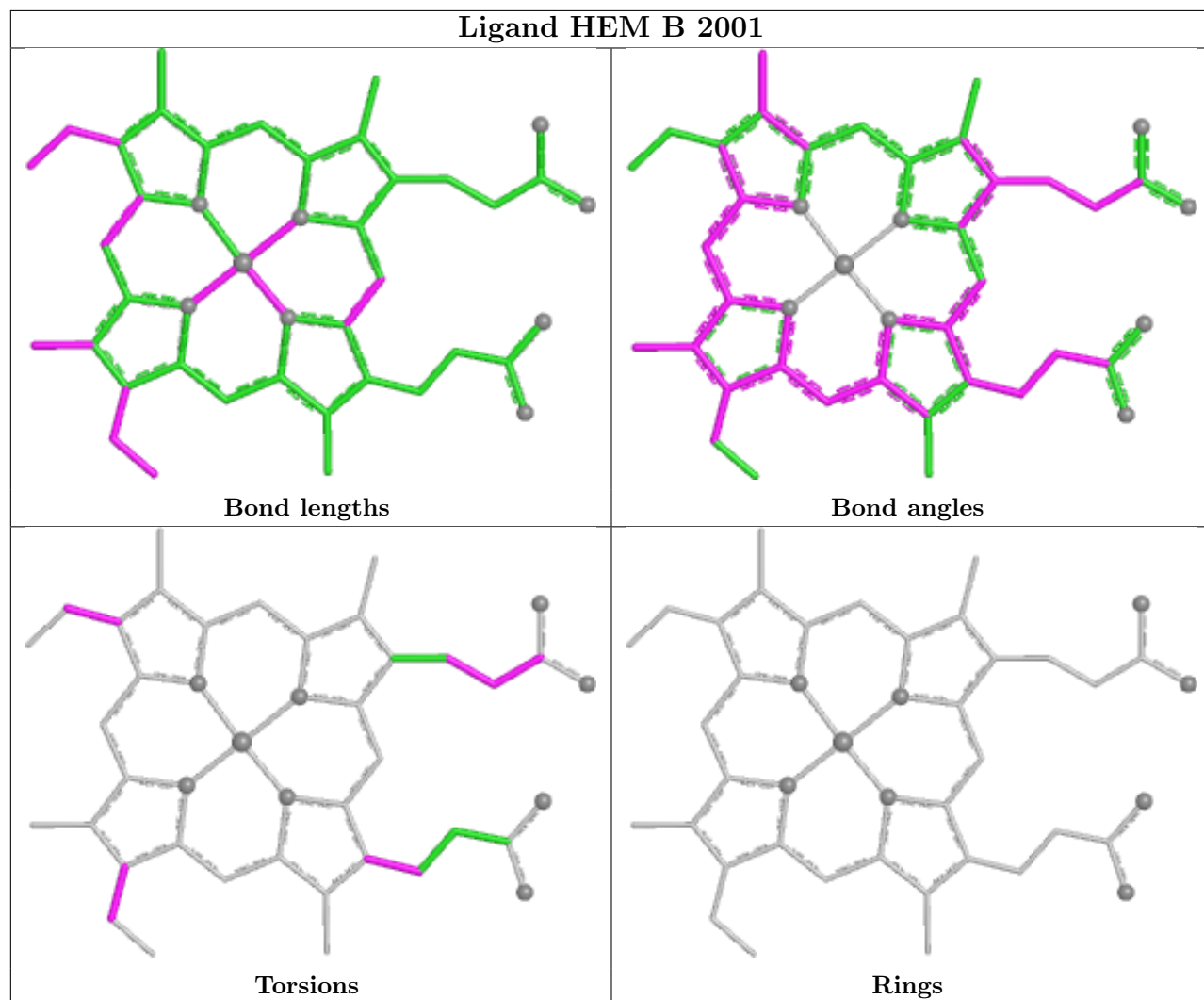
There are no ring outliers.

