



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:16 PM UTC

PDB ID : 4HHB / pdb_00004hhb
Title : THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT
1.74 ANGSTROMS RESOLUTION
Authors : Fermi, G.; Perutz, M.F.
Deposited on : 1984-03-07
Resolution : 1.74 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

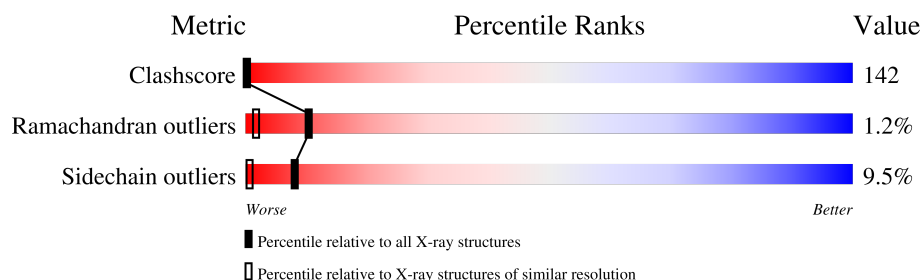
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	45% 28% 27%
1	C	141	40% 40% 18%
2	B	146	48% 30% 22%
2	D	146	38% 25% 34%

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	HEM	C	142	-	X	-	-
3	HEM	D	148	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4779 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.

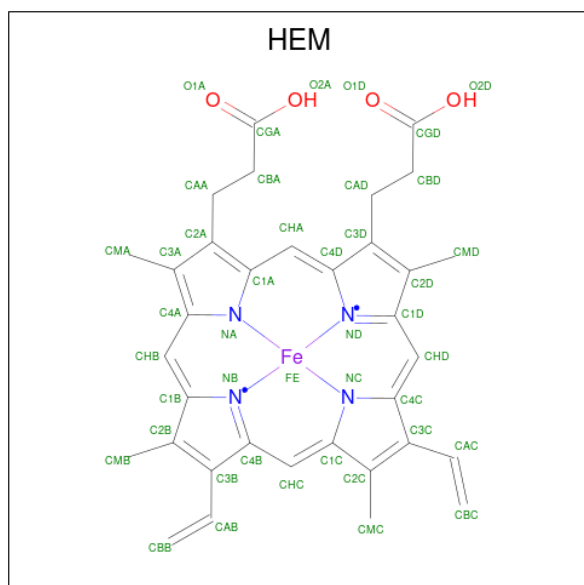
- Molecule 1 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

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



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	P		
			1	1	0	0
4	D	1	Total	P		
			1	1	0	0

- Molecule 5 is water.

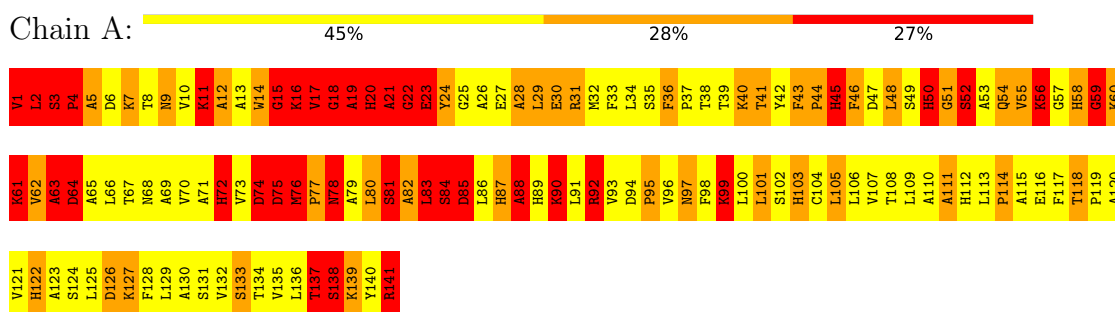
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O		
			56	56	0	0
5	B	57	Total	O		
			57	57	0	0
5	C	59	Total	O		
			59	59	0	0
5	D	49	Total	O		
			49	49	0	0

3 Residue-property plots

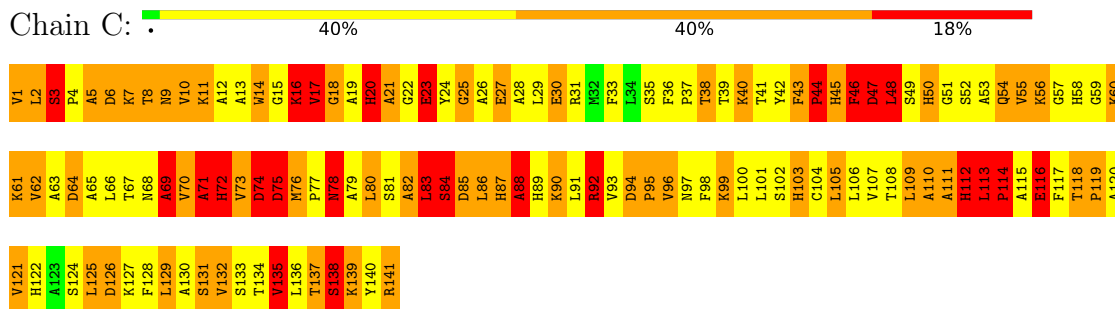
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

