



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:59 AM EDT

PDB ID : 1TH2 / pdb_00001th2
Title : crystal structure of NADPH depleted bovine liver catalase complexed with azide
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

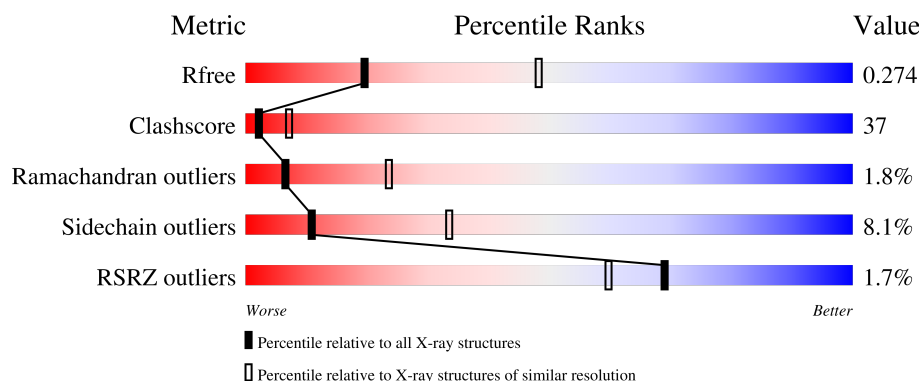
1 Overall quality at a glance

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	% 48% 41% 8% ..
1	B	506	% 36% 53% 8% ..
1	C	506	2% 38% 51% 9% ..
1	D	506	3% 45% 46% 7% ..

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
3	AZI	D	3000	-	X	-	-

2 Entry composition [i](#)

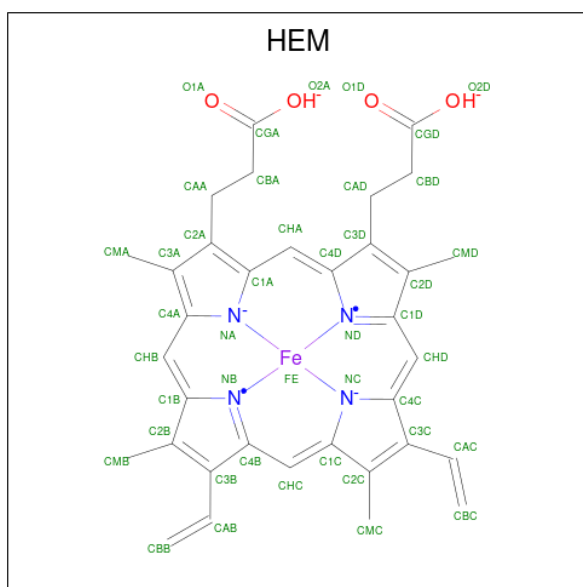
There are 4 unique types of molecules in this entry. The entry contains 17049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



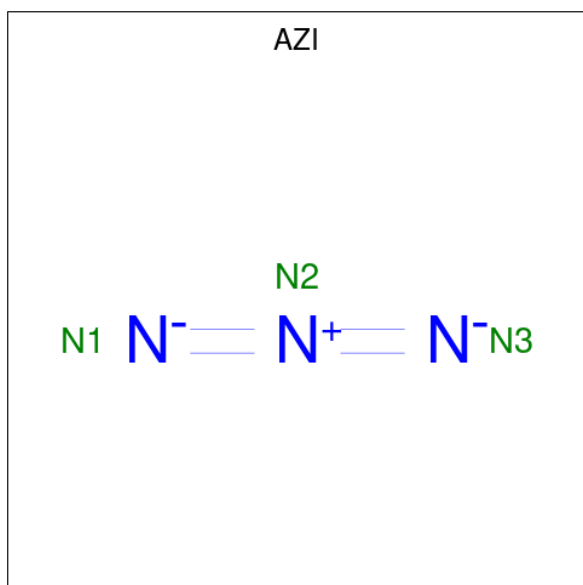
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	N		
			3	3	0	0

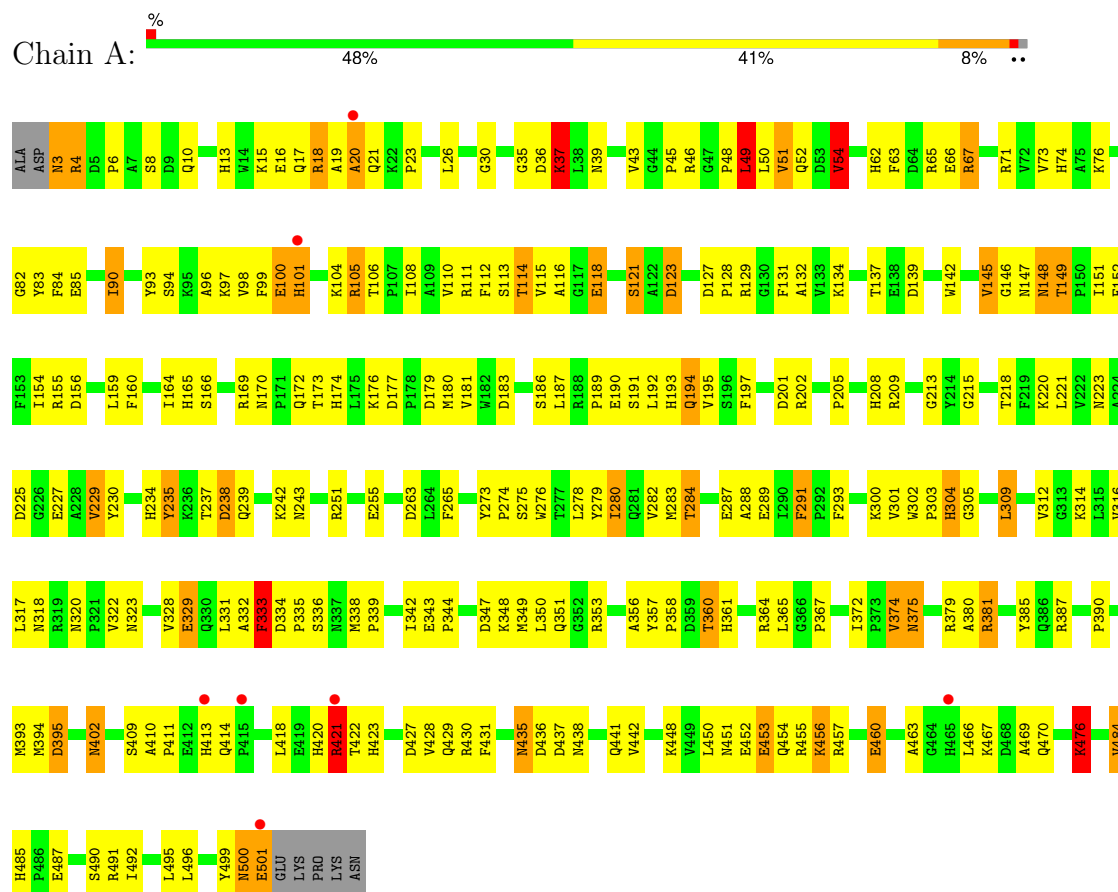
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	250	Total	O		
			250	250	0	0
4	B	182	Total	O		
			182	182	0	0
4	C	193	Total	O		
			193	193	0	0
4	D	181	Total	O		
			181	181	0	0

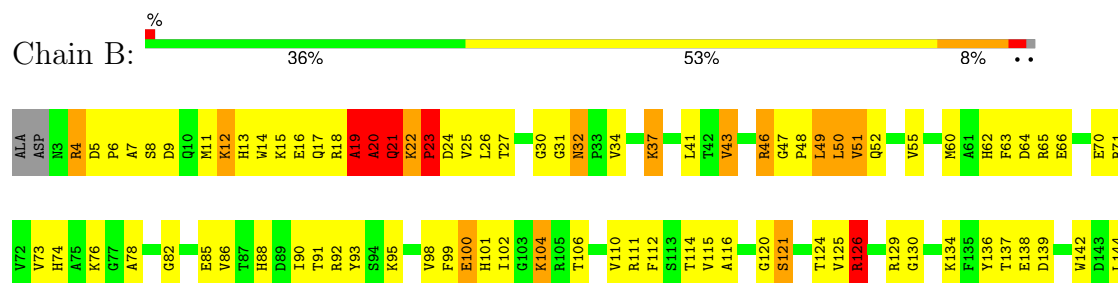
3 Residue-property plots [i](#)

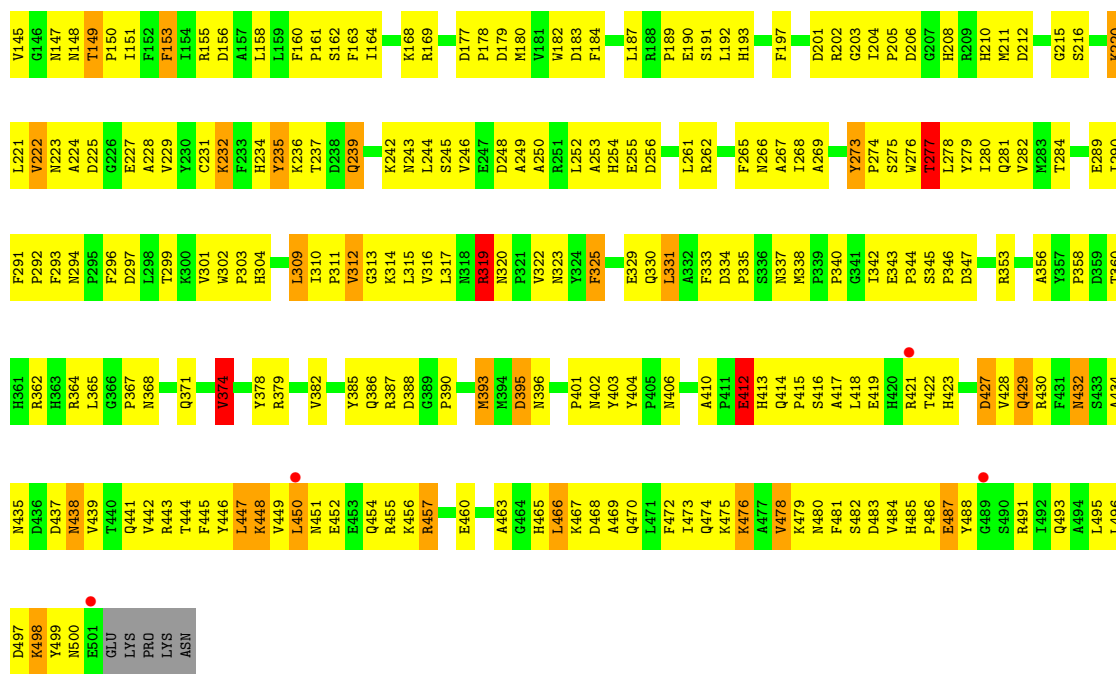
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Catalase

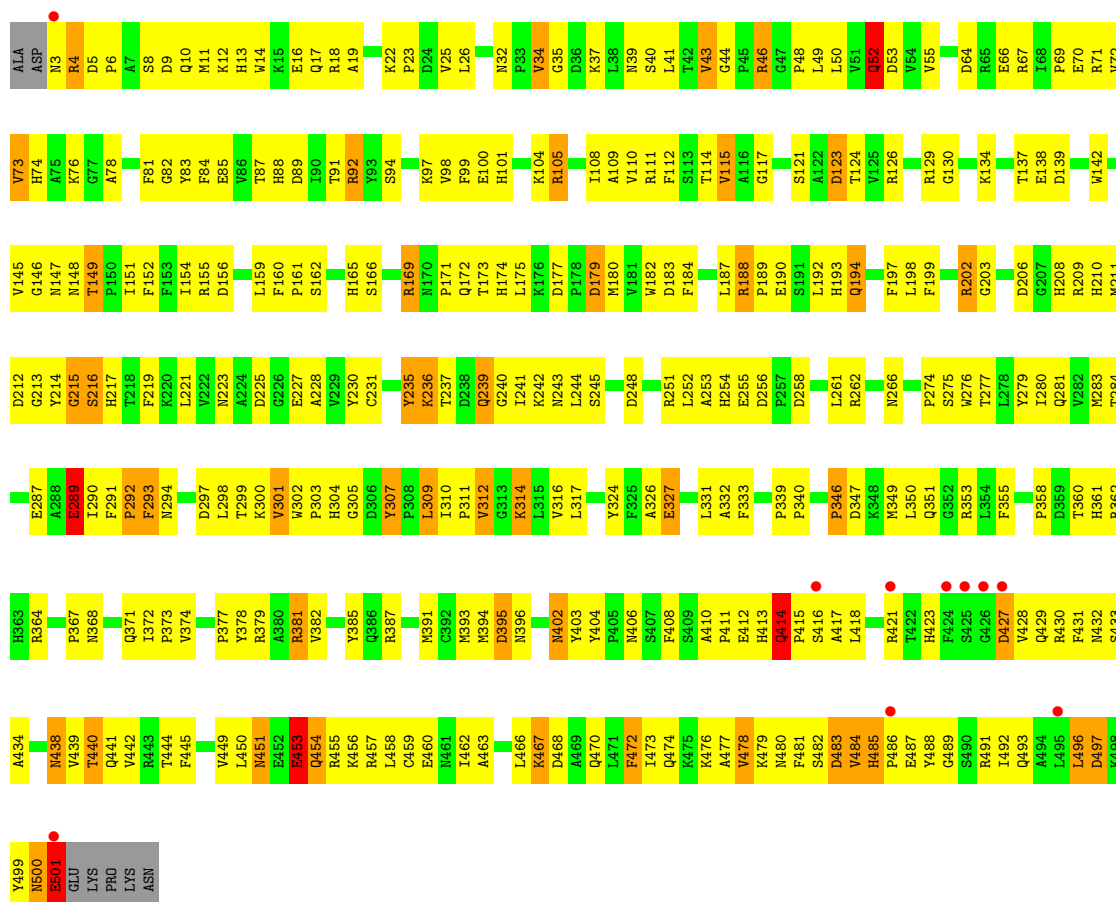


• Molecule 1: Catalase

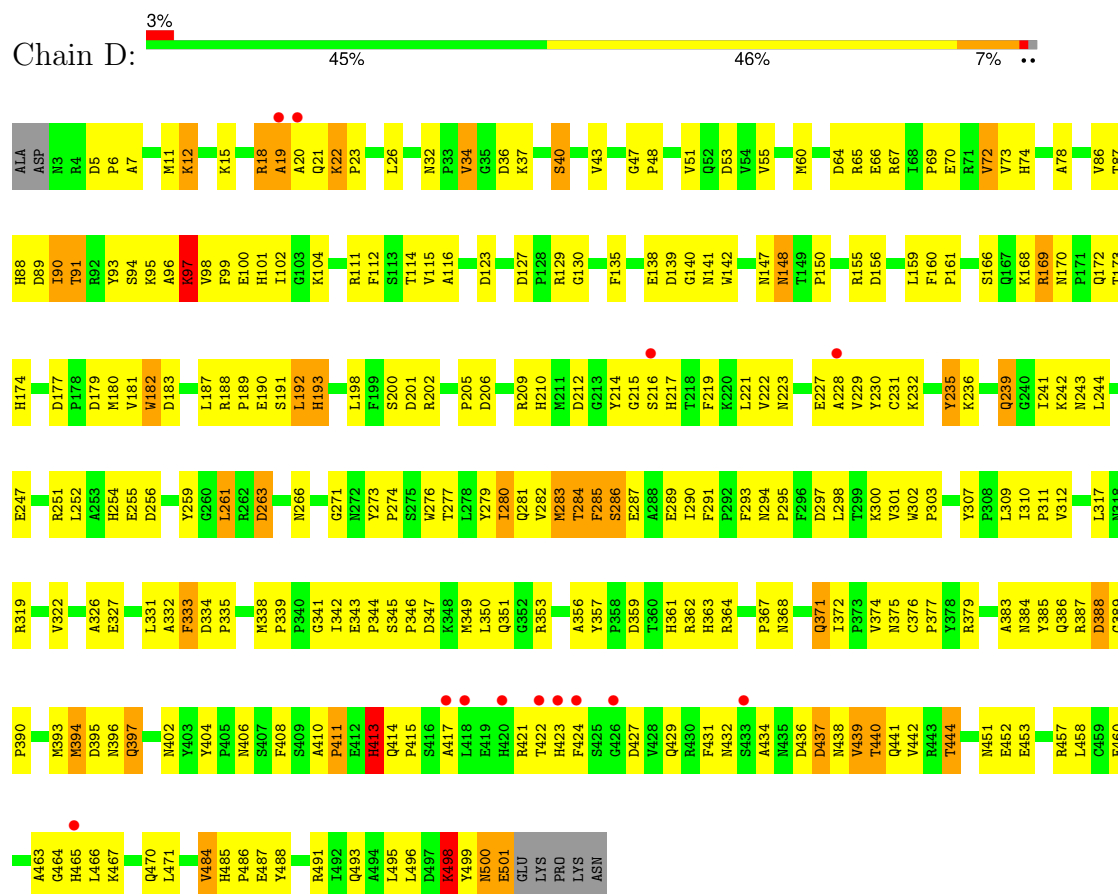




● Molecule 1: Catalase



● 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	86.27Å 140.93Å 230.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.09 – 2.80 39.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.9 (39.09-2.80) 87.8 (39.09-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.280 0.221 , 0.274	Depositor DCC
R_{free} test set	1859 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17049	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, AZI

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	0.82	8/4137 (0.2%)	1.99	74/5619 (1.3%)
1	B	0.92	6/4137 (0.1%)	1.79	57/5619 (1.0%)
1	C	0.89	10/4137 (0.2%)	1.71	63/5619 (1.1%)
1	D	0.75	1/4137 (0.0%)	1.25	17/5619 (0.3%)
All	All	0.85	25/16548 (0.2%)	1.70	211/22476 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3
1	B	1	7
1	C	2	3
All	All	4	13

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CD-NE	-30.70	1.03	1.46
1	D	413	HIS	CA-CB	-25.78	1.09	1.53
1	A	20	ALA	C-N	-21.63	1.04	1.33
1	C	202	ARG	NE-CZ	19.52	1.54	1.33
1	B	319	ARG	NE-CZ	18.30	1.53	1.33
1	C	292	PRO	C-N	15.99	1.55	1.33
1	C	414	GLN	CA-CB	-15.34	1.32	1.53
1	C	485	HIS	ND1-CE1	-13.55	1.19	1.32
1	C	292	PRO	CA-C	-12.56	1.36	1.52
1	B	374	VAL	CA-CB	12.49	1.69	1.54
1	A	280	ILE	CA-CB	11.95	1.67	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CB-CG	-11.46	1.18	1.52
1	C	413	HIS	CB-CG	11.08	1.65	1.50
1	A	421	ARG	CD-NE	-10.24	1.31	1.46
1	A	229	VAL	CA-CB	-10.16	1.40	1.55
1	C	485	HIS	CD2-NE2	-10.05	1.26	1.37
1	A	375	ASN	CA-CB	-7.36	1.41	1.53
1	A	304	HIS	CA-CB	-7.01	1.41	1.53
1	B	319	ARG	CA-CB	-6.96	1.39	1.53
1	C	485	HIS	CE1-NE2	6.02	1.38	1.32
1	C	453	GLU	CA-CB	5.90	1.63	1.53
1	A	49	LEU	CB-CG	-5.88	1.41	1.53
1	A	243	ASN	N-CA	5.54	1.52	1.45
1	B	450	LEU	CA-CB	-5.54	1.44	1.53
1	C	454	GLN	CB-CG	-5.05	1.37	1.52

