



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:04 AM UTC

PDB ID : 2PCB / pdb\_00002pcb  
Title : CRYSTAL STRUCTURE OF A COMPLEX BETWEEN ELECTRON TRANSFER PARTNERS, CYTOCHROME C PEROXIDASE AND CYTOCHROME C  
Authors : Pelletier, H.; Kraut, J.  
Deposited on : 1993-04-14  
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](mailto: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>.

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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

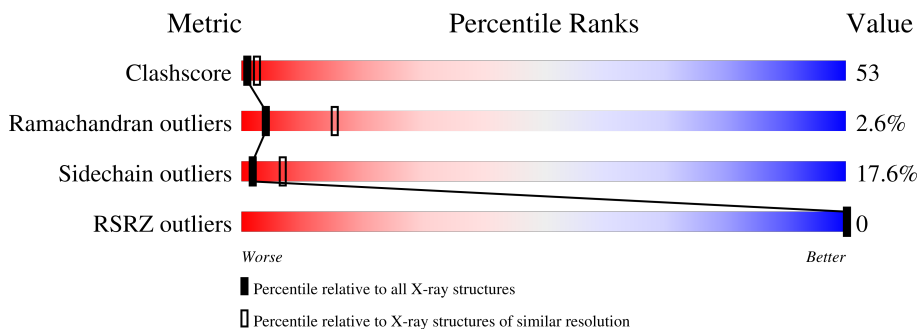
# 1 Overall quality at a glance

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))
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  $\geq 3$ , 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	296	
1	C	296	
2	B	104	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6031 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 CYTOCHROME C PEROXIDASE (CCP).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2371	1514	395	456	6	0	0	0
1	C	294	2371	1514	395	456	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	conflict	UNP P00431
A	152	GLY	ASP	conflict	UNP P00431
C	53	ILE	THR	conflict	UNP P00431
C	152	GLY	ASP	conflict	UNP P00431

- Molecule 2 is a protein called CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	104	823	524	144	151	4	0	0	0

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



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

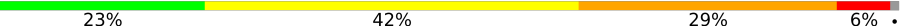
- Molecule 4 is water.

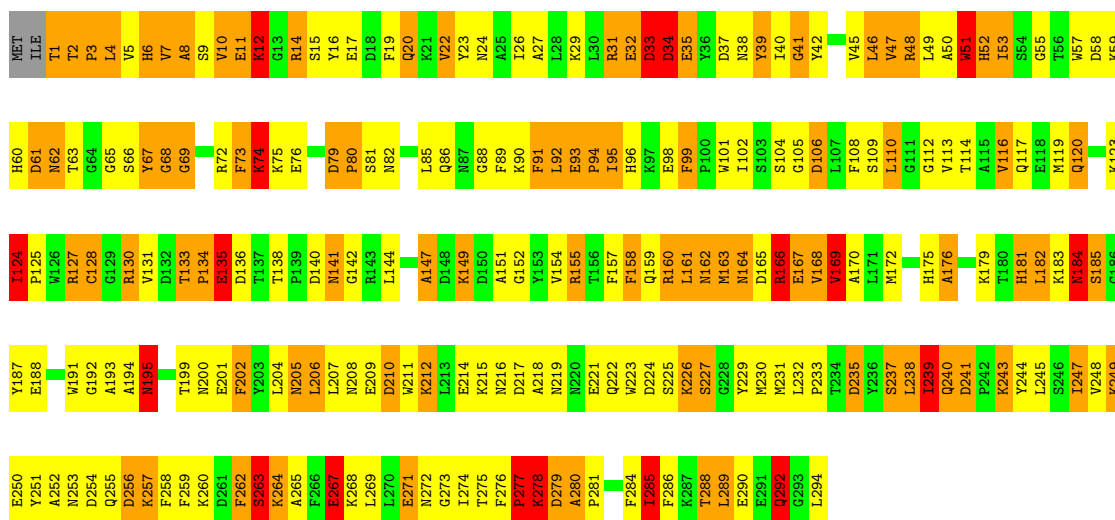
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	146	146	146	0	0
4	B	41	41	41	0	0
4	C	150	150	150	0	0

### 3 Residue-property plots

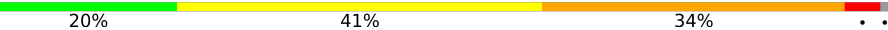
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

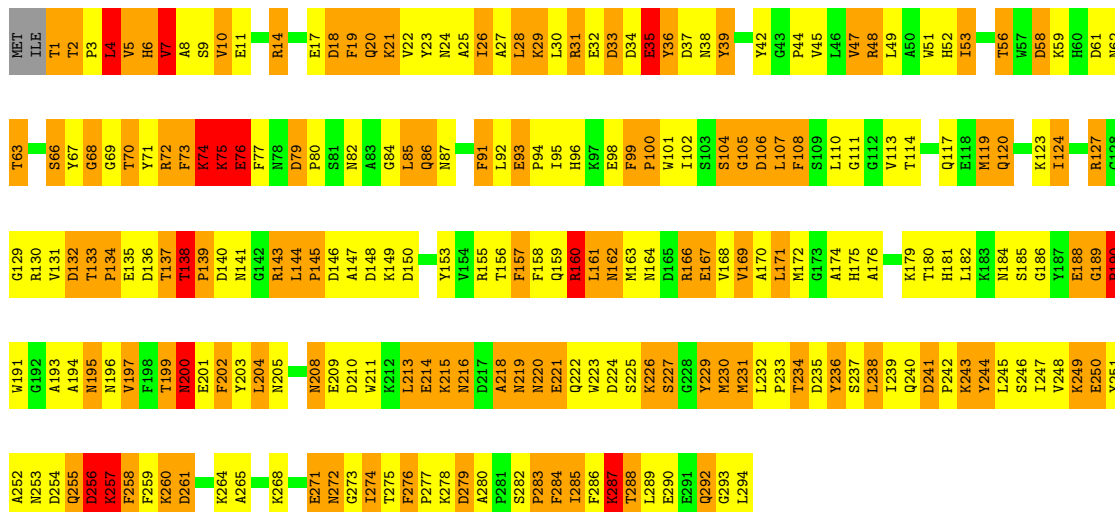
#### • Molecule 1: CYTOCHROME C PEROXIDASE (CCP)

Chain A: 



#### • Molecule 1: CYTOCHROME C PEROXIDASE (CCP)

Chain C: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.30Å 105.30Å 186.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80 6.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.80) 83.4 (6.00-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.82Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.178 , (Not available) 0.172 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 152.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.46	10/2438 (0.4%)	2.75	234/3302 (7.1%)
1	C	1.44	5/2438 (0.2%)	2.81	256/3302 (7.8%)
2	B	1.31	2/839 (0.2%)	2.70	73/1118 (6.5%)
All	All	1.43	17/5715 (0.3%)	2.77	563/7722 (7.3%)

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	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	LYS	CA-C	-11.24	1.47	1.53
1	A	192	GLY	N-CA	9.75	1.56	1.44
2	B	27	LYS	N-CA	9.11	1.51	1.46
1	A	193	ALA	C-O	7.28	1.32	1.24
1	C	106	ASP	N-CA	6.68	1.54	1.46
1	A	124	ILE	CA-CB	5.96	1.58	1.54
1	A	263	SER	N-CA	5.89	1.53	1.46
1	A	199	THR	CA-CB	5.59	1.61	1.53
1	A	224	ASP	N-CA	5.49	1.52	1.46
1	A	274	ILE	CA-CB	5.37	1.60	1.54
1	A	175	HIS	CG-CD2	5.33	1.41	1.35
2	B	24	GLY	CA-C	5.32	1.56	1.51
1	C	107	LEU	C-O	5.29	1.30	1.24
1	C	5	VAL	CA-C	5.24	1.59	1.52
1	A	123	LYS	C-N	-5.20	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	LYS	N-CA	5.03	1.52	1.46
1	A	134	PRO	C-N	-5.02	1.26	1.33