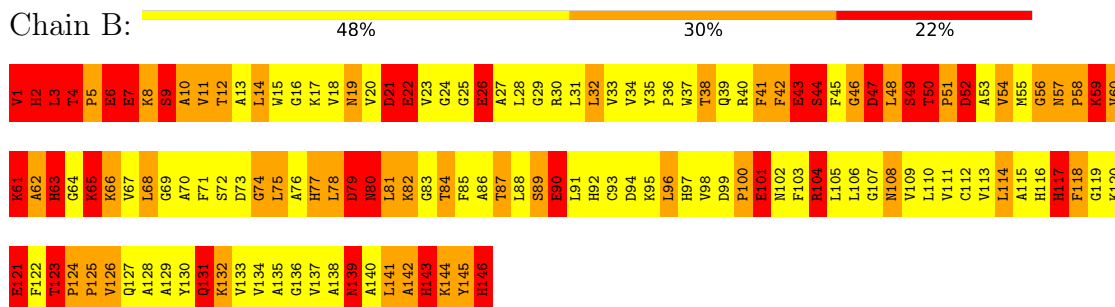
• Molecule 1: Hemoglobin subunit alpha



• Molecule 1: Hemoglobin subunit alpha



• Molecule 2: Hemoglobin subunit beta



• Molecule 2: Hemoglobin subunit beta





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.15Å 83.59Å 53.80Å 90.00° 99.34° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.74	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.74)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.135 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4779	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	9.87	528/1097 (48.1%)	7.13	602/1491 (40.4%)
1	C	9.98	511/1097 (46.6%)	7.37	563/1491 (37.8%)
2	B	11.66	521/1153 (45.2%)	7.56	637/1566 (40.7%)
2	D	12.76	567/1153 (49.2%)	8.54	658/1566 (42.0%)
All	All	11.16	2127/4500 (47.3%)	7.68	2460/6114 (40.2%)

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	50
1	C	2	45
2	B	2	49
2	D	5	62
All	All	10	206