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ASP	CA-CB-CG	42.17	154.78	112.60
1	D	413	HIS	CA-CB-CG	41.97	155.76	113.80
1	B	395	ASP	N-CA-CB	-38.66	54.12	110.56
1	A	3	ASN	CA-CB-CG	38.54	151.14	112.60
1	A	375	ASN	CA-CB-CG	37.08	149.68	112.60
1	A	402	ASN	CA-CB-CG	34.10	146.70	112.60
1	C	453	GLU	CB-CG-CD	32.78	168.33	112.60
1	C	292	PRO	N-CA-C	31.10	153.23	114.35
1	B	487	GLU	CB-CG-CD	28.79	161.53	112.60
1	B	126	ARG	CD-NE-CZ	28.55	164.37	124.40
1	D	453	GLU	CB-CG-CD	28.54	161.13	112.60
1	C	202	ARG	NE-CZ-NH2	-27.81	94.17	119.20
1	A	435	ASN	CA-CB-CG	27.34	139.94	112.60
1	A	418	LEU	N-CA-CB	26.03	149.52	109.69
1	C	292	PRO	CA-C-O	26.00	150.70	118.98
1	C	483	ASP	N-CA-CB	25.26	153.26	110.32
1	C	395	ASP	CA-CB-CG	-25.02	87.58	112.60
1	B	319	ARG	NE-CZ-NH1	-24.32	97.18	121.50
1	B	395	ASP	CA-CB-CG	24.08	136.68	112.60
1	A	456	LYS	CG-CD-CE	24.03	166.58	111.30
1	B	19	ALA	O-C-N	-23.43	91.43	122.59
1	B	412	GLU	CB-CG-CD	23.38	152.35	112.60
1	C	52	GLN	CB-CG-CD	23.17	151.99	112.60
1	B	374	VAL	CB-CA-C	-22.87	82.08	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	454	GLN	CB-CG-CD	22.15	150.26	112.60
1	A	395	ASP	N-CA-CB	21.96	143.77	110.61
1	B	20	ALA	CA-C-N	21.92	157.10	121.58
1	B	20	ALA	C-N-CA	21.92	157.10	121.58
1	A	421	ARG	CB-CG-CD	21.80	161.44	111.30
1	C	202	ARG	NE-CZ-NH1	20.87	142.37	121.50
1	C	292	PRO	CB-CA-C	-20.84	81.50	110.88
1	B	374	VAL	N-CA-CB	20.48	136.07	110.47
1	D	97	LYS	CG-CD-CE	20.24	157.84	111.30
1	A	421	ARG	CG-CD-NE	20.13	156.29	112.00
1	B	487	GLU	CA-CB-CG	19.86	153.81	114.10
1	C	501	GLU	CB-CA-C	19.82	147.76	110.10
1	A	20	ALA	O-C-N	19.68	145.99	122.17
1	A	229	VAL	CA-CB-CG2	19.40	143.38	110.40
1	A	54	VAL	CA-CB-CG2	-19.25	77.67	110.40
1	A	456	LYS	CB-CG-CD	18.91	154.81	111.30
1	A	118	GLU	N-CA-CB	-18.81	83.37	110.45
1	B	32	ASN	CB-CG-ND2	-18.60	88.50	116.40
1	C	453	GLU	N-CA-CB	18.48	141.73	110.49
1	B	476	LYS	CD-CE-NZ	18.44	170.92	111.90
1	C	414	GLN	CB-CA-C	18.31	134.14	110.34
1	C	414	GLN	CA-CB-CG	18.21	150.51	114.10
1	C	292	PRO	O-C-N	-18.02	92.81	122.36
1	A	97	LYS	CG-CD-CE	17.97	152.64	111.30
1	B	319	ARG	CA-CB-CG	17.78	149.66	114.10
1	A	500	ASN	CA-CB-CG	17.77	130.37	112.60
1	A	453	GLU	CB-CG-CD	17.51	142.37	112.60
1	C	454	GLN	N-CA-CB	-17.44	83.95	109.94
1	C	453	GLU	CA-CB-CG	17.37	148.84	114.10
1	B	23	PRO	CB-CA-C	-17.15	83.27	111.56
1	B	23	PRO	CA-C-O	-17.06	89.55	120.60
1	B	429	GLN	CA-CB-CG	16.40	146.90	114.10
1	C	501	GLU	CB-CG-CD	16.09	139.96	112.60
1	B	277	THR	CB-CA-C	16.09	137.01	110.79
1	B	478	VAL	N-CA-CB	-15.40	92.53	110.55
1	A	435	ASN	CB-CA-C	15.34	137.69	111.46
1	A	501	GLU	CB-CA-C	15.31	139.20	110.10
1	B	412	GLU	N-CA-CB	15.20	134.01	110.46
1	A	304	HIS	CA-CB-CG	14.99	128.79	113.80
1	A	375	ASN	CB-CA-C	14.86	139.72	109.55
1	A	500	ASN	N-CA-CB	-14.73	88.36	110.60
1	A	280	ILE	CB-CA-C	-14.61	91.50	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	PRO	O-C-N	-14.48	103.09	122.64
1	A	476	LYS	CG-CD-CE	14.31	144.22	111.30
1	D	453	GLU	CA-CB-CG	14.05	142.19	114.10
1	A	375	ASN	N-CA-CB	-13.81	88.89	110.44
1	A	490	SER	CA-CB-OG	13.73	138.56	111.10
1	B	478	VAL	CB-CA-C	13.48	129.22	111.97
1	A	381	ARG	CG-CD-NE	13.22	141.10	112.00
1	B	450	LEU	CA-CB-CG	13.05	161.97	116.30
1	A	421	ARG	CD-NE-CZ	13.00	142.61	124.40
1	A	284	THR	CA-CB-OG1	12.87	128.90	109.60
1	A	37	LYS	CG-CD-CE	12.71	140.52	111.30
1	A	418	LEU	CB-CA-C	-12.63	90.19	109.90
1	B	32	ASN	CB-CG-OD1	12.45	145.70	120.80
1	C	289	GLU	CB-CA-C	12.44	133.32	110.56
1	A	304	HIS	N-CA-CB	-12.40	89.54	110.49
1	B	19	ALA	CA-C-N	-12.33	97.99	121.54
1	B	19	ALA	C-N-CA	-12.33	97.99	121.54
1	C	289	GLU	CG-CD-OE2	-11.95	90.92	118.40
1	A	421	ARG	CA-CB-CG	11.62	137.33	114.10
1	B	412	GLU	CA-CB-CG	11.54	137.19	114.10
1	C	289	GLU	CA-CB-CG	11.44	136.98	114.10
1	A	49	LEU	CB-CG-CD2	11.40	144.91	110.70
1	B	478	VAL	CA-CB-CG1	-11.33	91.14	110.40
1	B	22	LYS	O-C-N	11.32	134.34	121.32
1	A	476	LYS	CD-CE-NZ	11.04	147.23	111.90
1	C	454	GLN	CB-CA-C	-10.87	93.42	110.81
1	D	394	MET	CB-CG-SD	10.87	145.29	112.70
1	A	456	LYS	CA-CB-CG	10.85	135.80	114.10
1	B	32	ASN	CA-CB-CG	-10.55	102.05	112.60
1	A	202	ARG	CD-NE-CZ	10.18	138.65	124.40
1	C	478	VAL	CB-CA-C	10.13	125.31	112.04
1	C	483	ASP	CB-CA-C	-10.12	88.97	110.32
1	B	22	LYS	CA-C-N	9.89	132.21	119.84
1	B	22	LYS	C-N-CA	9.89	132.21	119.84
1	D	356	ALA	N-CA-C	9.81	121.56	111.07
1	A	284	THR	CB-CA-C	-9.77	91.48	109.46
1	C	501	GLU	N-CA-CB	-9.77	93.89	110.50
1	A	304	HIS	CB-CA-C	9.73	129.78	110.42
1	B	319	ARG	CB-CG-CD	9.36	132.82	111.30
1	B	416	SER	N-CA-CB	-9.21	96.35	110.44
1	A	435	ASN	N-CA-CB	-9.09	97.98	111.43
1	B	478	VAL	CA-CB-CG2	9.00	125.70	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	413	HIS	CB-CG-ND1	-8.94	109.28	122.70
1	C	413	HIS	CB-CG-CD2	8.92	142.80	131.20
1	B	21	GLN	N-CA-C	8.88	122.59	107.93
1	A	356	ALA	N-CA-C	8.81	121.98	111.33
1	A	501	GLU	N-CA-CB	-8.67	95.76	110.50
1	A	284	THR	CA-CB-CG2	-8.61	95.86	110.50
1	A	243	ASN	CB-CA-C	-8.48	90.72	109.56
1	C	292	PRO	CA-C-N	8.47	138.19	123.03
1	C	292	PRO	C-N-CA	8.47	138.19	123.03
1	C	414	GLN	N-CA-CB	-8.43	96.10	110.43
1	B	319	ARG	NE-CZ-NH2	8.37	126.73	119.20
1	A	280	ILE	CA-CB-CG1	8.33	124.56	110.40
1	A	176	LYS	CG-CD-CE	8.32	130.44	111.30
1	C	55	VAL	N-CA-C	-8.26	102.49	110.42
1	A	280	ILE	CA-CB-CG2	-8.16	96.63	110.50
1	C	231	CYS	CA-CB-SG	-8.11	95.76	114.40
1	A	453	GLU	CA-CB-CG	7.99	130.08	114.10
1	D	484	VAL	N-CA-C	-7.80	103.31	111.58
1	A	342	ILE	N-CA-CB	7.72	123.41	111.99
1	A	342	ILE	CB-CA-C	-7.67	99.69	110.12
1	A	395	ASP	CB-CA-C	-7.61	97.32	110.17
1	D	89	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	176	LYS	CD-CE-NZ	-7.41	88.18	111.90
1	C	372	ILE	N-CA-C	-7.19	102.45	108.63
1	B	319	ARG	CB-CA-C	-7.16	94.84	109.38
1	C	115	VAL	N-CA-C	7.14	118.19	111.48
1	C	123	ASP	N-CA-C	7.12	119.12	111.36
1	B	55	VAL	N-CA-C	-7.10	103.61	110.42
1	B	215	GLY	N-CA-C	-7.07	106.06	115.32
1	C	236	LYS	CG-CD-CE	7.02	127.45	111.30
1	B	450	LEU	N-CA-CB	-7.01	98.99	110.41
1	C	289	GLU	CB-CG-CD	7.00	124.51	112.60
1	D	55	VAL	N-CA-C	-6.99	103.96	110.53
1	A	372	ILE	N-CA-C	-6.85	102.65	109.02
1	D	169	ARG	N-CA-C	6.83	120.13	110.50
1	B	450	LEU	CB-CA-C	6.75	121.06	109.51
1	D	452	GLU	N-CA-C	6.67	119.41	111.33
1	A	333	PHE	CA-CB-CG	6.64	120.44	113.80
1	B	374	VAL	CA-CB-CG1	-6.40	99.52	110.40
1	A	116	ALA	N-CA-C	6.36	119.52	111.69
1	A	215	GLY	N-CA-C	-6.34	106.80	114.66
1	A	113	SER	N-CA-C	6.26	116.71	107.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	ALA	N-CA-C	6.18	118.01	111.28
1	D	90	ILE	N-CA-C	-6.04	106.84	113.43
1	A	51	VAL	N-CA-C	-6.03	105.10	112.76
1	B	374	VAL	CA-CB-CG2	-6.02	100.16	110.40
1	A	114	THR	N-CA-C	-5.97	100.52	109.96
1	C	202	ARG	CD-NE-CZ	5.97	132.76	124.40
1	C	215	GLY	N-CA-C	-5.97	107.77	114.40
1	C	485	HIS	CA-C-N	5.95	127.27	119.84
1	C	485	HIS	C-N-CA	5.95	127.27	119.84
1	B	319	ARG	CG-CD-NE	-5.93	98.95	112.00
1	C	44	GLY	CA-C-N	5.93	126.08	119.32
1	C	44	GLY	C-N-CA	5.93	126.08	119.32
1	D	67	ARG	N-CA-C	5.90	119.26	109.46
1	A	54	VAL	CB-CA-C	5.88	121.75	112.16
1	B	92	ARG	N-CA-C	-5.84	106.20	113.15
1	B	169	ARG	N-CA-C	5.83	118.72	110.50
1	C	324	TYR	N-CA-C	5.82	117.30	111.07
1	C	394	MET	CB-CA-C	-5.82	108.21	115.89
1	C	188	ARG	CA-C-N	5.79	125.89	119.87
1	C	188	ARG	C-N-CA	5.79	125.89	119.87
1	B	116	ALA	N-CA-C	5.78	117.38	111.14
1	A	67	ARG	N-CA-C	5.78	119.66	109.96
1	B	22	LYS	C-N-CD	-5.77	101.36	125.00
1	A	500	ASN	CB-CA-C	5.75	121.26	112.00
1	A	291	PHE	CA-C-N	5.75	125.42	119.56
1	A	291	PHE	C-N-CA	5.75	125.42	119.56
1	C	124	THR	N-CA-C	5.72	118.51	108.56
1	C	484	VAL	N-CA-C	-5.68	105.31	110.82
1	B	319	ARG	N-CA-CB	5.65	121.24	111.13
1	C	281	GLN	N-CA-C	-5.57	100.62	109.76
1	C	307	TYR	CA-C-N	5.54	125.52	120.03
1	C	307	TYR	C-N-CA	5.54	125.52	120.03
1	A	289	GLU	CB-CG-CD	-5.51	103.22	112.60
1	B	432	ASN	N-CA-C	5.48	117.39	108.63
1	A	90	ILE	N-CA-C	-5.47	106.08	111.88
1	A	229	VAL	CB-CA-C	-5.45	100.68	110.48
1	A	484	VAL	N-CA-C	-5.43	105.82	111.58
1	C	478	VAL	N-CA-CB	-5.38	103.75	110.47
1	C	327	GLU	N-CA-C	5.37	119.93	112.90
1	C	117	GLY	N-CA-C	5.33	117.60	111.36
1	A	238	ASP	N-CA-C	-5.33	106.83	113.38
1	D	182	TRP	N-CA-C	5.32	118.23	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	378	TYR	N-CA-C	5.32	119.03	112.54
1	C	312	VAL	N-CA-C	5.31	115.81	111.62
1	A	197	PHE	N-CA-C	-5.30	105.40	111.07
1	B	273	TYR	N-CA-C	5.27	117.07	109.48
1	B	23	PRO	N-CA-C	5.17	123.13	112.47
1	A	121	SER	N-CA-C	5.17	116.95	110.24
1	D	388	ASP	N-CA-C	5.15	115.63	108.00
1	C	483	ASP	N-CA-C	-5.13	106.13	112.38
1	C	314	LYS	N-CA-C	5.12	117.83	109.59
1	C	114	THR	CA-C-N	-5.11	117.96	122.97
1	C	114	THR	C-N-CA	-5.11	117.96	122.97
1	D	498	LYS	N-CA-C	-5.11	105.36	111.03
1	D	434	ALA	N-CA-C	5.11	117.59	111.71
1	B	313	GLY	N-CA-C	5.11	118.59	111.19
1	C	67	ARG	N-CA-C	5.10	118.53	109.96
1	B	51	VAL	N-CA-C	-5.10	104.67	111.05
1	A	123	ASP	N-CA-C	5.04	116.85	111.36
1	C	101	HIS	N-CA-C	5.03	116.32	109.18
1	A	181	VAL	N-CA-C	5.01	115.44	110.23

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	395	ASP	CA
1	B	23	PRO	CA
1	C	453	GLU	CA
1	C	501	GLU	CA

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ALA	Mainchain
1	A	20	ALA	Mainchain
1	A	421	ARG	Sidechain
1	B	126	ARG	Sidechain
1	B	19	ALA	Peptide,Mainchain
1	B	22	LYS	Peptide
1	B	23	PRO	Peptide,Mainchain
1	B	319	ARG	Sidechain
1	C	289	GLU	Sidechain
1	C	292	PRO	Peptide,Mainchain

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	3839	278	0
1	B	4017	0	3838	365	0
1	C	4017	0	3839	356	0
1	D	4017	0	3839	305	0
2	A	43	0	30	17	0
2	B	43	0	30	19	0
2	C	43	0	30	9	0
2	D	43	0	30	2	0
3	D	3	0	0	1	0
4	A	250	0	0	17	0
4	B	182	0	0	17	0
4	C	193	0	0	13	0
4	D	181	0	0	20	0
All	All	17049	0	15475	1169	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 37.