All (563) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	ASP	CA-CB-CG	17.70	130.30	112.60
1	A	73	PHE	CA-CB-CG	14.81	128.62	113.80
1	A	241	ASP	CA-CB-CG	13.54	126.14	112.60
1	A	106	ASP	CA-CB-CG	13.14	125.74	112.60
1	A	218	ALA	CA-C-N	12.98	141.30	122.35
1	A	218	ALA	C-N-CA	12.98	141.30	122.35
1	C	209	GLU	CA-C-N	12.42	140.74	123.11
1	C	209	GLU	C-N-CA	12.42	140.74	123.11
1	C	149	LYS	N-CA-C	12.18	120.44	108.75
1	C	144	LEU	CB-CA-C	11.97	127.07	109.11
2	B	62	GLU	CB-CG-CD	11.83	132.70	112.60
1	A	223	TRP	CA-C-O	-11.78	107.26	120.69
1	A	164	ASN	CA-CB-CG	11.69	124.29	112.60
1	C	279	ASP	CA-CB-CG	-11.68	100.92	112.60
2	B	91	ARG	NE-CZ-NH1	11.30	132.80	121.50
1	A	208	ASN	CA-CB-CG	-11.30	101.30	112.60
1	C	201	GLU	CA-C-N	11.18	135.63	120.54
1	C	201	GLU	C-N-CA	11.18	135.63	120.54
2	B	103	ASN	CA-CB-CG	11.17	123.77	112.60
1	C	218	ALA	N-CA-C	-11.10	99.75	113.18
1	A	210	ASP	CA-CB-CG	-11.01	101.59	112.60
1	C	195	ASN	CA-CB-CG	-10.90	101.70	112.60
1	C	260	LYS	O-C-N	10.81	133.27	122.03
2	B	20	VAL	CB-CA-C	10.71	120.49	111.06
1	A	159	GLN	CA-CB-CG	10.64	135.37	114.10
1	C	18	ASP	CA-CB-CG	10.61	123.21	112.60
1	C	127	ARG	CA-C-O	-10.53	108.55	120.66
1	C	34	ASP	CA-CB-CG	10.52	123.12	112.60
1	C	119	MET	CA-C-O	10.31	132.11	119.95
1	C	7	VAL	CB-CA-C	10.27	124.81	110.84
1	C	271	GLU	CB-CG-CD	10.21	129.96	112.60
1	A	99	PHE	O-C-N	10.13	130.64	121.42
1	C	99	PHE	O-C-N	10.10	128.56	121.19
1	A	17	GLU	CB-CG-CD	10.06	129.70	112.60
1	C	166	ARG	CD-NE-CZ	-9.97	110.44	124.40
1	A	141	ASN	CA-CB-CG	9.90	122.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ASN	CA-CB-CG	9.83	122.43	112.60
1	A	154	VAL	CA-C-O	-9.77	110.50	120.85
1	C	91	PHE	CA-C-O	-9.76	110.65	120.70
1	C	215	LYS	CA-C-O	-9.72	110.97	121.56
1	C	148	ASP	CA-CB-CG	9.71	122.31	112.60
1	A	79	ASP	CA-C-O	9.66	128.83	119.75
1	A	155	ARG	NE-CZ-NH1	-9.66	111.84	121.50
1	A	79	ASP	CA-CB-CG	9.59	122.19	112.60
1	A	254	ASP	CA-CB-CG	-9.38	103.22	112.60
1	A	253	ASN	N-CA-C	9.37	124.04	112.23
1	A	14	ARG	CA-C-O	9.33	131.69	121.05
1	A	82	ASN	OD1-CG-ND2	9.32	131.92	122.60
1	C	32	GLU	CB-CG-CD	9.32	128.44	112.60
1	C	287	LYS	O-C-N	9.21	133.37	123.06
1	C	91	PHE	O-C-N	9.16	131.99	122.09
1	A	74	LYS	N-CA-CB	9.14	125.94	110.49
1	C	150	ASP	CA-C-O	-9.09	111.59	121.31
1	A	181	HIS	CA-CB-CG	-9.02	104.78	113.80
1	A	22	VAL	CB-CA-C	9.01	123.41	111.88
1	A	37	ASP	CA-C-N	9.01	135.50	122.35
1	A	37	ASP	C-N-CA	9.01	135.50	122.35
1	A	74	LYS	CA-C-O	-8.97	107.68	120.51
1	C	260	LYS	N-CA-CB	8.96	122.99	109.91
1	C	72	ARG	NE-CZ-NH2	-8.93	111.17	119.20
1	A	267	GLU	CB-CG-CD	8.92	127.76	112.60
1	C	169	VAL	CA-C-O	-8.91	111.04	120.57
1	A	194	ALA	CA-C-O	-8.90	111.42	121.39
1	A	184	ASN	N-CA-CB	8.89	125.26	110.33
1	A	158	PHE	CA-CB-CG	-8.85	104.95	113.80
1	A	33	ASP	CA-CB-CG	-8.80	103.80	112.60
1	A	98	GLU	CB-CG-CD	8.66	127.32	112.60
1	C	19	PHE	CA-CB-CG	-8.62	105.18	113.80
1	A	286	PHE	O-C-N	8.58	132.66	122.96
1	C	86	GLN	CA-C-O	8.55	129.76	120.10
1	C	61	ASP	N-CA-CB	-8.54	98.65	110.95
2	B	42	GLN	N-CA-C	8.40	122.02	111.69
1	C	221	GLU	CA-CB-CG	8.36	130.82	114.10
1	A	20	GLN	CB-CG-CD	8.35	126.80	112.60
2	B	62	GLU	CB-CA-C	8.33	124.14	110.81
1	C	31	ARG	CD-NE-CZ	-8.32	112.75	124.40
1	A	75	LYS	CA-CB-CG	8.32	130.74	114.10
1	C	284	PHE	CA-C-O	-8.30	111.59	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	HIS	CA-CB-CG	-8.30	105.50	113.80
1	A	69	GLY	CA-C-N	8.28	135.63	121.14
1	A	69	GLY	C-N-CA	8.28	135.63	121.14
1	C	141	ASN	CA-CB-CG	8.27	120.87	112.60
1	A	219	ASN	CB-CA-C	8.27	122.88	111.63
1	C	136	ASP	CA-CB-CG	-8.26	104.34	112.60
2	B	91	ARG	CD-NE-CZ	8.23	135.93	124.40
1	A	109	SER	CA-C-O	-8.22	111.71	120.42
1	A	41	GLY	CA-C-O	-8.22	112.15	122.59
1	A	53	ILE	CA-C-N	8.22	134.63	120.58
1	A	53	ILE	C-N-CA	8.22	134.63	120.58
1	A	273	GLY	CA-C-O	8.17	127.70	119.04
1	C	10	VAL	CA-C-O	-8.14	110.60	120.78
1	C	287	LYS	CA-CB-CG	8.13	130.36	114.10
1	A	39	TYR	CA-CB-CG	-8.12	99.29	113.90
1	C	35	GLU	CA-CB-CG	8.10	130.30	114.10
1	A	142	GLY	N-CA-C	8.08	128.34	115.08
1	A	40	ILE	O-C-N	8.07	132.50	121.84
1	C	137	THR	CA-C-O	8.03	128.73	119.18
1	C	20	GLN	OE1-CD-NE2	8.02	130.62	122.60
1	C	127	ARG	NE-CZ-NH1	-8.01	113.49	121.50
1	A	191	TRP	CA-C-N	-8.00	108.89	121.37
1	A	191	TRP	C-N-CA	-8.00	108.89	121.37
1	A	106	ASP	N-CA-C	-7.91	102.73	111.36
1	A	176	ALA	N-CA-C	-7.91	102.89	112.54
1	C	32	GLU	CA-CB-CG	7.90	129.90	114.10
1	C	264	LYS	CA-C-O	7.89	129.75	121.07
2	B	92	GLU	CA-CB-CG	7.88	129.86	114.10
1	C	260	LYS	CA-C-O	-7.85	112.76	121.00
1	A	278	LYS	CA-C-N	7.83	136.49	121.54
1	A	278	LYS	C-N-CA	7.83	136.49	121.54
1	C	220	ASN	CA-CB-CG	7.82	120.42	112.60
1	C	76	GLU	CA-C-O	7.82	128.42	119.27
2	B	59	TRP	CB-CA-C	7.78	124.38	111.31
1	A	184	ASN	CA-C-O	-7.78	109.24	120.13
1	C	150	ASP	O-C-N	7.77	131.31	122.99
1	C	273	GLY	N-CA-C	7.76	126.48	115.30
1	C	284	PHE	O-C-N	7.74	132.15	123.01
1	A	32	GLU	CA-CB-CG	7.71	129.53	114.10
1	A	61	ASP	CB-CA-C	7.69	123.37	109.99
2	B	47	THR	CB-CA-C	7.69	123.65	112.12
1	C	3	PRO	CA-C-N	7.67	134.12	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	PRO	C-N-CA	7.67	134.12	121.39
1	C	204	LEU	O-C-N	7.65	129.95	122.07
1	C	100	PRO	CA-C-O	7.60	130.52	119.34
2	B	24	GLY	N-CA-C	-7.60	96.37	111.34
1	C	74	LYS	O-C-N	7.57	132.66	122.59
1	A	184	ASN	O-C-N	7.56	132.10	122.19
1	A	152	GLY	O-C-N	7.55	132.52	122.70
1	C	174	ALA	O-C-N	7.54	132.46	122.43
1	C	120	GLN	CB-CG-CD	7.46	125.28	112.60
2	B	85	ILE	N-CA-C	-7.45	97.54	108.87
1	C	161	LEU	N-CA-C	-7.44	104.05	113.72
1	A	128	CYS	CA-C-O	-7.43	113.39	121.94
2	B	95	ILE	CB-CA-C	7.43	121.75	112.02
1	A	239	ILE	CA-C-O	-7.42	112.08	119.20
1	A	160	ARG	CD-NE-CZ	7.41	134.78	124.40
1	C	224	ASP	CA-C-O	-7.41	112.86	120.71
1	C	215	LYS	N-CA-C	-7.39	100.08	110.50
1	C	79	ASP	CA-CB-CG	7.38	119.98	112.60
1	C	91	PHE	N-CA-CB	7.38	120.77	110.07
1	C	196	ASN	O-C-N	7.37	128.70	121.85
1	A	154	VAL	O-C-N	7.33	129.38	121.83
1	A	34	ASP	CA-CB-CG	-7.33	105.27	112.60
1	A	22	VAL	N-CA-C	-7.30	102.70	110.36
1	C	171	LEU	CA-C-O	-7.29	113.06	121.07
1	C	211	TRP	O-C-N	7.29	132.66	123.19
1	C	272	ASN	OD1-CG-ND2	7.29	129.89	122.60
1	C	5	VAL	CB-CA-C	-7.28	99.28	110.50
1	C	87	ASN	CA-CB-CG	-7.26	105.34	112.60
2	B	82	PHE	CB-CA-C	7.25	124.03	109.68
2	B	57	ILE	CA-C-O	7.25	128.81	121.63
2	B	75	ILE	O-C-N	7.24	129.35	121.10
2	B	12	GLN	N-CA-C	7.23	118.81	111.07
1	C	158	PHE	CA-CB-CG	-7.21	106.58	113.80
1	A	131	VAL	CA-C-N	7.20	130.97	120.82
1	A	131	VAL	C-N-CA	7.20	130.97	120.82
1	C	253	ASN	CA-C-N	7.18	131.96	121.26
1	C	253	ASN	C-N-CA	7.18	131.96	121.26
1	A	253	ASN	OD1-CG-ND2	7.16	129.76	122.60
2	B	53	LYS	CB-CA-C	-7.14	98.54	110.68
1	C	38	ASN	O-C-N	7.14	131.64	122.86
1	C	75	LYS	CA-CB-CG	7.14	128.39	114.10
1	C	106	ASP	N-CA-CB	7.13	120.68	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	ALA	CA-C-N	7.13	130.70	120.79
1	C	170	ALA	C-N-CA	7.13	130.70	120.79
1	A	193	ALA	N-CA-C	7.12	120.09	111.40
1	A	155	ARG	NH1-CZ-NH2	7.12	128.55	119.30
1	A	120	GLN	CA-CB-CG	7.10	128.30	114.10
1	C	190	PRO	O-C-N	-7.09	113.06	122.64
1	C	120	GLN	CA-C-O	-7.08	112.07	120.57
1	C	61	ASP	O-C-N	7.08	129.95	122.23
1	A	209	GLU	CB-CG-CD	7.07	124.63	112.60
1	A	3	PRO	CA-C-O	7.07	133.47	120.60
1	C	278	LYS	CA-C-O	-7.04	112.31	120.20
1	C	10	VAL	O-C-N	7.03	131.36	122.57
2	B	91	ARG	N-CA-C	-7.02	103.71	111.36
1	C	210	ASP	O-C-N	7.02	131.97	123.13
1	C	26	ILE	O-C-N	7.01	129.16	121.94
1	C	68	GLY	N-CA-C	7.00	122.76	113.37
1	A	229	TYR	O-C-N	6.99	132.47	123.11
1	A	138	THR	CA-CB-CG2	6.97	122.36	110.50
1	A	20	GLN	CA-C-N	6.97	129.92	120.44
1	A	20	GLN	C-N-CA	6.97	129.92	120.44
1	A	202	PHE	CA-CB-CG	6.97	120.77	113.80
1	A	208	ASN	CA-C-O	-6.97	111.54	119.41
1	A	138	THR	O-C-N	6.95	127.22	121.31
1	A	46	LEU	N-CA-C	-6.92	102.96	111.40
1	A	240	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	A	223	TRP	O-C-N	6.91	131.13	123.04
1	C	20	GLN	O-C-N	6.91	130.08	122.20
2	B	80	MET	CA-C-N	6.90	130.18	122.59
2	B	80	MET	C-N-CA	6.90	130.18	122.59
1	C	138	THR	CA-C-O	6.88	126.22	119.75
1	A	27	ALA	O-C-N	6.88	130.73	122.27
1	C	36	TYR	CA-C-O	6.88	127.83	120.95
1	C	244	TYR	N-CA-C	-6.88	103.71	111.14
1	A	6	HIS	CA-C-O	-6.86	112.97	120.24
1	C	211	TRP	CA-C-O	-6.85	113.37	121.11
2	B	16	GLN	N-CA-C	-6.85	104.79	113.01
1	C	37	ASP	CA-C-O	-6.85	113.47	122.03
1	A	155	ARG	CA-C-O	6.83	127.99	120.82
1	C	258	PHE	O-C-N	-6.82	115.00	122.09
1	A	106	ASP	CB-CA-C	6.82	122.44	110.85
1	A	221	GLU	CA-C-O	-6.82	113.46	121.16
1	C	93	GLU	CA-C-O	6.82	124.85	118.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASP	CB-CA-C	6.81	120.32	109.62
1	C	240	GLN	OE1-CD-NE2	-6.81	115.79	122.60
1	C	113	VAL	N-CA-C	6.80	116.95	110.42
1	C	234	THR	CA-CB-OG1	6.79	119.79	109.60
1	C	226	LYS	O-C-N	6.78	129.93	122.20
1	C	145	PRO	O-C-N	6.77	131.16	123.04
1	C	226	LYS	CA-C-O	-6.76	112.62	120.20
1	C	231	MET	O-C-N	-6.76	114.41	123.19
1	C	265	ALA	O-C-N	6.75	129.03	122.07
2	B	57	ILE	CB-CA-C	6.74	121.69	110.30
1	C	104	SER	CA-C-O	6.72	128.09	120.90
1	C	253	ASN	N-CA-CB	-6.71	99.93	110.46
1	A	199	THR	CA-C-O	-6.69	114.25	121.14
1	C	197	VAL	N-CA-CB	6.69	121.89	111.99
2	B	85	ILE	CA-C-O	-6.67	112.55	121.02
1	A	95	ILE	CA-C-O	6.67	128.24	121.17
1	A	48	ARG	O-C-N	-6.65	112.96	122.41
1	C	117	GLN	O-C-N	6.64	129.00	122.09
1	A	39	TYR	O-C-N	6.63	131.85	121.91
2	B	24	GLY	O-C-N	6.62	127.52	123.35
1	C	276	PHE	CA-C-N	6.62	126.64	119.89
1	C	276	PHE	C-N-CA	6.62	126.64	119.89
1	A	285	ILE	O-C-N	6.62	128.93	122.97
1	C	148	ASP	CA-C-N	-6.62	116.05	123.13
1	C	148	ASP	C-N-CA	-6.62	116.05	123.13
1	C	196	ASN	N-CA-CB	6.61	121.95	110.65
1	A	52	HIS	CA-C-O	-6.60	112.80	120.20
1	A	31	ARG	CA-CB-CG	6.60	127.30	114.10
1	C	254	ASP	CB-CA-C	-6.60	102.40	111.51
1	A	262	PHE	CA-C-N	-6.60	111.34	120.38
1	A	262	PHE	C-N-CA	-6.60	111.34	120.38
2	B	86	LYS	CB-CA-C	6.58	119.69	109.03
1	A	230	MET	CA-C-N	6.58	131.69	121.76
1	A	230	MET	C-N-CA	6.58	131.69	121.76
1	C	56	THR	CA-C-N	6.58	130.05	120.71
1	C	56	THR	C-N-CA	6.58	130.05	120.71
1	C	224	ASP	O-C-N	6.55	131.53	123.21
1	C	160	ARG	NE-CZ-NH1	6.55	128.05	121.50
1	C	106	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	144	LEU	O-C-N	6.54	128.85	121.53
1	A	285	ILE	N-CA-C	-6.53	95.88	107.18
1	C	157	PHE	CA-C-O	6.53	127.88	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	LYS	N-CA-C	-6.52	99.95	110.32
1	C	264	LYS	CA-C-N	6.52	128.92	120.44
1	C	264	LYS	C-N-CA	6.52	128.92	120.44
1	A	128	CYS	N-CA-C	-6.52	102.12	110.53
1	C	190	PRO	CA-C-O	6.51	132.45	120.60
1	C	52	HIS	CA-CB-CG	-6.50	107.30	113.80
2	B	20	VAL	CA-C-O	6.50	124.75	119.29
1	C	175	HIS	CA-CB-CG	6.49	120.29	113.80
1	A	92	LEU	N-CA-C	6.48	118.43	111.36
2	B	70	ASN	N-CA-CB	-6.48	103.06	111.09
1	A	240	GLN	CA-CB-CG	6.48	127.05	114.10
1	C	213	LEU	CB-CA-C	6.47	120.39	109.84
1	C	166	ARG	CB-CA-C	6.46	121.51	110.79
1	A	117	GLN	O-C-N	-6.46	115.38	122.09
1	C	241	ASP	CB-CA-C	6.45	117.65	108.68
1	C	184	ASN	CA-CB-CG	6.44	119.04	112.60
2	B	2	ASP	CA-C-O	6.43	129.31	121.72
1	A	51	TRP	CA-C-N	-6.43	111.00	120.38
1	A	51	TRP	C-N-CA	-6.43	111.00	120.38
1	A	47	VAL	O-C-N	-6.42	115.41	121.90
1	A	76	GLU	CB-CG-CD	6.42	123.52	112.60
1	C	32	GLU	CA-C-O	-6.42	113.75	120.55
2	B	54	ASN	CB-CA-C	6.41	123.71	110.31
1	A	8	ALA	CA-C-O	-6.41	114.82	121.87
1	C	283	PRO	O-C-N	6.40	130.78	123.10
1	C	246	SER	CA-C-O	-6.39	112.62	119.97
1	A	51	TRP	CB-CA-C	6.39	121.52	110.79
1	A	140	ASP	CA-CB-CG	-6.38	106.22	112.60
1	C	39	TYR	N-CA-C	6.38	120.38	112.47
1	A	49	LEU	N-CA-C	-6.35	103.88	111.69
1	A	191	TRP	N-CA-C	-6.35	105.36	113.23
1	C	21	LYS	N-CA-C	-6.35	104.44	111.36
2	B	66	GLU	CB-CG-CD	6.34	123.38	112.60
1	C	101	TRP	CA-CB-CG	6.32	125.61	113.60
2	B	53	LYS	O-C-N	6.32	128.81	122.12
1	A	288	THR	CA-C-N	6.31	129.06	120.54
1	A	288	THR	C-N-CA	6.31	129.06	120.54
1	A	93	GLU	N-CA-C	6.29	122.07	113.77
1	A	238	LEU	CA-C-O	-6.29	113.15	120.20
1	A	116	VAL	CB-CA-C	6.27	119.65	111.81
1	C	117	GLN	CA-C-O	-6.27	114.19	120.90