All (2127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	ARG	NE-CZ	149.01	2.96	1.33
2	D	104	ARG	NE-CZ	113.64	2.58	1.33
1	A	92	ARG	NE-CZ	113.03	2.57	1.33
2	D	2	HIS	CG-ND1	100.10	2.48	1.38
2	B	2	HIS	ND1-CE1	85.56	2.18	1.32
2	B	26	GLU	CD-OE1	83.01	2.83	1.25
2	B	117	HIS	CD2-NE2	76.23	2.21	1.37
2	D	47	ASP	CA-C	75.94	2.43	1.52
2	B	104	ARG	NE-CZ	72.93	2.13	1.33
2	D	6	GLU	CD-OE2	70.65	2.59	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	143	HIS	ND1-CE1	66.61	1.99	1.32
2	D	146	HIS	ND1-CE1	-65.24	0.67	1.32
2	B	2	HIS	CD2-NE2	64.78	2.09	1.37
2	B	2	HIS	CG-CD2	63.51	2.05	1.35
2	D	52	ASP	CG-OD2	62.86	2.44	1.25
2	B	26	GLU	CD-OE2	62.05	2.43	1.25
1	C	23	GLU	CD-OE1	59.20	2.37	1.25
2	D	77	HIS	ND1-CE1	58.71	1.91	1.32
2	D	2	HIS	CE1-NE2	58.36	1.91	1.32
2	D	2	HIS	ND1-CE1	57.84	1.90	1.32
2	D	6	GLU	CA-C	55.99	2.31	1.52
2	D	5	PRO	CA-CB	55.55	2.31	1.54
2	D	2	HIS	CA-CB	53.36	2.21	1.53
2	D	73	ASP	CG-OD2	53.09	2.26	1.25
2	D	20	VAL	CA-CB	52.52	2.10	1.54
2	D	47	ASP	N-CA	52.29	2.09	1.46
2	B	146	HIS	ND1-CE1	51.88	1.84	1.32
2	B	117	HIS	CG-ND1	51.28	1.94	1.38
2	B	104	ARG	CZ-NH2	49.47	1.97	1.33
2	B	2	HIS	CB-CG	-47.38	0.83	1.50
1	C	20	HIS	ND1-CE1	46.46	1.79	1.32
2	B	2	HIS	CG-ND1	46.02	1.88	1.38
2	D	77	HIS	CD2-NE2	46.00	1.88	1.37
1	C	1	VAL	N-CA	45.98	2.33	1.46
2	B	22	GLU	CD-OE2	45.71	2.12	1.25
2	D	2	HIS	CG-CD2	45.45	1.85	1.35
2	D	143	HIS	CG-CD2	44.89	1.85	1.35
1	A	78	ASN	CG-OD1	44.08	2.07	1.23
2	B	77	HIS	CG-CD2	43.72	1.83	1.35
2	D	4	THR	C-N	-43.46	0.97	1.33
1	A	17	VAL	C-O	-43.41	0.75	1.24
2	D	146	HIS	CG-ND1	42.80	1.85	1.38
2	B	117	HIS	ND1-CE1	42.75	1.75	1.32
1	A	72	HIS	CG-ND1	42.65	1.85	1.38
1	A	21	ALA	CA-C	42.03	2.09	1.52
1	A	75	ASP	CG-OD2	41.45	2.04	1.25
2	B	1	VAL	C-N	-41.21	0.79	1.33
2	D	21	ASP	CA-C	-41.16	0.97	1.52
1	A	60	LYS	CE-NZ	39.88	2.69	1.49
2	B	104	ARG	CZ-NH1	39.28	1.87	1.32
1	A	90	LYS	CE-NZ	39.28	2.67	1.49
2	B	146	HIS	CB-CG	39.17	2.04	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	LEU	C-O	39.15	1.76	1.24
2	D	79	ASP	CG-OD1	39.02	1.99	1.25
1	C	92	ARG	CZ-NH1	38.98	1.87	1.32
2	D	79	ASP	CG-OD2	38.54	1.98	1.25
1	C	72	HIS	CG-ND1	38.00	1.80	1.38
2	D	58	PRO	CG-CD	-37.56	0.23	1.50
2	D	76	ALA	N-CA	37.39	1.94	1.46
1	C	138	SER	CA-CB	37.27	2.14	1.53
1	A	92	ARG	CZ-NH2	-36.68	0.85	1.33
1	C	112	HIS	CG-ND1	36.64	1.78	1.38
2	B	65	LYS	CE-NZ	36.58	2.59	1.49
2	D	50	THR	CA-CB	36.57	2.11	1.53
2	D	90	GLU	CG-CD	36.47	2.43	1.52
2	B	43	GLU	CG-CD	36.37	2.42	1.52
2	B	146	HIS	CG-ND1	-36.15	0.98	1.38
1	A	138	SER	CA-CB	36.02	2.12	1.53
1	A	17	VAL	CA-C	35.54	1.96	1.52
1	A	3	SER	C-N	35.11	1.62	1.33
2	D	117	HIS	CE1-NE2	-35.11	0.97	1.32
2	D	22	GLU	CG-CD	34.79	2.39	1.52
2	B	49	SER	C-O	34.44	1.79	1.23
2	B	139	ASN	CB-CG	-34.28	0.66	1.52
2	D	76	ALA	CA-C	-33.64	1.07	1.52
1	A	75	ASP	CB-CG	-33.54	0.68	1.52
2	D	132	LYS	CE-NZ	33.20	2.48	1.49
2	D	5	PRO	N-CA	32.87	1.84	1.47
2	D	117	HIS	CG-ND1	32.71	1.74	1.38