All (1169) 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:B:19:ALA:CB	1:B:20:ALA:HB3	1.14	1.55
1:B:19:ALA:HB1	1:B:20:ALA:CB	1.34	1.52
1:B:147:ASN:ND2	2:B:2001:HEM:CAC	1.83	1.42
1:D:111:ARG:NH1	4:D:3133:HOH:O	1.63	1.25
1:B:147:ASN:HD22	2:B:2001:HEM:CAC	1.50	1.17
1:B:19:ALA:CB	1:B:20:ALA:CB	2.05	1.16
1:A:380:ALA:O	4:A:2149:HOH:O	1.64	1.16
1:D:223:ASN:HD21	1:D:227:GLU:HB3	1.12	1.13
1:D:290:ILE:HD11	4:D:3107:HOH:O	1.49	1.13
2:B:2001:HEM:HBD2	4:B:2183:HOH:O	1.50	1.08
1:B:147:ASN:ND2	2:B:2001:HEM:HAC	1.67	1.07
1:B:13:HIS:CE1	4:B:2057:HOH:O	2.06	1.05
1:A:448:LYS:NZ	4:A:2167:HOH:O	1.91	1.04
1:B:15:LYS:HD2	1:D:408:PHE:HA	1.37	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ARG:NH2	4:D:3083:HOH:O	1.83	1.01
1:A:71:ARG:HG3	4:A:2051:HOH:O	1.61	1.00
1:D:102:ILE:HD12	1:D:102:ILE:H	1.26	1.00
1:C:402:ASN:H	1:C:402:ASN:HD22	1.00	1.00
1:B:4:ARG:HD2	1:B:8:SER:HB3	1.43	0.99
1:A:329:GLU:OE1	4:A:2002:HOH:O	1.79	0.99
1:C:18:ARG:HH12	1:C:23:PRO:HA	1.23	0.98
1:D:406:ASN:HD21	1:D:410:ALA:HB3	1.29	0.98
1:B:19:ALA:HB3	1:B:20:ALA:HB3	1.46	0.97
1:C:261:LEU:CD2	4:C:2021:HOH:O	2.11	0.97
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.29	0.96
1:A:15:LYS:HD2	1:C:408:PHE:HA	1.46	0.95
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.31	0.94
1:C:379:ARG:HD3	4:C:2120:HOH:O	1.67	0.94
1:B:393:MET:CE	1:D:372:ILE:HA	1.98	0.92
1:A:379:ARG:HD3	4:A:2084:HOH:O	1.70	0.91
1:C:78:ALA:HB2	1:C:261:LEU:HD22	1.52	0.91
1:A:353:ARG:HD2	2:A:2000:HEM:HBB2	1.53	0.90
1:A:223:ASN:HD21	1:A:227:GLU:HB2	1.36	0.90
1:A:360:THR:HG23	1:D:64:ASP:HB3	1.51	0.89
1:C:72:VAL:HG13	1:C:73:VAL:HG22	1.54	0.89
1:A:100:GLU:O	1:A:101:HIS:HB3	1.69	0.89
1:B:466:LEU:HD22	1:B:474:GLN:HG2	1.54	0.88
1:B:223:ASN:HD21	1:B:227:GLU:HB2	1.41	0.86
1:A:349:MET:HB3	2:A:2000:HEM:HBB1	1.58	0.85
1:B:457:ARG:HH11	1:B:457:ARG:HB2	1.41	0.85
1:C:223:ASN:HD21	1:C:227:GLU:HB2	1.41	0.85
1:C:453:GLU:HG2	4:C:2191:HOH:O	1.75	0.85
1:B:457:ARG:HB2	1:B:457:ARG:NH1	1.92	0.85
1:C:217:HIS:HE1	1:C:349:MET:HB3	1.41	0.85
1:D:223:ASN:ND2	1:D:227:GLU:HB3	1.93	0.84
1:C:156:ASP:HB3	1:C:159:LEU:HD23	1.59	0.84
1:A:229:VAL:HG11	1:A:282:VAL:HG13	1.57	0.83
1:A:145:VAL:O	2:A:2000:HEM:CBC	2.27	0.82
1:A:223:ASN:ND2	1:A:227:GLU:HB2	1.94	0.82
1:D:60:MET:HE3	1:D:60:MET:HA	1.61	0.82
1:B:13:HIS:HE1	4:B:2057:HOH:O	1.51	0.82
1:D:123:ASP:OD1	4:D:3036:HOH:O	1.97	0.82
1:B:112:PHE:HA	1:B:130:GLY:O	1.79	0.82
1:C:402:ASN:HD22	1:C:402:ASN:N	1.77	0.82
1:A:94:SER:HB2	1:A:221:LEU:HD22	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2001:HEM:CBD	4:B:2183:HOH:O	2.18	0.82
1:A:43:VAL:CG1	1:A:48:PRO:HD2	2.09	0.81
1:C:97:LYS:HD2	1:C:138:GLU:HB2	1.60	0.81
1:D:406:ASN:ND2	1:D:410:ALA:HB3	1.95	0.81
1:B:190:GLU:HA	1:B:438:ASN:HB3	1.60	0.81
1:C:190:GLU:HA	1:C:438:ASN:HB3	1.60	0.81
1:A:413:HIS:ND1	4:A:2158:HOH:O	2.11	0.81
1:C:432:ASN:ND2	1:C:434:ALA:H	1.78	0.81
1:A:35:GLY:HA2	1:C:414:GLN:O	1.80	0.81
1:C:492:ILE:HG22	1:C:496:LEU:HD23	1.62	0.80
1:A:49:LEU:HD13	1:B:51:VAL:HG11	1.60	0.80
1:D:465:HIS:HD2	4:D:3080:HOH:O	1.63	0.80
1:C:189:PRO:HB3	1:C:480:ASN:ND2	1.98	0.79
1:D:97:LYS:HA	1:D:100:GLU:HG3	1.63	0.79
1:B:147:ASN:ND2	2:B:2001:HEM:C3C	2.50	0.78
1:D:235:TYR:HA	1:D:277:THR:O	1.84	0.78
1:B:360:THR:OG1	1:C:64:ASP:HB3	1.84	0.78
1:B:147:ASN:HD22	2:B:2001:HEM:CBC	1.96	0.78
1:B:498:LYS:HE3	4:B:2180:HOH:O	1.84	0.78
1:B:294:ASN:HA	1:C:46:ARG:HH12	1.47	0.78
1:B:62:HIS:HE1	1:D:368:ASN:HD21	1.32	0.77
1:A:151:ILE:HG13	1:A:194:GLN:HG2	1.67	0.77
1:D:94:SER:HB2	1:D:221:LEU:HB3	1.67	0.77
1:A:186:SER:HB2	1:A:476:LYS:HG2	1.67	0.76
1:C:209:ARG:O	1:C:239:GLN:HG2	1.85	0.76
1:C:251:ARG:HG3	1:C:252:LEU:N	2.00	0.76
1:D:432:ASN:OD1	4:D:3028:HOH:O	2.02	0.76
1:A:360:THR:HG23	1:D:64:ASP:CB	2.15	0.76
1:D:458:LEU:HD21	1:D:488:TYR:OH	1.86	0.76
1:D:40:SER:OG	4:D:3015:HOH:O	2.05	0.75
1:B:208:HIS:O	1:B:211:MET:HG2	1.86	0.75
1:B:454:GLN:HA	1:B:457:ARG:NH1	2.02	0.75
1:A:460:GLU:HG3	1:A:495:LEU:HD21	1.69	0.75
1:C:217:HIS:CE1	1:C:349:MET:HB3	2.21	0.75
1:C:432:ASN:HD22	1:C:433:SER:N	1.84	0.75
1:B:19:ALA:CA	1:B:20:ALA:CB	2.47	0.74
1:B:338:MET:HE2	1:B:342:ILE:HG22	1.69	0.74
1:C:18:ARG:NH1	1:C:23:PRO:HA	2.01	0.74
1:C:209:ARG:O	1:C:239:GLN:CG	2.35	0.74
1:C:421:ARG:HA	4:C:2112:HOH:O	1.87	0.74
1:D:22:LYS:HE3	1:D:22:LYS:HA	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:SER:HB2	1:C:221:LEU:HD22	1.70	0.74
1:C:402:ASN:H	1:C:402:ASN:ND2	1.82	0.73
1:B:229:VAL:HG23	1:B:284:THR:HA	1.70	0.73
1:C:9:ASP:OD1	1:C:12:LYS:HD3	1.87	0.73
1:D:43:VAL:CG1	1:D:48:PRO:HD2	2.19	0.73
1:B:71:ARG:HG2	2:B:2001:HEM:O1A	1.89	0.72
1:D:439:VAL:HG23	1:D:440:THR:N	2.04	0.72
1:B:6:PRO:HG2	1:B:266:ASN:OD1	1.90	0.72
1:C:152:PHE:O	1:C:299:THR:HG22	1.90	0.72
1:C:298:LEU:HD22	1:C:349:MET:HG2	1.70	0.72
1:D:376:CYS:SG	4:D:3175:HOH:O	2.47	0.72
1:A:349:MET:HE3	2:A:2000:HEM:HBB1	1.72	0.72
1:D:170:ASN:ND2	1:D:172:GLN:H	1.87	0.72
1:B:129:ARG:CB	1:B:211:MET:HE1	2.20	0.72
1:B:205:PRO:HG3	1:B:211:MET:HE3	1.70	0.72
1:C:71:ARG:HD2	1:C:111:ARG:NH2	2.05	0.72
1:B:294:ASN:HA	1:C:46:ARG:NH1	2.05	0.72
1:D:499:TYR:C	1:D:501:GLU:H	1.95	0.71
1:A:146:GLY:HA2	2:A:2000:HEM:HBC1	1.72	0.71
1:B:367:PRO:HG3	1:D:65:ARG:HD3	1.72	0.71
1:B:406:ASN:ND2	1:B:410:ALA:HB3	2.04	0.71
1:A:451:ASN:H	1:A:454:GLN:HE21	1.35	0.71
1:C:216:SER:HB2	2:C:2002:HEM:CBC	2.20	0.71
1:A:460:GLU:HA	1:A:495:LEU:HD21	1.72	0.71
1:B:4:ARG:HD2	1:B:8:SER:CB	2.19	0.71
1:B:419:GLU:CD	1:B:419:GLU:H	1.99	0.71
1:B:248:ASP:O	1:B:252:LEU:HD13	1.90	0.71
1:C:151:ILE:HG13	1:C:194:GLN:HG2	1.72	0.71
1:B:139:ASP:O	1:D:32:ASN:HA	1.91	0.70
1:A:93:TYR:CE1	1:A:282:VAL:HG11	2.27	0.70
1:A:413:HIS:CE1	4:A:2158:HOH:O	2.44	0.70
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.56	0.70
1:C:402:ASN:HD21	1:D:180:MET:HE3	1.55	0.70
1:A:332:ALA:HB1	1:A:361:HIS:CD2	2.26	0.70
1:B:34:VAL:HG11	1:B:37:LYS:HB3	1.72	0.70
1:B:147:ASN:HD21	2:B:2001:HEM:CAC	1.95	0.70
1:B:456:LYS:O	1:B:460:GLU:HG3	1.91	0.70
1:A:422:THR:HG22	1:A:423:HIS:N	2.06	0.70
1:C:280:ILE:HG23	1:C:312:VAL:HG21	1.73	0.70
1:C:481:PHE:O	1:C:484:VAL:HB	1.92	0.70
1:C:92:ARG:H	1:C:92:ARG:HD3	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:HIS:CD2	1:A:487:GLU:HB3	2.26	0.69
1:C:162:SER:HB3	1:D:404:TYR:H	1.57	0.69
1:A:18:ARG:NH2	1:A:21:GLN:HE21	1.90	0.69
1:C:479:LYS:CE	4:C:2192:HOH:O	2.40	0.69
1:A:329:GLU:OE1	1:A:329:GLU:HA	1.92	0.69
1:C:410:ALA:HB1	1:C:411:PRO:HD2	1.74	0.69
1:C:485:HIS:CE1	1:C:487:GLU:H	2.10	0.69
1:D:193:HIS:HA	1:D:442:VAL:HG22	1.73	0.69
1:A:487:GLU:O	1:A:491:ARG:HG3	1.93	0.69
1:C:304:HIS:HB3	4:C:2101:HOH:O	1.92	0.69
1:B:456:LYS:HB2	1:B:491:ARG:NH2	2.07	0.69
1:D:78:ALA:HB2	1:D:261:LEU:HG	1.73	0.69
1:D:338:MET:HE2	1:D:342:ILE:HG22	1.75	0.69
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.58	0.69
1:A:421:ARG:HG3	1:B:429:GLN:HG2	1.75	0.69
1:A:148:ASN:C	1:A:148:ASN:HD22	2.01	0.68
1:D:280:ILE:HD11	1:D:310:ILE:HB	1.75	0.68
1:A:429:GLN:NE2	1:B:421:ARG:HD2	2.09	0.68
1:A:460:GLU:HA	1:A:495:LEU:CD2	2.24	0.68
1:B:323:ASN:HD21	1:D:396:ASN:HD22	1.40	0.68
1:C:193:HIS:HA	1:C:442:VAL:HG22	1.76	0.68
1:D:18:ARG:O	1:D:19:ALA:HB3	1.92	0.68
1:D:112:PHE:HA	1:D:130:GLY:O	1.92	0.68
1:D:138:GLU:HA	1:D:379:ARG:O	1.93	0.68
1:C:179:ASP:O	1:C:183:ASP:HB2	1.94	0.68
1:A:349:MET:HE3	2:A:2000:HEM:CBB	2.24	0.68
1:A:360:THR:HG22	1:D:64:ASP:O	1.93	0.68
1:D:72:VAL:HG12	4:D:3056:HOH:O	1.93	0.67
1:C:112:PHE:HA	1:C:130:GLY:O	1.93	0.67
1:C:298:LEU:CD2	1:C:349:MET:HG2	2.24	0.67
1:C:237:THR:HA	1:C:276:TRP:CD1	2.29	0.67
1:A:193:HIS:HA	1:A:442:VAL:HG22	1.76	0.67
1:B:385:TYR:CE2	1:B:404:TYR:HB2	2.30	0.67
1:D:155:ARG:NH2	1:D:438:ASN:OD1	2.27	0.67
1:A:421:ARG:NH2	1:B:430:ARG:H	1.92	0.67
1:B:268:ILE:HB	1:B:320:ASN:ND2	2.10	0.67
1:C:142:TRP:HB2	1:C:339:PRO:CD	2.25	0.67
1:B:266:ASN:O	1:B:267:ALA:C	2.38	0.67
1:B:301:VAL:HG22	1:B:441:GLN:OE1	1.95	0.67
1:B:358:PRO:O	1:B:362:ARG:HG3	1.93	0.67
1:C:499:TYR:C	1:C:501:GLU:H	2.03	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:O	1:B:47:GLY:HA3	1.94	0.67
1:C:451:ASN:H	1:C:454:GLN:HE21	1.42	0.67
1:D:101:HIS:HE1	4:D:3076:HOH:O	1.78	0.67
1:A:90:ILE:HD13	1:A:312:VAL:HG22	1.76	0.67
1:B:432:ASN:HA	1:C:39:ASN:OD1	1.94	0.67
1:D:43:VAL:HG13	1:D:48:PRO:HD2	1.77	0.67
1:B:180:MET:HG3	1:C:11:MET:HE2	1.75	0.66
1:D:90:ILE:HD13	1:D:312:VAL:HG13	1.77	0.66
1:A:353:ARG:HG2	2:A:2000:HEM:C2B	2.30	0.66
1:B:323:ASN:ND2	1:D:396:ASN:HB3	2.10	0.66
1:C:358:PRO:O	1:C:362:ARG:HG3	1.95	0.66
1:D:232:LYS:O	1:D:280:ILE:HA	1.95	0.66
1:B:202:ARG:NH1	4:B:2050:HOH:O	2.28	0.66
1:B:19:ALA:HB3	1:B:21:GLN:HE21	1.61	0.66
1:D:95:LYS:HG2	1:D:222:VAL:O	1.96	0.66
1:D:415:PRO:HB3	4:D:3177:HOH:O	1.95	0.66
1:C:110:VAL:HG21	1:C:317:LEU:HD21	1.77	0.65
1:C:169:ARG:HH11	1:C:169:ARG:HG2	1.61	0.65
1:C:310:ILE:N	1:C:310:ILE:HD12	2.11	0.65
1:D:170:ASN:HD22	1:D:173:THR:H	1.44	0.65
1:C:50:LEU:HD22	1:D:48:PRO:HB2	1.78	0.65
1:B:216:SER:OG	2:B:2001:HEM:HBC1	1.96	0.65
1:B:268:ILE:HB	1:B:320:ASN:HD21	1.61	0.65
1:A:155:ARG:NH1	1:A:436:ASP:HB2	2.12	0.65
1:B:125:VAL:HG22	1:B:126:ARG:N	2.11	0.65
1:C:126:ARG:HD2	1:C:198:LEU:O	1.96	0.65
1:A:414:GLN:O	1:C:35:GLY:HA2	1.97	0.65
1:A:172:GLN:NE2	1:D:322:VAL:HA	2.12	0.65
1:B:323:ASN:HD21	1:D:396:ASN:ND2	1.94	0.65
1:B:129:ARG:HB2	1:B:211:MET:HE1	1.78	0.64
1:C:355:PHE:O	1:C:358:PRO:HD2	1.96	0.64
1:D:286:SER:O	1:D:289:GLU:HB3	1.96	0.64
1:A:74:HIS:HA	1:A:114:THR:O	1.97	0.64
1:D:439:VAL:HG23	1:D:440:THR:H	1.62	0.64
1:B:37:LYS:O	1:B:37:LYS:HG3	1.96	0.64
1:C:154:ILE:HD12	1:C:159:LEU:HB2	1.79	0.64
1:A:430:ARG:NH1	1:D:53:ASP:OD2	2.24	0.64
1:D:115:VAL:HB	1:D:127:ASP:OD2	1.98	0.64
1:A:160:PHE:CE2	1:A:164:ILE:HG13	2.32	0.64
1:A:67:ARG:HH21	1:D:168:LYS:HE3	1.61	0.64
1:B:382:VAL:HG13	1:B:382:VAL:O	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LYS:HE2	4:C:2192:HOH:O	1.98	0.64
1:B:19:ALA:CA	1:B:20:ALA:HB2	2.26	0.64
1:A:30:GLY:O	1:C:377:PRO:HB3	1.98	0.64
1:A:193:HIS:CA	1:A:442:VAL:HG22	2.28	0.64
1:C:472:PHE:C	1:C:472:PHE:CD1	2.76	0.64
1:A:357:TYR:OH	2:A:2000:HEM:NB	2.30	0.63
1:C:14:TRP:O	1:C:18:ARG:HB2	1.99	0.63
1:B:422:THR:HG22	1:B:423:HIS:N	2.13	0.63
1:B:5:ASP:HB2	1:B:6:PRO:HD2	1.80	0.63
1:B:485:HIS:HD2	1:B:486:PRO:HD2	1.63	0.63
1:A:422:THR:HG22	1:A:423:HIS:H	1.62	0.63
1:B:41:LEU:HD11	1:C:428:VAL:HG12	1.81	0.63
1:B:91:THR:C	1:B:93:TYR:H	2.07	0.63
1:B:412:GLU:OE2	1:D:23:PRO:HG2	1.99	0.63
1:B:498:LYS:HD3	1:B:499:TYR:N	2.13	0.63
1:A:71:ARG:HD2	1:A:111:ARG:NH2	2.12	0.63
1:B:148:ASN:HB3	1:B:211:MET:HE2	1.78	0.63
1:B:454:GLN:HA	1:B:457:ARG:HH12	1.63	0.63
1:C:105:ARG:HG2	1:C:105:ARG:HH11	1.63	0.63
1:A:187:LEU:HD23	1:A:476:LYS:HE2	1.80	0.63
1:A:451:ASN:H	1:A:454:GLN:NE2	1.97	0.63
1:B:9:ASP:CB	4:B:2057:HOH:O	2.47	0.63
1:D:413:HIS:CD2	1:D:415:PRO:HD3	2.33	0.63
1:A:429:GLN:HE22	1:B:421:ARG:HD2	1.63	0.62
1:B:252:LEU:HD12	1:B:252:LEU:N	2.12	0.62
1:A:148:ASN:C	1:A:148:ASN:ND2	2.57	0.62
1:C:4:ARG:H	1:C:4:ARG:HD2	1.64	0.62
1:A:364:ARG:NE	2:A:2000:HEM:O1A	2.31	0.62
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.81	0.62
1:D:6:PRO:HD2	1:D:266:ASN:OD1	1.98	0.62
1:C:492:ILE:HG22	1:C:496:LEU:CD2	2.28	0.62
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.81	0.62
1:D:285:PHE:HD1	1:D:285:PHE:H	1.47	0.62
1:B:9:ASP:CG	4:B:2057:HOH:O	2.42	0.62
1:B:221:LEU:O	1:B:228:ALA:HA	1.99	0.62
1:D:102:ILE:H	1:D:102:ILE:CD1	2.03	0.62
1:B:26:LEU:HD21	1:B:37:LYS:CD	2.29	0.62
1:B:64:ASP:HB3	1:C:360:THR:HB	1.82	0.61
1:A:332:ALA:N	1:A:375:ASN:OD1	2.32	0.61
1:B:95:LYS:HB3	1:B:224:ALA:N	2.15	0.61
1:B:447:LEU:HD22	1:B:485:HIS:ND1	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:LYS:HE2	1:B:483:ASP:OD2	2.00	0.61
1:A:442:VAL:HG12	1:A:484:VAL:HG11	1.82	0.61
1:C:223:ASN:ND2	1:C:227:GLU:HB2	2.14	0.61
1:C:304:HIS:CD2	1:C:309:LEU:HD13	2.36	0.61
1:C:414:GLN:HE22	1:C:417:ALA:N	1.99	0.61
1:D:436:ASP:O	1:D:437:ASP:HB3	2.00	0.61
1:D:232:LYS:HB2	1:D:281:GLN:HB2	1.82	0.61
1:C:72:VAL:CG1	1:C:73:VAL:HG22	2.30	0.61
1:C:450:LEU:HG	1:C:454:GLN:HB3	1.83	0.61
1:C:456:LYS:O	1:C:460:GLU:HG3	2.01	0.60
1:C:497:ASP:HA	1:C:500:ASN:HD22	1.66	0.60
1:B:310:ILE:HD12	1:B:310:ILE:N	2.16	0.60
1:C:414:GLN:NE2	1:C:417:ALA:H	1.99	0.60
1:C:470:GLN:NE2	1:C:472:PHE:HE2	2.00	0.60
1:A:46:ARG:NH1	1:D:295:PRO:HD3	2.16	0.60
1:A:421:ARG:CG	1:B:429:GLN:HG2	2.30	0.60
1:B:90:ILE:O	1:B:93:TYR:HB2	2.00	0.60
1:C:169:ARG:HG2	1:C:174:HIS:O	2.00	0.60
1:C:499:TYR:O	1:C:501:GLU:HB3	2.01	0.60
1:D:327:GLU:O	1:D:374:VAL:HG21	2.02	0.60
1:A:177:ASP:OD1	1:A:179:ASP:HB2	2.02	0.60
1:C:165:HIS:HB3	1:D:402:ASN:ND2	2.16	0.60
1:A:229:VAL:HG12	1:A:230:TYR:N	2.16	0.60
1:C:300:LYS:HA	1:C:441:GLN:OE1	2.02	0.60
1:C:466:LEU:O	1:C:466:LEU:HD12	2.02	0.60
1:D:290:ILE:O	1:D:291:PHE:C	2.44	0.60
1:D:347:ASP:HB3	1:D:350:LEU:HB3	1.83	0.60
1:A:360:THR:HG23	1:D:64:ASP:CA	2.32	0.60
1:B:401:PRO:HB2	1:B:410:ALA:HB2	1.83	0.60
1:A:23:PRO:HB2	1:C:412:GLU:HG3	1.84	0.60
1:B:168:LYS:O	4:B:2073:HOH:O	2.16	0.60
1:A:187:LEU:C	1:A:189:PRO:HD3	2.26	0.59
1:B:19:ALA:HB1	1:B:20:ALA:HB3	0.61	0.59
1:D:74:HIS:O	1:D:111:ARG:NH2	2.34	0.59
1:B:455:ARG:HG3	1:B:455:ARG:HH11	1.68	0.59
1:B:404:TYR:OH	1:B:413:HIS:HD2	1.85	0.59
1:C:277:THR:OG1	1:C:314:LYS:HE2	2.03	0.59
1:B:32:ASN:HA	1:D:139:ASP:O	2.02	0.59
1:C:177:ASP:HB3	1:C:180:MET:HG3	1.84	0.59
1:C:213:GLY:HA3	1:C:235:TYR:CD2	2.38	0.59
1:C:485:HIS:CE1	1:C:487:GLU:HB3	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:LYS:O	1:D:501:GLU:N	2.34	0.59
1:D:187:LEU:O	1:D:188:ARG:HD2	2.02	0.59
1:B:95:LYS:HD3	1:B:224:ALA:HA	1.84	0.59
1:C:139:ASP:HB3	1:C:340:PRO:HD2	1.84	0.59
1:B:65:ARG:HD3	1:D:367:PRO:HB3	1.85	0.59
1:B:235:TYR:N	1:B:235:TYR:CD1	2.71	0.59
1:C:166:SER:HA	1:C:180:MET:HE3	1.85	0.59
1:D:499:TYR:C	1:D:501:GLU:N	2.60	0.59
1:A:301:VAL:O	1:A:303:PRO:HD3	2.02	0.59
1:B:138:GLU:HA	1:B:379:ARG:O	2.03	0.59
2:B:2001:HEM:HBC2	2:B:2001:HEM:CMC	2.32	0.59
1:D:294:ASN:HB3	1:D:297:ASP:HB2	1.85	0.58
1:A:51:VAL:HG12	1:B:51:VAL:HA	1.84	0.58
1:A:237:THR:HA	1:A:276:TRP:CD1	2.38	0.58
1:A:364:ARG:NH1	1:A:365:LEU:HD21	2.17	0.58
1:B:294:ASN:ND2	1:C:46:ARG:HD2	2.19	0.58
1:C:97:LYS:CD	1:C:138:GLU:HB2	2.30	0.58
1:C:252:LEU:HA	1:C:255:GLU:HB2	1.85	0.58
1:C:488:TYR:O	1:C:492:ILE:HG12	2.03	0.58
1:B:223:ASN:ND2	1:B:227:GLU:HB2	2.16	0.58
1:C:235:TYR:HA	1:C:277:THR:O	2.04	0.58
1:C:470:GLN:NE2	1:C:472:PHE:CE2	2.71	0.58
1:A:149:THR:HG21	1:A:194:GLN:OE1	2.03	0.58
1:B:101:HIS:O	1:B:104:LYS:HB2	2.03	0.58
1:B:239:GLN:HE22	1:B:275:SER:H	1.51	0.58
1:B:444:THR:O	1:B:448:LYS:HB3	2.04	0.58
1:A:283:MET:HE3	1:A:302:TRP:CE2	2.39	0.58
1:A:360:THR:CG2	1:D:64:ASP:O	2.51	0.58
1:A:187:LEU:O	1:A:189:PRO:HD3	2.03	0.58
1:B:164:ILE:O	1:B:168:LYS:HG3	2.04	0.58
1:A:331:LEU:HD13	1:A:374:VAL:CG2	2.33	0.58
1:B:90:ILE:HD13	1:B:312:VAL:HB	1.84	0.58
1:B:250:ALA:O	1:B:253:ALA:HB3	2.04	0.58
1:B:446:TYR:HA	1:B:450:LEU:HD12	1.86	0.58
1:C:193:HIS:CA	1:C:442:VAL:HG22	2.34	0.58
1:A:331:LEU:HD13	1:A:374:VAL:HG22	1.85	0.58
1:B:50:LEU:HD22	1:B:50:LEU:N	2.18	0.58
1:D:310:ILE:HD12	1:D:310:ILE:N	2.19	0.58
1:D:212:ASP:OD1	1:D:236:LYS:HA	2.04	0.57
1:B:134:LYS:HB2	1:B:333:PHE:CE1	2.39	0.57
1:C:209:ARG:O	1:C:239:GLN:HG3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2154:HOH:O	1:C:326:ALA:HB1	2.03	0.57
1:A:145:VAL:O	2:A:2000:HEM:HBC1	2.03	0.57
1:C:46:ARG:CG	1:C:46:ARG:HH11	2.18	0.57
1:C:169:ARG:HD3	1:C:174:HIS:CE1	2.39	0.57
1:B:428:VAL:HG23	1:B:428:VAL:O	2.04	0.57
1:D:116:ALA:O	1:D:168:LYS:NZ	2.31	0.57
1:A:421:ARG:CZ	1:B:430:ARG:H	2.18	0.57
1:C:262:ARG:HG3	1:C:266:ASN:ND2	2.20	0.57
1:A:300:LYS:HA	1:A:441:GLN:OE1	2.05	0.57
1:B:76:LYS:HE3	1:B:121:SER:O	2.03	0.57
1:C:261:LEU:HD23	4:C:2021:HOH:O	1.88	0.57
1:A:96:ALA:HB3	1:A:99:PHE:CD2	2.40	0.57
1:B:485:HIS:CD2	1:B:486:PRO:HD2	2.39	0.57
1:C:217:HIS:CD2	1:C:350:LEU:HB2	2.40	0.57
1:C:216:SER:CB	2:C:2002:HEM:CBC	2.82	0.57
1:B:368:ASN:O	1:B:371:GLN:HB2	2.04	0.56
1:C:151:ILE:CG2	1:C:301:VAL:HG12	2.35	0.56
1:C:217:HIS:CG	1:C:350:LEU:HB2	2.40	0.56
1:A:428:VAL:HG12	1:A:428:VAL:O	2.05	0.56
1:C:209:ARG:HD2	1:C:274:PRO:HB3	1.85	0.56
1:D:86:VAL:HG23	1:D:104:LYS:O	2.05	0.56
1:D:193:HIS:CA	1:D:442:VAL:HG22	2.35	0.56
1:B:192:LEU:HD21	1:B:480:ASN:HB3	1.87	0.56
1:B:388:ASP:HB2	1:D:66:GLU:HG2	1.87	0.56
1:C:423:HIS:HB2	1:D:427:ASP:OD1	2.05	0.56
1:D:227:GLU:HB2	4:D:3088:HOH:O	2.04	0.56
1:D:242:LYS:NZ	4:D:3092:HOH:O	2.37	0.56
1:A:100:GLU:CD	1:A:104:LYS:HZ2	2.13	0.56
1:A:108:ILE:HA	1:A:134:LYS:O	2.06	0.56
1:A:485:HIS:HD2	1:A:487:GLU:HB3	1.67	0.56
1:B:111:ARG:NH1	4:B:2004:HOH:O	2.38	0.56
1:A:93:TYR:HD1	1:A:229:VAL:HG21	1.70	0.56
1:C:151:ILE:HG23	1:C:301:VAL:HG12	1.87	0.56
1:C:421:ARG:HE	1:D:429:GLN:NE2	2.02	0.56
1:B:367:PRO:HG2	1:B:390:PRO:CG	2.35	0.56
1:C:347:ASP:HB3	1:C:350:LEU:HB3	1.87	0.56
1:A:82:GLY:HA3	1:A:316:VAL:O	2.06	0.56
1:C:213:GLY:HA3	1:C:235:TYR:CE2	2.41	0.56
1:C:478:VAL:HG11	1:C:493:GLN:HB2	1.86	0.56
1:A:323:ASN:HD21	1:C:396:ASN:HD22	1.54	0.56
1:B:265:PHE:CZ	1:C:173:THR:HG22	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:GLU:OE2	1:B:491:ARG:NH2	2.38	0.56
1:D:441:GLN:HA	1:D:444:THR:CG2	2.35	0.56
1:C:142:TRP:HB2	1:C:339:PRO:CG	2.36	0.56
1:C:202:ARG:HA	1:C:243:ASN:OD1	2.05	0.56
1:C:423:HIS:HA	1:D:427:ASP:HA	1.88	0.55
1:B:304:HIS:CE1	1:B:309:LEU:HD11	2.41	0.55
1:C:499:TYR:C	1:C:501:GLU:N	2.62	0.55
1:D:217:HIS:CD2	1:D:353:ARG:HH11	2.24	0.55
1:B:393:MET:HE1	1:D:372:ILE:HA	1.88	0.55
1:C:43:VAL:HG21	1:D:43:VAL:HG21	1.88	0.55
1:C:332:ALA:HB1	1:C:361:HIS:CE1	2.42	0.55
1:B:98:VAL:HG13	1:B:99:PHE:CD1	2.41	0.55
1:B:358:PRO:HD3	4:B:2005:HOH:O	2.07	0.55
1:B:479:LYS:O	1:B:482:SER:HB2	2.06	0.55
1:D:422:THR:HG22	1:D:423:HIS:N	2.22	0.55
1:B:234:HIS:O	1:B:278:LEU:HD12	2.06	0.55
1:C:476:LYS:NZ	1:C:476:LYS:HB3	2.21	0.55
1:A:100:GLU:O	1:A:100:GLU:HG2	2.07	0.55
1:C:142:TRP:HB2	1:C:339:PRO:HD3	1.88	0.55
1:A:13:HIS:O	1:A:17:GLN:HB2	2.07	0.55
1:A:123:ASP:OD2	4:A:2028:HOH:O	2.18	0.55
1:C:432:ASN:HD22	1:C:432:ASN:C	2.11	0.55
1:C:438:ASN:N	1:C:438:ASN:OD1	2.40	0.55
1:D:206:ASP:HB2	1:D:244:LEU:HG	1.89	0.55
1:D:96:ALA:C	1:D:98:VAL:H	2.15	0.55
1:D:280:ILE:CD1	1:D:310:ILE:HB	2.35	0.55
1:D:331:LEU:HD21	1:D:374:VAL:HG22	1.89	0.55
1:C:146:GLY:HA3	1:C:235:TYR:OH	2.07	0.54
1:B:364:ARG:NH2	1:B:365:LEU:HD21	2.21	0.54
1:C:235:TYR:N	1:C:235:TYR:CD1	2.75	0.54
1:C:462:ILE:HD13	1:C:481:PHE:CZ	2.42	0.54
1:D:291:PHE:HD1	1:D:293:PHE:O	1.90	0.54
1:A:322:VAL:HA	1:D:172:GLN:HE21	1.71	0.54
1:B:145:VAL:HG21	1:B:335:PRO:HD3	1.90	0.54
1:C:487:GLU:O	1:C:491:ARG:HB2	2.07	0.54
1:A:291:PHE:HD2	1:A:293:PHE:O	1.90	0.54
1:B:41:LEU:O	1:B:50:LEU:HD23	2.07	0.54
1:C:110:VAL:CG2	1:C:317:LEU:HD21	2.36	0.54
1:D:34:VAL:O	1:D:34:VAL:HG23	2.06	0.54
1:B:62:HIS:CD2	1:D:386:GLN:HB3	2.43	0.54
1:B:155:ARG:NH1	1:B:299:THR:OG1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:SER:HB2	2:C:2002:HEM:HBC2	1.89	0.54
1:C:429:GLN:HG2	1:C:431:PHE:CZ	2.42	0.54
1:C:432:ASN:HD21	1:C:434:ALA:H	1.54	0.54
1:D:287:GLU:O	1:D:290:ILE:N	2.40	0.54
1:D:442:VAL:HG12	1:D:484:VAL:HG11	1.89	0.54
1:B:151:ILE:HD13	1:B:193:HIS:ND1	2.23	0.54
1:C:287:GLU:HA	1:C:290:ILE:HG12	1.89	0.54
1:B:422:THR:HG22	1:B:423:HIS:H	1.71	0.54
2:B:2001:HEM:HBC2	2:B:2001:HEM:HMC2	1.90	0.54
1:D:94:SER:HB2	1:D:221:LEU:HD22	1.90	0.54
1:D:34:VAL:O	1:D:34:VAL:CG2	2.56	0.54
1:A:66:GLU:HG2	1:C:387:ARG:O	2.08	0.54
1:B:155:ARG:NH2	1:B:438:ASN:OD1	2.41	0.54
1:D:102:ILE:HD12	1:D:102:ILE:N	2.09	0.54
1:D:170:ASN:HD22	1:D:172:GLN:H	1.56	0.54
1:D:309:LEU:HD12	1:D:309:LEU:N	2.23	0.54
1:D:437:ASP:OD2	1:D:440:THR:HB	2.08	0.54
1:A:466:LEU:HD12	1:A:466:LEU:O	2.07	0.54
1:C:466:LEU:HD21	1:C:477:ALA:CB	2.38	0.54
1:A:251:ARG:NH1	1:A:251:ARG:HB3	2.23	0.53
1:B:160:PHE:CE2	1:B:164:ILE:HG13	2.43	0.53
1:B:256:ASP:OD2	1:B:262:ARG:HD2	2.08	0.53
1:C:97:LYS:HD2	1:C:138:GLU:CD	2.33	0.53
1:D:5:ASP:OD2	1:D:7:ALA:HB3	2.07	0.53
1:D:301:VAL:O	1:D:303:PRO:HD3	2.09	0.53
1:A:49:LEU:O	1:B:51:VAL:HG13	2.09	0.53
1:B:16:GLU:C	1:B:18:ARG:H	2.14	0.53
1:D:97:LYS:CA	1:D:100:GLU:HG3	2.37	0.53
1:B:43:VAL:O	1:B:43:VAL:HG22	2.08	0.53
1:B:189:PRO:O	1:B:192:LEU:HG	2.08	0.53
1:B:252:LEU:H	1:B:252:LEU:CD1	2.22	0.53
1:C:109:ALA:HB3	1:C:134:LYS:HB3	1.90	0.53
1:C:293:PHE:CD1	1:C:293:PHE:N	2.77	0.53
1:D:285:PHE:N	1:D:285:PHE:CD1	2.76	0.53
1:B:110:VAL:HG21	1:B:317:LEU:HD21	1.89	0.53
1:C:212:ASP:OD2	1:C:236:LYS:HA	2.09	0.53
1:A:335:PRO:O	1:A:338:MET:HE2	2.08	0.53
1:C:22:LYS:HD3	1:C:23:PRO:O	2.07	0.53
1:D:189:PRO:C	1:D:191:SER:H	2.17	0.53
1:A:71:ARG:HH11	1:A:71:ARG:CG	2.21	0.53
1:A:191:SER:HB2	1:A:195:VAL:HG23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:MET:HE2	1:C:180:MET:HG2	1.90	0.53
1:B:266:ASN:O	1:B:269:ALA:N	2.41	0.53
1:B:446:TYR:CE1	1:B:455:ARG:HG2	2.44	0.53
1:C:261:LEU:HD22	4:C:2021:HOH:O	1.92	0.53
1:D:383:ALA:HB1	1:D:411:PRO:HG3	1.90	0.53
1:A:192:LEU:HD12	1:A:438:ASN:O	2.08	0.53
1:C:245:SER:HB3	1:C:248:ASP:OD1	2.09	0.53
1:C:221:LEU:O	1:C:228:ALA:HA	2.09	0.53
1:D:90:ILE:HD11	1:D:99:PHE:CG	2.44	0.53
1:A:427:ASP:OD1	1:B:423:HIS:HB2	2.09	0.53
4:A:2159:HOH:O	1:B:423:HIS:CE1	2.62	0.53
1:B:46:ARG:HG3	1:C:294:ASN:HD21	1.73	0.53
1:A:15:LYS:HD2	1:C:408:PHE:CA	2.32	0.53
1:B:82:GLY:HA3	1:B:316:VAL:O	2.09	0.53
1:B:345:SER:HB2	1:B:346:PRO:HD2	1.91	0.53
1:D:460:GLU:HA	1:D:495:LEU:HD13	1.91	0.53
1:B:26:LEU:HD21	1:B:37:LYS:HG2	1.90	0.52
1:B:134:LYS:HB2	1:B:333:PHE:HE1	1.74	0.52
1:C:466:LEU:HD21	1:C:477:ALA:HB3	1.91	0.52
1:A:156:ASP:OD1	1:D:40:SER:OG	2.26	0.52
1:B:160:PHE:N	1:B:161:PRO:HD2	2.25	0.52
1:B:212:ASP:OD1	1:B:236:LYS:HA	2.09	0.52
1:C:206:ASP:HA	1:C:244:LEU:HG	1.90	0.52
1:C:216:SER:CB	2:C:2002:HEM:HBC2	2.39	0.52
1:A:387:ARG:O	1:C:66:GLU:HG2	2.10	0.52
1:B:206:ASP:OD1	1:B:244:LEU:HD21	2.10	0.52
1:C:154:ILE:HD11	1:C:349:MET:HE1	1.91	0.52
1:D:18:ARG:O	1:D:19:ALA:CB	2.57	0.52
1:A:18:ARG:NH2	1:A:21:GLN:NE2	2.56	0.52
1:A:492:ILE:O	1:A:496:LEU:HB2	2.09	0.52
1:B:252:LEU:N	1:B:252:LEU:CD1	2.72	0.52
1:B:265:PHE:CE1	1:C:173:THR:HG22	2.44	0.52
1:C:78:ALA:HB2	1:C:261:LEU:CD2	2.35	0.52
1:C:108:ILE:HA	1:C:134:LYS:O	2.10	0.52
1:C:428:VAL:HG21	1:D:424:PHE:HD2	1.75	0.52
1:C:485:HIS:ND1	1:C:485:HIS:C	2.68	0.52
1:B:15:LYS:CD	1:D:408:PHE:HA	2.25	0.52
1:B:25:VAL:HG11	1:D:414:GLN:HG3	1.91	0.52
1:C:327:GLU:HA	1:C:374:VAL:HG11	1.92	0.52
1:D:88:HIS:CD2	1:D:311:PRO:HG2	2.45	0.52
1:D:422:THR:HG22	1:D:423:HIS:H	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASP:HB2	1:A:227:GLU:HG3	1.92	0.52
1:A:451:ASN:N	1:A:454:GLN:NE2	2.57	0.52
1:B:385:TYR:CD2	1:B:404:TYR:HB2	2.44	0.52
1:D:359:ASP:HA	1:D:362:ARG:HH11	1.75	0.52
1:A:155:ARG:HD3	4:A:2014:HOH:O	2.09	0.52
1:B:73:VAL:HG22	1:B:164:ILE:HG21	1.92	0.52
1:B:236:LYS:O	1:B:276:TRP:HA	2.08	0.52
1:D:135:PHE:HB2	1:D:142:TRP:HB3	1.91	0.52
1:A:450:LEU:HA	1:A:454:GLN:HE22	1.75	0.52
1:A:450:LEU:HA	1:A:454:GLN:NE2	2.24	0.52
1:B:148:ASN:CB	1:B:211:MET:HE2	2.40	0.52
1:B:442:VAL:HG12	1:B:484:VAL:HG11	1.91	0.52
1:C:155:ARG:NH1	1:C:297:ASP:OD2	2.37	0.52
1:A:30:GLY:O	1:C:377:PRO:CB	2.58	0.52
1:A:101:HIS:CE1	1:A:104:LYS:HB2	2.45	0.52
1:A:172:GLN:HE21	1:D:322:VAL:HA	1.73	0.52
1:B:447:LEU:HD23	1:B:447:LEU:H	1.75	0.52
1:D:169:ARG:HD3	1:D:174:HIS:O	2.10	0.52
1:D:335:PRO:CD	1:D:357:TYR:CG	2.93	0.52
1:B:304:HIS:CD2	1:B:309:LEU:HD21	2.44	0.52
1:A:251:ARG:O	1:A:255:GLU:HG3	2.10	0.51
1:B:65:ARG:O	1:D:389:GLY:HA2	2.10	0.51
1:B:231:CYS:HA	1:B:281:GLN:O	2.10	0.51
1:B:340:PRO:HG3	1:B:417:ALA:HB1	1.92	0.51
1:C:406:ASN:ND2	1:C:410:ALA:HB3	2.13	0.51
1:A:323:ASN:ND2	1:C:396:ASN:HD22	2.07	0.51
1:C:280:ILE:HG23	1:C:312:VAL:CG2	2.37	0.51
1:B:234:HIS:O	1:B:278:LEU:HA	2.10	0.51
1:C:479:LYS:HE3	4:C:2192:HOH:O	2.05	0.51
1:D:414:GLN:O	1:D:417:ALA:N	2.39	0.51
1:D:465:HIS:CD2	4:D:3080:HOH:O	2.47	0.51
1:A:334:ASP:OD1	1:A:361:HIS:CE1	2.63	0.51
1:B:18:ARG:O	1:B:19:ALA:C	2.53	0.51
1:B:25:VAL:CG1	1:D:414:GLN:HG3	2.40	0.51
1:C:280:ILE:CG2	1:C:312:VAL:HG21	2.38	0.51
1:A:274:PRO:HD2	1:A:317:LEU:O	2.11	0.51
1:A:283:MET:SD	1:A:288:ALA:HA	2.51	0.51
1:B:23:PRO:O	1:B:24:ASP:C	2.51	0.51
1:B:88:HIS:HB2	1:B:312:VAL:HA	1.91	0.51
1:A:423:HIS:HA	1:B:427:ASP:HA	1.91	0.51
1:C:10:GLN:CD	1:C:10:GLN:C	2.78	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ASN:HB3	1:C:297:ASP:HB2	1.93	0.51
1:D:201:ASP:O	1:D:243:ASN:HB3	2.10	0.51
1:D:206:ASP:CB	1:D:244:LEU:HG	2.41	0.51
1:D:286:SER:O	1:D:290:ILE:HG13	2.10	0.51
1:D:290:ILE:CD1	4:D:3107:HOH:O	2.30	0.51
1:D:440:THR:HG22	1:D:441:GLN:N	2.26	0.51
1:A:422:THR:CG2	1:A:423:HIS:N	2.73	0.51
1:B:99:PHE:O	1:B:100:GLU:C	2.54	0.51
1:B:125:VAL:CG2	1:B:126:ARG:N	2.73	0.51
1:B:418:LEU:HD21	1:D:36:ASP:HB3	1.93	0.51
1:C:82:GLY:HA3	1:C:316:VAL:O	2.11	0.51
1:C:414:GLN:NE2	1:C:417:ALA:N	2.58	0.51
1:B:74:HIS:ND1	1:B:114:THR:O	2.44	0.51
1:B:439:VAL:O	1:B:442:VAL:HB	2.11	0.51
1:A:239:GLN:HE22	1:A:275:SER:H	1.59	0.51
1:B:20:ALA:C	1:B:21:GLN:HG3	2.33	0.51
1:D:189:PRO:C	1:D:191:SER:N	2.67	0.51
1:D:293:PHE:HZ	1:D:440:THR:HG21	1.75	0.51
1:A:213:GLY:HA3	1:A:235:TYR:CE2	2.46	0.50
1:B:393:MET:HE2	1:D:371:GLN:O	2.11	0.50
1:B:466:LEU:HD21	1:B:474:GLN:HA	1.93	0.50
1:C:467:LYS:HD2	1:C:467:LYS:O	2.11	0.50
1:D:215:GLY:O	1:D:217:HIS:N	2.44	0.50
1:B:275:SER:HA	1:B:315:LEU:O	2.12	0.50
1:D:96:ALA:HB3	1:D:99:PHE:CD2	2.46	0.50
1:D:335:PRO:HD3	1:D:357:TYR:CG	2.46	0.50
1:A:23:PRO:HB2	1:C:412:GLU:CG	2.40	0.50
1:A:453:GLU:HG2	1:A:457:ARG:HH12	1.76	0.50
1:B:43:VAL:HG13	1:B:48:PRO:HD2	1.92	0.50
1:C:152:PHE:HA	1:C:194:GLN:HG3	1.93	0.50
1:A:45:PRO:HD3	1:D:431:PHE:CE2	2.47	0.50
1:A:51:VAL:HG22	1:B:49:LEU:HB3	1.93	0.50
1:B:296:PHE:CE1	1:B:346:PRO:HD2	2.47	0.50
1:B:393:MET:HE3	1:D:372:ILE:HA	1.90	0.50
1:B:470:GLN:NE2	1:B:472:PHE:HE1	2.10	0.50
1:C:432:ASN:ND2	1:C:432:ASN:C	2.69	0.50
1:D:177:ASP:O	1:D:181:VAL:HG23	2.11	0.50