1	A	193	ALA	O-C-N	-6.26	114.59	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ILE	N-CA-CB	6.25	120.86	110.86
2	B	81	ILE	N-CA-CB	6.24	118.38	111.89
1	C	155	ARG	N-CA-C	-6.24	104.11	111.03
1	A	141	ASN	N-CA-C	-6.23	102.14	110.24
2	B	104	GLU	CA-CB-CG	6.23	126.55	114.10
1	A	280	ALA	O-C-N	6.22	128.47	121.94
1	C	167	GLU	CB-CG-CD	6.22	123.17	112.60
2	B	23	GLY	CA-C-O	6.21	127.45	119.68
1	A	37	ASP	N-CA-C	6.20	119.73	111.30
1	C	208	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	C	133	THR	CA-C-N	6.19	126.16	120.03
1	C	133	THR	C-N-CA	6.19	126.16	120.03
1	C	110	LEU	CA-C-O	-6.19	113.86	120.42
1	A	61	ASP	N-CA-CB	-6.18	101.59	110.80
1	A	67	TYR	N-CA-C	6.17	117.70	110.97
1	C	148	ASP	CA-C-O	-6.17	112.31	119.59
1	C	271	GLU	CA-CB-CG	6.17	126.44	114.10
1	C	105	GLY	CA-C-O	-6.16	112.23	119.50
1	C	290	GLU	O-C-N	6.14	128.72	122.09
1	C	111	GLY	O-C-N	-6.14	116.30	122.19
1	C	58	ASP	CB-CG-OD2	-6.13	104.29	118.40
1	C	287	LYS	CB-CG-CD	6.11	125.36	111.30
1	A	163	MET	CA-CB-CG	6.11	126.31	114.10
1	A	131	VAL	CA-C-O	-6.10	113.98	120.39
1	A	161	LEU	CA-C-O	-6.09	114.10	120.32
1	C	286	PHE	CA-CB-CG	6.09	119.89	113.80
1	C	208	ASN	CB-CA-C	6.08	122.70	109.99
1	C	127	ARG	CD-NE-CZ	-6.08	115.89	124.40
1	C	185	SER	N-CA-C	6.07	122.79	113.19
2	B	50	ASP	O-C-N	6.07	130.67	122.59
1	C	87	ASN	CA-C-O	-6.07	114.45	120.82
1	C	105	GLY	N-CA-C	-6.07	106.82	114.16
2	B	70	ASN	N-CA-C	6.06	120.96	108.71
1	C	132	ASP	CA-CB-CG	6.06	118.66	112.60
1	C	184	ASN	N-CA-C	-6.06	105.92	113.55
1	A	265	ALA	O-C-N	6.05	129.71	122.27
1	C	32	GLU	CG-CD-OE1	6.05	132.32	118.40
1	A	46	LEU	CB-CA-C	6.04	120.94	110.79
1	C	288	THR	O-C-N	6.04	129.86	123.03
1	A	214	GLU	O-C-N	6.04	130.47	123.17
1	A	135	GLU	CA-CB-CG	6.03	126.17	114.10
2	B	17	CYS	N-CA-C	6.02	123.40	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	THR	O-C-N	6.02	131.17	123.11
1	A	205	ASN	N-CA-C	-6.01	104.72	111.28
1	C	181	HIS	O-C-N	6.01	130.30	123.27
1	C	160	ARG	CD-NE-CZ	6.00	132.80	124.40
1	C	48	ARG	N-CA-C	-6.00	103.50	111.24
1	A	248	VAL	O-C-N	5.99	127.78	121.91
1	A	280	ALA	CA-C-N	5.99	126.46	119.99
1	A	280	ALA	C-N-CA	5.99	126.46	119.99
1	A	169	VAL	O-C-N	5.97	127.66	121.87
1	C	99	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A	68	GLY	CA-C-O	-5.94	112.49	119.50
2	B	72	LYS	O-C-N	5.93	128.43	122.03
1	A	223	TRP	CA-CB-CG	-5.93	102.34	113.60
1	A	66	SER	CA-C-N	5.91	128.46	120.65
1	A	66	SER	C-N-CA	5.91	128.46	120.65
1	A	162	ASN	CA-C-N	-5.91	113.84	122.65
1	A	162	ASN	C-N-CA	-5.91	113.84	122.65
2	B	26	HIS	CA-C-O	-5.91	113.86	120.54
1	A	166	ARG	CA-C-N	5.89	130.55	120.71
1	A	166	ARG	C-N-CA	5.89	130.55	120.71
1	A	24	ASN	CB-CG-ND2	5.89	125.23	116.40
1	A	176	ALA	O-C-N	5.88	130.32	122.43
1	C	213	LEU	O-C-N	-5.88	116.16	123.04
1	C	184	ASN	O-C-N	5.88	130.94	122.13
1	A	94	PRO	O-C-N	5.87	129.27	122.23
1	A	14	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	A	22	VAL	O-C-N	-5.86	116.08	121.94
1	A	264	LYS	CA-C-O	5.83	127.49	121.07
1	A	105	GLY	CA-C-N	-5.83	112.01	120.29
1	A	105	GLY	C-N-CA	-5.83	112.01	120.29
1	C	58	ASP	CA-CB-CG	-5.82	106.78	112.60
1	A	237	SER	CA-CB-OG	-5.81	99.48	111.10
1	C	108	PHE	O-C-N	-5.81	115.96	122.12
1	C	56	THR	N-CA-C	-5.78	105.72	112.89
1	C	205	ASN	CB-CG-OD1	5.78	132.36	120.80
1	A	159	GLN	CB-CA-C	5.78	121.77	110.67
2	B	41	GLY	N-CA-C	-5.78	103.36	113.76
1	C	257	LYS	N-CA-C	-5.77	104.91	111.14
2	B	27	LYS	N-CA-C	-5.76	104.05	108.78
1	A	133	THR	CA-C-O	5.76	127.63	120.54
1	A	68	GLY	O-C-N	5.76	129.19	122.68
1	C	284	PHE	CB-CA-C	-5.75	99.81	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	68	LEU	CB-CA-C	5.74	122.42	110.32
1	A	211	TRP	CA-CB-CG	-5.72	102.73	113.60
1	A	40	ILE	N-CA-C	-5.71	104.77	111.00
2	B	46	PHE	CA-CB-CG	5.71	119.51	113.80
1	C	145	PRO	CA-C-O	-5.70	114.62	122.15
1	C	73	PHE	O-C-N	5.70	129.65	123.10
1	A	95	ILE	CB-CG1-CD1	5.68	125.74	113.80
1	C	254	ASP	N-CA-C	5.68	117.23	107.28
1	C	202	PHE	O-C-N	5.68	128.00	122.09
1	C	134	PRO	N-CD-CG	-5.66	94.72	103.20
1	C	25	ALA	CA-C-N	5.65	127.77	120.70
1	C	25	ALA	C-N-CA	5.65	127.77	120.70
2	B	13	LYS	CA-C-O	-5.65	112.84	119.05
1	A	155	ARG	CB-CA-C	-5.64	102.02	110.88
1	A	167	GLU	CB-CG-CD	5.62	122.16	112.60
1	A	226	LYS	CA-C-O	5.62	126.51	119.59
1	A	210	ASP	N-CA-CB	5.62	118.75	110.49
2	B	91	ARG	CA-C-O	5.61	126.37	120.42
2	B	91	ARG	NH1-CZ-NH2	-5.61	112.00	119.30
1	C	137	THR	N-CA-C	-5.61	106.43	113.28
1	C	9	SER	CA-C-O	-5.61	114.31	120.70
1	C	26	ILE	N-CA-C	-5.61	104.86	110.30
1	A	45	VAL	CA-C-N	-5.60	111.36	120.71
1	A	45	VAL	C-N-CA	-5.60	111.36	120.71
1	A	35	GLU	O-C-N	5.60	130.31	122.36
1	A	195	ASN	CB-CG-ND2	5.59	124.79	116.40
2	B	53	LYS	CA-CB-CG	5.59	125.28	114.10
1	C	221	GLU	CB-CG-CD	5.58	122.09	112.60
1	C	238	LEU	CB-CA-C	5.58	120.05	110.79
1	A	113	VAL	CA-CB-CG1	-5.57	100.93	110.40
2	B	38	ARG	CD-NE-CZ	5.56	132.18	124.40
1	C	162	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	256	ASP	N-CA-CB	5.55	118.76	110.22
1	C	20	GLN	CB-CA-C	-5.55	99.70	110.46
1	C	86	GLN	O-C-N	-5.55	115.73	122.22
2	B	23	GLY	CA-C-N	-5.54	117.36	122.29
2	B	23	GLY	C-N-CA	-5.54	117.36	122.29
1	C	259	PHE	CA-CB-CG	-5.54	108.26	113.80
2	B	38	ARG	N-CA-CB	5.54	120.91	111.66
1	C	106	ASP	CB-CA-C	5.54	120.09	110.79
1	A	76	GLU	CA-CB-CG	5.54	125.17	114.10
1	A	279	ASP	O-C-N	5.54	129.95	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	ASN	N-CA-C	-5.54	102.29	110.48
2	B	61	GLU	N-CA-CB	5.52	119.83	110.49
1	C	19	PHE	CA-C-O	-5.52	115.20	121.00
1	C	293	GLY	N-CA-C	-5.51	106.59	115.08
1	C	290	GLU	CA-C-O	-5.50	115.03	120.70
1	C	9	SER	O-C-N	5.50	130.16	123.01
1	A	2	THR	O-C-N	5.50	127.64	121.32
1	A	130	ARG	N-CA-C	-5.49	102.15	110.28
1	A	157	PHE	CA-C-O	-5.49	115.03	120.90
1	C	176	ALA	CA-C-N	5.49	130.22	122.09
1	C	176	ALA	C-N-CA	5.49	130.22	122.09
1	A	263	SER	CA-C-O	5.49	126.55	120.63
1	C	204	LEU	CB-CA-C	-5.49	102.27	110.88
1	C	214	GLU	CA-CB-CG	5.49	125.07	114.10
1	A	12	LYS	N-CA-CB	5.48	119.75	110.49
1	C	216	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	179	LYS	CA-C-N	-5.47	113.35	122.64
1	A	179	LYS	C-N-CA	-5.47	113.35	122.64
1	C	127	ARG	O-C-N	5.44	129.91	123.27
1	C	227	SER	CA-C-N	-5.44	116.99	123.08
1	C	227	SER	C-N-CA	-5.44	116.99	123.08
1	C	120	GLN	N-CA-CB	-5.43	104.21	112.47
1	A	157	PHE	O-C-N	5.43	127.74	122.09
2	B	25	LYS	N-CA-C	-5.42	103.33	110.43
1	A	80	PRO	N-CA-C	-5.42	106.80	113.84
1	A	248	VAL	CA-CB-CG2	5.41	119.60	110.40
1	A	264	LYS	O-C-N	-5.40	116.30	122.08
2	B	3	VAL	N-CA-C	-5.39	98.13	109.34
1	A	208	ASN	N-CA-C	5.39	119.98	113.41
1	A	241	ASP	CA-C-N	5.39	124.72	118.85
1	A	241	ASP	C-N-CA	5.39	124.72	118.85
1	A	217	ASP	CA-CB-CG	5.38	117.98	112.60
2	B	85	ILE	O-C-N	5.38	129.07	122.83
1	A	165	ASP	N-CA-C	5.38	117.90	111.71
2	B	26	HIS	O-C-N	5.38	129.35	123.22
2	B	85	ILE	CA-C-N	-5.38	113.11	122.36
2	B	85	ILE	C-N-CA	-5.38	113.11	122.36
1	A	217	ASP	CA-C-O	-5.37	112.07	119.05
2	B	53	LYS	CA-C-O	5.36	126.42	120.63
1	C	213	LEU	N-CA-CB	-5.36	101.64	109.95
1	C	156	THR	CA-C-O	-5.36	114.84	120.63
1	C	124	ILE	O-C-N	5.34	127.19	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	HIS	CA-CB-CG	5.34	119.14	113.80
1	C	219	ASN	CB-CG-ND2	-5.34	108.40	116.40
1	C	170	ALA	CA-C-O	5.33	126.25	120.55
1	C	258	PHE	CA-C-O	5.33	126.60	120.90
1	A	120	GLN	N-CA-C	-5.32	106.74	113.23
1	A	157	PHE	N-CA-CB	5.32	117.87	109.94
1	A	24	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	249	LYS	CA-C-O	5.32	126.19	120.55
1	C	34	ASP	N-CA-C	5.31	119.24	112.87
1	C	137	THR	CA-C-N	5.31	127.88	120.65
1	C	137	THR	C-N-CA	5.31	127.88	120.65
1	C	255	GLN	CA-C-O	5.30	126.36	120.63
1	A	104	SER	O-C-N	5.30	127.74	122.12
1	C	101	TRP	O-C-N	5.30	128.42	122.22
2	B	18	HIS	O-C-N	5.30	129.31	123.33
1	A	185	SER	CA-C-O	-5.29	113.16	119.35
1	C	31	ARG	NH1-CZ-NH2	5.29	126.18	119.30
1	A	99	PHE	CA-CB-CG	-5.29	108.51	113.80
1	C	75	LYS	CB-CG-CD	5.29	123.46	111.30
1	C	139	PRO	CB-CA-C	5.28	117.88	110.60
1	A	147	ALA	O-C-N	5.27	128.62	122.24
1	C	226	LYS	N-CA-CB	5.27	118.47	110.14
1	C	104	SER	O-C-N	-5.27	116.61	122.09
1	A	240	GLN	CG-CD-OE1	5.27	131.34	120.80
2	B	82	PHE	O-C-N	-5.26	117.25	123.41
1	C	2	THR	CB-CA-C	5.26	115.78	109.31
1	C	200	ASN	O-C-N	5.26	129.06	122.22
1	C	256	ASP	CA-C-O	-5.25	115.28	120.90
1	A	277	PRO	CA-C-O	5.25	130.15	120.60
1	A	14	ARG	O-C-N	-5.25	116.82	123.01
2	B	38	ARG	CA-C-O	5.25	127.00	121.33
1	A	79	ASP	O-C-N	-5.24	116.64	121.30
1	C	72	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	C	127	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	A	229	TYR	N-CA-C	-5.22	101.60	109.85
1	C	6	HIS	CA-C-N	-5.22	116.35	122.93
1	C	6	HIS	C-N-CA	-5.22	116.35	122.93
1	A	31	ARG	NE-CZ-NH2	-5.22	114.51	119.20
2	B	62	GLU	CA-CB-CG	5.21	124.52	114.10
1	C	236	TYR	CA-C-O	5.21	125.79	119.49
2	B	62	GLU	CG-CD-OE1	5.20	130.36	118.40
1	A	184	ASN	OD1-CG-ND2	5.20	127.80	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	ILE	CA-C-O	-5.19	115.73	121.29
1	A	55	GLY	CA-C-O	-5.19	112.86	119.09
1	C	63	THR	CA-CB-OG1	-5.19	101.82	109.60
1	C	214	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	33	ASP	CA-C-O	-5.17	113.11	120.51
1	A	50	ALA	O-C-N	5.17	128.05	122.11
1	C	149	LYS	O-C-N	-5.17	117.36	121.65
1	A	89	PHE	CA-CB-CG	5.16	118.96	113.80
1	C	250	GLU	CA-CB-CG	5.16	124.43	114.10
1	A	192	GLY	CA-C-N	5.16	129.33	120.71
1	A	192	GLY	C-N-CA	5.16	129.33	120.71
1	A	62	ASN	CB-CG-ND2	5.16	124.14	116.40
1	C	19	PHE	CA-C-N	5.16	127.91	120.38
1	C	19	PHE	C-N-CA	5.16	127.91	120.38
1	A	235	ASP	N-CA-C	-5.16	106.50	112.89
1	A	164	ASN	CA-C-O	-5.15	115.35	121.89
1	A	3	PRO	CA-C-N	5.15	130.87	122.07
1	A	3	PRO	C-N-CA	5.15	130.87	122.07
1	A	226	LYS	N-CA-C	-5.14	107.17	112.93
1	C	235	ASP	CA-C-N	5.14	128.82	120.60
1	C	235	ASP	C-N-CA	5.14	128.82	120.60
1	A	98	GLU	N-CA-CB	5.14	117.76	110.16
1	C	28	LEU	CA-C-O	-5.13	114.30	120.10
1	A	170	ALA	CA-C-O	-5.13	114.98	120.42
1	C	4	LEU	N-CA-CB	-5.13	102.50	110.29
1	C	120	GLN	CA-CB-CG	-5.12	103.86	114.10
1	C	1	THR	CA-CB-CG2	5.12	119.21	110.50
1	A	288	THR	N-CA-C	-5.12	103.77	110.53
1	C	276	PHE	O-C-N	5.11	126.94	121.12
1	A	119	MET	N-CA-CB	5.11	118.97	110.91
1	A	277	PRO	O-C-N	-5.10	115.75	122.64
1	A	206	LEU	CA-C-O	5.10	126.18	120.82
1	C	61	ASP	N-CA-C	-5.10	105.83	113.89
1	C	189	GLY	CA-C-N	5.09	126.20	119.84
1	C	189	GLY	C-N-CA	5.09	126.20	119.84
1	A	14	ARG	CB-CA-C	5.08	118.12	109.53
1	C	14	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	C	199	THR	N-CA-CB	5.08	120.00	110.87
2	B	94	LEU	O-C-N	5.07	129.12	122.33
1	C	170	ALA	N-CA-C	5.06	117.57	111.40
1	A	85	LEU	CA-C-O	-5.05	113.16	119.38
2	B	16	GLN	N-CA-CB	5.05	119.23	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46	PHE	CA-C-O	5.05	126.40	120.80
1	A	46	LEU	CA-C-N	-5.04	112.35	120.62
1	A	46	LEU	C-N-CA	-5.04	112.35	120.62
1	A	155	ARG	CD-NE-CZ	-5.04	117.35	124.40
1	A	149	LYS	N-CA-C	5.04	117.85	109.94
1	A	292	GLN	N-CA-C	-5.04	106.82	113.17
1	C	216	ASN	OD1-CG-ND2	-5.03	117.57	122.60
2	B	88	LYS	N-CA-CB	5.03	117.69	110.40
2	B	55	LYS	N-CA-C	-5.02	105.32	111.75
1	C	256	ASP	CA-CB-CG	-5.02	107.58	112.60
1	A	163	MET	CB-CG-SD	5.02	127.76	112.70
1	A	17	GLU	CG-CD-OE1	5.02	129.94	118.40
1	A	46	LEU	CA-C-O	-5.01	115.19	120.55
1	C	219	ASN	OD1-CG-ND2	5.01	127.61	122.60
1	C	249	LYS	CA-CB-CG	5.01	124.12	114.10
1	C	210	ASP	CB-CA-C	-5.01	102.63	110.79
1	A	3	PRO	N-CA-C	5.01	122.78	112.47
1	C	30	LEU	N-CA-C	-5.01	105.90	111.36
1	C	238	LEU	CA-C-N	-5.01	113.46	121.02
1	C	238	LEU	C-N-CA	-5.01	113.46	121.02
1	C	38	ASN	CA-C-O	-5.00	115.93	122.14
1	C	30	LEU	CA-CB-CG	5.00	133.81	116.30
1	C	159	GLN	CB-CA-C	5.00	120.77	110.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	166	ARG	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2371	0	2252	184	0
1	C	2371	0	2252	210	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	823	0	849	195	0
3	A	43	0	30	5	0
3	B	43	0	30	18	0
3	C	43	0	30	2	0
4	A	146	0	0	27	2
4	B	41	0	0	15	1
4	C	150	0	0	26	1
All	All	6031	0	5443	591	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