5 monomers are involved in 89 short contacts:

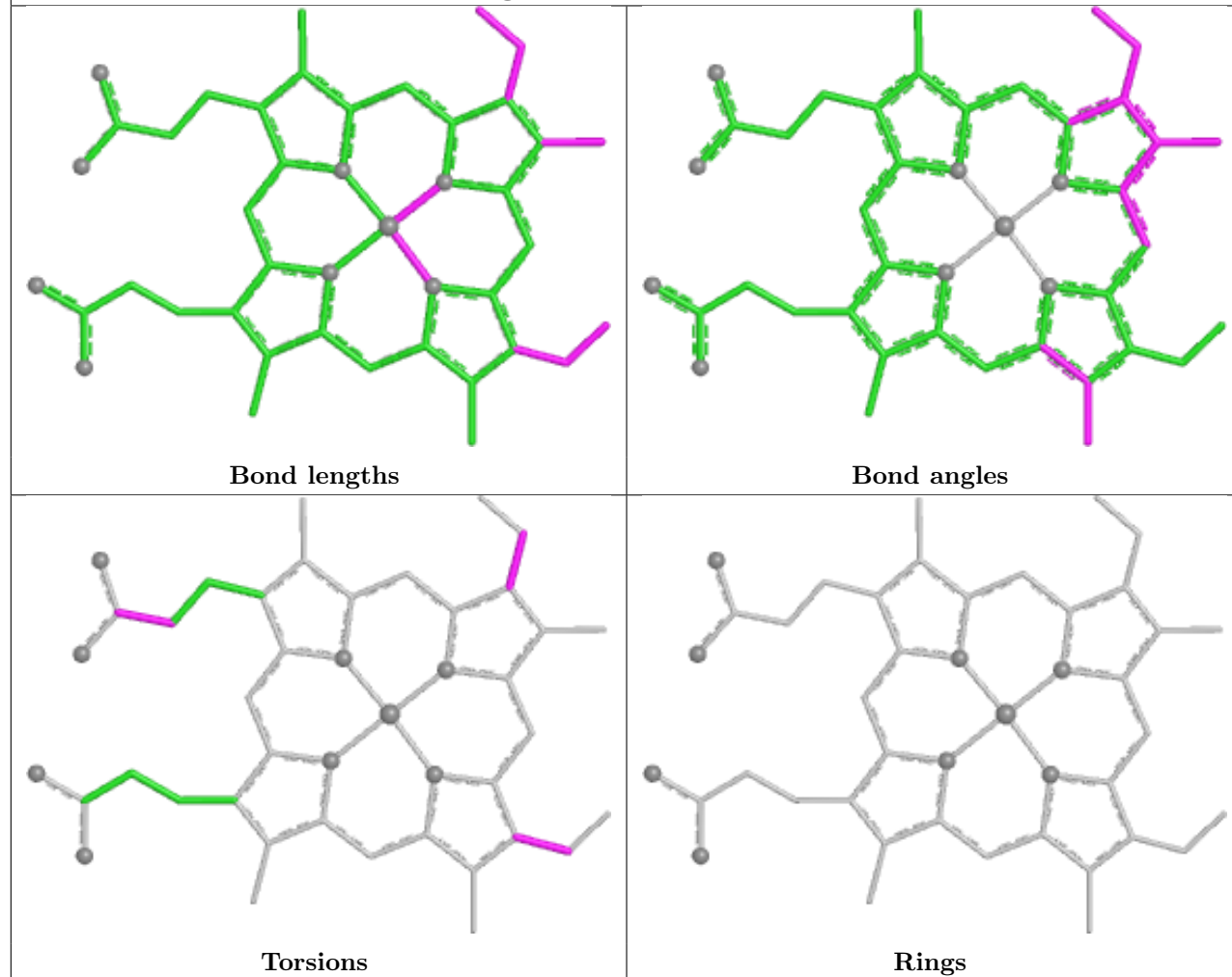
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	HEM	25	0
2	A	3000	CYN	6	0
3	A	2000	HEM	17	0
3	D	2003	HEM	21	0
3	C	2002	HEM	26	0