1:D:499:TYR:O	1:D:501:GLU:N	2.45	0.50
1:A:422:THR:CG2	1:A:423:HIS:H	2.25	0.50
1:B:367:PRO:HD2	1:B:390:PRO:HG2	1.92	0.50
1:B:478:VAL:O	1:B:479:LYS:C	2.54	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:TYR:C	1:C:216:SER:H	2.19	0.50
1:C:377:PRO:HG2	1:C:382:VAL:CG2	2.41	0.50
1:A:45:PRO:HD3	1:D:431:PHE:CZ	2.46	0.50
1:B:15:LYS:O	1:B:18:ARG:HB2	2.11	0.50
1:B:323:ASN:ND2	1:D:396:ASN:HD22	2.07	0.50
1:C:97:LYS:HD2	1:C:138:GLU:OE2	2.11	0.50
1:C:453:GLU:CD	1:C:456:LYS:HD3	2.36	0.50
1:D:222:VAL:HG21	1:D:343:GLU:OE2	2.11	0.50
1:D:441:GLN:HA	1:D:444:THR:HG22	1.93	0.50
1:C:371:GLN:OE1	1:C:393:MET:N	2.43	0.50
1:A:273:TYR:CD1	1:A:318:ASN:HA	2.47	0.50
1:B:442:VAL:HG11	1:B:484:VAL:HG21	1.93	0.50
1:C:350:LEU:O	1:C:353:ARG:N	2.45	0.50
1:A:349:MET:HB3	2:A:2000:HEM:CBB	2.37	0.50
1:B:329:GLU:O	1:B:364:ARG:NH2	2.40	0.50
1:B:447:LEU:O	1:B:448:LYS:HB2	2.11	0.50
1:A:106:THR:HG21	1:A:137:THR:HG22	1.94	0.49
1:B:16:GLU:O	1:B:18:ARG:N	2.45	0.49
1:C:152:PHE:HB3	1:C:298:LEU:HD23	1.92	0.49
1:C:402:ASN:HD21	1:D:180:MET:CE	2.25	0.49
1:A:155:ARG:NH2	1:A:190:GLU:HB2	2.27	0.49
1:B:279:TYR:CD1	1:B:311:PRO:HA	2.47	0.49
1:B:445:PHE:HA	1:B:449:VAL:HG23	1.94	0.49
1:C:451:ASN:H	1:C:454:GLN:NE2	2.07	0.49
1:C:482:SER:OG	1:C:489:GLY:HA3	2.11	0.49
1:D:280:ILE:HG23	1:D:312:VAL:HG21	1.93	0.49
1:A:229:VAL:HG11	1:A:282:VAL:CG1	2.38	0.49
1:C:440:THR:HG22	1:C:441:GLN:N	2.27	0.49
1:B:322:VAL:O	1:C:172:GLN:HB2	2.12	0.49
1:C:451:ASN:OD1	1:C:451:ASN:C	2.55	0.49
1:D:183:ASP:O	1:D:187:LEU:HG	2.12	0.49
1:B:12:LYS:HD3	1:C:470:GLN:OE1	2.12	0.49
1:B:149:THR:OG1	1:B:150:PRO:HD2	2.13	0.49
1:B:206:ASP:OD1	1:B:244:LEU:HD11	2.12	0.49
1:B:220:LYS:HD2	1:B:228:ALA:HB1	1.93	0.49
1:C:126:ARG:CD	1:C:198:LEU:O	2.60	0.49
1:A:65:ARG:HD3	1:C:367:PRO:HG3	1.94	0.49
1:B:26:LEU:CD2	1:B:37:LYS:HG2	2.43	0.49
1:B:156:ASP:OD1	1:C:40:SER:OG	2.25	0.49
1:C:70:GLU:HG2	4:C:2147:HOH:O	2.13	0.49
1:C:216:SER:HB2	2:C:2002:HEM:HBC1	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:HA	1:A:194:GLN:HG3	1.94	0.49
1:B:243:ASN:O	1:B:244:LEU:HD23	2.13	0.49
1:D:427:ASP:CB	1:D:429:GLN:HE21	2.26	0.49
1:B:345:SER:C	1:B:347:ASP:H	2.20	0.49
1:B:393:MET:HE1	1:D:372:ILE:HG12	1.94	0.49
1:B:497:ASP:HA	1:B:500:ASN:HD22	1.77	0.49
1:D:15:LYS:O	1:D:18:ARG:HB3	2.13	0.49
1:D:463:ALA:O	1:D:467:LYS:CG	2.60	0.49
1:A:367:PRO:HG2	1:A:390:PRO:HD2	1.95	0.49
1:B:147:ASN:CG	2:B:2001:HEM:HAC	2.33	0.49
1:B:16:GLU:C	1:B:18:ARG:N	2.71	0.49
1:B:46:ARG:HD2	1:C:294:ASN:ND2	2.28	0.49
1:B:100:GLU:HB3	1:B:104:LYS:HG3	1.94	0.49
1:C:183:ASP:OD2	1:D:408:PHE:HE1	1.96	0.49
1:A:48:PRO:HB2	1:B:50:LEU:HD12	1.94	0.48
1:A:265:PHE:CE2	1:D:173:THR:HG22	2.48	0.48
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.95	0.48
1:B:395:ASP:OD2	4:B:2107:HOH:O	2.19	0.48
1:C:189:PRO:HB3	1:C:480:ASN:HD22	1.78	0.48
1:A:421:ARG:HH22	1:B:430:ARG:H	1.61	0.48
1:B:74:HIS:CE1	1:B:115:VAL:HG22	2.48	0.48
1:B:254:HIS:HB3	1:C:254:HIS:HB3	1.95	0.48
1:C:410:ALA:HB1	1:C:411:PRO:CD	2.41	0.48
1:D:345:SER:C	1:D:347:ASP:H	2.21	0.48
1:D:439:VAL:CG2	1:D:440:THR:N	2.72	0.48
1:A:18:ARG:HH11	1:A:18:ARG:CG	2.25	0.48
1:C:71:ARG:CD	1:C:111:ARG:NH2	2.75	0.48
1:B:447:LEU:HD22	1:B:485:HIS:HD1	1.77	0.48
1:C:13:HIS:O	1:C:17:GLN:HG2	2.14	0.48
1:C:46:ARG:NH1	1:C:46:ARG:HG2	2.29	0.48
1:D:93:TYR:CE1	1:D:282:VAL:HG11	2.48	0.48
1:A:190:GLU:HA	1:A:438:ASN:HB3	1.96	0.48
1:A:353:ARG:HG2	2:A:2000:HEM:C3B	2.48	0.48
1:A:393:MET:HG3	1:C:393:MET:SD	2.54	0.48
1:A:421:ARG:NH2	1:B:430:ARG:N	2.59	0.48
1:D:20:ALA:O	1:D:21:GLN:C	2.56	0.48
1:A:50:LEU:HD13	1:B:50:LEU:HD13	1.95	0.48
1:A:148:ASN:HD22	1:A:149:THR:N	2.11	0.48
1:C:297:ASP:OD1	1:C:299:THR:N	2.46	0.48
1:D:256:ASP:OD2	1:D:259:TYR:HA	2.14	0.48
1:D:436:ASP:O	1:D:437:ASP:CB	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:495:LEU:O	1:D:498:LYS:HB2	2.13	0.48
1:A:351:GLN:HE22	1:C:52:GLN:HE21	1.61	0.48
1:B:64:ASP:HB3	1:C:360:THR:CB	2.42	0.48
1:B:183:ASP:O	1:B:187:LEU:HG	2.12	0.48
1:C:92:ARG:H	1:C:92:ARG:CD	2.25	0.48
1:C:287:GLU:C	1:C:289:GLU:N	2.69	0.48
1:D:332:ALA:HB1	1:D:361:HIS:CE1	2.49	0.48
1:A:187:LEU:CD2	1:A:476:LYS:HE2	2.43	0.48
1:A:367:PRO:HG2	1:A:390:PRO:CG	2.43	0.48
1:C:391:MET:HE3	1:C:393:MET:CE	2.42	0.48
1:B:41:LEU:HD23	1:C:430:ARG:HG3	1.95	0.48
1:C:457:ARG:O	1:C:458:LEU:C	2.57	0.48
1:D:333:PHE:N	1:D:333:PHE:CD1	2.82	0.48
1:D:421:ARG:HH11	1:D:421:ARG:HG2	1.78	0.48
1:A:193:HIS:HB2	4:A:2023:HOH:O	2.13	0.48
2:B:2001:HEM:O2D	4:B:2183:HOH:O	2.18	0.48
1:C:284:THR:OG1	1:C:287:GLU:HG3	2.13	0.48
1:C:453:GLU:O	1:C:456:LYS:HB3	2.14	0.48
1:D:96:ALA:C	1:D:98:VAL:N	2.72	0.48
1:A:62:HIS:O	1:A:63:PHE:C	2.57	0.47
1:A:421:ARG:HH22	1:B:430:ARG:N	2.12	0.47
1:C:123:ASP:OD2	1:C:258:ASP:HA	2.14	0.47
1:D:235:TYR:N	1:D:235:TYR:CD1	2.81	0.47
1:A:500:ASN:O	1:A:501:GLU:C	2.57	0.47
1:B:279:TYR:HA	1:B:310:ILE:O	2.14	0.47
1:B:304:HIS:NE2	1:B:309:LEU:HD21	2.29	0.47
1:B:470:GLN:NE2	1:B:472:PHE:CE1	2.82	0.47
1:C:12:LYS:O	1:C:16:GLU:HG3	2.14	0.47
1:D:87:THR:HA	1:D:102:ILE:HG23	1.95	0.47
1:D:231:CYS:HA	1:D:281:GLN:O	2.13	0.47
1:D:281:GLN:O	1:D:302:TRP:HZ3	1.97	0.47
1:A:343:GLU:HB3	1:A:344:PRO:HD2	1.95	0.47
1:B:223:ASN:C	1:B:225:ASP:H	2.21	0.47
1:B:404:TYR:OH	1:B:413:HIS:CD2	2.67	0.47
1:C:105:ARG:HH11	1:C:105:ARG:CG	2.26	0.47
1:C:134:LYS:HB2	1:C:333:PHE:CE2	2.50	0.47
1:A:62:HIS:HE1	1:C:387:ARG:O	1.98	0.47
1:B:142:TRP:HA	1:B:337:ASN:O	2.13	0.47
1:C:85:GLU:CD	1:C:105:ARG:HH12	2.22	0.47
1:C:214:TYR:C	1:C:216:SER:N	2.70	0.47
1:D:141:ASN:OD1	1:D:377:PRO:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:HIS:NE2	4:A:2079:HOH:O	2.35	0.47
1:B:14:TRP:CH2	1:B:18:ARG:HD2	2.49	0.47
1:B:474:GLN:O	1:B:478:VAL:HG23	2.14	0.47
1:C:251:ARG:CG	1:C:252:LEU:N	2.74	0.47
1:D:210:HIS:CD2	1:D:242:LYS:HB2	2.50	0.47
1:A:51:VAL:CG2	1:B:49:LEU:HB3	2.45	0.47
1:A:343:GLU:HB3	1:A:344:PRO:CD	2.44	0.47
1:A:367:PRO:HG2	1:A:390:PRO:CD	2.45	0.47
1:A:409:SER:O	1:C:23:PRO:HB3	2.14	0.47
1:B:11:MET:CE	1:C:180:MET:HG2	2.44	0.47
1:B:434:ALA:C	1:B:435:ASN:HD22	2.23	0.47
1:C:83:TYR:CD1	1:C:83:TYR:C	2.93	0.47
1:C:89:ASP:OD1	1:C:89:ASP:C	2.57	0.47
1:C:349:MET:HE3	2:C:2002:HEM:CAB	2.43	0.47
1:C:467:LYS:HE2	1:C:468:ASP:OD2	2.14	0.47
1:C:499:TYR:O	1:C:501:GLU:N	2.47	0.47
1:D:70:GLU:HG2	4:D:3026:HOH:O	2.14	0.47
1:D:251:ARG:HG3	4:D:3021:HOH:O	2.14	0.47
1:D:500:ASN:O	1:D:501:GLU:C	2.57	0.47
1:A:71:ARG:HH12	1:A:329:GLU:CD	2.22	0.47
1:A:160:PHE:C	1:A:160:PHE:CD2	2.93	0.47
1:C:139:ASP:HB3	1:C:340:PRO:CD	2.44	0.47
1:D:148:ASN:N	1:D:148:ASN:HD22	2.13	0.47
1:A:50:LEU:C	1:A:52:GLN:N	2.69	0.47
1:A:186:SER:HB2	1:A:476:LYS:CG	2.41	0.47
1:B:210:HIS:CB	1:B:242:LYS:HB3	2.45	0.47
1:C:215:GLY:O	1:C:217:HIS:N	2.48	0.47
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.96	0.47
1:B:62:HIS:HD2	4:B:2182:HOH:O	1.98	0.47
2:B:2001:HEM:HAA1	2:B:2001:HEM:HHA	1.64	0.47
1:C:485:HIS:HE1	1:C:487:GLU:HB3	1.80	0.47
1:B:210:HIS:CE1	1:B:239:GLN:HB3	2.51	0.46
1:C:46:ARG:NH1	1:C:46:ARG:CG	2.78	0.46
1:D:205:PRO:HA	1:D:243:ASN:HA	1.97	0.46
1:A:191:SER:O	1:A:192:LEU:C	2.59	0.46
1:A:284:THR:OG1	1:A:287:GLU:HG3	2.15	0.46
1:B:360:THR:OG1	1:C:64:ASP:CB	2.58	0.46
1:B:450:LEU:HA	1:B:454:GLN:OE1	2.15	0.46
1:C:152:PHE:O	1:C:299:THR:CG2	2.63	0.46
1:D:43:VAL:O	1:D:47:GLY:HA3	2.16	0.46
1:D:74:HIS:CE1	1:D:115:VAL:HG22	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:CE2	1:A:164:ILE:CG1	2.98	0.46
1:A:467:LYS:HD2	1:A:499:TYR:CD1	2.50	0.46
1:B:182:TRP:NE1	1:B:465:HIS:ND1	2.52	0.46
1:C:6:PRO:HD2	1:C:266:ASN:OD1	2.15	0.46
1:C:129:ARG:HB2	1:C:148:ASN:CG	2.40	0.46
1:D:90:ILE:HD13	1:D:312:VAL:CG1	2.44	0.46
1:A:65:ARG:NH1	1:C:362:ARG:HD2	2.31	0.46
1:A:160:PHE:CZ	1:A:164:ILE:HD11	2.51	0.46
1:B:66:GLU:HB3	1:D:388:ASP:HB2	1.96	0.46
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.97	0.46
1:B:393:MET:HE2	1:D:372:ILE:HA	1.90	0.46
1:C:451:ASN:O	1:C:455:ARG:HB2	2.15	0.46
1:D:347:ASP:O	1:D:351:GLN:HG2	2.15	0.46
1:B:26:LEU:HD12	1:D:384:ASN:HA	1.98	0.46
2:B:2001:HEM: CBD	2:B:2001:HEM:HMD2	2.45	0.46
1:C:206:ASP:OD2	1:C:242:LYS:HE3	2.15	0.46
1:D:334:ASP:OD1	1:D:361:HIS:ND1	2.48	0.46
1:A:6:PRO:O	4:A:2055:HOH:O	2.20	0.46
1:B:291:PHE:CD1	1:B:292:PRO:HD2	2.50	0.46
1:B:472:PHE:CZ	1:B:473:ILE:HG13	2.51	0.46
1:C:87:THR:C	1:C:88:HIS:ND1	2.74	0.46
1:C:349:MET:HE3	2:C:2002:HEM:HAB	1.96	0.46
1:C:381:ARG:NH1	1:C:381:ARG:HG2	2.29	0.46
1:D:385:TYR:HB3	1:D:402:ASN:O	2.15	0.46
1:A:393:MET:SD	1:C:393:MET:HG3	2.56	0.46
1:C:4:ARG:HD3	1:C:8:SER:HB2	1.97	0.46
1:C:69:PRO:O	1:C:364:ARG:HG3	2.16	0.46
1:D:219:PHE:O	1:D:230:TYR:HA	2.15	0.46
1:D:451:ASN:OD1	1:D:451:ASN:C	2.58	0.46
1:C:74:HIS:O	1:C:111:ARG:NH2	2.46	0.46
1:C:177:ASP:CB	1:C:180:MET:HG3	2.45	0.46
1:D:148:ASN:HD22	1:D:148:ASN:H	1.62	0.46
1:D:223:ASN:HD21	1:D:227:GLU:CB	2.03	0.46
1:D:493:GLN:HA	1:D:496:LEU:HD12	1.97	0.46
1:B:273:TYR:HA	1:B:274:PRO:HD3	1.78	0.46
1:B:338:MET:HE2	1:B:342:ILE:CG2	2.41	0.46
1:B:382:VAL:O	1:B:382:VAL:CG1	2.63	0.46
1:A:83:TYR:CD1	1:A:105:ARG:HD2	2.51	0.46
1:B:74:HIS:O	1:B:111:ARG:NH2	2.49	0.46
1:D:501:GLU:C	1:D:501:GLU:OE1	2.58	0.46
1:A:39:ASN:CG	1:D:432:ASN:HA	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LYS:NZ	1:A:121:SER:O	2.49	0.45
1:B:485:HIS:O	1:B:488:TYR:HB3	2.15	0.45
1:C:177:ASP:CG	1:C:180:MET:HG3	2.41	0.45
1:C:239:GLN:CD	1:C:239:GLN:H	2.23	0.45
1:D:217:HIS:ND1	1:D:298:LEU:HD13	2.31	0.45
1:A:17:GLN:HG3	4:A:2067:HOH:O	2.16	0.45
1:A:452:GLU:O	1:A:453:GLU:C	2.58	0.45
1:B:476:LYS:O	1:B:479:LYS:HB3	2.17	0.45
1:C:212:ASP:OD2	1:C:236:LYS:HD3	2.17	0.45
1:C:474:GLN:NE2	1:C:496:LEU:HD12	2.30	0.45
1:D:127:ASP:O	1:D:129:ARG:NH1	2.49	0.45
1:D:182:TRP:CD2	1:D:466:LEU:HD13	2.51	0.45
1:A:279:TYR:HB2	1:A:309:LEU:HD12	1.98	0.45
1:A:469:ALA:O	1:A:470:GLN:C	2.59	0.45
1:D:188:ARG:HB3	1:D:190:GLU:CD	2.41	0.45
1:D:372:ILE:HB	1:D:375:ASN:HD22	1.81	0.45
1:A:73:VAL:O	1:A:74:HIS:HB2	2.15	0.45
1:B:443:ARG:HG3	1:B:447:LEU:HD21	1.99	0.45
1:C:190:GLU:CA	1:C:438:ASN:HD22	2.30	0.45
1:D:74:HIS:HA	1:D:114:THR:O	2.16	0.45
1:A:112:PHE:CG	1:A:208:HIS:HB3	2.51	0.45
1:A:460:GLU:HG3	1:A:495:LEU:CD2	2.44	0.45
1:A:467:LYS:HD2	1:A:499:TYR:CG	2.52	0.45
1:B:26:LEU:HD21	1:B:37:LYS:CG	2.46	0.45
1:B:180:MET:HG3	1:C:11:MET:CE	2.46	0.45
1:B:223:ASN:C	1:B:225:ASP:N	2.73	0.45
1:B:223:ASN:OD1	1:B:225:ASP:HB3	2.16	0.45
1:C:284:THR:HG1	1:C:287:GLU:HG3	1.82	0.45
1:C:439:VAL:O	1:C:440:THR:C	2.58	0.45
1:C:463:ALA:O	1:C:467:LYS:HB3	2.16	0.45
1:D:90:ILE:HD11	1:D:99:PHE:CD2	2.52	0.45
1:A:71:ARG:CG	1:A:71:ARG:NH1	2.77	0.45
1:A:85:GLU:OE1	1:A:105:ARG:NH1	2.50	0.45
1:A:131:PHE:N	1:A:146:GLY:O	2.38	0.45
1:B:63:PHE:O	1:B:66:GLU:HG3	2.16	0.45
1:B:110:VAL:CG2	1:B:317:LEU:HD21	2.47	0.45
1:B:450:LEU:HD22	1:B:454:GLN:HG3	1.99	0.45
1:C:4:ARG:H	1:C:4:ARG:CD	2.28	0.45
1:C:149:THR:HG21	1:C:194:GLN:OE1	2.16	0.45
1:C:239:GLN:NE2	1:C:275:SER:O	2.45	0.45
1:C:251:ARG:C	1:C:253:ALA:N	2.72	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:HD13	1:D:484:VAL:HG23	1.99	0.45
1:D:209:ARG:HG2	1:D:274:PRO:HB3	1.98	0.45
1:A:37:LYS:HE3	1:C:404:TYR:CD2	2.51	0.45
1:A:84:PHE:O	1:A:105:ARG:HA	2.16	0.45
1:B:24:ASP:O	1:D:411:PRO:HA	2.15	0.45
1:B:497:ASP:HA	1:B:500:ASN:HB2	1.98	0.45
1:C:219:PHE:O	1:C:230:TYR:HA	2.16	0.45
1:C:391:MET:O	1:C:393:MET:HE2	2.16	0.45
1:C:485:HIS:HA	1:C:486:PRO:HD2	1.69	0.45
1:D:18:ARG:HG2	1:D:18:ARG:HH11	1.81	0.45
1:D:90:ILE:HG21	1:D:312:VAL:HG13	1.98	0.45
1:D:166:SER:HA	1:D:180:MET:HE2	1.99	0.45
1:D:276:TRP:CZ3	1:D:317:LEU:HD12	2.51	0.45
1:A:74:HIS:O	1:A:111:ARG:NH2	2.50	0.45
1:C:73:VAL:HB	1:C:74:HIS:HD2	1.80	0.45
1:D:284:THR:OG1	1:D:287:GLU:HG3	2.17	0.45
1:A:132:ALA:HB1	1:A:333:PHE:CD2	2.52	0.45
1:A:421:ARG:NH1	1:B:430:ARG:H	2.15	0.45
1:B:91:THR:C	1:B:93:TYR:N	2.72	0.45
1:C:26:LEU:HD21	1:C:37:LYS:HD3	1.98	0.45
1:A:54:VAL:H	1:A:54:VAL:HG22	1.63	0.45
1:B:62:HIS:CE1	1:D:368:ASN:HD21	2.23	0.45
1:B:248:ASP:C	1:B:252:LEU:HD13	2.41	0.45
1:B:343:GLU:HB3	1:B:344:PRO:HD2	1.97	0.45
1:B:467:LYS:CG	1:B:468:ASP:N	2.80	0.45
1:C:169:ARG:HG2	1:C:169:ARG:NH1	2.31	0.45
1:C:450:LEU:HA	1:C:454:GLN:HE21	1.82	0.45
1:D:189:PRO:O	1:D:191:SER:N	2.50	0.45
1:D:331:LEU:HG	1:D:374:VAL:HG21	1.99	0.45
1:A:50:LEU:C	1:A:52:GLN:H	2.24	0.44
1:A:74:HIS:CB	2:A:2000:HEM:HAD1	2.47	0.44
1:B:353:ARG:HG2	2:B:2001:HEM:C3B	2.52	0.44
1:D:69:PRO:O	1:D:364:ARG:HG3	2.17	0.44
1:A:349:MET:CB	2:A:2000:HEM:HBB1	2.40	0.44
1:B:129:ARG:HG2	1:B:211:MET:HE1	2.00	0.44
1:B:252:LEU:O	1:B:253:ALA:C	2.59	0.44
1:B:277:THR:OG1	1:B:314:LYS:NZ	2.48	0.44
1:C:97:LYS:O	1:C:100:GLU:HB2	2.17	0.44
1:C:155:ARG:HD3	1:C:297:ASP:OD2	2.17	0.44
1:A:43:VAL:HG13	1:A:43:VAL:O	2.18	0.44
1:A:456:LYS:O	1:A:460:GLU:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:MET:HE1	1:C:161:PRO:HD3	1.99	0.44
1:B:475:LYS:O	1:B:476:LYS:C	2.60	0.44
1:C:84:PHE:O	1:C:105:ARG:HA	2.17	0.44
1:C:283:MET:HB3	1:C:302:TRP:CH2	2.53	0.44
1:C:283:MET:HE2	1:C:307:TYR:CZ	2.52	0.44
1:D:43:VAL:HG13	1:D:43:VAL:O	2.18	0.44
1:A:98:VAL:HB	1:A:137:THR:HG21	1.99	0.44
1:A:209:ARG:HD3	1:A:274:PRO:HG3	2.00	0.44
1:B:129:ARG:CG	1:B:211:MET:HE1	2.48	0.44
1:B:235:TYR:N	1:B:235:TYR:HD1	2.14	0.44
1:C:192:LEU:HD13	1:C:484:VAL:CG2	2.47	0.44
1:C:210:HIS:O	1:C:241:ILE:HA	2.18	0.44
1:D:150:PRO:HB3	1:D:214:TYR:CD2	2.53	0.44
1:D:206:ASP:HA	1:D:244:LEU:HG	1.99	0.44
1:D:414:GLN:HB3	1:D:417:ALA:HB3	2.00	0.44
1:A:284:THR:HG23	1:A:287:GLU:OE1	2.17	0.44
1:A:332:ALA:HB1	1:A:361:HIS:NE2	2.32	0.44
1:A:67:ARG:NH2	1:D:168:LYS:HE3	2.30	0.44
1:B:367:PRO:CG	1:D:65:ARG:HD3	2.46	0.44
1:B:427:ASP:OD1	1:B:427:ASP:N	2.48	0.44
1:A:234:HIS:O	1:A:278:LEU:HD12	2.18	0.44
1:A:238:ASP:OD2	1:A:314:LYS:NZ	2.51	0.44
1:B:481:PHE:HD1	1:B:488:TYR:CE2	2.36	0.44
1:D:87:THR:C	1:D:88:HIS:ND1	2.76	0.44
1:D:343:GLU:HB3	1:D:344:PRO:HD2	2.00	0.44
1:A:4:ARG:HH22	1:D:179:ASP:CG	2.25	0.44
1:B:334:ASP:O	1:B:337:ASN:HB2	2.18	0.44
2:B:2001:HEM:CBD	2:B:2001:HEM:CMD	2.95	0.44
1:D:280:ILE:HG23	1:D:312:VAL:CG2	2.48	0.44
1:D:439:VAL:CG2	1:D:440:THR:H	2.27	0.44
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.53	0.44
1:A:429:GLN:O	1:A:431:PHE:CD2	2.71	0.44
1:A:463:ALA:O	1:A:467:LYS:HB3	2.18	0.44
1:B:120:GLY:HA3	1:C:121:SER:N	2.32	0.44
1:C:34:VAL:HG21	1:C:37:LYS:HB2	1.99	0.44
1:C:41:LEU:HB3	1:C:53:ASP:HB2	1.99	0.44
1:C:171:PRO:HG2	4:D:3020:HOH:O	2.17	0.44
1:D:439:VAL:O	1:D:440:THR:C	2.61	0.44
1:A:164:ILE:O	1:A:165:HIS:C	2.60	0.43
1:A:353:ARG:NH2	1:A:357:TYR:OH	2.43	0.43
1:C:197:PHE:CD1	1:C:197:PHE:C	2.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TYR:CD1	1:A:83:TYR:C	2.95	0.43
1:A:348:LYS:NZ	4:A:2006:HOH:O	2.35	0.43
1:B:206:ASP:CG	1:B:244:LEU:HD21	2.43	0.43
1:C:5:ASP:HB2	1:C:6:PRO:HD2	1.99	0.43
1:C:279:TYR:CD1	1:C:311:PRO:HA	2.53	0.43
1:D:427:ASP:HB3	1:D:429:GLN:HE21	1.83	0.43
1:D:458:LEU:HD21	1:D:488:TYR:HH	1.82	0.43
1:A:43:VAL:O	1:A:43:VAL:HG22	2.17	0.43
1:A:111:ARG:HD2	1:A:328:VAL:HG12	2.00	0.43
1:A:303:PRO:C	1:A:305:GLY:N	2.76	0.43
1:B:229:VAL:HG21	1:B:282:VAL:CG1	2.48	0.43
1:C:70:GLU:O	1:C:71:ARG:C	2.61	0.43
1:C:280:ILE:O	1:C:280:ILE:HG13	2.16	0.43
1:C:467:LYS:HE2	1:C:468:ASP:CG	2.43	0.43
1:D:367:PRO:HG2	1:D:390:PRO:HG2	1.99	0.43
1:D:397:GLN:HE21	1:D:397:GLN:HB2	1.56	0.43
1:A:13:HIS:HA	1:A:16:GLU:HB2	2.01	0.43
1:A:127:ASP:C	1:A:128:PRO:O	2.59	0.43
1:B:4:ARG:NH2	1:C:470:GLN:HG3	2.33	0.43
1:B:432:ASN:O	4:B:2163:HOH:O	2.21	0.43
1:C:183:ASP:O	1:C:187:LEU:HG	2.17	0.43
1:C:217:HIS:CE1	1:C:350:LEU:N	2.87	0.43
1:C:476:LYS:HB3	1:C:476:LYS:HZ2	1.83	0.43
1:D:160:PHE:CG	2:D:2003:HEM:HAB	2.53	0.43
1:D:209:ARG:O	1:D:239:GLN:HB2	2.18	0.43
1:D:271:GLY:HA2	1:D:273:TYR:CE1	2.53	0.43
1:D:298:LEU:HD22	1:D:349:MET:CB	2.49	0.43
1:A:139:ASP:O	1:C:32:ASN:HA	2.18	0.43
1:A:160:PHE:O	1:A:164:ILE:HG12	2.18	0.43
1:B:100:GLU:HB3	1:B:101:HIS:H	1.55	0.43
1:B:467:LYS:HG3	1:B:468:ASP:N	2.33	0.43
1:C:427:ASP:OD2	1:D:421:ARG:HD2	2.19	0.43
1:A:129:ARG:HG3	1:A:205:PRO:HG3	1.99	0.43
1:A:147:ASN:ND2	2:A:2000:HEM:C3C	2.86	0.43
1:A:235:TYR:CD1	1:A:235:TYR:N	2.86	0.43
1:B:472:PHE:CE2	1:B:473:ILE:HG13	2.54	0.43
1:C:22:LYS:HD3	1:C:22:LYS:C	2.42	0.43
1:C:139:ASP:CB	1:C:340:PRO:HD2	2.49	0.43
1:D:60:MET:O	1:D:64:ASP:OD1	2.35	0.43
1:D:371:GLN:OE1	1:D:393:MET:N	2.49	0.43
1:D:464:GLY:O	1:D:467:LYS:HE3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:GLN:O	1:D:471:LEU:C	2.62	0.43
1:A:110:VAL:CG2	1:A:317:LEU:HD21	2.48	0.43
1:B:100:GLU:CB	1:B:104:LYS:HG3	2.49	0.43
1:B:469:ALA:HB1	1:B:473:ILE:HG21	2.01	0.43
1:C:304:HIS:HA	1:C:307:TYR:O	2.18	0.43
1:D:73:VAL:O	1:D:74:HIS:HB2	2.18	0.43
1:A:395:ASP:OD1	1:C:327:GLU:OE2	2.36	0.43
1:B:78:ALA:HB2	1:B:261:LEU:HG	2.01	0.43
1:B:90:ILE:O	1:B:93:TYR:N	2.51	0.43
1:B:487:GLU:O	1:B:491:ARG:HB2	2.19	0.43
1:C:347:ASP:O	1:C:351:GLN:HG2	2.18	0.43
1:D:441:GLN:O	1:D:444:THR:HG23	2.19	0.43
1:A:23:PRO:CB	1:C:412:GLU:CG	2.96	0.43
1:A:421:ARG:CZ	1:B:429:GLN:HB3	2.48	0.43
1:B:11:MET:HB3	1:D:408:PHE:CD2	2.54	0.43
1:D:252:LEU:HD22	1:D:259:TYR:CD1	2.53	0.43
1:D:287:GLU:C	1:D:289:GLU:N	2.74	0.43
1:D:387:ARG:HG2	1:D:387:ARG:HH11	1.82	0.43
1:A:46:ARG:HH12	1:D:295:PRO:HD3	1.83	0.43
1:A:452:GLU:N	1:A:455:ARG:NH1	2.67	0.43
1:A:496:LEU:O	1:A:499:TYR:N	2.51	0.43
1:B:62:HIS:HE1	1:D:368:ASN:ND2	2.08	0.43
1:B:387:ARG:O	1:D:66:GLU:HG3	2.19	0.43
1:C:84:PHE:HA	1:C:314:LYS:O	2.19	0.43
1:C:145:VAL:CG1	1:C:353:ARG:HH22	2.32	0.43
1:D:209:ARG:NH2	1:D:263:ASP:OD1	2.35	0.43
1:A:273:TYR:HA	1:A:274:PRO:HD3	1.87	0.42
1:B:163:PHE:HB2	1:B:184:PHE:CE2	2.54	0.42
1:D:206:ASP:CA	1:D:244:LEU:HG	2.49	0.42
1:A:427:ASP:OD2	1:B:421:ARG:NH2	2.52	0.42
1:B:451:ASN:O	1:B:452:GLU:C	2.61	0.42
1:C:18:ARG:HD3	1:C:18:ARG:O	2.19	0.42
1:C:98:VAL:HG13	1:C:99:PHE:CD1	2.54	0.42
1:A:303:PRO:O	1:A:304:HIS:C	2.61	0.42
1:B:50:LEU:C	1:B:52:GLN:N	2.76	0.42
1:B:145:VAL:CG1	1:B:353:ARG:NH2	2.82	0.42
1:B:248:ASP:O	1:B:249:ALA:C	2.62	0.42
1:B:275:SER:C	1:B:276:TRP:CE3	2.97	0.42
1:B:445:PHE:HA	1:B:449:VAL:CG2	2.49	0.42
1:C:252:LEU:O	1:C:256:ASP:N	2.43	0.42
1:D:96:ALA:O	1:D:98:VAL:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:ASP:OD2	1:D:241:ILE:HD11	2.19	0.42
1:A:39:ASN:HA	1:D:156:ASP:OD2	2.19	0.42
1:B:31:GLY:C	1:D:140:GLY:HA3	2.45	0.42
1:B:98:VAL:HG13	1:B:99:PHE:CE1	2.54	0.42
4:B:2002:HOH:O	1:D:395:ASP:HB2	2.19	0.42
1:A:169:ARG:HD2	1:A:174:HIS:CE1	2.54	0.42
1:B:232:LYS:HD3	1:B:302:TRP:CD2	2.54	0.42
1:B:414:GLN:HA	1:B:415:PRO:HD2	1.92	0.42
1:D:91:THR:C	1:D:93:TYR:H	2.26	0.42
1:D:368:ASN:HD22	1:D:368:ASN:HA	1.63	0.42
1:A:218:THR:HG23	1:A:302:TRP:CZ2	2.54	0.42
1:B:279:TYR:C	1:B:280:ILE:HG23	2.44	0.42
1:B:396:ASN:HB2	1:D:326:ALA:HB2	2.00	0.42
1:C:287:GLU:C	1:C:289:GLU:H	2.26	0.42
1:C:303:PRO:C	1:C:305:GLY:N	2.77	0.42
1:C:395:ASP:O	1:C:395:ASP:CG	2.61	0.42
1:C:414:GLN:NE2	1:C:416:SER:HB3	2.35	0.42
1:A:99:PHE:O	1:A:101:HIS:N	2.52	0.42
1:A:166:SER:HA	1:A:180:MET:HE2	2.01	0.42
1:B:177:ASP:HA	1:B:178:PRO:HD2	1.92	0.42
1:B:418:LEU:HD21	1:D:36:ASP:CB	2.49	0.42
1:C:217:HIS:HD1	1:C:298:LEU:HD13	1.84	0.42
1:C:290:ILE:CD1	4:C:2164:HOH:O	2.67	0.42
1:C:291:PHE:HD2	1:C:293:PHE:O	2.03	0.42
1:C:414:GLN:HE21	1:C:414:GLN:C	2.28	0.42
1:C:444:THR:HG22	1:C:444:THR:O	2.20	0.42
1:D:239:GLN:N	1:D:239:GLN:OE1	2.52	0.42
1:A:454:GLN:C	1:A:456:LYS:N	2.76	0.42
1:B:129:ARG:CZ	1:B:205:PRO:HD2	2.49	0.42
1:B:428:VAL:O	1:B:428:VAL:CG2	2.67	0.42
1:D:285:PHE:HD1	1:D:285:PHE:N	2.12	0.42
1:B:261:LEU:N	1:B:261:LEU:HD12	2.35	0.42
1:B:393:MET:HE1	1:D:372:ILE:CG1	2.49	0.42
1:B:485:HIS:O	1:B:488:TYR:CB	2.68	0.42
1:C:25:VAL:HG23	4:C:2049:HOH:O	2.20	0.42
1:C:81:PHE:CD1	1:C:81:PHE:N	2.88	0.42
1:C:169:ARG:HH11	1:C:169:ARG:CG	2.30	0.42
1:C:237:THR:OG1	1:C:239:GLN:HG2	2.20	0.42
1:C:403:TYR:O	1:C:406:ASN:HB3	2.19	0.42
1:D:11:MET:O	1:D:12:LYS:C	2.62	0.42
1:A:351:GLN:HE22	1:C:52:GLN:NE2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:CG1	1:B:48:PRO:HD2	2.50	0.42
1:B:331:LEU:HD21	1:B:374:VAL:HG11	2.02	0.42
1:B:451:ASN:H	1:B:454:GLN:HG2	1.85	0.42
1:C:49:LEU:HD23	1:D:51:VAL:HG11	2.02	0.42
1:C:82:GLY:C	1:C:108:ILE:HG12	2.44	0.42
1:C:126:ARG:HE	1:C:203:GLY:HA3	1.84	0.42
1:C:182:TRP:CG	1:C:466:LEU:HD13	2.54	0.42
1:D:192:LEU:HD13	1:D:484:VAL:CG2	2.50	0.42
1:D:293:PHE:CD1	1:D:300:LYS:HE2	2.55	0.42
1:D:388:ASP:OD1	1:D:388:ASP:N	2.51	0.42
1:A:4:ARG:HD3	1:A:8:SER:HB2	2.02	0.41
1:A:85:GLU:OE1	1:A:105:ARG:HD3	2.20	0.41
1:B:95:LYS:HG2	1:B:222:VAL:O	2.20	0.41
1:B:291:PHE:HD2	1:B:293:PHE:O	2.03	0.41
1:B:325:PHE:CE2	1:D:388:ASP:HA	2.55	0.41
1:C:71:ARG:HG3	1:C:71:ARG:HH11	1.85	0.41
1:C:179:ASP:OD1	1:C:473:ILE:HD12	2.19	0.41
1:C:459:CYS:HA	1:C:492:ILE:CD1	2.50	0.41
1:D:229:VAL:HA	1:D:285:PHE:HE1	1.84	0.41
1:D:487:GLU:O	1:D:491:ARG:HB2	2.20	0.41
1:A:183:ASP:O	1:A:187:LEU:HG	2.19	0.41
1:A:320:ASN:HD22	1:A:320:ASN:HA	1.62	0.41
1:A:344:PRO:HB3	1:A:350:LEU:HD21	2.00	0.41
1:B:5:ASP:OD2	1:B:7:ALA:HB3	2.20	0.41
1:B:112:PHE:CD1	1:B:208:HIS:HB3	2.55	0.41
1:B:149:THR:HB	1:B:197:PHE:CE2	2.55	0.41
1:B:493:GLN:O	1:B:496:LEU:HB2	2.20	0.41
1:D:221:LEU:HA	1:D:341:GLY:O	2.19	0.41
1:A:67:ARG:O	1:D:363:HIS:HE1	2.02	0.41
1:B:110:VAL:HG12	1:B:111:ARG:N	2.35	0.41
1:B:302:TRP:O	1:B:303:PRO:C	2.64	0.41
1:C:184:PHE:O	1:C:188:ARG:HB2	2.21	0.41
1:C:290:ILE:O	1:C:291:PHE:C	2.62	0.41
1:D:421:ARG:HG2	1:D:421:ARG:NH1	2.36	0.41
1:A:385:TYR:CD1	1:A:385:TYR:N	2.87	0.41
1:A:454:GLN:O	1:A:455:ARG:C	2.62	0.41
1:C:199:PHE:CE2	1:C:462:ILE:HA	2.56	0.41
1:D:254:HIS:CE1	1:D:255:GLU:HG3	2.55	0.41
1:A:169:ARG:CD	1:A:174:HIS:CE1	3.03	0.41
1:A:173:THR:O	1:A:174:HIS:HB3	2.20	0.41
1:A:220:LYS:HD2	1:A:420:HIS:HD2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LYS:O	1:B:37:LYS:CG	2.66	0.41
1:B:41:LEU:HD22	1:C:429:GLN:C	2.45	0.41
1:B:145:VAL:CG1	1:B:353:ARG:HH22	2.33	0.41
1:C:43:VAL:CG1	1:C:48:PRO:HD2	2.51	0.41
1:D:279:TYR:HA	1:D:310:ILE:O	2.19	0.41
1:A:154:ILE:HG13	1:A:349:MET:CE	2.51	0.41
1:A:357:TYR:O	1:A:361:HIS:ND1	2.54	0.41
1:C:74:HIS:CE1	1:C:115:VAL:HG22	2.55	0.41
1:B:245:SER:O	1:B:246:VAL:C	2.64	0.41
1:B:279:TYR:O	1:B:280:ILE:CG2	2.69	0.41
1:B:403:TYR:CD1	1:B:403:TYR:N	2.89	0.41
2:B:2001:HEM:HBD2	2:B:2001:HEM:HMD2	2.02	0.41
1:C:89:ASP:OD1	1:C:91:THR:HB	2.20	0.41
1:C:129:ARG:HG2	1:C:211:MET:SD	2.61	0.41
1:A:129:ARG:HB2	1:A:148:ASN:HB3	2.03	0.41
1:A:334:ASP:OD1	1:A:361:HIS:ND1	2.53	0.41
1:A:492:ILE:O	1:A:496:LEU:N	2.54	0.41
2:A:2000:HEM:HBA1	2:A:2000:HEM:HHA	2.01	0.41
1:B:486:PRO:C	1:B:488:TYR:H	2.27	0.41
1:C:368:ASN:O	1:C:371:GLN:HB2	2.21	0.41
1:D:18:ARG:HH11	1:D:18:ARG:CG	2.34	0.41
1:D:139:ASP:HB3	1:D:339:PRO:HB3	2.02	0.41
1:D:283:MET:HG3	1:D:307:TYR:CE1	2.55	0.41
1:D:319:ARG:NH2	4:D:3023:HOH:O	2.49	0.41
1:D:335:PRO:HD2	1:D:357:TYR:HB2	2.03	0.41
1:A:10:GLN:CD	1:A:10:GLN:C	2.88	0.41
1:A:94:SER:CB	1:A:221:LEU:HD22	2.40	0.41
1:A:151:ILE:HD12	1:A:193:HIS:CG	2.56	0.41
1:A:170:ASN:OD1	1:A:172:GLN:N	2.38	0.41
1:A:451:ASN:OD1	1:A:451:ASN:C	2.63	0.41
1:B:93:TYR:CE1	1:B:282:VAL:HG11	2.55	0.41
1:B:106:THR:HG21	1:B:137:THR:HG22	2.03	0.41
1:B:438:ASN:ND2	4:B:2048:HOH:O	2.53	0.41
1:B:446:TYR:HB3	1:B:447:LEU:HD23	2.02	0.41
1:C:16:GLU:O	1:C:19:ALA:HB3	2.20	0.41
1:C:414:GLN:HA	1:C:415:PRO:HD2	1.83	0.41
1:D:188:ARG:HB3	1:D:190:GLU:OE1	2.21	0.41
1:A:284:THR:HG23	1:A:284:THR:H	1.61	0.41
1:A:364:ARG:CZ	1:A:365:LEU:HD21	2.50	0.41
1:B:191:SER:O	1:B:192:LEU:C	2.63	0.41
1:B:386:GLN:C	1:B:387:ARG:HG2	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PHE:CD1	2:C:2002:HEM:HAB	2.56	0.41
1:C:428:VAL:HG21	1:D:424:PHE:CD2	2.55	0.41
1:D:198:LEU:C	1:D:200:SER:H	2.29	0.41
1:A:410:ALA:HB1	1:A:411:PRO:HD2	2.02	0.40
1:B:145:VAL:HG22	1:B:333:PHE:HB3	2.03	0.40
1:C:223:ASN:OD1	1:C:225:ASP:N	2.50	0.40
1:C:346:PRO:O	1:C:347:ASP:C	2.64	0.40
1:D:251:ARG:HA	1:D:254:HIS:NE2	2.36	0.40
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.83	0.40
2:A:2000:HEM:HMD2	4:A:2005:HOH:O	2.21	0.40
1:B:15:LYS:HD2	1:D:408:PHE:CA	2.27	0.40
1:B:70:GLU:O	1:B:71:ARG:C	2.65	0.40
1:B:177:ASP:OD1	1:B:177:ASP:C	2.64	0.40
1:C:43:VAL:HG13	1:C:48:PRO:HD2	2.03	0.40
1:C:440:THR:O	1:C:441:GLN:C	2.64	0.40
1:C:482:SER:C	1:C:484:VAL:N	2.78	0.40
1:D:189:PRO:HD2	4:D:3167:HOH:O	2.21	0.40
1:D:221:LEU:O	1:D:228:ALA:HA	2.22	0.40
1:D:414:GLN:O	1:D:415:PRO:C	2.65	0.40
1:B:30:GLY:O	1:D:377:PRO:HG3	2.21	0.40
1:B:37:LYS:HE2	1:B:37:LYS:HB2	1.94	0.40
1:B:153:PHE:CD1	1:B:153:PHE:N	2.90	0.40
1:B:158:LEU:HD12	1:C:39:ASN:C	2.46	0.40
1:C:105:ARG:CG	1:C:105:ARG:NH1	2.83	0.40
1:C:208:HIS:HA	1:C:211:MET:HE2	2.03	0.40
1:D:34:VAL:HG21	1:D:37:LYS:HB2	2.03	0.40
1:D:182:TRP:NE1	1:D:465:HIS:ND1	2.52	0.40
1:B:25:VAL:O	1:B:27:THR:HG23	2.21	0.40
1:B:86:VAL:HB	1:B:102:ILE:HA	2.02	0.40
1:B:163:PHE:HD1	1:B:184:PHE:CE2	2.39	0.40
1:B:463:ALA:O	1:B:467:LYS:HB3	2.21	0.40
1:C:217:HIS:ND1	1:C:298:LEU:HD13	2.37	0.40
1:C:444:THR:O	1:C:449:VAL:HG23	2.21	0.40
1:D:357:TYR:CD1	1:D:357:TYR:N	2.89	0.40
1:D:413:HIS:O	1:D:414:GLN:HG2	2.21	0.40
1:D:485:HIS:HA	1:D:486:PRO:HD2	1.89	0.40
1:A:100:GLU:O	1:A:100:GLU:CG	2.69	0.40
1:A:155:ARG:HH21	1:A:190:GLU:HB2	1.86	0.40
1:A:347:ASP:OD1	1:A:349:MET:HB2	2.22	0.40
1:B:27:THR:O	1:D:384:ASN:HB3	2.21	0.40
1:B:136:TYR:CD2	1:B:378:TYR:CE1	3.09	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:PRO:HD2	1:B:317:LEU:O	2.22	0.40
1:C:22:LYS:HD3	1:C:23:PRO:N	2.37	0.40
1:C:360:THR:HG21	2:C:2002:HEM:HBA1	2.03	0.40
1:C:385:TYR:CZ	1:C:404:TYR:HB2	2.56	0.40
1:C:445:PHE:CD1	1:C:449:VAL:HB	2.57	0.40
1:D:293:PHE:CZ	1:D:440:THR:HG21	2.56	0.40
3:D:3000:AZI:N2	2:D:2003:HEM:NC	2.69	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%)	441 (89%)	52 (10%)	4 (1%)	16	44
1	B	497/506 (98%)	413 (83%)	72 (14%)	12 (2%)	4	17
1	C	497/506 (98%)	435 (88%)	56 (11%)	6 (1%)	10	34
1	D	497/506 (98%)	429 (86%)	54 (11%)	14 (3%)	4	14
All	All	1988/2024 (98%)	1718 (86%)	234 (12%)	36 (2%)	6	23