All (591) 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)
2:B:14:CYS:SG	3:B:105:HEM:HAB	1.79	1.22
2:B:14:CYS:SG	3:B:105:HEM:CAB	2.33	1.17
1:C:147:ALA:O	1:C:233:PRO:HD2	1.51	1.06
2:B:50:ASP:HA	2:B:53:LYS:HE2	1.42	1.02
1:C:164:ASN:ND2	1:C:167:GLU:HG3	1.74	1.02
1:C:84:GLY:H	1:C:86:GLN:NE2	1.57	1.01
2:B:41:GLY:HA2	2:B:48:TYR:CE1	1.96	1.00
1:A:195:ASN:HD22	1:A:195:ASN:H	1.09	1.00
2:B:79:LYS:HG3	3:B:105:HEM:O2D	1.63	0.98
1:C:74:LYS:HB2	1:C:74:LYS:NZ	1.77	0.97
1:A:292:GLN:HB2	1:A:294:LEU:CD1	1.96	0.96
1:C:84:GLY:H	1:C:86:GLN:HE22	1.04	0.94
1:C:26:ILE:HG22	1:C:114:THR:HG21	1.48	0.92
1:C:28:LEU:HD13	1:C:289:LEU:HD13	1.50	0.91
2:B:19:THR:HG23	2:B:27:LYS:HD3	1.53	0.91
1:C:4:LEU:HG	4:C:657:HOH:O	1.70	0.91
1:A:185:SER:HB3	3:A:295:HEM:HBA1	1.52	0.91
2:B:34:GLY:O	2:B:38:ARG:HD3	1.70	0.90
1:C:74:LYS:HB2	1:C:74:LYS:HZ1	1.33	0.90
1:C:63:THR:HA	4:C:623:HOH:O	1.72	0.90
1:C:272:ASN:HA	4:C:692:HOH:O	1.72	0.90
2:B:9:ILE:CD1	2:B:90:GLU:HG3	2.04	0.88
1:C:244:TYR:O	1:C:248:VAL:HG23	1.72	0.88
2:B:53:LYS:HB2	2:B:54:ASN:ND2	1.89	0.87
1:C:69:GLY:O	1:C:72:ARG:HG2	1.75	0.87
1:C:28:LEU:HD13	1:C:289:LEU:CD1	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ASN:HD22	2:B:54:ASN:N	1.69	0.86
1:C:230:MET:HE2	1:C:230:MET:O	1.73	0.86
1:C:69:GLY:HA2	4:C:630:HOH:O	1.75	0.86
2:B:65:MET:HE1	2:B:92:GLU:CG	2.05	0.86
1:A:176:ALA:O	4:A:303:HOH:O	1.92	0.86
1:A:35:GLU:HB2	4:A:356:HOH:O	1.72	0.86
2:B:65:MET:HE1	2:B:92:GLU:HG2	1.58	0.86
2:B:3:VAL:HG12	2:B:97:TYR:HA	1.56	0.86
1:A:10:VAL:HG13	1:A:128:CYS:SG	2.16	0.85
2:B:57:ILE:HD13	2:B:63:THR:HG21	1.58	0.85
2:B:41:GLY:HA2	2:B:48:TYR:CD1	2.12	0.84
1:A:33:ASP:N	1:A:33:ASP:OD1	2.07	0.83
1:A:216:ASN:HD22	1:A:222:GLN:NE2	1.75	0.83
1:C:20:GLN:HE22	1:C:287:LYS:H	1.22	0.83
2:B:25:LYS:HE3	2:B:27:LYS:HE2	1.61	0.83
1:C:31:ARG:HD2	4:C:608:HOH:O	1.80	0.82
1:C:215:LYS:HE3	1:C:221:GLU:OE1	1.80	0.81
1:A:292:GLN:HB2	1:A:294:LEU:HD13	1.61	0.81
1:A:1:THR:HG23	1:A:2:THR:H	1.44	0.81
1:C:20:GLN:NE2	1:C:287:LYS:H	1.79	0.81
1:C:75:LYS:HB2	4:C:619:HOH:O	1.81	0.80
1:C:161:LEU:O	1:C:162:ASN:HB3	1.82	0.80
2:B:70:ASN:OD1	2:B:72:LYS:HG3	1.81	0.80
2:B:26:HIS:CD2	2:B:31:ASN:H	2.01	0.79
2:B:41:GLY:HA2	2:B:48:TYR:CZ	2.17	0.79
2:B:9:ILE:HD11	2:B:90:GLU:HG3	1.65	0.79
1:C:191:TRP:HD1	1:C:231:MET:HE2	1.48	0.78
2:B:39:LYS:O	2:B:42:GLN:HB2	1.83	0.78
1:C:26:ILE:CG2	1:C:114:THR:HG21	2.13	0.78
2:B:90:GLU:HB2	4:B:475:HOH:O	1.82	0.78
2:B:82:PHE:O	4:B:325:HOH:O	2.02	0.77
1:C:169:VAL:HG22	1:C:238:LEU:HD22	1.65	0.76
1:A:271:GLU:HG2	1:A:276:PHE:HE2	1.49	0.76
1:A:256:ASP:HB2	4:A:446:HOH:O	1.84	0.75
1:A:216:ASN:HD22	1:A:222:GLN:HE21	1.33	0.75
1:A:147:ALA:O	1:A:233:PRO:HD2	1.86	0.75
2:B:66:GLU:OE1	2:B:74:TYR:HE2	1.70	0.74
1:A:22:VAL:HG11	1:A:102:ILE:HD13	1.69	0.74
2:B:59:TRP:CE3	2:B:59:TRP:HA	2.22	0.74
1:C:216:ASN:HD22	1:C:222:GLN:NE2	1.85	0.74
1:A:163:MET:HE2	1:A:167:GLU:HB3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ASP:HB2	2:B:5:LYS:H	1.52	0.73
1:A:32:GLU:HG3	4:A:359:HOH:O	1.88	0.72
1:A:68:GLY:HA3	1:A:133:THR:OG1	1.88	0.72
2:B:50:ASP:CA	2:B:53:LYS:HE2	2.19	0.72
1:C:223:TRP:O	1:C:230:MET:HA	1.89	0.72
2:B:3:VAL:HG12	2:B:97:TYR:CA	2.18	0.72
2:B:65:MET:CE	2:B:92:GLU:HG2	2.19	0.72
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.52	0.72
1:A:22:VAL:HG11	1:A:102:ILE:CD1	2.20	0.72
2:B:59:TRP:CZ3	2:B:64:LEU:HD23	2.25	0.71
1:C:53:ILE:HG22	1:C:71:TYR:HB2	1.71	0.71
2:B:49:THR:O	2:B:53:LYS:NZ	2.23	0.71
2:B:54:ASN:ND2	2:B:54:ASN:N	2.37	0.71
1:A:1:THR:HG23	1:A:2:THR:N	2.04	0.71
2:B:64:LEU:HB2	2:B:95:ILE:CD1	2.20	0.70
2:B:39:LYS:HA	2:B:57:ILE:O	1.91	0.70
1:A:99:PHE:O	1:A:102:ILE:HG22	1.91	0.70
1:C:225:SER:O	4:C:441:HOH:O	2.10	0.70
2:B:39:LYS:C	2:B:42:GLN:NE2	2.50	0.70
1:C:96:HIS:CD2	1:C:107:LEU:HD22	2.26	0.70
1:A:53:ILE:HD13	1:A:108:PHE:HB2	1.73	0.70
2:B:57:ILE:CD1	2:B:63:THR:HG21	2.22	0.70
1:A:195:ASN:H	1:A:195:ASN:ND2	1.86	0.69
1:A:240:GLN:HG2	4:A:396:HOH:O	1.91	0.69
2:B:82:PHE:CE2	2:B:84:GLY:HA2	2.28	0.69
1:C:200:ASN:ND2	1:C:255:GLN:OE1	2.26	0.69
2:B:17:CYS:SG	3:B:105:HEM:CAC	2.81	0.69
1:C:7:VAL:HA	1:C:275:THR:O	1.93	0.69
1:C:66:SER:HB2	1:C:130:ARG:HD3	1.73	0.69
1:C:67:TYR:HD2	1:C:274:ILE:HG23	1.57	0.69
1:A:47:VAL:HG22	1:A:116:VAL:HG23	1.75	0.69
1:C:146:ASP:O	1:C:234:THR:HG21	1.93	0.69
1:A:14:ARG:HG2	1:A:101:TRP:CZ3	2.27	0.69
1:A:125:PRO:HB2	1:A:267:GLU:OE1	1.92	0.68
2:B:26:HIS:CD2	2:B:31:ASN:N	2.62	0.68
1:C:93:GLU:N	1:C:94:PRO:HD2	2.08	0.68
2:B:32:LEU:O	2:B:102:THR:CG2	2.42	0.68
2:B:66:GLU:HG2	2:B:74:TYR:CD2	2.28	0.68
1:A:195:ASN:HD22	1:A:195:ASN:N	1.89	0.68
1:C:84:GLY:N	1:C:86:GLN:HE22	1.87	0.68
2:B:64:LEU:HB2	2:B:95:ILE:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:PHE:HA	4:B:357:HOH:O	1.94	0.68
1:C:71:TYR:HA	1:C:76:GLU:CG	2.24	0.68
1:C:8:ALA:HB1	1:C:129:GLY:HA3	1.76	0.67
1:A:216:ASN:ND2	1:A:222:GLN:HE21	1.91	0.67
1:A:271:GLU:HB3	4:A:447:HOH:O	1.93	0.67
1:C:84:GLY:N	1:C:86:GLN:NE2	2.39	0.67
1:A:163:MET:CE	1:A:268:LYS:HZ2	2.07	0.67
1:A:47:VAL:HG22	1:A:116:VAL:CG2	2.24	0.67
1:A:128:CYS:SG	4:A:492:HOH:O	2.52	0.67
3:B:105:HEM:HHD	3:B:105:HEM:HBC2	1.77	0.67
2:B:16:GLN:OE1	2:B:16:GLN:N	2.28	0.67
2:B:36:PHE:HA	2:B:59:TRP:O	1.96	0.66
1:A:11:GLU:O	1:A:14:ARG:HB2	1.96	0.66
2:B:53:LYS:HB2	2:B:54:ASN:HD22	1.61	0.66
1:C:143:ARG:CG	4:C:672:HOH:O	2.42	0.66
1:A:62:ASN:HB2	4:A:382:HOH:O	1.96	0.66
1:C:58:ASP:HB2	1:C:143:ARG:NH1	2.10	0.66
2:B:26:HIS:HD2	2:B:31:ASN:N	1.93	0.66
1:C:29:LYS:HG2	1:C:91:PHE:CZ	2.31	0.66
2:B:9:ILE:HD13	2:B:90:GLU:CG	2.26	0.65
1:C:119:MET:O	1:C:120:GLN:HB2	1.95	0.65
1:A:155:ARG:NH2	1:A:243:LYS:HE3	2.11	0.65
2:B:9:ILE:CD1	2:B:90:GLU:CG	2.74	0.65
1:C:292:GLN:HB3	1:C:294:LEU:HD12	1.79	0.65
2:B:3:VAL:HA	2:B:97:TYR:HB2	1.79	0.64
1:A:53:ILE:HD13	1:A:108:PHE:CB	2.28	0.64
1:A:59:LYS:HD2	1:A:162:ASN:HD21	1.62	0.64
2:B:39:LYS:HB3	2:B:42:GLN:NE2	2.12	0.64
1:A:106:ASP:OD1	1:A:130:ARG:NH1	2.31	0.64
1:C:75:LYS:HE3	1:C:140:ASP:HA	1.80	0.64
1:A:31:ARG:CZ	1:A:289:LEU:HD23	2.28	0.64
1:A:278:LYS:HG2	1:A:279:ASP:N	2.11	0.64
1:C:279:ASP:OD1	1:C:279:ASP:N	2.29	0.64
2:B:31:ASN:OD1	2:B:32:LEU:N	2.31	0.64
2:B:9:ILE:HG22	2:B:94:LEU:HD22	1.79	0.63
2:B:49:THR:C	2:B:53:LYS:NZ	2.56	0.63
2:B:14:CYS:HB3	3:B:105:HEM:C3B	2.33	0.63
1:C:76:GLU:HB3	1:C:138:THR:CG2	2.29	0.63
2:B:3:VAL:HG12	2:B:97:TYR:N	2.13	0.63
1:C:104:SER:HB3	1:C:108:PHE:CE2	2.33	0.63
2:B:49:THR:C	2:B:53:LYS:HZ1	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ILE:HA	1:C:95:ILE:HD11	1.81	0.62
2:B:48:TYR:HA	2:B:79:LYS:HZ1	1.64	0.62
2:B:66:GLU:OE1	2:B:74:TYR:CE2	2.52	0.62
1:A:281:PRO:HD3	4:A:338:HOH:O	1.98	0.62
2:B:53:LYS:C	2:B:54:ASN:HD22	2.07	0.62
1:C:67:TYR:CD2	1:C:274:ILE:HG23	2.35	0.62
1:C:134:PRO:HD2	1:C:137:THR:CG2	2.29	0.62
1:A:200:ASN:HA	4:A:423:HOH:O	1.98	0.62
2:B:38:ARG:O	2:B:59:TRP:N	2.33	0.62
1:C:230:MET:HE2	1:C:230:MET:C	2.25	0.62
1:C:22:VAL:O	1:C:23:TYR:C	2.42	0.62
1:A:155:ARG:HA	1:A:244:TYR:OH	1.99	0.62
2:B:66:GLU:HG2	2:B:74:TYR:HD2	1.64	0.62
2:B:17:CYS:SG	3:B:105:HEM:CBC	2.88	0.61
2:B:30:PRO:HG3	2:B:46:PHE:CD2	2.34	0.61
1:C:282:SER:HB3	1:C:283:PRO:HD2	1.82	0.61
1:C:23:TYR:HD1	1:C:24:ASN:HD22	1.48	0.61
1:A:72:ARG:NH2	1:A:73:PHE:CZ	2.68	0.61
2:B:59:TRP:HA	2:B:59:TRP:HE3	1.65	0.61
1:A:172:MET:SD	3:A:295:HEM:CBB	2.89	0.61
1:A:294:LEU:O	4:A:361:HOH:O	2.16	0.61
2:B:14:CYS:CB	3:B:105:HEM:CAB	2.79	0.61
1:C:10:VAL:HG12	1:C:11:GLU:O	1.99	0.61
1:C:26:ILE:HA	1:C:95:ILE:CD1	2.30	0.61
1:A:281:PRO:CD	4:A:338:HOH:O	2.49	0.61
2:B:16:GLN:CD	2:B:16:GLN:H	2.09	0.61
1:C:135:GLU:HG3	1:C:135:GLU:O	1.99	0.60
1:C:248:VAL:O	1:C:252:ALA:HB2	2.02	0.60
2:B:80:MET:HB2	3:B:105:HEM:C1D	2.37	0.60
1:A:96:HIS:HE1	1:A:102:ILE:O	1.83	0.60
1:C:7:VAL:HG22	4:C:728:HOH:O	2.01	0.60
1:A:271:GLU:HG2	1:A:276:PHE:CE2	2.33	0.60
1:C:213:LEU:HD13	1:C:223:TRP:CE2	2.37	0.60
1:A:292:GLN:C	1:A:294:LEU:HD12	2.27	0.59
1:C:48:ARG:O	1:C:49:LEU:C	2.46	0.59
1:A:225:SER:OG	1:A:227:SER:HB2	2.03	0.59
1:C:261:ASP:OD1	1:C:261:ASP:N	2.35	0.59
1:A:4:LEU:HD12	1:A:6:HIS:CE1	2.38	0.59
2:B:40:THR:HG21	2:B:55:LYS:HB3	1.85	0.59
1:C:195:ASN:N	1:C:195:ASN:OD1	2.29	0.59
1:A:255:GLN:NE2	1:A:259:PHE:CZ	2.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LEU:O	2:B:66:GLU:N	2.36	0.59
2:B:70:ASN:HB3	2:B:73:LYS:HB3	1.84	0.59
1:C:92:LEU:C	1:C:94:PRO:HD2	2.28	0.59
1:C:143:ARG:O	1:C:157:PHE:CE1	2.55	0.59
1:A:166:ARG:HH21	1:A:257:LYS:HE3	1.67	0.58
1:C:134:PRO:HD2	1:C:137:THR:HG21	1.85	0.58
1:A:169:VAL:HG12	1:A:251:TYR:CE2	2.38	0.58
1:C:99:PHE:N	1:C:100:PRO:HD3	2.17	0.58
1:C:99:PHE:O	1:C:102:ILE:HG22	2.02	0.58
1:A:201:GLU:O	1:A:202:PHE:C	2.46	0.58
1:A:216:ASN:ND2	1:A:222:GLN:NE2	2.47	0.58
2:B:25:LYS:HE3	2:B:27:LYS:CE	2.33	0.58
2:B:55:LYS:O	2:B:55:LYS:HD3	2.03	0.58
1:A:93:GLU:HB3	1:A:94:PRO:HD3	1.84	0.58
2:B:2:ASP:N	2:B:2:ASP:OD1	2.36	0.58
1:C:70:THR:HB	1:C:138:THR:HG23	1.86	0.58
1:C:250:GLU:OE2	1:C:257:LYS:HE3	2.04	0.58
1:A:124:ILE:HD13	1:A:263:SER:HA	1.85	0.58
2:B:14:CYS:HB3	3:B:105:HEM:CAB	2.33	0.58
2:B:21:GLU:CD	2:B:21:GLU:H	2.12	0.57
1:C:143:ARG:O	1:C:157:PHE:HE1	1.86	0.57
2:B:3:VAL:CG1	2:B:97:TYR:HA	2.31	0.57
2:B:14:CYS:SG	3:B:105:HEM:CBB	2.91	0.57
2:B:82:PHE:HE2	2:B:84:GLY:HA2	1.68	0.57
1:C:282:SER:HB3	1:C:283:PRO:CD	2.34	0.57
2:B:7:LYS:CD	4:B:415:HOH:O	2.52	0.57
2:B:9:ILE:HD13	2:B:90:GLU:HG2	1.86	0.57
1:C:230:MET:HE3	1:C:231:MET:C	2.29	0.57
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.69	0.57
2:B:55:LYS:O	2:B:57:ILE:HG23	2.04	0.57
1:C:26:ILE:HG13	1:C:95:ILE:HD13	1.87	0.57
1:C:130:ARG:HG3	1:C:130:ARG:NH1	2.20	0.57
1:C:28:LEU:HD13	1:C:289:LEU:HD11	1.87	0.57
2:B:9:ILE:CG2	2:B:94:LEU:HD22	2.34	0.56
2:B:14:CYS:HB3	3:B:105:HEM:C4B	2.40	0.56
2:B:61:GLU:OE2	2:B:99:LYS:HE3	2.05	0.56
3:B:105:HEM:HHC	3:B:105:HEM:HBB2	1.86	0.56
1:C:20:GLN:HE22	1:C:287:LYS:N	1.96	0.56
1:A:80:PRO:HD3	1:A:141:ASN:ND2	2.20	0.56
1:A:128:CYS:HB2	4:A:492:HOH:O	2.04	0.56
2:B:14:CYS:HB3	3:B:105:HEM:CHC	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASN:HD22	1:C:222:GLN:HE21	1.54	0.56
1:C:24:ASN:O	1:C:28:LEU:HD22	2.05	0.56
2:B:64:LEU:CB	2:B:95:ILE:HD11	2.35	0.56
2:B:68:LEU:C	2:B:91:ARG:HD2	2.31	0.56
2:B:20:VAL:O	2:B:33:HIS:HB2	2.06	0.55
1:C:236:TYR:CE2	1:C:239:ILE:HD11	2.40	0.55
2:B:74:TYR:O	2:B:75:ILE:HG12	2.07	0.55
1:C:93:GLU:N	1:C:94:PRO:CD	2.70	0.55
2:B:42:GLN:HB3	4:B:468:HOH:O	2.06	0.55
1:C:204:LEU:O	1:C:208:ASN:HB2	2.07	0.55
1:A:16:TYR:CG	1:A:16:TYR:O	2.60	0.55
1:A:169:VAL:HG12	1:A:251:TYR:HE2	1.68	0.55
1:A:163:MET:HE3	1:A:268:LYS:HZ2	1.70	0.55
1:A:46:LEU:O	1:A:47:VAL:C	2.50	0.55
2:B:8:LYS:HG3	4:B:415:HOH:O	2.07	0.55
1:A:134:PRO:O	1:A:136:ASP:N	2.40	0.55
1:A:212:LYS:HE2	4:A:445:HOH:O	2.06	0.55
1:C:164:ASN:HD21	1:C:167:GLU:HG3	1.68	0.55
2:B:94:LEU:O	2:B:98:LEU:HG	2.07	0.54
1:C:191:TRP:CD1	1:C:231:MET:HE2	2.36	0.54
1:A:158:PHE:HB3	1:A:163:MET:HB2	1.88	0.54
2:B:59:TRP:CE3	2:B:64:LEU:HD23	2.42	0.54
1:A:128:CYS:CB	4:A:492:HOH:O	2.56	0.54
1:A:163:MET:CE	1:A:167:GLU:HB3	2.36	0.54
1:C:72:ARG:NH2	1:C:133:THR:O	2.41	0.54
2:B:82:PHE:CE2	2:B:84:GLY:CA	2.91	0.54
1:A:277:PRO:HG2	4:A:487:HOH:O	2.07	0.54
1:C:271:GLU:O	1:C:274:ILE:HG13	2.08	0.54
1:C:292:GLN:CB	1:C:294:LEU:HD12	2.38	0.54
1:A:1:THR:CG2	1:A:2:THR:N	2.70	0.54
1:A:172:MET:SD	3:A:295:HEM:HBB2	2.47	0.54
1:A:257:LYS:O	1:A:258:PHE:C	2.50	0.54
1:C:82:ASN:O	1:C:85:LEU:HB2	2.07	0.54
1:A:15:SER:O	1:A:19:PHE:HD2	1.91	0.54
2:B:32:LEU:O	2:B:102:THR:HG22	2.08	0.54
2:B:81:ILE:HG12	4:B:456:HOH:O	2.08	0.54
1:C:166:ARG:HB2	1:C:247:ILE:HD13	1.90	0.54
1:A:59:LYS:HD2	1:A:162:ASN:ND2	2.23	0.54
1:A:147:ALA:HB1	1:A:232:LEU:HD13	1.90	0.54
2:B:65:MET:N	2:B:95:ILE:CD1	2.71	0.54
2:B:66:GLU:CD	2:B:74:TYR:CE2	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASP:O	1:A:245:LEU:HB2	2.08	0.53
2:B:16:GLN:N	2:B:16:GLN:CD	2.65	0.53
1:C:48:ARG:HD3	1:C:85:LEU:HD21	1.88	0.53
2:B:59:TRP:CE3	2:B:64:LEU:CD2	2.91	0.53
3:B:105:HEM:CBB	3:B:105:HEM:HHC	2.38	0.53
1:C:26:ILE:HG22	1:C:114:THR:CG2	2.31	0.53
1:A:51:TRP:O	1:A:52:HIS:C	2.46	0.53
2:B:62:GLU:HB2	4:B:352:HOH:O	2.09	0.53
1:C:203:TYR:HD1	1:C:248:VAL:HG13	1.74	0.53
2:B:30:PRO:HG3	2:B:46:PHE:CG	2.44	0.53
1:A:34:ASP:HA	4:A:411:HOH:O	2.08	0.52
1:A:271:GLU:O	1:A:272:ASN:C	2.52	0.52
1:C:105:GLY:O	1:C:130:ARG:HD2	2.09	0.52
1:A:181:HIS:C	1:A:187:TYR:O	2.53	0.52
2:B:65:MET:N	2:B:95:ILE:HD11	2.24	0.52
1:C:133:THR:HB	1:C:134:PRO:CD	2.38	0.52
1:A:73:PHE:CE2	1:A:135:GLU:HA	2.45	0.52
2:B:14:CYS:C	2:B:16:GLN:N	2.64	0.52
1:A:182:LEU:N	1:A:187:TYR:O	2.43	0.52
1:C:33:ASP:OD1	1:C:33:ASP:N	2.43	0.52
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.23	0.52
2:B:80:MET:HB2	3:B:105:HEM:C4D	2.44	0.52
1:C:257:LYS:O	1:C:261:ASP:OD1	2.27	0.52