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

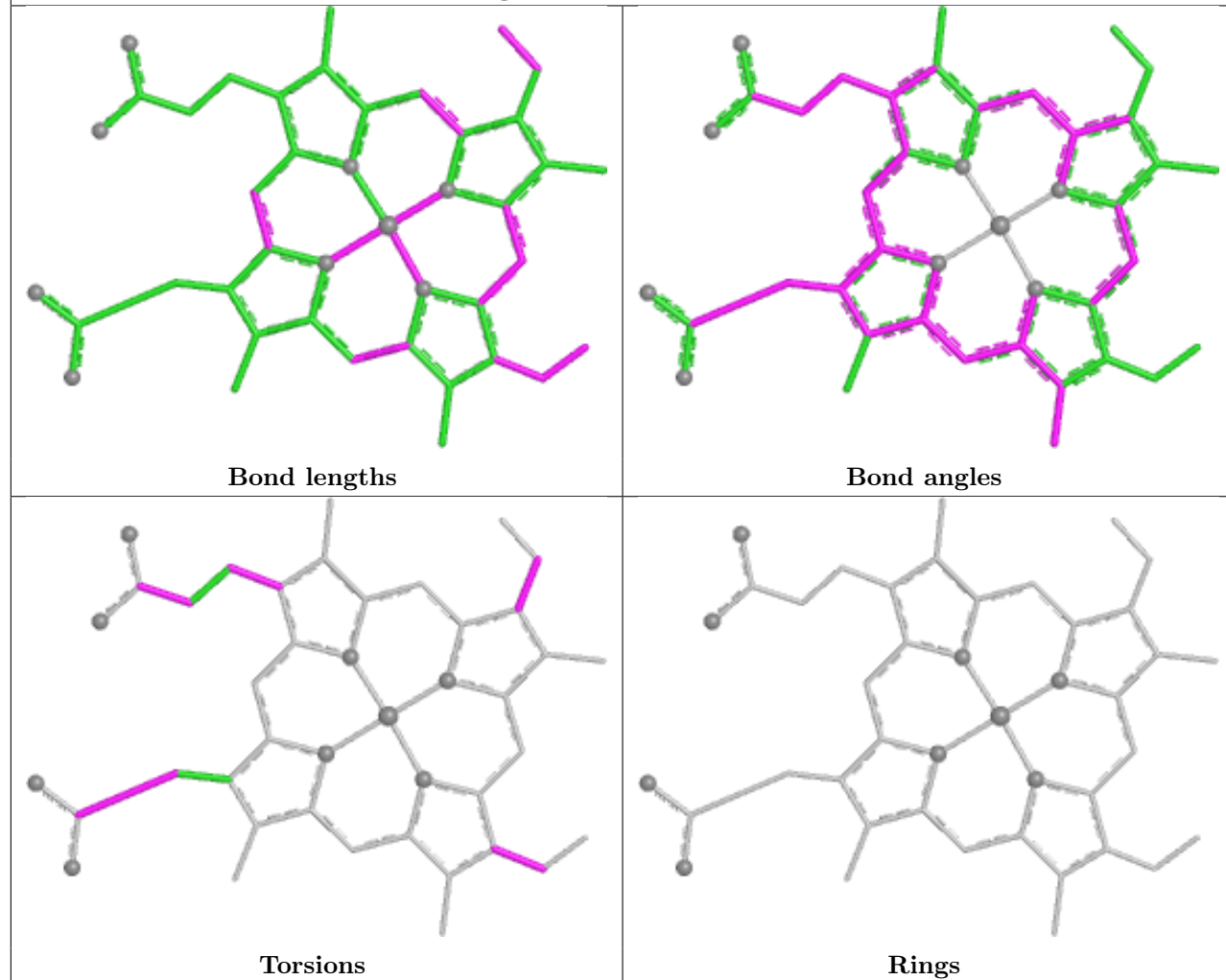
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