2	B	139	ASN	CG-ND2	32.61	2.01	1.33
2	B	121	GLU	CD-OE1	32.59	1.87	1.25
2	D	117	HIS	ND1-CE1	32.43	1.65	1.32
2	B	7	GLU	CA-CB	-32.39	0.98	1.53
2	B	65	LYS	CG-CD	32.39	2.49	1.52
2	B	2	HIS	CA-CB	32.12	2.01	1.53
1	A	15	GLY	C-O	32.09	1.67	1.23
2	D	2	HIS	CB-CG	-31.86	1.05	1.50
2	D	45	PHE	C-N	-31.72	0.87	1.33
2	B	65	LYS	CB-CG	-31.42	0.58	1.52
1	A	50	HIS	CA-CB	31.34	2.02	1.53
2	D	63	HIS	ND1-CE1	31.07	1.63	1.32
2	D	43	GLU	CA-C	30.09	1.94	1.52
1	A	75	ASP	CG-OD1	29.91	1.82	1.25
2	D	143	HIS	ND1-CE1	29.86	1.62	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	82	LYS	CD-CE	29.82	2.42	1.52
2	D	53	ALA	C-O	-29.69	0.89	1.24
1	A	20	HIS	CG-ND1	29.68	1.71	1.38
1	A	15	GLY	C-N	-29.57	0.92	1.33
1	A	20	HIS	CE1-NE2	-29.47	1.03	1.32
2	B	143	HIS	CG-ND1	29.46	1.70	1.38
1	C	1	VAL	CB-CG2	29.16	2.48	1.52
1	A	112	HIS	ND1-CE1	29.13	1.61	1.32
1	C	56	LYS	CD-CE	29.11	2.39	1.52
2	D	20	VAL	CA-C	-29.08	1.19	1.52
2	B	9	SER	N-CA	-28.97	1.10	1.46
1	C	22	GLY	CA-C	-28.84	1.20	1.52
1	C	70	VAL	C-N	-28.81	0.99	1.33
2	B	2	HIS	CE1-NE2	28.80	1.61	1.32
2	B	12	THR	CB-CG2	-28.61	0.58	1.52
2	B	82	LYS	CE-NZ	28.56	2.35	1.49
2	D	26	GLU	CD-OE1	28.50	1.79	1.25
1	C	78	ASN	CA-C	-28.37	1.14	1.52
2	B	66	LYS	CD-CE	28.23	2.37	1.52
2	B	47	ASP	CG-OD2	28.13	1.78	1.25
2	B	59	LYS	CD-CE	28.09	2.36	1.52
2	D	77	HIS	CE1-NE2	-27.93	1.04	1.32
2	B	65	LYS	CD-CE	27.62	2.35	1.52
1	A	50	HIS	C-N	-27.59	0.96	1.33
2	B	117	HIS	CG-CD2	27.51	1.66	1.35
2	D	146	HIS	CE1-NE2	27.48	1.60	1.32
2	B	82	LYS	CD-CE	-27.41	0.70	1.52
2	B	2	HIS	CA-C	27.29	1.84	1.52
1	C	92	ARG	CD-NE	-27.27	1.08	1.46
1	A	81	SER	CA-CB	27.24	2.00	1.53
2	B	22	GLU	CD-OE1	27.23	1.77	1.25
2	D	104	ARG	CD-NE	27.11	1.84	1.46
1	C	116	GLU	CB-CG	27.11	2.33	1.52
2	D	13	ALA	CA-CB	-27.01	1.11	1.53
2	D	55	MET	CA-C	26.98	1.90	1.52
1	A	127	LYS	CB-CG	-26.93	0.71	1.52
2	D	120	LYS	CE-NZ	26.78	2.29	1.49
1	C	92	ARG	CZ-NH2	-26.78	0.98	1.33
2	B	1	VAL	CA-C	26.70	2.09	1.52
1	A	75	ASP	CA-CB	26.64	1.97	1.53
2	B	74	GLY	C-N	26.62	1.70	1.33
1	C	50	HIS	CG-ND1	26.41	1.67	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	ASP	CG-OD1	-26.23	0.75	1.25
2	B	8	LYS	CE-NZ	26.12	2.27	1.49
1	C	99	LYS	CB-CG	-26.06	0.74	1.52
1	C	72	HIS	ND1-CE1	-25.88	1.06	1.32
2	D	2	HIS	C-O	25.73	1.54	1.23
2	B	145	TYR	C-N	-25.66	0.97	1.33
1	A	71	ALA	CA-C	-25.59	1.19	1.52
1	C	23	GLU	CG-CD	25.47	2.15	1.52
2	D	22	GLU	CB-CG	-25.47	0.76	1.52
2	D	49	SER	CA-C	25.39	1.86	1.52
2	B	9	SER	CA-C	25.36	1.87	1.52
1	A	78	ASN	CB-CG	-25.34	0.88	1.52
1	A	85	ASP	CG-OD2	25.32	1.73	1.25
2	B	87	THR	CA-CB	25.29	1.95	1.53
1	A	52	SER	CA-C	-25.22	1.21	1.52
1	C	114	PRO	CA-C	25.21	1.91	1.52
2	D	12	THR	CA-CB	25.18	1.93	1.53
2	B	63	HIS	ND1-CE1	25.14	1.57	1.32
2	B	73	ASP	CA-C	-25.10	1.20	1.52
1	C	74	ASP	C-O	-25.09	0.91	1.24
1	C	15	GLY	C-O	25.09	1.57	1.23
2	D	66	LYS	CD-CE	24.95	2.27	1.52
1	C	56	LYS	CG-CD	24.92	2.27	1.52
2	D	65	LYS	CG-CD	24.88	2.27	1.52