2:B:98:LEU:O	2:B:99:LYS:C	2.53	0.52
1:A:16:TYR:HD1	1:A:284:PHE:CD1	2.28	0.52
1:C:73:PHE:O	1:C:77:PHE:N	2.41	0.52
1:A:202:PHE:HZ	1:A:235:ASP:HB3	1.74	0.52
1:C:166:ARG:CA	1:C:247:ILE:HD13	2.40	0.52
1:A:280:ALA:HA	4:A:338:HOH:O	2.10	0.52
2:B:41:GLY:HA2	2:B:48:TYR:CG	2.45	0.52
2:B:25:LYS:CE	2:B:27:LYS:HE2	2.34	0.51
2:B:70:ASN:OD1	2:B:72:LYS:CG	2.54	0.51
1:C:73:PHE:O	1:C:77:PHE:HB2	2.11	0.51
2:B:69:GLU:HA	2:B:85:ILE:O	2.11	0.51
1:A:3:PRO:HB3	1:A:61:ASP:O	2.09	0.51
1:C:71:TYR:CE2	1:C:77:PHE:CE1	2.98	0.51
1:A:155:ARG:HH22	1:A:241:ASP:CG	2.19	0.51
2:B:56:GLY:O	2:B:57:ILE:HG22	2.10	0.51
1:C:133:THR:HB	1:C:137:THR:HG21	1.92	0.51
1:C:182:LEU:HD11	1:C:218:ALA:HB2	1.93	0.51
2:B:41:GLY:HA2	2:B:48:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:GLU:O	2:B:63:THR:C	2.52	0.51
1:C:58:ASP:HB2	1:C:143:ARG:HH12	1.74	0.51
1:C:145:PRO:HA	1:C:153:TYR:OH	2.10	0.51
1:C:179:LYS:HE3	1:C:180:THR:O	2.10	0.51
1:C:238:LEU:HD23	1:C:244:TYR:CD2	2.45	0.51
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.93	0.51
1:C:4:LEU:CG	4:C:657:HOH:O	2.45	0.51
2:B:7:LYS:HD3	4:B:415:HOH:O	2.09	0.51
2:B:50:ASP:O	2:B:54:ASN:HB2	2.11	0.51
1:C:39:TYR:HD2	4:C:429:HOH:O	1.93	0.51
1:A:275:THR:O	1:A:277:PRO:HD3	2.12	0.50
2:B:94:LEU:O	2:B:94:LEU:HD12	2.11	0.50
2:B:31:ASN:OD1	2:B:31:ASN:C	2.54	0.50
2:B:39:LYS:C	2:B:42:GLN:HE21	2.18	0.50
2:B:57:ILE:C	2:B:57:ILE:HD12	2.36	0.50
1:C:204:LEU:O	1:C:208:ASN:N	2.38	0.50
1:A:46:LEU:C	1:A:48:ARG:N	2.69	0.50
1:C:249:LYS:O	1:C:252:ALA:HB3	2.12	0.50
2:B:78:THR:OG1	2:B:79:LYS:N	2.45	0.50
1:C:191:TRP:NE1	1:C:230:MET:HE1	2.25	0.50
2:B:12:GLN:NE2	4:B:413:HOH:O	2.33	0.50
2:B:32:LEU:O	2:B:102:THR:HB	2.11	0.50
1:A:204:LEU:O	1:A:205:ASN:C	2.55	0.50
1:C:139:PRO:HB3	1:C:143:ARG:HH21	1.76	0.50
1:A:26:ILE:HB	1:A:114:THR:HG21	1.93	0.49
2:B:64:LEU:O	2:B:65:MET:C	2.55	0.49
1:A:26:ILE:CG2	1:A:114:THR:HG21	2.42	0.49
2:B:40:THR:HB	2:B:52:ASN:O	2.13	0.49
1:C:256:ASP:HB3	4:C:680:HOH:O	2.13	0.49
1:C:26:ILE:CG1	1:C:95:ILE:HD13	2.42	0.49
1:A:58:ASP:CG	1:A:160:ARG:HD2	2.38	0.49
1:C:120:GLN:HB2	1:C:197:VAL:HG23	1.95	0.49
2:B:26:HIS:HB3	4:B:354:HOH:O	2.13	0.49
1:C:105:GLY:HA2	4:C:630:HOH:O	2.13	0.49
1:A:15:SER:O	1:A:19:PHE:CD2	2.65	0.49
2:B:54:ASN:O	2:B:55:LYS:C	2.54	0.49
2:B:87:LYS:HB3	2:B:87:LYS:HE2	1.66	0.49
1:C:144:LEU:CD1	4:C:612:HOH:O	2.60	0.49
1:A:47:VAL:CG2	1:A:116:VAL:CG2	2.91	0.49
1:A:79:ASP:OD2	4:A:432:HOH:O	2.20	0.49
1:A:164:ASN:O	1:A:168:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:MET:O	1:C:120:GLN:CB	2.60	0.49
1:C:179:LYS:HB3	1:C:190:PRO:HB3	1.94	0.49
1:A:58:ASP:OD1	1:A:60:HIS:ND1	2.46	0.49
1:A:184:ASN:ND2	3:A:295:HEM:O2A	2.46	0.49
2:B:85:ILE:C	2:B:86:LYS:HD3	2.38	0.49
2:B:33:HIS:HA	2:B:102:THR:O	2.13	0.48
1:C:166:ARG:HA	1:C:247:ILE:HD13	1.94	0.48
2:B:64:LEU:CB	2:B:95:ILE:CD1	2.89	0.48
2:B:66:GLU:CD	2:B:74:TYR:HE2	2.19	0.48
1:C:272:ASN:CA	4:C:692:HOH:O	2.45	0.48
1:A:212:LYS:HD3	4:A:445:HOH:O	2.12	0.48
2:B:57:ILE:CD1	2:B:58:THR:O	2.61	0.48
1:C:93:GLU:HB3	1:C:94:PRO:HD3	1.95	0.48
1:A:237:SER:O	1:A:238:LEU:C	2.55	0.48
2:B:3:VAL:O	2:B:7:LYS:HB2	2.13	0.48
1:C:23:TYR:OH	1:C:288:THR:HG22	2.13	0.48
2:B:60:LYS:HB3	2:B:63:THR:OG1	2.14	0.48
1:A:166:ARG:NH2	1:A:250:GLU:OE2	2.46	0.48
2:B:56:GLY:C	2:B:57:ILE:CG2	2.87	0.48
2:B:54:ASN:C	2:B:56:GLY:N	2.69	0.48
1:C:143:ARG:HG3	4:C:672:HOH:O	2.13	0.48
1:A:163:MET:HE3	1:A:268:LYS:NZ	2.28	0.48
1:C:27:ALA:HB1	1:C:289:LEU:HG	1.96	0.48
1:C:134:PRO:O	1:C:137:THR:OG1	2.24	0.48
1:C:214:GLU:O	1:C:221:GLU:HA	2.13	0.48
2:B:7:LYS:HD2	4:B:415:HOH:O	2.10	0.47
1:C:44:PRO:HD2	4:C:712:HOH:O	2.13	0.47
1:A:73:PHE:CE1	1:A:135:GLU:HB2	2.50	0.47
1:C:42:TYR:CG	1:C:91:PHE:CD2	3.02	0.47
2:B:49:THR:O	2:B:52:ASN:N	2.38	0.47
1:C:186:GLY:O	1:C:220:ASN:ND2	2.41	0.47
1:C:62:ASN:CG	1:C:62:ASN:O	2.57	0.47
1:A:155:ARG:NH2	1:A:241:ASP:OD1	2.42	0.47
1:A:202:PHE:CD1	1:A:231:MET:HE1	2.49	0.47
1:A:11:GLU:O	1:A:12:LYS:C	2.57	0.47
1:A:68:GLY:CA	1:A:133:THR:OG1	2.62	0.47
1:A:202:PHE:CZ	1:A:235:ASP:HB3	2.49	0.47
1:C:48:ARG:NH1	1:C:85:LEU:HG	2.29	0.47
1:C:213:LEU:HD13	1:C:223:TRP:NE1	2.29	0.47
1:A:29:LYS:HE3	4:A:437:HOH:O	2.15	0.47
1:A:182:LEU:HB2	1:A:188:GLU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:PHE:CD1	2:B:10:PHE:C	2.92	0.47
2:B:26:HIS:CB	4:B:354:HOH:O	2.62	0.47
2:B:69:GLU:HB2	2:B:91:ARG:NH2	2.29	0.47
2:B:80:MET:HB2	3:B:105:HEM:ND	2.29	0.47
1:C:42:TYR:O	1:C:45:VAL:HG12	2.15	0.47
1:C:134:PRO:HD2	1:C:137:THR:HG23	1.96	0.47
1:C:166:ARG:O	1:C:167:GLU:C	2.56	0.47
2:B:3:VAL:HG11	2:B:100:LYS:CD	2.44	0.47
2:B:48:TYR:HA	2:B:79:LYS:NZ	2.28	0.47
2:B:48:TYR:CA	2:B:79:LYS:HZ1	2.28	0.47
2:B:70:ASN:HD22	2:B:73:LYS:NZ	2.12	0.47
1:A:290:GLU:O	1:A:290:GLU:HG3	2.14	0.47
1:C:133:THR:HB	1:C:134:PRO:HD3	1.95	0.47
1:A:20:GLN:O	1:A:23:TYR:HB3	2.15	0.47
1:C:232:LEU:O	1:C:233:PRO:C	2.55	0.47
1:A:34:ASP:OD1	1:A:34:ASP:N	2.48	0.46
1:A:69:GLY:O	1:A:72:ARG:HD3	2.15	0.46
2:B:3:VAL:O	2:B:7:LYS:N	2.47	0.46
2:B:22:LYS:HA	2:B:31:ASN:HD21	1.80	0.46
1:C:144:LEU:HD11	4:C:612:HOH:O	2.13	0.46
1:A:271:GLU:C	4:A:447:HOH:O	2.58	0.46
2:B:14:CYS:C	2:B:16:GLN:H	2.23	0.46
1:C:79:ASP:HA	1:C:80:PRO:HD3	1.82	0.46
1:C:182:LEU:HB2	1:C:188:GLU:HG2	1.97	0.46
1:A:243:LYS:HE3	1:A:243:LYS:HB2	1.51	0.46
1:C:6:HIS:HB3	1:C:67:TYR:CE2	2.51	0.46
1:C:236:TYR:O	1:C:239:ILE:HG13	2.15	0.46
1:A:1:THR:O	1:A:3:PRO:HD3	2.15	0.46
1:A:166:ARG:NH2	1:A:257:LYS:HE3	2.28	0.46
2:B:36:PHE:HE1	2:B:98:LEU:HB3	1.80	0.46
1:C:131:VAL:O	1:C:132:ASP:C	2.58	0.46
2:B:13:LYS:NZ	4:B:383:HOH:O	2.49	0.46
1:C:276:PHE:HA	1:C:277:PRO:HD2	1.64	0.46
2:B:26:HIS:CD2	2:B:30:PRO:HA	2.50	0.46
2:B:74:TYR:C	2:B:75:ILE:CG1	2.88	0.46
1:C:4:LEU:CB	4:C:657:HOH:O	2.63	0.46
1:A:59:LYS:CD	1:A:162:ASN:ND2	2.79	0.46
2:B:3:VAL:HG11	2:B:100:LYS:HG3	1.97	0.46
2:B:40:THR:HG23	2:B:57:ILE:H	1.79	0.46
1:A:10:VAL:HA	4:A:492:HOH:O	2.16	0.46
1:A:34:ASP:OD2	2:B:90:GLU:OE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLY:O	1:A:116:VAL:HG23	2.16	0.46
1:A:262:PHE:O	1:A:263:SER:C	2.58	0.46
1:C:241:ASP:HA	1:C:242:PRO:HD3	1.74	0.46
1:A:4:LEU:O	1:A:62:ASN:ND2	2.48	0.46
1:A:7:VAL:HG23	1:A:8:ALA:O	2.15	0.46
1:C:200:ASN:HD22	1:C:200:ASN:H	1.63	0.46
1:C:215:LYS:HD3	1:C:219:ASN:O	2.15	0.46
1:A:232:LEU:HB2	1:A:235:ASP:OD2	2.15	0.45
2:B:56:GLY:O	2:B:57:ILE:CG2	2.64	0.45
1:C:19:PHE:CD2	1:C:284:PHE:HE2	2.33	0.45
1:C:71:TYR:HA	1:C:76:GLU:HG2	1.94	0.45
1:C:138:THR:HA	1:C:139:PRO:HD3	1.83	0.45
1:A:243:LYS:O	1:A:247:ILE:HG13	2.16	0.45
2:B:27:LYS:HD2	2:B:27:LYS:N	2.32	0.45
1:C:71:TYR:CE2	1:C:77:PHE:HE1	2.35	0.45
2:B:74:TYR:C	2:B:75:ILE:HG13	2.42	0.45
1:A:2:THR:O	1:A:2:THR:HG23	2.17	0.45
1:A:42:TYR:CD2	1:A:91:PHE:CD2	3.04	0.45
2:B:31:ASN:ND2	4:B:349:HOH:O	2.23	0.45
1:C:172:MET:HE1	3:C:295:HEM:CBB	2.46	0.45
2:B:38:ARG:O	2:B:58:THR:HA	2.16	0.45
1:C:68:GLY:O	1:C:72:ARG:NH1	2.50	0.45
1:C:216:ASN:OD1	1:C:218:ALA:HB3	2.17	0.45
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.69	0.45
2:B:89:THR:O	2:B:92:GLU:HB2	2.17	0.45
1:A:47:VAL:CG2	1:A:116:VAL:HG22	2.47	0.45
1:A:288:THR:O	1:A:292:GLN:HG3	2.17	0.45
2:B:70:ASN:HD22	2:B:73:LYS:HZ3	1.65	0.45
1:A:11:GLU:OE2	1:A:106:ASP:OD2	2.35	0.45
2:B:75:ILE:HA	2:B:76:PRO:HD2	1.74	0.45
1:C:127:ARG:CD	1:C:271:GLU:OE2	2.65	0.45
1:A:278:LYS:C	1:A:280:ALA:H	2.24	0.45
2:B:4:GLU:OE1	2:B:4:GLU:HA	2.17	0.45
1:C:24:ASN:O	1:C:28:LEU:CD2	2.65	0.45
1:C:86:GLN:CD	1:C:86:GLN:H	2.25	0.45
1:A:53:ILE:CD1	1:A:108:PHE:HB2	2.44	0.44
1:A:110:LEU:O	1:A:110:LEU:HD23	2.16	0.44
2:B:33:HIS:CD2	2:B:103:ASN:HA	2.52	0.44
2:B:39:LYS:HB3	2:B:42:GLN:HE22	1.80	0.44
2:B:79:LYS:NZ	3:B:105:HEM:CGD	2.80	0.44
1:C:127:ARG:HG3	1:C:271:GLU:OE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ARG:HG2	4:C:672:HOH:O	2.13	0.44
1:A:207:LEU:HD12	1:A:252:ALA:CB	2.46	0.44
1:C:6:HIS:HB3	1:C:67:TYR:CD2	2.53	0.44
2:B:53:LYS:HZ2	2:B:53:LYS:HG3	1.42	0.44
1:C:280:ALA:HA	4:C:622:HOH:O	2.16	0.44
1:C:216:ASN:ND2	1:C:222:GLN:NE2	2.61	0.44
1:A:151:ALA:CA	1:A:237:SER:HB3	2.47	0.44
3:A:295:HEM:HMC1	3:A:295:HEM:HBC2	2.00	0.44
2:B:57:ILE:HD12	2:B:58:THR:O	2.18	0.44
2:B:66:GLU:CG	2:B:74:TYR:CD2	3.00	0.44
1:C:14:ARG:HB3	1:C:18:ASP:HB2	1.99	0.44
1:A:91:PHE:CD1	1:A:91:PHE:C	2.95	0.44
1:A:147:ALA:O	1:A:233:PRO:HB2	2.18	0.44
1:A:210:ASP:HB3	4:A:439:HOH:O	2.16	0.44
1:A:4:LEU:HD12	1:A:6:HIS:HE1	1.83	0.44
1:C:70:THR:C	1:C:72:ARG:N	2.75	0.44
1:C:130:ARG:NH2	4:C:664:HOH:O	2.51	0.44
1:C:193:ALA:HB2	1:C:229:TYR:OH	2.18	0.44
1:A:53:ILE:O	1:A:65:GLY:O	2.36	0.43
1:A:206:LEU:HG	1:A:239:ILE:CG2	2.48	0.43
2:B:50:ASP:HA	2:B:53:LYS:CE	2.30	0.43
1:C:24:ASN:HD22	1:C:24:ASN:N	2.15	0.43
1:A:127:ARG:O	1:A:130:ARG:NH1	2.47	0.43
1:A:155:ARG:HH11	1:A:155:ARG:HD2	1.37	0.43
2:B:22:LYS:HB2	2:B:33:HIS:ND1	2.34	0.43
1:C:56:THR:HA	1:C:143:ARG:HB2	2.00	0.43
1:A:3:PRO:HG3	1:A:61:ASP:HA	2.00	0.43
1:A:57:TRP:HB3	1:A:161:LEU:HD22	1.99	0.43
1:C:8:ALA:HB3	1:C:276:PHE:CD1	2.53	0.43
1:C:143:ARG:HB3	1:C:160:ARG:NH2	2.34	0.43
1:A:15:SER:OG	1:A:16:TYR:N	2.51	0.43
1:A:200:ASN:O	1:A:201:GLU:C	2.61	0.43
1:A:67:TYR:HA	1:A:130:ARG:HB3	2.01	0.43
2:B:39:LYS:HB3	2:B:42:GLN:CD	2.44	0.43
1:C:243:LYS:HG3	4:C:639:HOH:O	2.18	0.43
1:C:19:PHE:CD2	1:C:284:PHE:CE2	3.07	0.43
1:A:48:ARG:NH1	4:A:364:HOH:O	2.49	0.43
1:C:74:LYS:HB3	1:C:75:LYS:H	1.25	0.43
1:A:2:THR:HA	1:A:3:PRO:HD3	1.80	0.43
1:A:130:ARG:NH1	1:A:130:ARG:CG	2.80	0.43
1:A:74:LYS:HB2	1:A:74:LYS:HE3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ALA:HA	1:A:281:PRO:HD3	1.53	0.42
1:A:110:LEU:C	1:A:110:LEU:CD2	2.92	0.42
2:B:10:PHE:HA	2:B:14:CYS:SG	2.60	0.42
2:B:63:THR:HG22	2:B:74:TYR:OH	2.20	0.42
1:A:79:ASP:HA	1:A:141:ASN:ND2	2.34	0.42
1:C:42:TYR:CD2	1:C:91:PHE:CD2	3.08	0.42
1:C:144:LEU:HA	1:C:145:PRO:HD3	1.81	0.42
1:A:204:LEU:HD21	1:A:252:ALA:O	2.19	0.42
2:B:74:TYR:O	2:B:75:ILE:CG1	2.67	0.42
1:C:91:PHE:CD1	1:C:91:PHE:C	2.97	0.42
2:B:62:GLU:HA	2:B:65:MET:HB2	2.02	0.42
1:C:31:ARG:NE	4:C:740:HOH:O	2.48	0.42
1:A:241:ASP:O	1:A:245:LEU:CB	2.68	0.42
2:B:68:LEU:HB2	2:B:91:ARG:CG	2.50	0.42
2:B:59:TRP:CE3	2:B:64:LEU:HD21	2.55	0.42
1:C:53:ILE:HG22	1:C:71:TYR:CB	2.44	0.42
1:C:106:ASP:OD1	1:C:130:ARG:NH1	2.49	0.42
1:C:238:LEU:HD23	1:C:238:LEU:HA	1.81	0.42
2:B:65:MET:H	2:B:95:ILE:CD1	2.32	0.41
1:C:4:LEU:CA	4:C:657:HOH:O	2.68	0.41
1:C:241:ASP:HB3	1:C:244:TYR:HB2	2.00	0.41
1:C:42:TYR:CD2	1:C:91:PHE:HD2	2.39	0.41
1:C:127:ARG:HH11	1:C:127:ARG:HD2	1.53	0.41
1:C:71:TYR:HA	1:C:76:GLU:CD	2.45	0.41
1:A:41:GLY:HA3	4:A:398:HOH:O	2.20	0.41
2:B:25:LYS:HE3	2:B:27:LYS:HB3	2.01	0.41
1:C:71:TYR:O	1:C:77:PHE:HD1	2.03	0.41
1:C:164:ASN:HD22	1:C:167:GLU:HG3	1.71	0.41
1:C:251:TYR:HB3	1:C:258:PHE:HB2	2.03	0.41
1:A:14:ARG:HG2	1:A:101:TRP:CE3	2.56	0.41
1:A:79:ASP:HA	1:A:80:PRO:HD3	1.82	0.41
1:A:147:ALA:CB	1:A:232:LEU:HD13	2.50	0.41
2:B:53:LYS:NZ	2:B:53:LYS:H	2.18	0.41
2:B:67:TYR:O	2:B:71:PRO:HD3	2.19	0.41
2:B:68:LEU:CB	2:B:91:ARG:HD2	2.50	0.41
2:B:95:ILE:O	2:B:96:ALA:C	2.64	0.41
1:A:72:ARG:NH2	1:A:73:PHE:HZ	2.14	0.41
1:A:151:ALA:N	1:A:237:SER:HB3	2.36	0.41
1:C:68:GLY:O	1:C:132:ASP:HA	2.21	0.41
1:C:189:GLY:HA2	1:C:190:PRO:HD3	1.87	0.41
1:C:199:THR:HB	1:C:200:ASN:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:THR:CG2	2:B:25:LYS:O	2.69	0.41
2:B:29:GLY:HA2	2:B:30:PRO:HD3	1.84	0.41
2:B:72:LYS:HB3	2:B:72:LYS:HE3	1.89	0.41
1:C:179:LYS:HA	1:C:191:TRP:CZ3	2.56	0.41
1:A:12:LYS:NZ	1:A:12:LYS:HB2	2.36	0.41
1:A:38:ASN:C	1:A:39:TYR:CD2	2.99	0.41
1:A:245:LEU:HD12	1:A:245:LEU:O	2.21	0.41
1:A:257:LYS:CD	1:A:257:LYS:C	2.93	0.41
2:B:62:GLU:O	2:B:65:MET:N	2.54	0.41
1:C:23:TYR:C	1:C:23:TYR:CD1	2.99	0.41
1:C:35:GLU:O	1:C:36:TYR:C	2.63	0.41
1:C:98:GLU:C	1:C:100:PRO:HD3	2.45	0.41
1:C:127:ARG:HG2	1:C:283:PRO:HB3	2.02	0.41
1:C:194:ALA:HB1	1:C:197:VAL:HG12	2.02	0.41
1:C:195:ASN:OD1	1:C:195:ASN:C	2.62	0.41
1:C:202:PHE:HB3	4:C:683:HOH:O	2.20	0.41
2:B:27:LYS:N	2:B:27:LYS:CD	2.84	0.41
2:B:56:GLY:C	2:B:57:ILE:HG23	2.45	0.41
1:A:32:GLU:HB3	1:A:33:ASP:OD1	2.21	0.40
1:A:73:PHE:CD2	1:A:135:GLU:HA	2.56	0.40
2:B:2:ASP:HB2	2:B:5:LYS:N	2.29	0.40
2:B:40:THR:O	2:B:53:LYS:HA	2.21	0.40
1:C:214:GLU:O	1:C:222:GLN:N	2.49	0.40
1:A:92:LEU:O	1:A:95:ILE:HB	2.21	0.40
1:A:22:VAL:HG22	1:A:99:PHE:CG	2.56	0.40
1:A:249:LYS:NZ	4:A:462:HOH:O	2.53	0.40
1:C:163:MET:HE1	1:C:268:LYS:HG2	2.03	0.40
1:A:11:GLU:H	1:A:11:GLU:HG2	1.50	0.40
1:A:88:GLY:O	1:A:92:LEU:HG	2.21	0.40
1:A:264:LYS:NZ	1:C:35:GLU:OE1	2.55	0.40
1:C:1:THR:HG23	1:C:2:THR:H	1.87	0.40
1:C:47:VAL:HG22	3:C:295:HEM:HMD3	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:444:HOH:O	4:A:444:HOH:O[8_665]	1.51	0.69
4:A:376:HOH:O	4:C:607:HOH:O[6_455]	1.61	0.59
1:C:279:ASP:CA	4:B:466:HOH:O[8_655]	2.09	0.11