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLU
1	B	19	ALA
1	B	20	ALA
1	B	23	PRO
1	B	100	GLU
1	B	124	THR
1	D	413	HIS
1	A	101	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	331	LEU
1	B	437	ASP
1	B	448	LYS
1	C	216	SER
1	C	440	THR
1	D	19	ALA
1	D	216	SER
1	D	411	PRO
1	D	440	THR
1	B	17	GLN
1	B	121	SER
1	D	12	LYS
1	D	91	THR
1	D	97	LYS
1	D	500	ASN
1	A	437	ASP
1	B	203	GLY
1	C	373	PRO
1	C	500	ASN
1	B	325	PHE
1	D	192	LEU
1	D	394	MET
1	D	437	ASP
1	A	201	ASP
1	C	240	GLY
1	C	346	PRO
1	D	346	PRO
1	D	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%)	388 (90%)	43 (10%)	7	24
1	C	431/437 (99%)	393 (91%)	38 (9%)	9	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	431/437 (99%)	404 (94%)	27 (6%)	16	45
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	3	ASN
1	A	4	ARG
1	A	18	ARG
1	A	26	LEU
1	A	36	ASP
1	A	37	LYS
1	A	49	LEU
1	A	54	VAL
1	A	105	ARG
1	A	118	GLU
1	A	145	VAL
1	A	148	ASN
1	A	149	THR
1	A	159	LEU
1	A	194	GLN
1	A	235	TYR
1	A	242	LYS
1	A	263	ASP
1	A	280	ILE
1	A	309	LEU
1	A	329	GLU
1	A	333	PHE
1	A	336	SER
1	A	360	THR
1	A	374	VAL
1	A	381	ARG
1	A	394	MET
1	A	402	ASN
1	A	421	ARG
1	A	435	ASN
1	A	460	GLU
1	A	476	LYS
1	B	4	ARG
1	B	12	LYS
1	B	21	GLN
1	B	37	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	43	VAL
1	B	46	ARG
1	B	49	LEU
1	B	50	LEU
1	B	85	GLU
1	B	104	LYS
1	B	126	ARG
1	B	144	LEU
1	B	149	THR
1	B	153	PHE
1	B	162	SER
1	B	179	ASP
1	B	201	ASP
1	B	204	ILE
1	B	220	LYS
1	B	222	VAL
1	B	232	LYS
1	B	235	TYR
1	B	237	THR
1	B	239	GLN
1	B	255	GLU
1	B	277	THR
1	B	289	GLU
1	B	290	ILE
1	B	309	LEU
1	B	312	VAL
1	B	319	ARG
1	B	330	GLN
1	B	374	VAL
1	B	393	MET
1	B	402	ASN
1	B	412	GLU
1	B	427	ASP
1	B	438	ASN
1	B	447	LEU
1	B	457	ARG
1	B	466	LEU
1	B	495	LEU
1	B	498	LYS
1	C	3	ASN
1	C	4	ARG
1	C	34	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	43	VAL
1	C	46	ARG
1	C	52	GLN
1	C	73	VAL
1	C	76	LYS
1	C	92	ARG
1	C	104	LYS
1	C	105	ARG
1	C	137	THR
1	C	147	ASN
1	C	149	THR
1	C	169	ARG
1	C	175	LEU
1	C	179	ASP
1	C	194	GLN
1	C	235	TYR
1	C	239	GLN
1	C	293	PHE
1	C	301	VAL
1	C	309	LEU
1	C	331	LEU
1	C	381	ARG
1	C	402	ASN
1	C	414	GLN
1	C	418	LEU
1	C	427	ASP
1	C	438	ASN
1	C	451	ASN
1	C	453	GLU
1	C	467	LYS
1	C	472	PHE
1	C	483	ASP
1	C	496	LEU
1	C	497	ASP
1	C	501	GLU
1	D	18	ARG
1	D	22	LYS
1	D	26	LEU
1	D	34	VAL
1	D	40	SER
1	D	72	VAL
1	D	147	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	148	ASN
1	D	159	LEU
1	D	193	HIS
1	D	235	TYR
1	D	239	GLN
1	D	247	GLU
1	D	261	LEU
1	D	263	ASP
1	D	280	ILE
1	D	283	MET
1	D	284	THR
1	D	285	PHE
1	D	286	SER
1	D	333	PHE
1	D	371	GLN
1	D	397	GLN
1	D	444	THR
1	D	457	ARG
1	D	498	LYS
1	D	501	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	62	HIS
1	A	148	ASN
1	A	167	GLN
1	A	194	GLN
1	A	234	HIS
1	A	239	GLN
1	A	254	HIS
1	A	320	ASN
1	A	337	ASN
1	A	420	HIS
1	A	429	GLN
1	A	454	GLN
1	B	13	HIS
1	B	17	GLN
1	B	21	GLN
1	B	32	ASN
1	B	62	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	147	ASN
1	B	172	GLN
1	B	239	GLN
1	B	272	ASN
1	B	304	HIS
1	B	320	ASN
1	B	323	ASN
1	B	337	ASN
1	B	363	HIS
1	B	396	ASN
1	B	402	ASN
1	B	413	HIS
1	B	429	GLN
1	B	435	ASN
1	B	461	ASN
1	B	470	GLN
1	B	474	GLN
1	B	500	ASN
1	C	17	GLN
1	C	21	GLN
1	C	52	GLN
1	C	147	ASN
1	C	172	GLN
1	C	208	HIS
1	C	402	ASN
1	C	413	HIS
1	C	414	GLN
1	C	420	HIS
1	C	432	ASN
1	C	435	ASN
1	C	438	ASN
1	C	454	GLN
1	C	461	ASN
1	C	474	GLN
1	C	480	ASN
1	C	500	ASN
1	D	21	GLN
1	D	32	ASN
1	D	52	GLN
1	D	147	ASN
1	D	148	ASN
1	D	170	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	193	HIS
1	D	208	HIS
1	D	210	HIS
1	D	243	ASN
1	D	304	HIS
1	D	337	ASN
1	D	363	HIS
1	D	368	ASN
1	D	397	GLN
1	D	413	HIS
1	D	420	HIS
1	D	429	GLN
1	D	432	ASN
1	D	480	ASN
1	D	500	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	2003	3,1	50,50,50	1.45	7 (14%)	67,82,82	3.44	12 (17%)
2	HEM	A	2000	1	50,50,50	1.56	8 (16%)	67,82,82	3.51	13 (19%)
2	HEM	B	2001	1	50,50,50	1.89	8 (16%)	67,82,82	3.99	16 (23%)
3	AZI	D	3000	2	2,2,2	7.55	2 (100%)	0,1,1	-	-
2	HEM	C	2002	1	50,50,50	1.34	5 (10%)	67,82,82	1.48	6 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	2000	1	-	12/14/54/54	-
2	HEM	D	2003	3,1	-	8/14/54/54	-
2	HEM	B	2001	1	-	3/14/54/54	-
2	HEM	C	2002	1	-	5/14/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3000	AZI	N3-N2	8.45	1.40	1.23
2	B	2001	HEM	CHB-C4A	8.28	1.58	1.39
3	D	3000	AZI	N1-N2	6.52	1.36	1.23
2	A	2000	HEM	FE-NB	5.58	2.12	1.94
2	C	2002	HEM	CBC-CAC	5.07	1.54	1.30
2	B	2001	HEM	CBC-CAC	4.78	1.53	1.30
2	D	2003	HEM	CBC-CAC	4.49	1.51	1.30
2	B	2001	HEM	CHC-C1C	3.85	1.45	1.38
2	A	2000	HEM	CMC-C2C	-3.39	1.43	1.50
2	A	2000	HEM	FE-NA	3.36	2.06	1.95
2	C	2002	HEM	CAB-C3B	-3.25	1.38	1.47
2	B	2001	HEM	CAB-C3B	-3.24	1.38	1.47
2	D	2003	HEM	CAB-C3B	-3.21	1.38	1.47
2	A	2000	HEM	FE-ND	3.21	2.04	1.94
2	D	2003	HEM	CHC-C4B	3.19	1.46	1.39
2	D	2003	HEM	FE-NB	3.19	2.04	1.94
2	A	2000	HEM	CAB-C3B	-3.17	1.38	1.47
2	B	2001	HEM	FE-NC	3.05	2.05	1.95
2	C	2002	HEM	FE-ND	3.01	2.04	1.94
2	D	2003	HEM	FE-NA	2.99	2.05	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	HEM	FE-NA	2.96	2.04	1.95
2	A	2000	HEM	CBC-CAC	2.65	1.43	1.30
2	D	2003	HEM	CHD-C1D	2.64	1.45	1.39
2	B	2001	HEM	CBD-CGD	-2.60	1.44	1.50
2	C	2002	HEM	CBB-CAB	2.57	1.42	1.30
2	A	2000	HEM	CBB-CAB	2.57	1.42	1.30
2	D	2003	HEM	CBB-CAB	2.54	1.42	1.30
2	B	2001	HEM	CBB-CAB	2.53	1.42	1.30
2	C	2002	HEM	FE-NC	2.49	2.03	1.95
2	A	2000	HEM	CAA-C2A	2.44	1.57	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2003	HEM	CMD-C2D-C1D	-19.11	95.17	125.03
2	A	2000	HEM	CBA-CAA-C2A	16.67	158.61	112.53
2	B	2001	HEM	CBA-CAA-C2A	16.48	158.09	112.53
2	B	2001	HEM	CHC-C1C-NC	-15.10	108.01	124.45
2	A	2000	HEM	CAD-CBD-CGD	13.56	149.63	113.67
2	B	2001	HEM	CAA-CBA-CGA	13.11	148.43	113.67
2	D	2003	HEM	CMD-C2D-C3D	10.36	154.17	126.15
2	D	2003	HEM	CMC-C2C-C1C	10.12	142.56	124.73
2	B	2001	HEM	CHC-C1C-C2C	-9.75	105.21	125.49
2	A	2000	HEM	CAA-CBA-CGA	9.08	137.75	113.67
2	D	2003	HEM	CMC-C2C-C3C	-8.79	107.16	128.43
2	A	2000	HEM	CAA-C2A-C1A	-8.09	109.14	124.94
2	A	2000	HEM	CAA-C2A-C3A	7.23	143.28	127.07
2	C	2002	HEM	CBC-CAC-C3C	6.87	161.86	127.53
2	B	2001	HEM	O2D-CGD-CBD	-6.62	93.10	114.00
2	A	2000	HEM	CMC-C2C-C1C	-6.58	113.14	124.73
2	B	2001	HEM	O1D-CGD-CBD	6.44	143.53	123.09
2	B	2001	HEM	CAA-C2A-C1A	-6.29	112.66	124.94
2	B	2001	HEM	CBD-CAD-C3D	6.29	129.91	112.53
2	B	2001	HEM	CAD-C3D-C2D	-6.15	116.36	127.87
2	D	2003	HEM	CBC-CAC-C3C	6.06	157.79	127.53
2	C	2002	HEM	CAC-C3C-C2C	-5.07	111.95	128.43
2	B	2001	HEM	CAA-C2A-C3A	4.53	137.24	127.07
2	D	2003	HEM	C1C-CHC-C4B	-4.42	116.62	126.02
2	A	2000	HEM	CAC-C3C-C4C	-4.22	114.75	124.82
2	A	2000	HEM	CAC-C3C-C2C	-4.07	115.19	128.43
2	A	2000	HEM	CMC-C2C-C3C	3.78	137.57	128.43
2	A	2000	HEM	CBC-CAC-C3C	3.70	146.02	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2002	HEM	CAC-C3C-C4C	3.59	133.40	124.82
2	D	2003	HEM	CHC-C4B-C3B	-3.27	118.55	125.07
2	A	2000	HEM	CBD-CAD-C3D	2.99	120.79	112.53
2	D	2003	HEM	CHC-C4B-NB	2.88	127.52	124.42
2	B	2001	HEM	CAD-CBD-CGD	-2.51	107.02	113.67
2	D	2003	HEM	CMB-C2B-C1B	2.47	128.90	125.03
2	B	2001	HEM	CMB-C2B-C1B	2.46	128.88	125.03
2	D	2003	HEM	CAC-C3C-C2C	-2.46	120.43	128.43
2	A	2000	HEM	CMB-C2B-C1B	2.44	128.85	125.03
2	C	2002	HEM	CMB-C2B-C1B	2.44	128.85	125.03
2	B	2001	HEM	CHB-C4A-NA	-2.39	119.53	123.86
2	B	2001	HEM	CAD-C3D-C4D	2.39	128.85	124.70
2	B	2001	HEM	CMC-C2C-C3C	-2.38	122.66	128.43
2	C	2002	HEM	CMC-C2C-C1C	-2.22	120.82	124.73
2	D	2003	HEM	CAC-C3C-C4C	2.20	130.07	124.82
2	B	2001	HEM	CBC-CAC-C3C	-2.08	117.13	127.53
2	A	2000	HEM	CHC-C1C-C2C	-2.06	121.19	125.49
2	C	2002	HEM	CHC-C1C-C2C	-2.06	121.20	125.49
2	D	2003	HEM	CHC-C1C-C2C	-2.03	121.26	125.49