1	C	20	HIS	CE1-NE2	24.77	1.57	1.32
2	D	43	GLU	CB-CG	-24.75	0.78	1.52
2	B	146	HIS	CG-CD2	24.75	1.63	1.35
1	A	23	GLU	CD-OE1	24.72	1.72	1.25
1	C	99	LYS	CD-CE	24.71	2.26	1.52
1	A	18	GLY	CA-C	24.59	1.86	1.51
1	A	73	VAL	CA-C	-24.46	1.21	1.52
1	A	92	ARG	CG-CD	24.38	2.25	1.52
2	B	5	PRO	N-CD	24.31	1.81	1.47
2	B	76	ALA	C-O	-24.28	0.91	1.24
2	B	63	HIS	CG-ND1	24.27	1.65	1.38
2	D	52	ASP	N-CA	24.27	1.76	1.46
1	C	20	HIS	CG-ND1	24.20	1.64	1.38
1	C	72	HIS	CG-CD2	24.20	1.62	1.35
2	D	26	GLU	CD-OE2	24.07	1.71	1.25
2	B	143	HIS	CE1-NE2	24.05	1.56	1.32
2	B	71	PHE	C-N	-24.01	1.05	1.33
1	A	74	ASP	CG-OD1	-23.80	0.80	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	LYS	CE-NZ	23.72	2.20	1.49
1	C	30	GLU	CD-OE2	-23.67	0.80	1.25
1	C	7	LYS	N-CA	23.66	1.75	1.46
2	D	47	ASP	CA-CB	23.61	1.94	1.53
2	D	1	VAL	CA-C	23.57	2.02	1.52
1	A	44	PRO	CA-C	23.56	1.83	1.52
2	B	1	VAL	C-O	23.55	1.70	1.23
1	C	16	LYS	CD-CE	23.54	2.23	1.52
2	D	139	ASN	CG-OD1	23.53	1.68	1.23
1	C	7	LYS	CA-C	-23.52	1.19	1.52
1	A	61	LYS	CD-CE	-23.51	0.81	1.52
2	D	73	ASP	CA-C	-23.42	1.21	1.52
1	A	23	GLU	CG-CD	23.28	2.10	1.52
1	C	82	ALA	C-N	23.28	1.69	1.33
1	A	52	SER	N-CA	23.28	1.75	1.46
2	B	81	LEU	C-N	23.26	1.66	1.34
1	A	137	THR	CA-CB	23.17	1.91	1.53
1	A	50	HIS	CG-CD2	23.16	1.61	1.35
2	D	80	ASN	N-CA	23.07	1.75	1.46
1	A	72	HIS	CD2-NE2	22.95	1.63	1.37
2	B	44	SER	C-O	22.86	1.50	1.24
2	D	79	ASP	CA-C	22.80	1.83	1.52
1	C	50	HIS	CE1-NE2	22.79	1.55	1.32
2	D	65	LYS	CD-CE	22.78	2.20	1.52
2	D	22	GLU	CA-C	22.61	1.83	1.52
1	C	115	ALA	CA-C	-22.60	1.21	1.52
2	D	21	ASP	C-O	22.59	1.50	1.24
2	D	80	ASN	CG-OD1	22.55	1.66	1.23
2	B	76	ALA	C-N	22.50	1.64	1.33
2	D	144	LYS	CE-NZ	22.50	2.16	1.49
2	D	18	VAL	CA-CB	-22.45	1.26	1.54
1	A	22	GLY	CA-C	-22.42	1.20	1.51
2	D	117	HIS	CG-CD2	22.41	1.60	1.35
1	C	40	LYS	CD-CE	-22.30	0.85	1.52
2	B	79	ASP	CG-OD2	22.20	1.67	1.25
2	B	5	PRO	N-CA	-22.20	1.19	1.47
1	C	10	VAL	CA-C	22.20	1.81	1.52
1	C	11	LYS	CA-C	-22.13	1.24	1.52
2	B	6	GLU	CG-CD	22.11	2.07	1.52
2	B	6	GLU	CD-OE1	22.09	1.67	1.25
2	B	121	GLU	CG-CD	22.09	2.07	1.52
2	B	58	PRO	N-CD	21.98	1.78	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	26	GLU	CB-CG	21.97	2.18	1.52
2	D	101	GLU	CG-CD	21.96	2.06	1.52
2	B	90	GLU	CG-CD	21.96	2.06	1.52
2	B	66	LYS	N-CA	-21.94	1.18	1.46
2	B	142	ALA	CA-C	21.79	1.82	1.52
2	D	46	GLY	CA-C	21.79	1.82	1.51
2	B	8	LYS	CB-CG	-21.75	0.87	1.52
2	D	80	ASN	CA-CB	-21.66	1.16	1.53
2	B	80	ASN	CA-C	21.64	1.80	1.53
1	C	87	HIS	CA-C	21.64	1.82	1.52
1	A	26	ALA	N-CA	-21.55	1.20	1.46
1	A	67	THR	CB-OG1	-21.50	1.09	1.43
1	C	16	LYS	CA-C	21.48	1.82	1.52
2	D	95	LYS	CG-CD	21.48	2.16	1.52
2	D	97	HIS	ND1-CE1	21.37	1.53	1.32
2	D	48	LEU	N-CA	21.28	1.72	1.46
1	A	14	TRP	NE1-CE2	-21.24	1.14	1.37
2	D	126	VAL	CA-CB	21.21	1.81	1.54
1	C	72	HIS	CA-C	-21.18	1.19	1.52
1	C	1	VAL	CB-CG1	21.13	2.22	1.52
2	B	43	GLU	CD-OE1	-21.09	0.85	1.25
2	D	4	THR	CA-CB	20.97	1.82	1.53
1	A	122	HIS	ND1-CE1	20.93	1.53	1.32