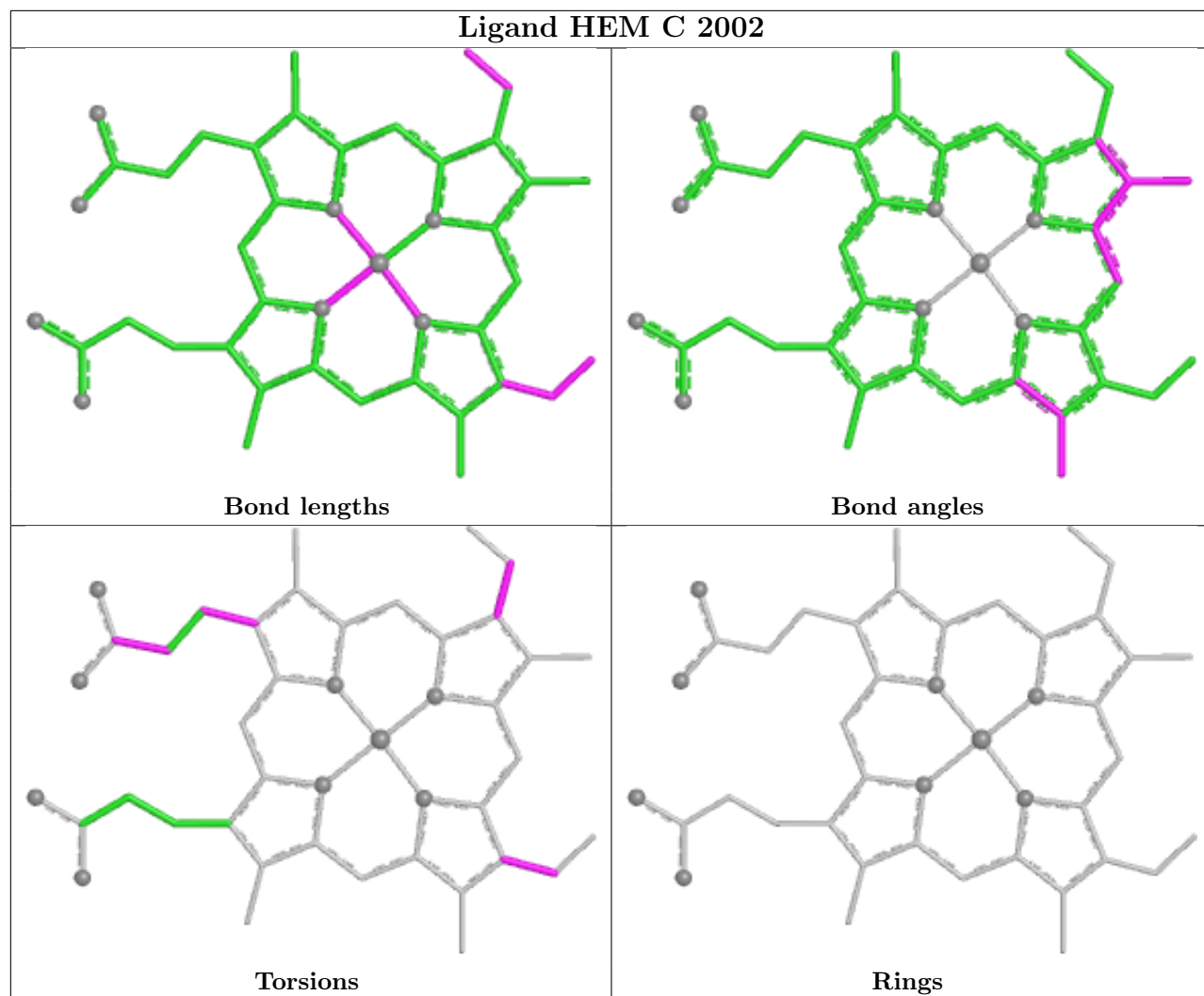


Ligand HEM A 2000



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 [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%)	-0.38	2 (0%) 88 84	9, 29, 55, 85	0
1	B	499/506 (98%)	-0.16	3 (0%) 85 80	12, 37, 64, 97	0
1	C	499/506 (98%)	-0.17	6 (1%) 76 68	12, 33, 65, 90	1 (0%)
1	D	499/506 (98%)	-0.16	4 (0%) 82 75	10, 35, 69, 89	0
All	All	1996/2024 (98%)	-0.22	15 (0%) 82 75	9, 34, 64, 97	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	20	ALA	3.2
1	D	426	GLY	2.7
1	A	20	ALA	2.7
1	C	501	GLU	2.3
1	D	424	PHE	2.3
1	C	3	ASN	2.3
1	C	425	SER	2.2
1	C	209	ARG	2.1
1	B	3	ASN	2.1
1	A	19	ALA	2.1
1	B	100	GLU	2.1
1	C	434	ALA	2.1
1	B	501	GLU	2.1
1	D	418	LEU	2.0
1	C	426	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