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	HEM	C4C-C3C-CAC-CBC
2	A	2000	HEM	C2D-C3D-CAD-CBD
2	B	2001	HEM	C2D-C3D-CAD-CBD
2	B	2001	HEM	C4D-C3D-CAD-CBD
2	C	2002	HEM	C2B-C3B-CAB-CBB
2	D	2003	HEM	C2B-C3B-CAB-CBB
2	D	2003	HEM	C4B-C3B-CAB-CBB
2	D	2003	HEM	C2C-C3C-CAC-CBC
2	A	2000	HEM	C3A-C2A-CAA-CBA
2	A	2000	HEM	C2B-C3B-CAB-CBB
2	A	2000	HEM	C4B-C3B-CAB-CBB
2	C	2002	HEM	C4B-C3B-CAB-CBB
2	D	2003	HEM	C4C-C3C-CAC-CBC
2	A	2000	HEM	C4D-C3D-CAD-CBD
2	A	2000	HEM	C1A-C2A-CAA-CBA
2	B	2001	HEM	C2B-C3B-CAB-CBB
2	D	2003	HEM	CAD-CBD-CGD-O1D
2	A	2000	HEM	C3D-CAD-CBD-CGD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	2003	HEM	CAD-CBD-CGD-O2D
2	A	2000	HEM	CAA-CBA-CGA-O1A
2	A	2000	HEM	CAD-CBD-CGD-O1D
2	A	2000	HEM	CAA-CBA-CGA-O2A
2	C	2002	HEM	CAD-CBD-CGD-O2D
2	D	2003	HEM	CAA-CBA-CGA-O2A
2	C	2002	HEM	CAD-CBD-CGD-O1D
2	D	2003	HEM	CAA-CBA-CGA-O1A
2	A	2000	HEM	CAD-CBD-CGD-O2D
2	C	2002	HEM	CAA-CBA-CGA-O2A