2	B	117	HIS	CE1-NE2	20.78	1.53	1.32
1	C	2	LEU	CA-C	20.58	1.79	1.52
2	D	90	GLU	CD-OE1	20.53	1.64	1.25
2	B	4	THR	CA-C	-20.50	1.27	1.52
1	A	2	LEU	CA-C	20.46	1.77	1.52
2	D	139	ASN	CA-CB	-20.44	1.20	1.53
1	C	68	ASN	C-O	20.37	1.48	1.24
1	A	45	HIS	C-N	20.36	1.62	1.33
2	B	101	GLU	CG-CD	20.28	2.02	1.52
2	D	95	LYS	C-N	20.27	1.64	1.33
1	A	50	HIS	C-O	20.27	1.48	1.23
2	D	18	VAL	N-CA	20.22	1.70	1.46
1	A	45	HIS	CE1-NE2	20.12	1.52	1.32
2	D	76	ALA	C-O	20.12	1.49	1.24
1	C	72	HIS	CB-CG	-20.11	1.22	1.50
2	B	8	LYS	C-O	19.90	1.47	1.24
1	C	8	THR	CA-CB	19.85	1.84	1.53
1	C	23	GLU	CD-OE2	-19.80	0.87	1.25
2	D	19	ASN	CA-C	-19.77	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	LYS	C-N	19.73	1.59	1.33
2	D	121	GLU	CG-CD	19.68	2.01	1.52
2	B	50	THR	N-CA	-19.53	1.29	1.46
2	D	43	GLU	CA-CB	-19.51	1.18	1.53
2	D	83	GLY	C-O	19.48	1.50	1.23
2	D	73	ASP	CA-CB	19.45	1.86	1.53
2	D	8	LYS	CA-CB	19.44	1.85	1.53
1	A	30	GLU	CG-CD	19.43	2.00	1.52
2	B	50	THR	CA-CB	-19.41	1.28	1.53
2	D	78	LEU	CG-CD2	-19.40	0.88	1.52
2	D	6	GLU	CB-CG	-19.37	0.94	1.52
2	D	19	ASN	CG-OD1	19.29	1.60	1.23
1	C	72	HIS	CA-CB	19.20	1.85	1.53
1	A	106	LEU	CB-CG	-19.19	1.15	1.53
1	C	90	LYS	CE-NZ	19.14	2.06	1.49
2	D	17	LYS	C-N	19.01	1.61	1.33
1	C	20	HIS	CD2-NE2	-18.85	1.17	1.37
1	C	70	VAL	N-CA	18.82	1.68	1.46
1	C	114	PRO	N-CA	18.82	1.72	1.47
1	C	71	ALA	CA-C	-18.81	1.28	1.52
1	C	103	HIS	CG-ND1	18.78	1.58	1.38
2	B	5	PRO	CA-C	18.75	1.78	1.52
2	B	41	PHE	CA-C	18.72	1.77	1.52
2	B	10	ALA	CA-C	18.69	1.78	1.52
2	B	139	ASN	CG-OD1	18.61	1.58	1.23
2	D	43	GLU	CD-OE1	18.60	1.60	1.25
1	A	72	HIS	CA-CB	18.57	1.78	1.53
2	D	53	ALA	CA-C	18.55	1.76	1.52
2	B	90	GLU	CA-CB	18.54	1.84	1.53
2	D	146	HIS	CD2-NE2	18.54	1.58	1.37
2	B	143	HIS	CA-C	18.53	1.76	1.52
1	C	61	LYS	CA-C	18.52	1.76	1.52
2	B	40	ARG	NE-CZ	18.51	1.53	1.33
1	A	58	HIS	CA-C	18.49	1.76	1.52
1	C	49	SER	C-N	18.44	1.58	1.33
1	A	74	ASP	C-N	-18.43	0.93	1.34
2	B	145	TYR	CA-C	18.42	1.75	1.52
2	B	81	LEU	N-CA	18.35	1.68	1.46
2	D	12	THR	N-CA	18.26	1.68	1.46
2	D	2	HIS	CD2-NE2	18.25	1.57	1.37
2	D	19	ASN	CG-ND2	18.22	1.71	1.33
1	C	25	GLY	C-O	18.22	1.47	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	82	LYS	CA-C	-18.21	1.28	1.52
1	C	133	SER	C-O	18.20	1.45	1.24
2	D	59	LYS	CG-CD	-18.20	0.97	1.52
1	C	118	THR	CA-CB	18.17	1.75	1.53
2	D	6	GLU	CG-CD	18.16	1.97	1.52
2	D	40	ARG	C-O	18.16	1.46	1.24
1	A	17	VAL	C-N	18.15	1.59	1.33
2	B	6	GLU	C-O	18.14	1.47	1.24
2	D	116	HIS	CE1-NE2	18.14	1.50	1.32
1	C	105	LEU	CG-CD2	18.12	2.12	1.52
1	A	4	PRO	N-CA	-18.11	1.32	1.47
2	D	66	LYS	CG-CD	18.11	2.06	1.52
2	B	77	HIS	ND1-CE1	-18.09	1.14	1.32
2	D	117	HIS	CB-CG	-18.09	1.24	1.50
2	B	6	GLU	CA-C	18.07	1.77	1.52
2	D	18	VAL	CA-C	18.00	1.73	1.52
1	C	71	ALA	N-CA	18.00	1.67	1.46
1	A	56	LYS	CG-CD	17.92	2.06	1.52
1	C	70	VAL	CA-C	17.84	1.74	1.52
1	C	38	THR	CA-CB	17.78	1.81	1.53
2	D	50	THR	N-CA	17.77	1.71	1.46