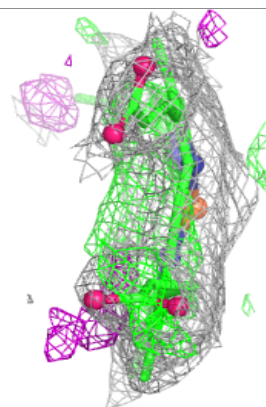
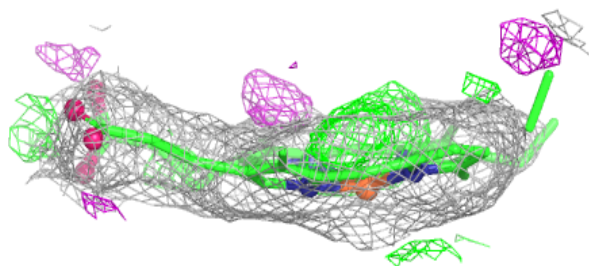
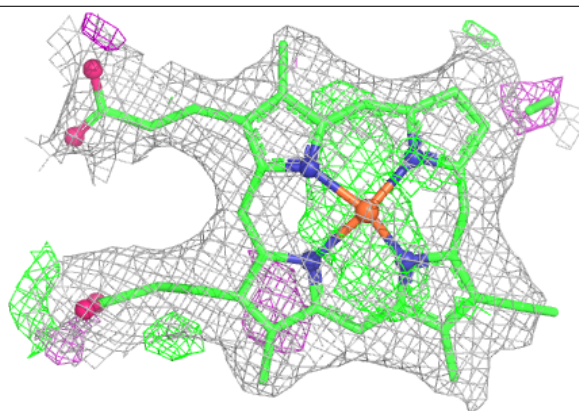
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CYN	D	3001	2/2	0.92	0.13	57,57,57,63	0
3	HEM	B	2001	43/43	0.93	0.15	20,37,58,100	0
3	HEM	D	2003	43/43	0.93	0.16	21,48,68,78	0
3	HEM	C	2002	43/43	0.94	0.13	22,37,54,101	0
3	HEM	A	2000	43/43	0.97	0.09	7,26,38,101	0
2	CYN	A	3000	2/2	0.98	0.08	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.

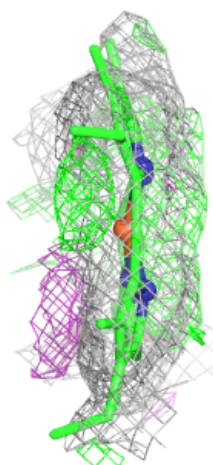
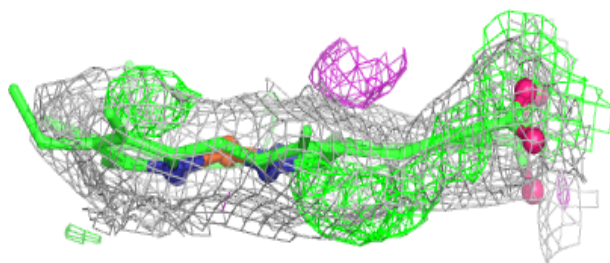
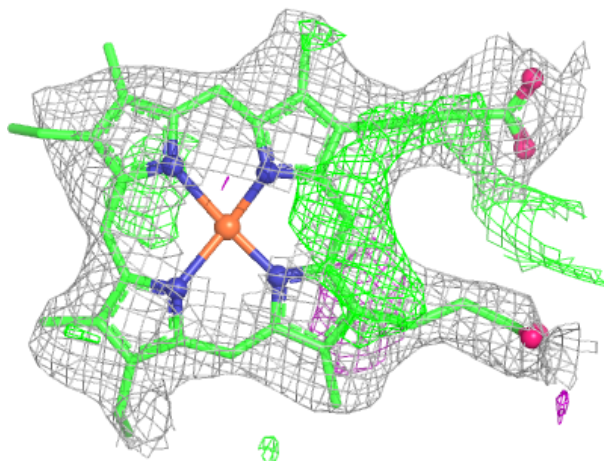
Electron density around HEM B 2001:

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



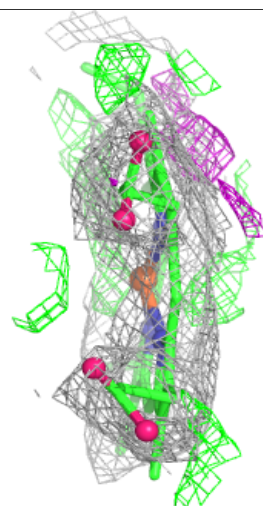
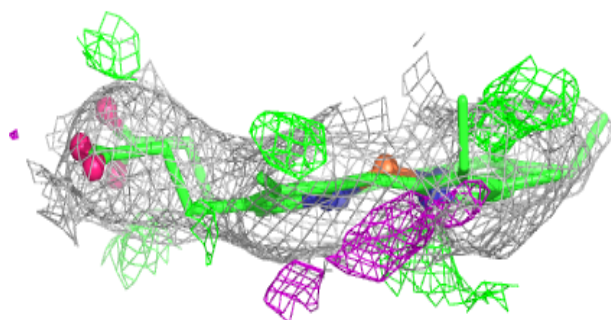
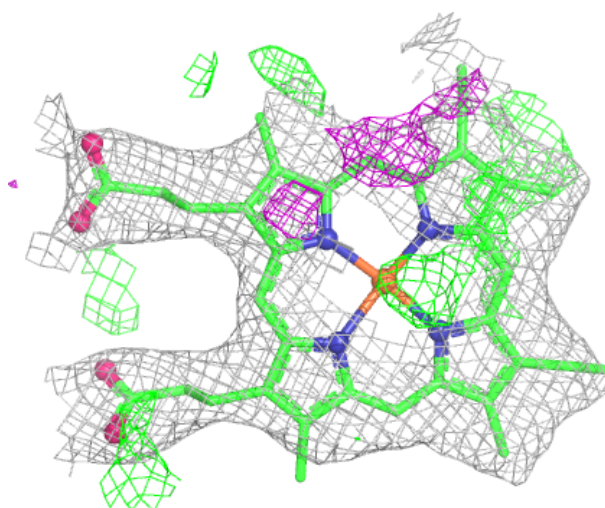
Electron density around HEM D 2003:

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



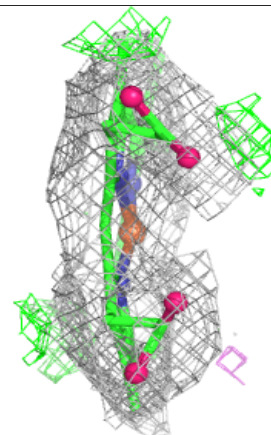
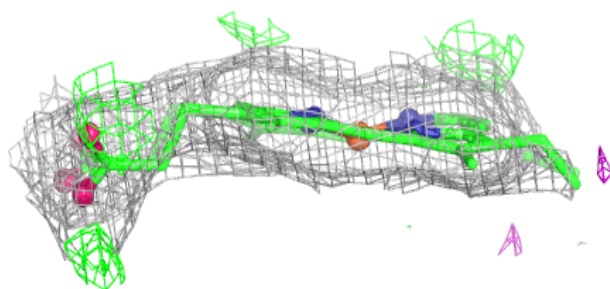
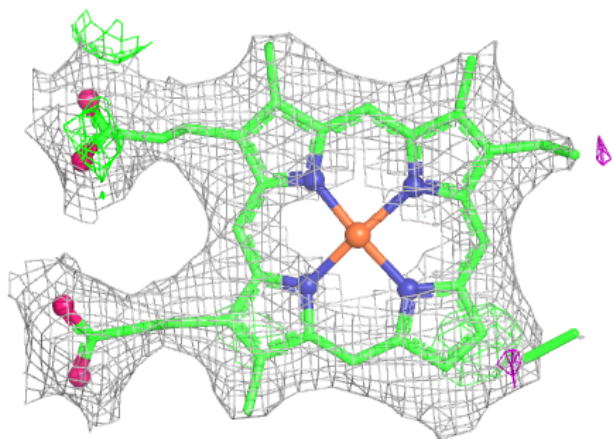
Electron density around HEM C 2002:

$2mF_o-DF_c$ (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.