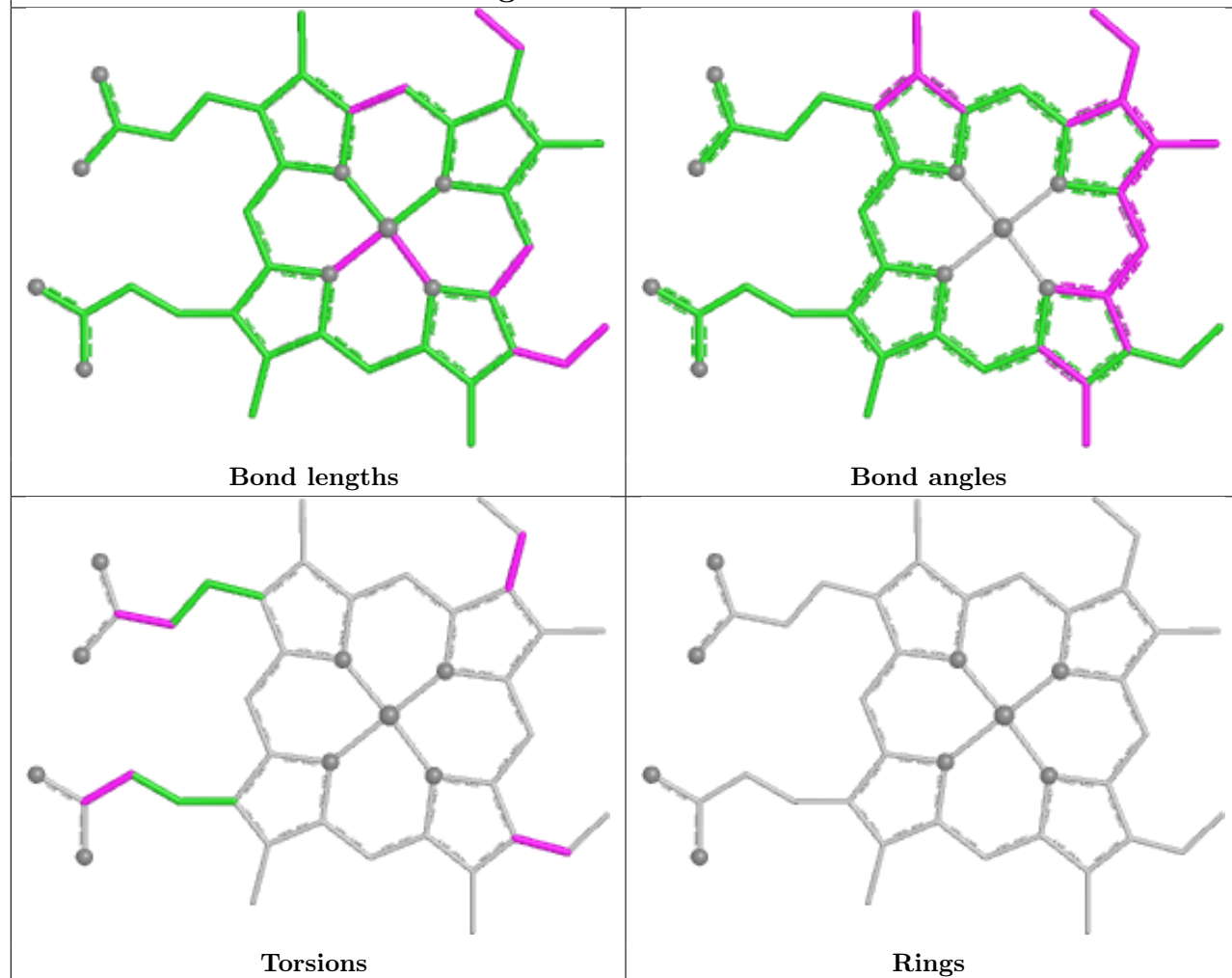
There are no ring outliers.