1	C	12	ALA	C-N	17.73	1.55	1.33
2	D	43	GLU	CD-OE2	17.72	1.59	1.25
1	C	45	HIS	ND1-CE1	-17.70	1.14	1.32
2	D	21	ASP	CG-OD1	17.70	1.58	1.25
1	C	30	GLU	CG-CD	17.66	1.96	1.52
2	D	53	ALA	C-N	17.66	1.56	1.33
1	A	49	SER	C-N	17.66	1.58	1.33
2	B	54	VAL	CA-C	-17.65	1.31	1.52
1	C	56	LYS	CA-C	-17.60	1.29	1.52
2	B	40	ARG	CZ-NH2	17.56	1.56	1.33
1	A	64	ASP	CB-CG	17.55	1.96	1.52
1	C	60	LYS	CE-NZ	17.54	2.02	1.49
1	A	84	SER	CA-CB	17.52	1.82	1.53
2	D	78	LEU	C-O	-17.48	1.01	1.24
1	A	99	LYS	CG-CD	-17.44	1.00	1.52
2	D	73	ASP	CG-OD1	17.43	1.58	1.25
1	A	71	ALA	C-O	17.39	1.44	1.24
2	D	59	LYS	CA-C	17.37	1.76	1.52
2	B	90	GLU	CD-OE1	-17.33	0.92	1.25
2	B	65	LYS	CA-CB	17.33	1.80	1.53
2	B	143	HIS	CB-CG	17.32	1.74	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	47	ASP	CA-C	17.32	1.75	1.52
1	A	47	ASP	C-N	-17.31	1.13	1.33
2	D	73	ASP	C-N	17.28	1.61	1.33
2	D	8	LYS	N-CA	17.27	1.68	1.46
2	B	2	HIS	C-O	17.27	1.43	1.24
1	C	131	SER	CA-C	17.25	1.76	1.52
2	B	59	LYS	CG-CD	-17.24	1.00	1.52
1	C	52	SER	CA-C	-17.18	1.28	1.52
1	C	54	GLN	CA-C	17.17	1.75	1.52
2	D	60	VAL	N-CA	17.16	1.67	1.46
1	A	47	ASP	CA-C	17.13	1.74	1.52
2	D	10	ALA	CA-C	17.12	1.75	1.52
1	A	62	VAL	CA-C	17.12	1.75	1.52
2	D	92	HIS	CA-C	17.08	1.76	1.52
1	A	14	TRP	CA-CB	17.08	1.83	1.53
2	D	83	GLY	C-N	17.07	1.55	1.33
1	A	77	PRO	CA-C	-17.04	1.28	1.52
2	D	8	LYS	CD-CE	17.04	2.03	1.52
1	A	74	ASP	CG-OD2	17.02	1.57	1.25
2	D	58	PRO	N-CD	16.90	1.71	1.47
2	D	94	ASP	N-CA	16.88	1.68	1.46
1	C	84	SER	CA-CB	16.87	1.79	1.53
1	A	29	LEU	CA-CB	16.86	1.79	1.53
1	A	37	PRO	N-CD	-16.86	1.24	1.47
1	C	137	THR	CA-C	16.85	1.74	1.52
1	C	73	VAL	CA-CB	16.84	1.80	1.54
1	A	4	PRO	C-N	16.84	1.59	1.33
2	D	7	GLU	CA-C	16.81	1.75	1.52
2	B	144	LYS	CE-NZ	16.79	1.99	1.49
1	A	87	HIS	CA-C	16.70	1.75	1.52
1	C	15	GLY	C-N	-16.69	1.09	1.33
2	B	47	ASP	N-CA	16.67	1.67	1.46
2	D	6	GLU	C-O	-16.63	1.02	1.24
1	A	19	ALA	C-O	16.62	1.47	1.24
1	A	88	ALA	CA-C	16.62	1.73	1.52
1	A	17	VAL	N-CA	-16.59	1.27	1.46
1	C	68	ASN	CG-OD1	-16.57	0.92	1.23
2	D	95	LYS	CE-NZ	16.55	1.99	1.49
1	A	33	PHE	CA-C	-16.53	1.30	1.52
2	D	60	VAL	CA-C	-16.52	1.33	1.52
2	B	79	ASP	C-O	-16.52	1.02	1.24
2	D	30	ARG	CD-NE	-16.52	1.23	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	95	LYS	CA-C	-16.50	1.31	1.52
2	D	17	LYS	CE-NZ	16.42	1.98	1.49
2	B	49	SER	CA-C	-16.41	1.31	1.53
2	D	1	VAL	N-CA	16.40	1.77	1.46
2	D	6	GLU	CD-OE1	-16.39	0.94	1.25
2	B	143	HIS	CG-CD2	-16.37	1.17	1.35
2	D	19	ASN	C-O	16.36	1.44	1.24
1	C	4	PRO	N-CA	-16.35	1.26	1.47
1	C	72	HIS	C-O	16.32	1.45	1.24
1	A	20	HIS	CD2-NE2	16.26	1.55	1.37
1	A	16	LYS	CG-CD	16.26	2.01	1.52
1	C	61	LYS	CE-NZ	16.25	1.98	1.49
2	B	144	LYS	CD-CE	16.22	2.01	1.52
2	D	135	ALA	CA-C	16.20	1.73	1.52
1	A	134	THR	CB-OG1	-16.18	1.17	1.43
1	A	89	HIS	CG-CD2	16.16	1.53	1.35
2	B	124	PRO	N-CD	16.16	1.70	1.47
2	B	45	PHE	CG-CD2	-16.12	1.04	1.38
2	B	6	GLU	CB-CG	-16.10	1.04	1.52
2	B	92	HIS	ND1-CE1	16.10	1.48	1.32