## 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	292/296 (99%)	264 (90%)	23 (8%)	5 (2%)	7	25
1	C	292/296 (99%)	258 (88%)	29 (10%)	5 (2%)	7	25
2	B	102/104 (98%)	75 (74%)	19 (19%)	8 (8%)	1	2
All	All	686/696 (99%)	597 (87%)	71 (10%)	18 (3%)	4	15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	GLU
1	A	277	PRO
2	B	61	GLU
2	B	65	MET
2	B	100	LYS
2	B	101	ALA
1	C	85	LEU
2	B	96	ALA
2	B	97	TYR
1	C	229	TYR
1	A	12	LYS
2	B	48	TYR
1	C	59	LYS
1	C	74	LYS
1	A	34	ASP
1	C	190	PRO
1	A	33	ASP
2	B	84	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/254 (99%)	210 (83%)	42 (17%)	2	8
1	C	252/254 (99%)	214 (85%)	38 (15%)	3	10
2	B	86/86 (100%)	62 (72%)	24 (28%)	0	1
All	All	590/594 (99%)	486 (82%)	104 (18%)	2	7

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	4	LEU
1	A	5	VAL
1	A	7	VAL
1	A	9	SER
1	A	10	VAL
1	A	11	GLU
1	A	12	LYS
1	A	51	TRP
1	A	74	LYS
1	A	81	SER
1	A	86	GLN
1	A	90	LYS
1	A	91	PHE
1	A	110	LEU
1	A	120	GLN
1	A	124	ILE
1	A	135	GLU
1	A	149	LYS
1	A	168	VAL
1	A	169	VAL
1	A	182	LEU
1	A	183	LYS
1	A	184	ASN
1	A	195	ASN
1	A	212	LYS
1	A	215	LYS
1	A	226	LYS
1	A	227	SER
1	A	239	ILE
1	A	243	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	247	ILE
1	A	257	LYS
1	A	260	LYS
1	A	263	SER
1	A	267	GLU
1	A	269	LEU
1	A	271	GLU
1	A	278	LYS
1	A	285	ILE
1	A	289	LEU
1	A	292	GLN
2	B	2	ASP
2	B	11	VAL
2	B	14	CYS
2	B	16	GLN
2	B	21	GLU
2	B	27	LYS
2	B	31	ASN
2	B	39	LYS
2	B	42	GLN
2	B	50	ASP
2	B	52	ASN
2	B	53	LYS
2	B	54	ASN
2	B	55	LYS
2	B	57	ILE
2	B	58	THR
2	B	63	THR
2	B	69	GLU
2	B	72	LYS
2	B	73	LYS
2	B	79	LYS
2	B	86	LYS
2	B	91	ARG
2	B	100	LYS
1	C	4	LEU
1	C	5	VAL
1	C	7	VAL
1	C	17	GLU
1	C	21	LYS
1	C	29	LYS
1	C	33	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	35	GLU
1	C	47	VAL
1	C	51	TRP
1	C	53	ILE
1	C	66	SER
1	C	70	THR
1	C	74	LYS
1	C	75	LYS
1	C	76	GLU
1	C	124	ILE
1	C	138	THR
1	C	143	ARG
1	C	160	ARG
1	C	168	VAL
1	C	171	LEU
1	C	188	GLU
1	C	200	ASN
1	C	226	LYS
1	C	227	SER
1	C	230	MET
1	C	237	SER
1	C	243	LYS
1	C	245	LEU
1	C	256	ASP
1	C	257	LYS
1	C	260	LYS
1	C	261	ASP
1	C	274	ILE
1	C	285	ILE
1	C	287	LYS
1	C	292	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	6	HIS
1	A	38	ASN
1	A	96	HIS
1	A	117	GLN
1	A	141	ASN
1	A	162	ASN
1	A	195	ASN