5 monomers are involved in 47 short contacts:

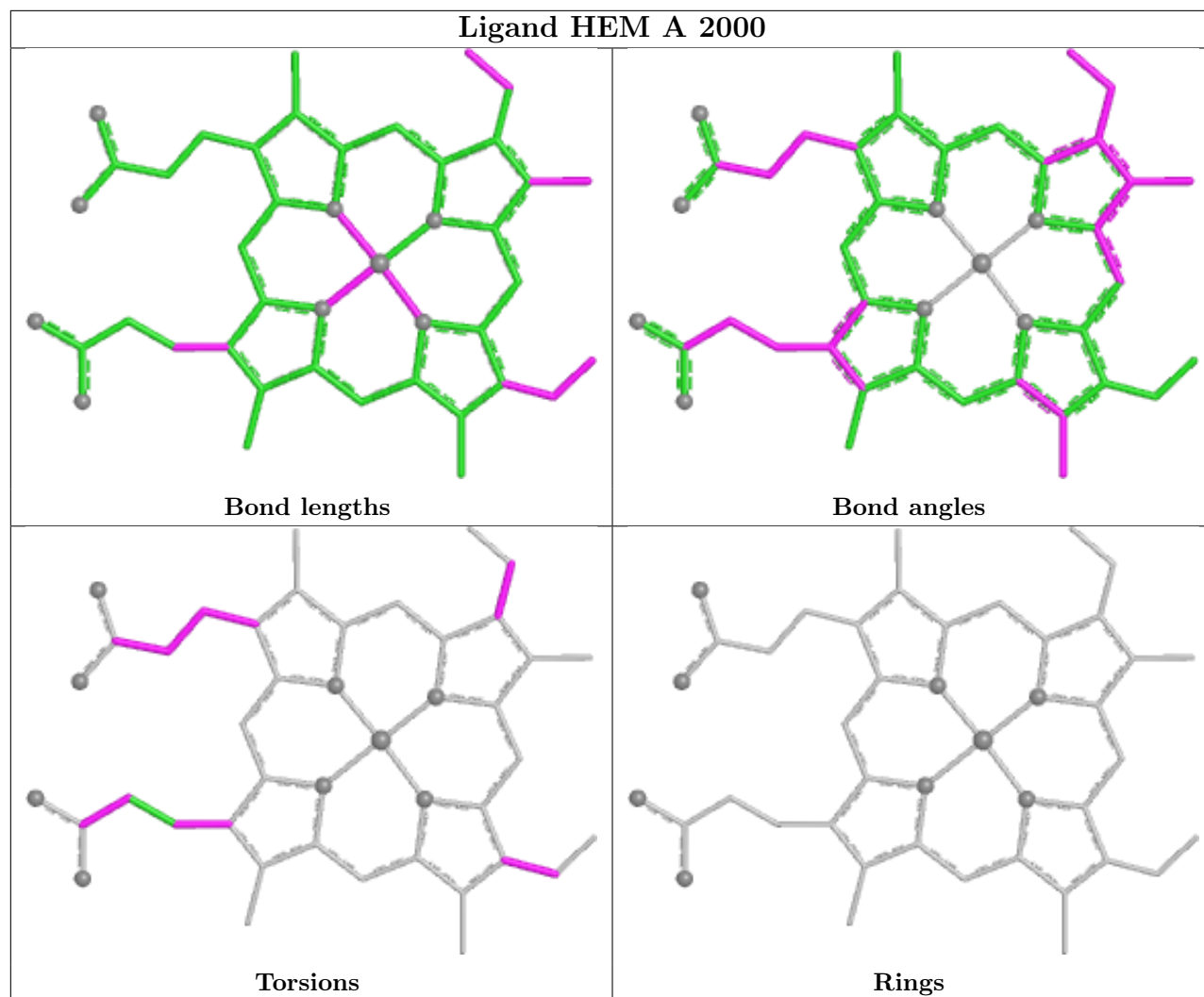
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2003	HEM	2	0
2	A	2000	HEM	17	0
2	B	2001	HEM	19	0
3	D	3000	AZI	1	0
2	C	2002	HEM	9	0

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

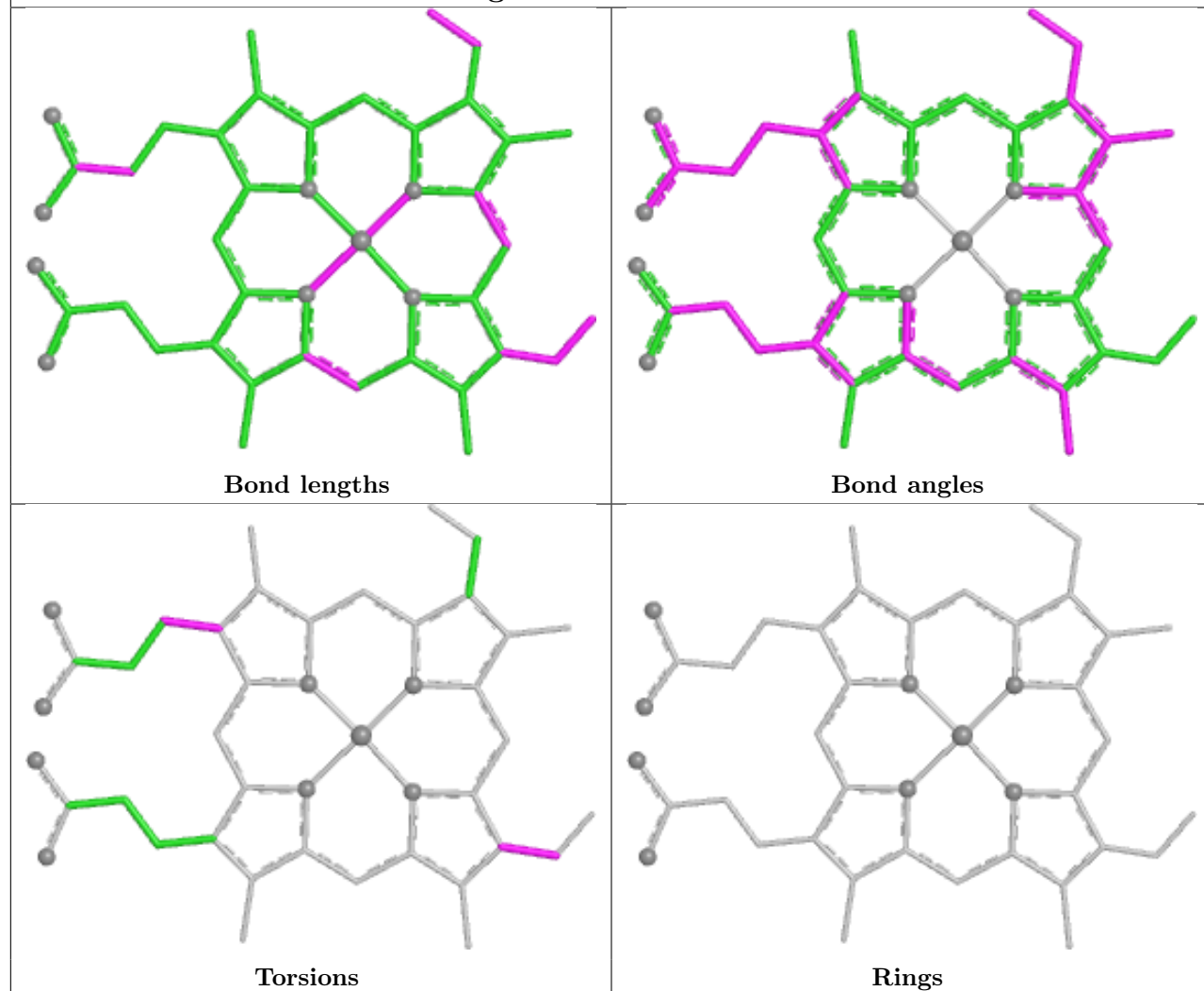
Ligand HEM D 2003

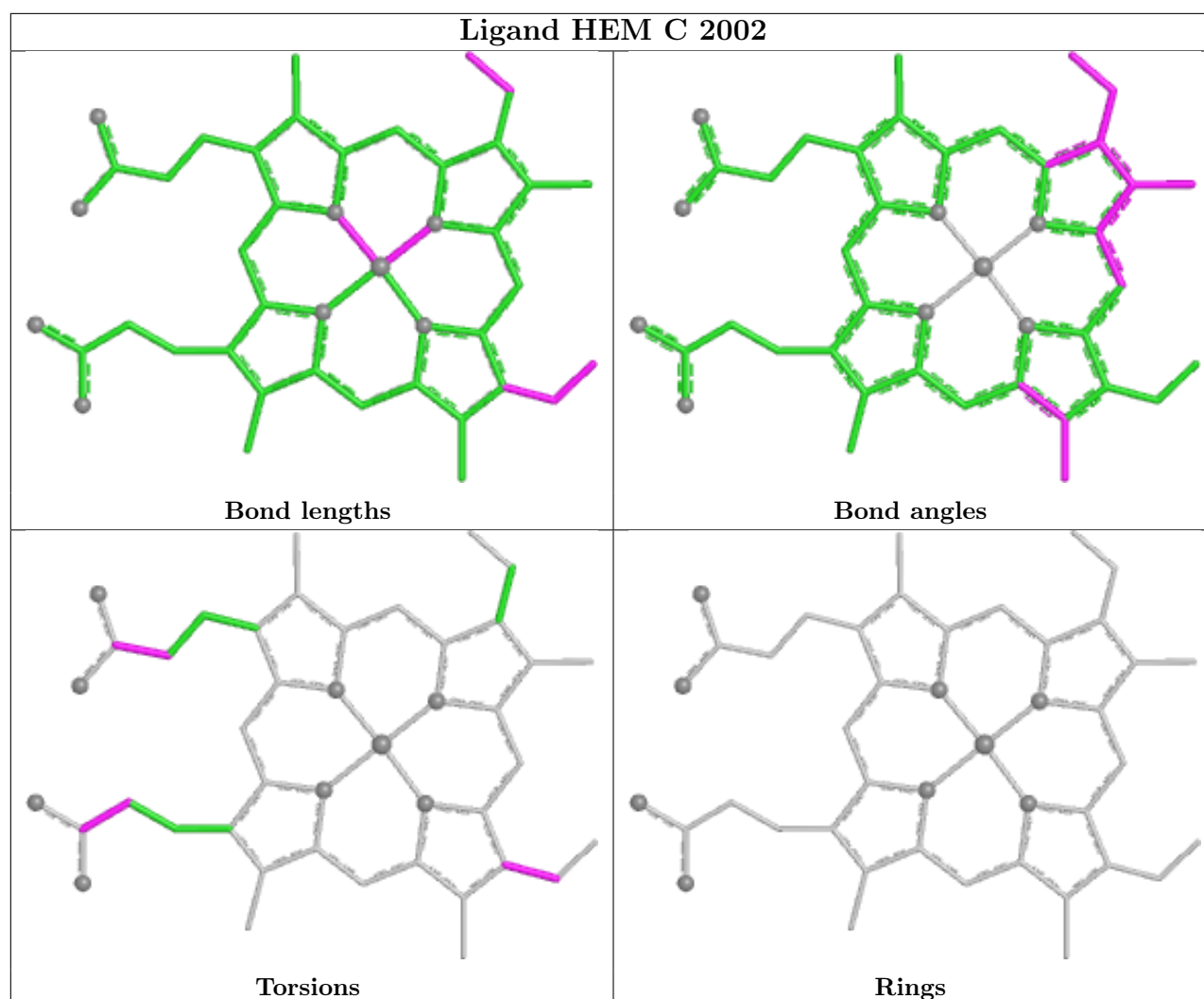


Ligand HEM A 2000



Ligand HEM B 2001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	20:ALA	C	21:GLN	N	1.04

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%)	0.01	7 (1%) 73 64	14, 43, 76, 97	0
1	B	499/506 (98%)	0.28	4 (0%) 82 75	22, 52, 83, 100	0
1	C	499/506 (98%)	0.20	10 (2%) 65 56	19, 48, 86, 100	1 (0%)
1	D	499/506 (98%)	0.26	13 (2%) 57 47	20, 51, 87, 99	0
All	All	1996/2024 (98%)	0.19	34 (1%) 69 60	14, 48, 83, 100	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	424	PHE	3.4
1	C	427	ASP	3.4
1	C	426	GLY	3.3
1	D	420	HIS	3.0
1	D	417	ALA	3.0
1	C	424	PHE	3.0
1	A	20	ALA	3.0
1	A	501	GLU	2.9
1	D	465	HIS	2.8
1	A	415	PRO	2.5
1	D	423	HIS	2.5
1	D	422	THR	2.5
1	D	216	SER	2.4
1	C	486	PRO	2.4
1	C	425	SER	2.4
1	D	433	SER	2.4
1	A	101	HIS	2.4
1	D	426	GLY	2.3
1	B	450	LEU	2.3
1	A	421	ARG	2.3
1	B	421	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	416	SER	2.3
1	B	501	GLU	2.2
1	D	418	LEU	2.2
1	D	19	ALA	2.2
1	C	3	ASN	2.2
1	A	413	HIS	2.1
1	C	495	LEU	2.1
1	B	489	GLY	2.1
1	D	228	ALA	2.1
1	C	501	GLU	2.1
1	A	465	HIS	2.0
1	C	421	ARG	2.0
1	D	20	ALA	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](#)

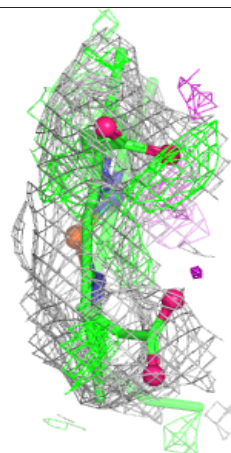
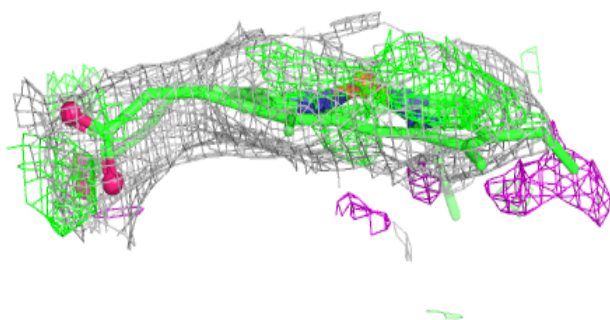
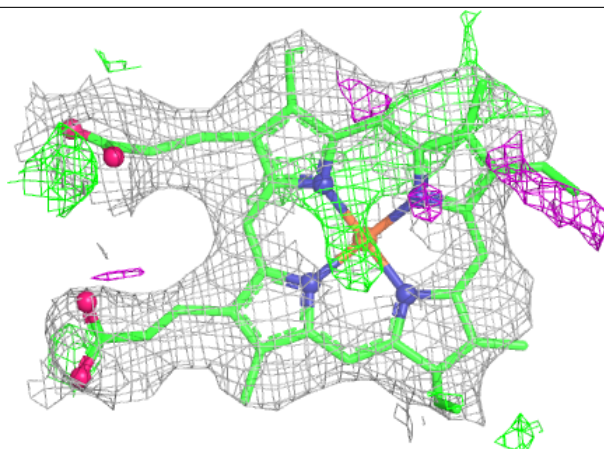
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	AZI	D	3000	3/3	0.87	0.14	58,58,67,76	0
2	HEM	A	2000	43/43	0.93	0.17	36,55,79,91	0
2	HEM	B	2001	43/43	0.94	0.14	34,47,74,93	0
2	HEM	D	2003	43/43	0.95	0.13	44,60,77,81	0
2	HEM	C	2002	43/43	0.95	0.12	20,53,70,77	0

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

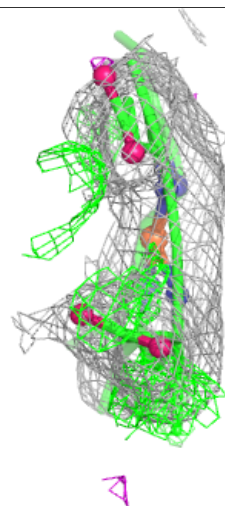
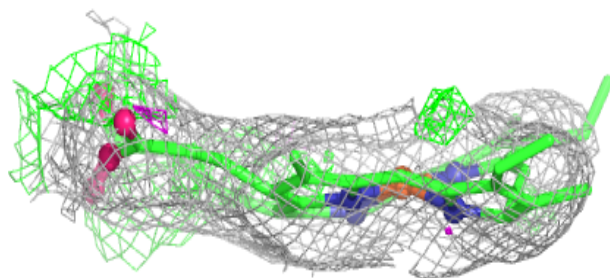
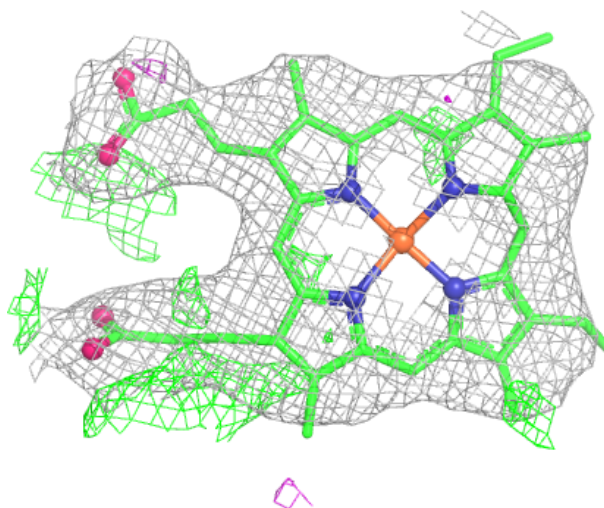
Electron density around HEM A 2000:

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



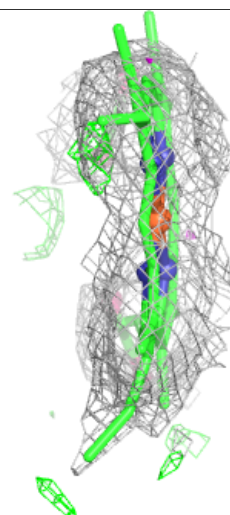
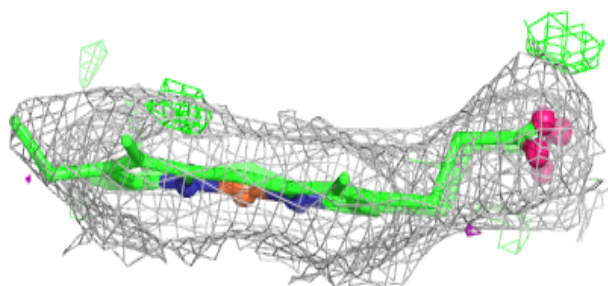
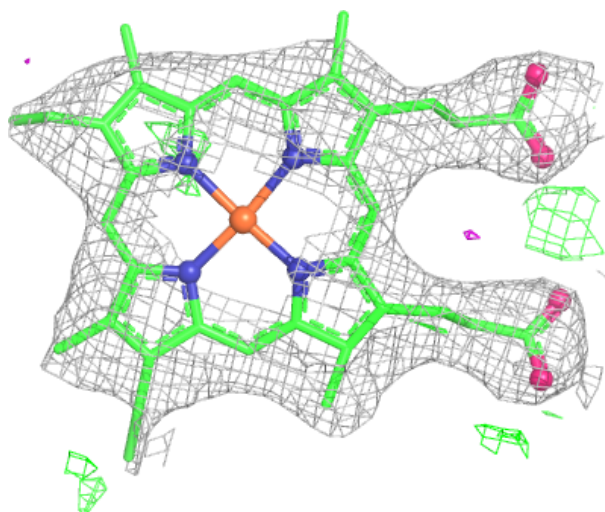
Electron density around HEM B 2001:

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



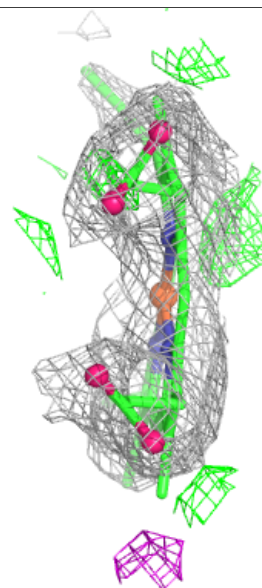
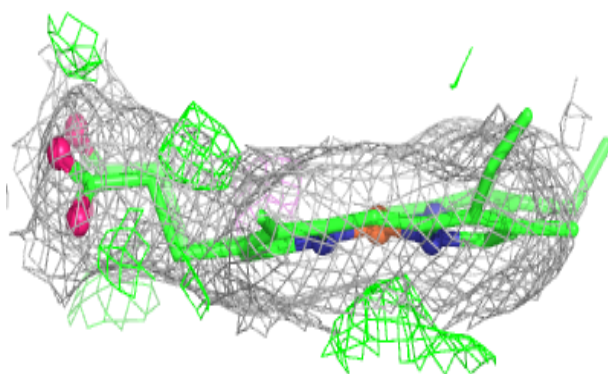
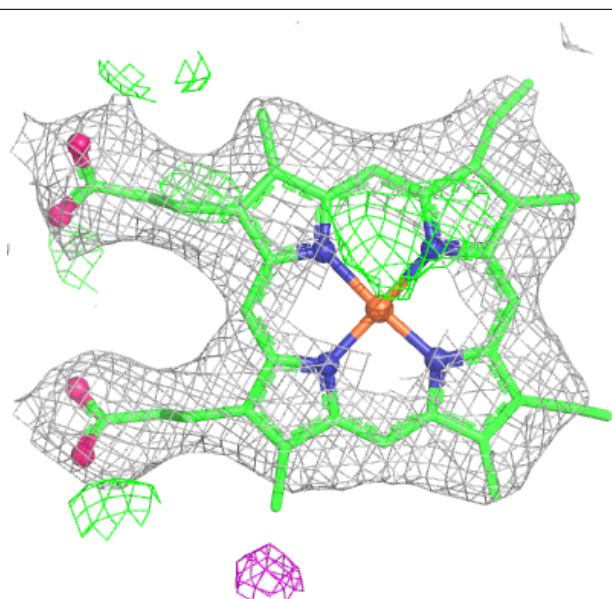
Electron density around HEM D 2003:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.