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Mol	Chain	Res	Type
1	A	205	ASN
1	A	222	GLN
2	B	26	HIS
2	B	42	GLN
2	B	54	ASN
2	B	103	ASN
1	C	20	GLN
1	C	24	ASN
1	C	86	GLN
1	C	87	ASN
1	C	162	ASN
1	C	200	ASN
1	C	208	ASN
1	C	219	ASN
1	C	222	GLN
1	C	292	GLN

### 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](#)

3 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	105	2	50,50,50	1.26	5 (10%)	67,82,82	1.29	8 (11%)
3	HEM	C	295	4,1	50,50,50	1.39	7 (14%)	67,82,82	1.40	11 (16%)
3	HEM	A	295	1	50,50,50	1.26	5 (10%)	67,82,82	1.20	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	105	2	-	5/14/54/54	-
3	HEM	C	295	4,1	-	2/14/54/54	-
3	HEM	A	295	1	-	6/14/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	295	HEM	FE-ND	3.70	2.06	1.94
3	C	295	HEM	CAB-C3B	2.87	1.55	1.47
3	A	295	HEM	CAB-C3B	2.85	1.55	1.47
3	B	105	HEM	CMD-C2D	2.84	1.56	1.50
3	C	295	HEM	CAD-C3D	2.74	1.58	1.51
3	A	295	HEM	FE-ND	2.72	2.03	1.94
3	B	105	HEM	CAB-C3B	2.65	1.54	1.47
3	A	295	HEM	FE-NC	2.52	2.03	1.95
3	C	295	HEM	FE-NC	2.48	2.03	1.95
3	A	295	HEM	FE-NB	2.41	2.02	1.94
3	B	105	HEM	FE-NB	2.41	2.02	1.94
3	C	295	HEM	CAA-C2A	2.33	1.57	1.51
3	B	105	HEM	CAC-C3C	2.32	1.53	1.47
3	C	295	HEM	CMC-C2C	2.27	1.55	1.50
3	A	295	HEM	CMC-C2C	2.22	1.55	1.50
3	C	295	HEM	CAC-C3C	2.06	1.52	1.47
3	B	105	HEM	CMC-C2C	2.05	1.55	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	295	HEM	O1A-CGA-CBA	-4.01	110.37	123.09
3	C	295	HEM	CAD-CBD-CGD	3.78	123.70	113.67
3	B	105	HEM	CHC-C4B-NB	3.77	128.49	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	295	HEM	O2A-CGA-CBA	3.68	125.62	114.00
3	A	295	HEM	O2A-CGA-O1A	3.08	131.24	123.33
3	C	295	HEM	O1D-CGD-CBD	-2.86	114.02	123.09
3	B	105	HEM	CHD-C4C-NC	-2.77	121.44	124.45
3	B	105	HEM	CBD-CAD-C3D	2.69	119.96	112.53
3	C	295	HEM	CAA-CBA-CGA	2.67	120.76	113.67
3	B	105	HEM	CMA-C3A-C2A	2.65	131.25	125.62
3	B	105	HEM	CMA-C3A-C4A	-2.53	121.57	125.42
3	B	105	HEM	CHC-C1C-NC	2.52	127.19	124.45
3	B	105	HEM	CHD-C4C-C3C	2.50	129.43	125.21
3	C	295	HEM	O2A-CGA-O1A	-2.47	116.97	123.33
3	A	295	HEM	O2D-CGD-O1D	2.30	129.25	123.33
3	C	295	HEM	CBA-CAA-C2A	2.28	118.85	112.53
3	C	295	HEM	CHA-C4D-ND	2.20	127.09	124.37
3	C	295	HEM	C1A-CHA-C4D	-2.17	121.14	126.25
3	A	295	HEM	O1D-CGD-CBD	-2.17	116.22	123.09
3	A	295	HEM	C4D-C3D-C2D	2.12	109.98	106.89
3	C	295	HEM	C3B-C2B-C1B	2.12	108.00	106.41
3	C	295	HEM	CHA-C1A-NA	2.12	127.70	123.86
3	C	295	HEM	C4C-CHD-C1D	-2.10	121.56	126.02
3	B	105	HEM	C1C-CHC-C4B	-2.02	121.73	126.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

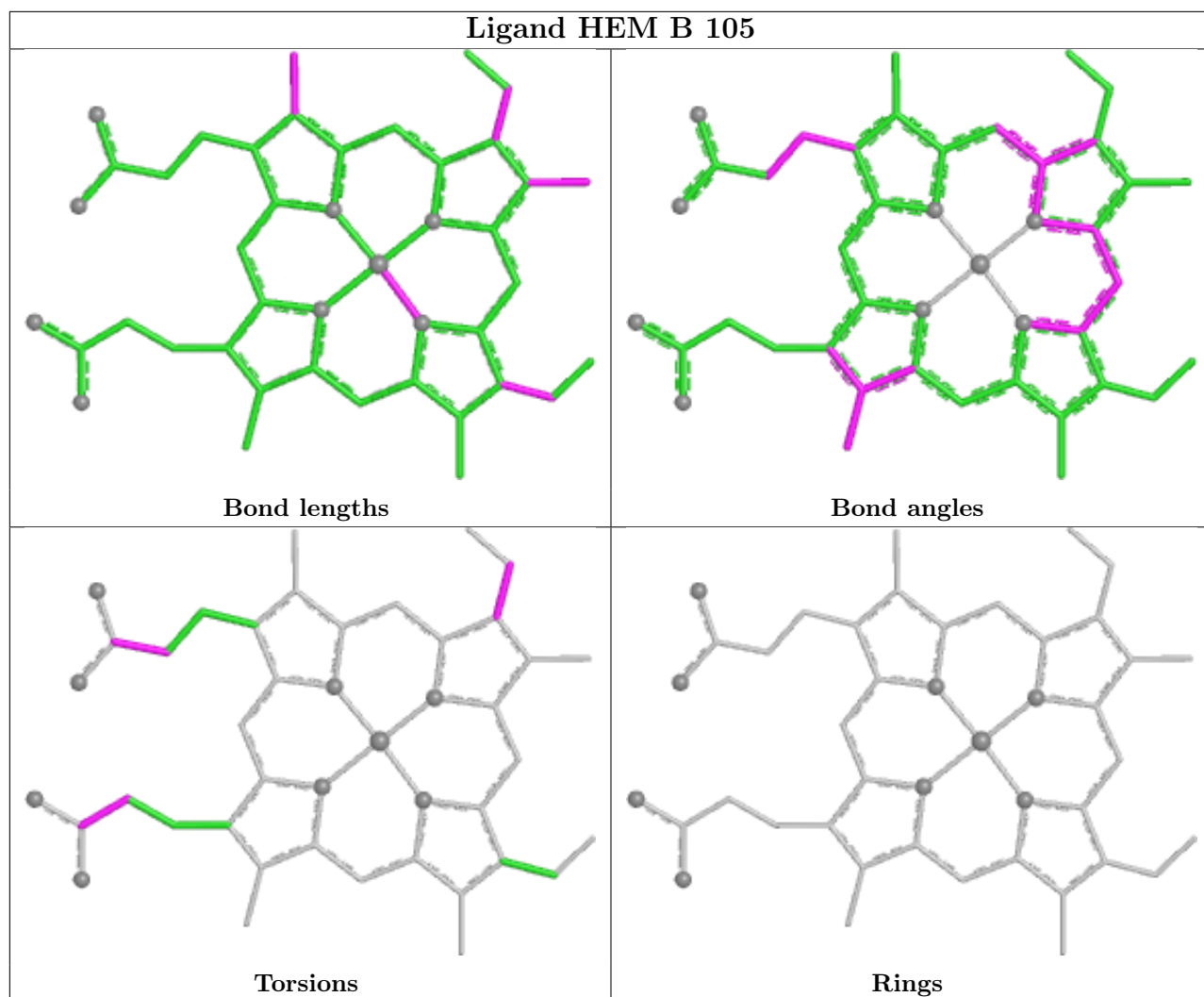
Mol	Chain	Res	Type	Atoms
3	A	295	HEM	C2B-C3B-CAB-CBB
3	A	295	HEM	C4B-C3B-CAB-CBB
3	B	105	HEM	C4C-C3C-CAC-CBC
3	B	105	HEM	CAA-CBA-CGA-O1A
3	A	295	HEM	CAA-CBA-CGA-O2A
3	B	105	HEM	CAA-CBA-CGA-O2A
3	C	295	HEM	CAD-CBD-CGD-O2D
3	A	295	HEM	CAD-CBD-CGD-O2D
3	B	105	HEM	CAD-CBD-CGD-O2D
3	B	105	HEM	CAD-CBD-CGD-O1D
3	C	295	HEM	CAD-CBD-CGD-O1D
3	A	295	HEM	CAA-CBA-CGA-O1A
3	A	295	HEM	CAD-CBD-CGD-O1D

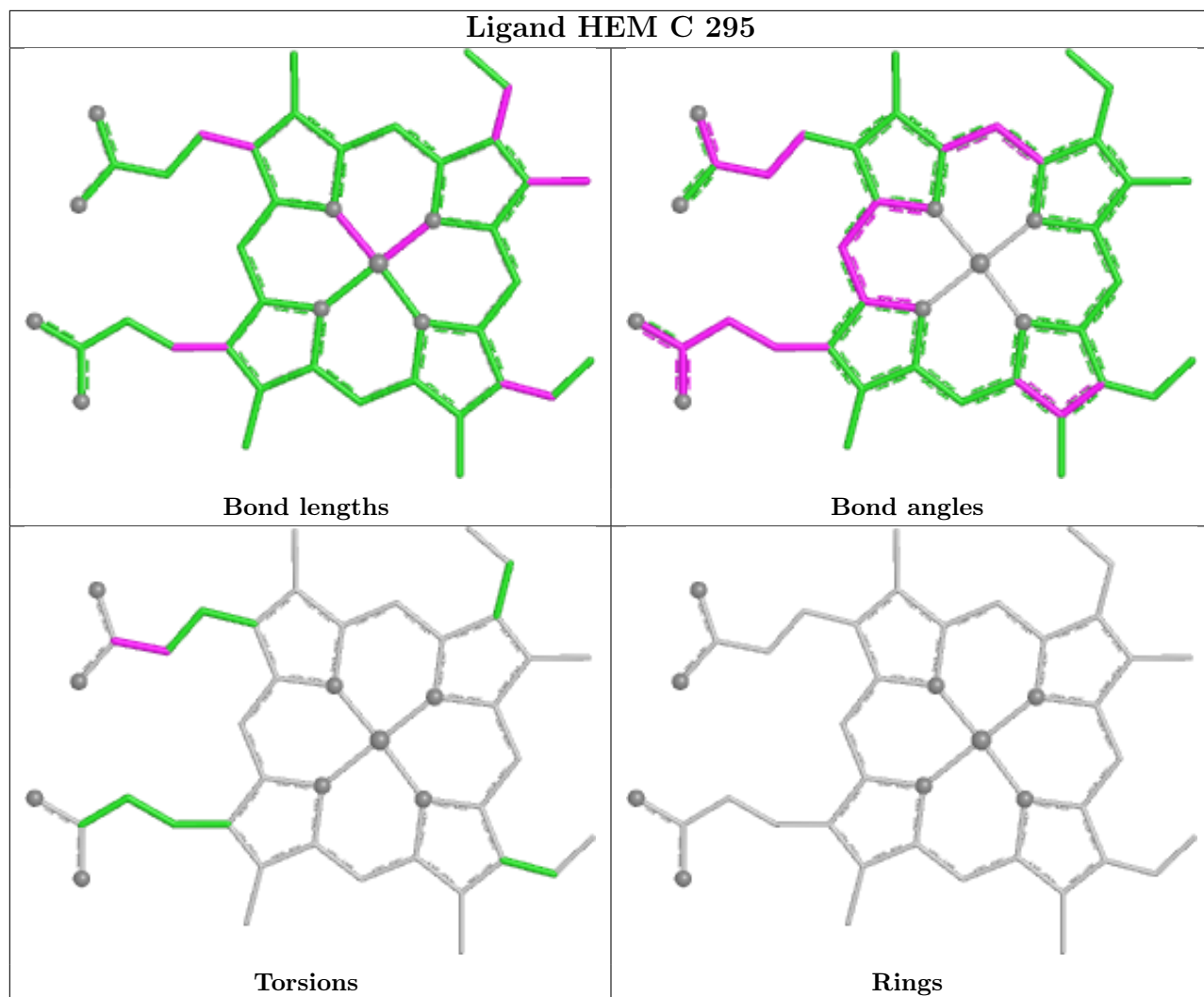
There are no ring outliers.

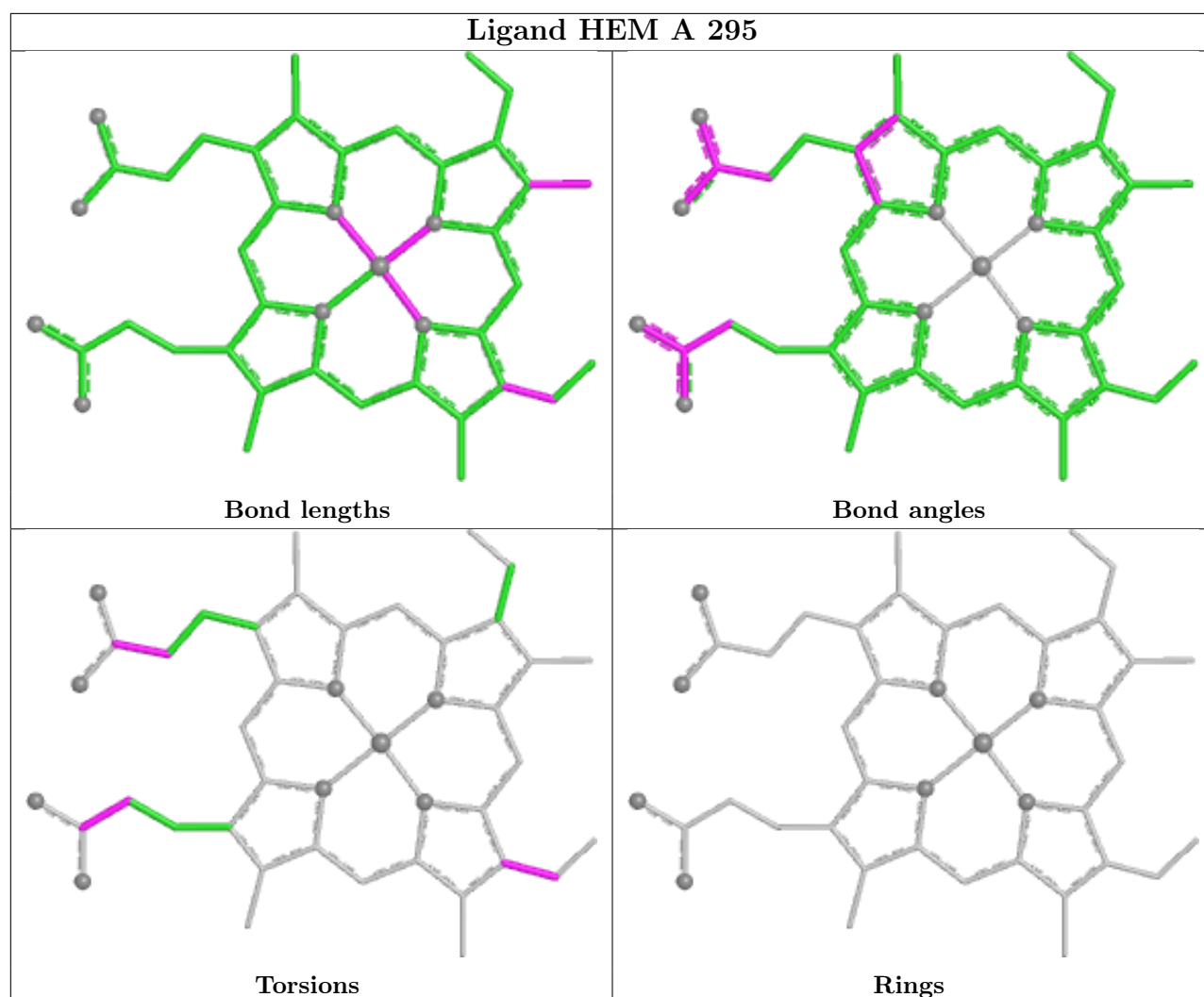
3 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	105	HEM	18	0
3	C	295	HEM	2	0
3	A	295	HEM	5	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.







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	294/296 (99%)	-1.28	0 100 100	10, 25, 47, 92	0
1	C	294/296 (99%)	-1.32	0 100 100	12, 26, 44, 62	0
2	B	104/104 (100%)	-0.38	0 100 100	29, 68, 92, 107	0
All	All	692/696 (99%)	-1.16	0 100 100	10, 27, 75, 107	0

There are no RSRZ outliers to report.

### 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.

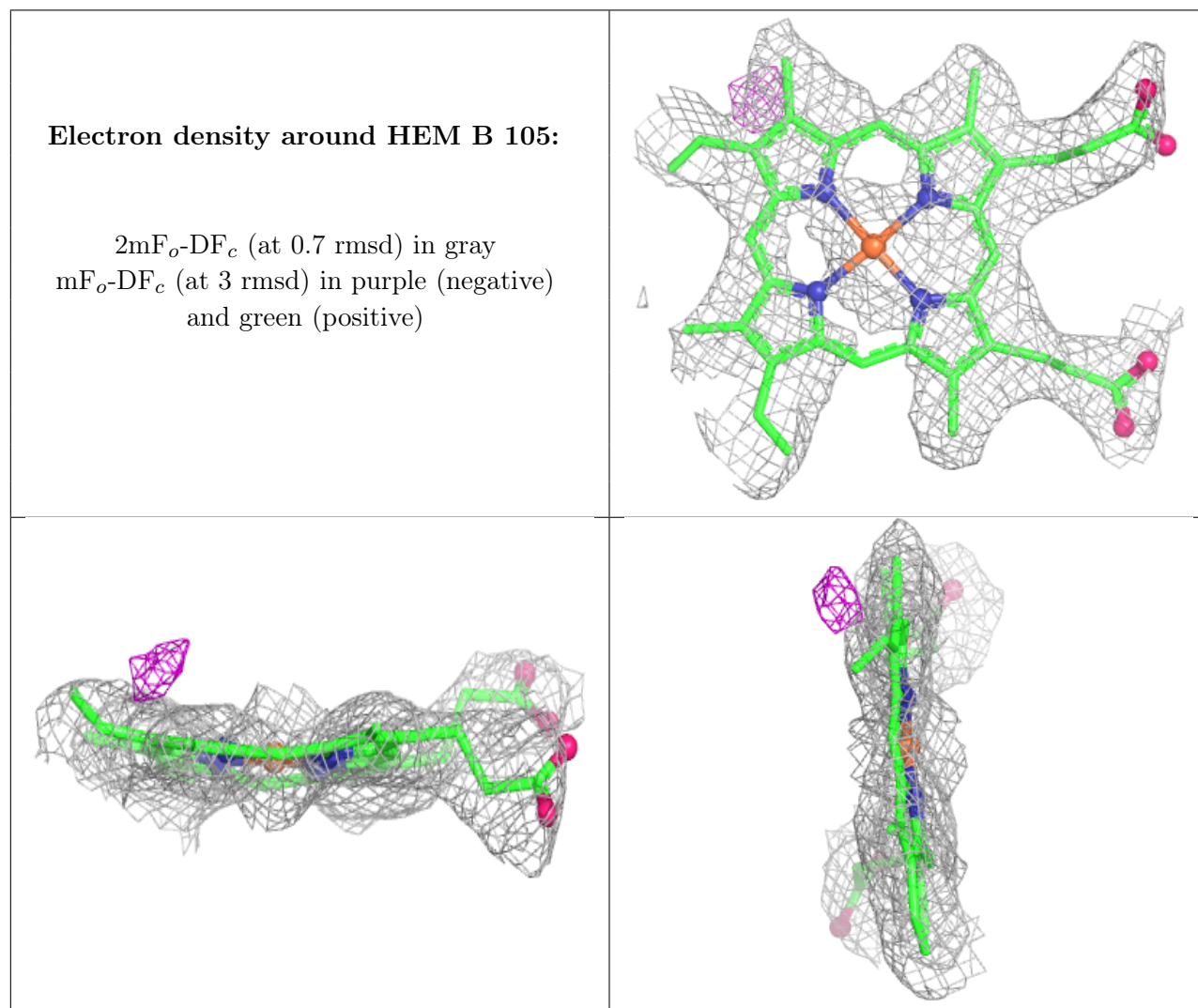
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	HEM	B	105	43/43	0.94	0.06	41,47,58,65	0
3	HEM	A	295	43/43	0.98	0.04	13,26,35,38	0
3	HEM	C	295	43/43	0.98	0.05	15,23,26,28	0

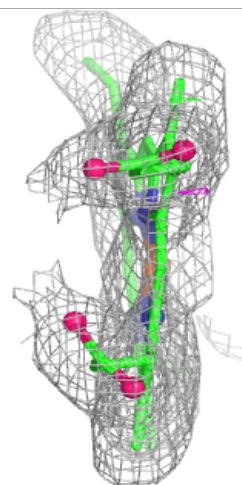
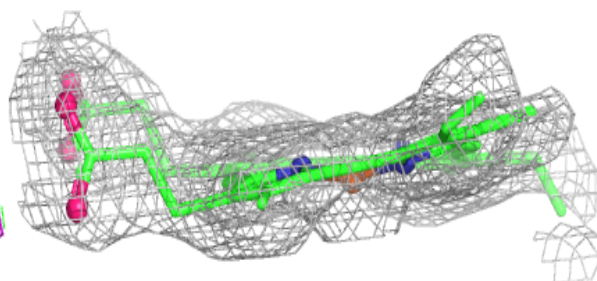
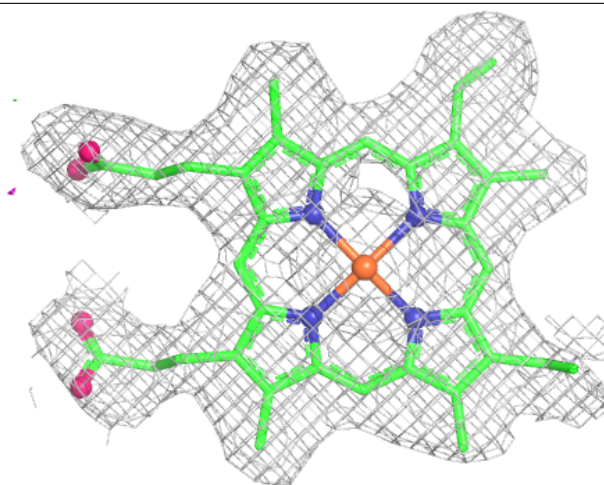
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

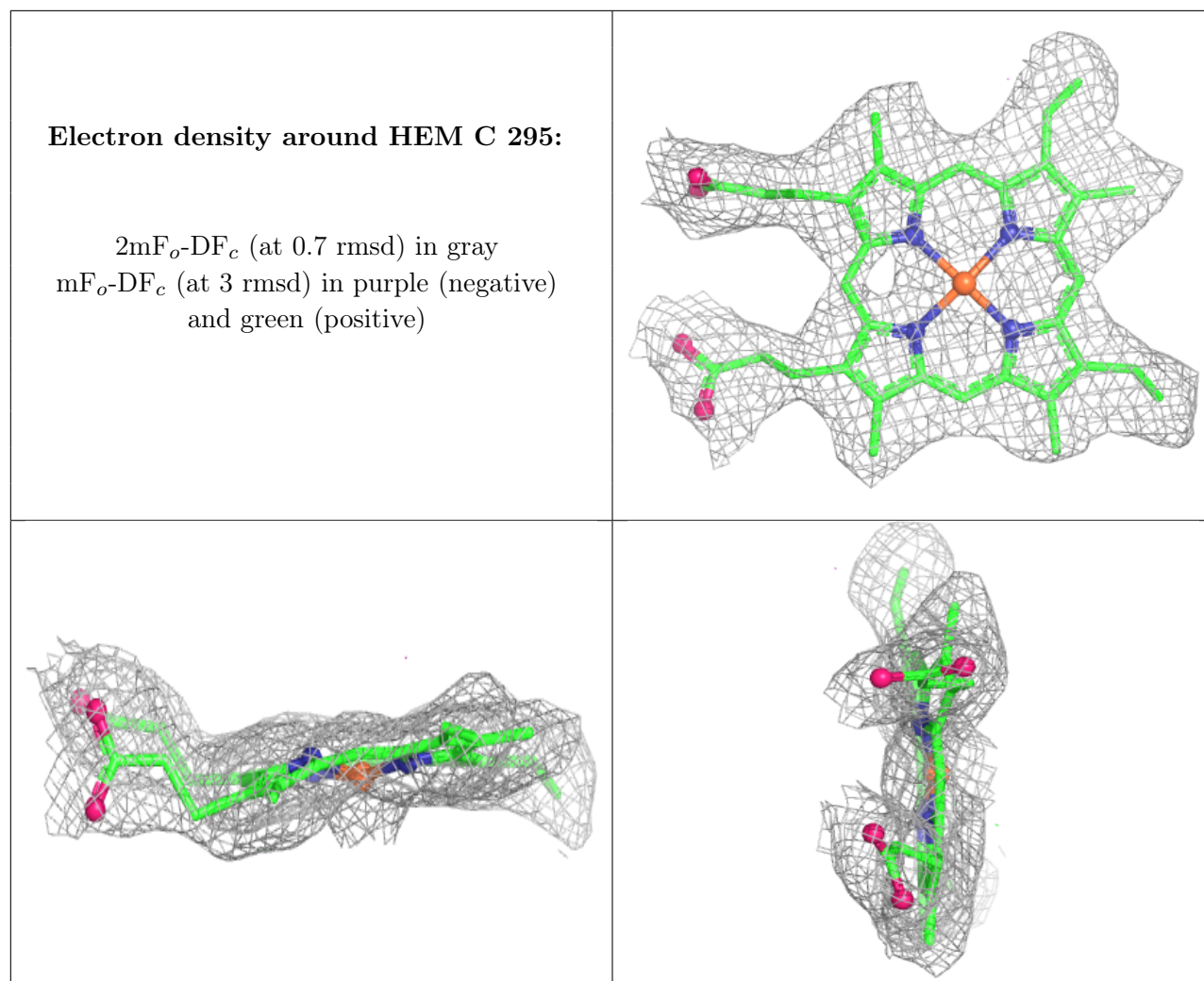
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around HEM A 295:**

$2mF_o-DF_c$  (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.