1	A	59	GLY	CA-C	-16.08	1.32	1.52
2	D	43	GLU	CG-CD	16.07	1.92	1.52
2	D	102	ASN	C-O	16.00	1.44	1.24
2	D	63	HIS	CA-CB	-15.98	1.27	1.53
2	B	116	HIS	ND1-CE1	15.94	1.48	1.32
2	B	43	GLU	CA-CB	-15.93	1.26	1.53
1	A	20	HIS	CG-CD2	15.91	1.53	1.35
1	A	49	SER	CB-OG	-15.84	1.10	1.42
2	B	9	SER	CA-CB	15.83	1.79	1.53
2	D	78	LEU	N-CA	-15.83	1.25	1.46
2	D	67	VAL	CA-CB	15.83	1.76	1.54
2	B	20	VAL	CA-C	-15.81	1.30	1.52
2	D	121	GLU	CA-CB	15.78	1.79	1.53
1	C	71	ALA	CA-CB	-15.75	1.28	1.53
2	B	6	GLU	CD-OE2	-15.73	0.95	1.25
1	C	128	PHE	CA-C	15.72	1.73	1.52
2	D	80	ASN	CA-C	15.69	1.73	1.52
2	D	92	HIS	CG-ND1	15.68	1.55	1.38
2	B	44	SER	C-N	15.67	1.55	1.33
2	B	69	GLY	C-N	15.66	1.53	1.33
1	C	49	SER	CB-OG	-15.66	1.10	1.42
1	A	12	ALA	C-O	15.62	1.45	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	HIS	CE1-NE2	-15.62	1.17	1.32
2	B	81	LEU	CA-C	-15.60	1.32	1.52
2	B	102	ASN	CG-OD1	-15.60	0.94	1.23
1	A	137	THR	CB-CG2	-15.57	1.01	1.52
2	D	19	ASN	C-N	-15.57	1.15	1.33
2	B	46	GLY	C-N	-15.56	1.07	1.33
1	A	139	LYS	CE-NZ	15.55	1.96	1.49
2	D	78	LEU	CA-CB	15.53	1.79	1.53
1	A	31	ARG	CD-NE	15.53	1.68	1.46
2	B	40	ARG	CD-NE	-15.51	1.24	1.46
1	C	127	LYS	C-O	15.50	1.42	1.24
2	D	93	CYS	C-O	-15.50	1.05	1.24
1	C	46	PHE	CD2-CE2	-15.50	0.92	1.38
1	A	1	VAL	N-CA	-15.48	1.16	1.46
2	D	77	HIS	C-N	15.47	1.55	1.33
1	A	122	HIS	N-CA	15.46	1.66	1.46
2	D	26	GLU	CG-CD	15.44	1.90	1.52
1	A	88	ALA	C-O	-15.42	1.06	1.24
1	A	134	THR	CA-C	-15.42	1.31	1.52
1	C	76	MET	CA-C	-15.41	1.33	1.52
1	A	83	LEU	CB-CG	-15.39	1.22	1.53
2	B	1	VAL	CB-CG1	15.37	2.03	1.52
2	D	66	LYS	CE-NZ	15.36	1.95	1.49
2	D	41	PHE	CA-C	15.33	1.73	1.52
1	A	13	ALA	CA-C	15.32	1.73	1.52
1	C	114	PRO	CA-CB	-15.29	1.32	1.53
1	A	2	LEU	C-N	-15.25	1.01	1.33
1	C	69	ALA	N-CA	15.25	1.64	1.46
1	A	96	VAL	CB-CG2	-15.24	1.02	1.52
2	B	80	ASN	N-CA	15.22	1.73	1.46
2	B	87	THR	CB-CG2	15.20	2.02	1.52
1	C	92	ARG	C-O	-15.20	1.04	1.23
2	D	110	LEU	C-N	15.20	1.53	1.33
1	A	56	LYS	C-N	15.18	1.55	1.33
1	A	137	THR	N-CA	15.17	1.65	1.46
1	C	19	ALA	C-O	15.15	1.44	1.24
1	A	77	PRO	C-O	15.14	1.43	1.24
2	D	82	LYS	CE-NZ	15.14	1.94	1.49
1	A	127	LYS	CG-CD	15.13	1.97	1.52
2	D	58	PRO	C-O	15.11	1.43	1.24
1	C	49	SER	CA-C	-15.11	1.32	1.52
2	D	50	THR	CA-C	15.08	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	VAL	CA-CB	-15.04	1.36	1.54
2	D	53	ALA	CA-CB	-15.04	1.29	1.53
2	B	66	LYS	CA-C	15.03	1.72	1.52
2	B	51	PRO	C-O	15.01	1.41	1.24
2	B	46	GLY	C-O	15.01	1.44	1.23
1	C	8	THR	CA-C	-14.99	1.33	1.52
1	C	20	HIS	CB-CG	14.98	1.71	1.50
2	D	8	LYS	CE-NZ	14.93	1.94	1.49
2	D	20	VAL	N-CA	14.86	1.63	1.46
1	C	47	ASP	CA-CB	14.85	1.72	1.53
2	D	8	LYS	CA-C	-14.76	1.32	1.52
2	B	2	HIS	C-N	-14.76	1.12	1.33
1	A	11	LYS	CD-CE	14.73	1.96	1.52
2	B	145	TYR	CA-CB	-14.73	1.29	1.53
1	A	90	LYS	N-CA	-14.72	1.27	1.46
2	D	45	PHE	CA-C	14.68	1.72	1.52
2	D	94	ASP	CG-OD2	14.66	1.53	1.25
1	C	1	VAL	CA-C	14.62	1.83	1.52
1	A	94	ASP	CA-C	14.60	1.69	1.53
2	B	121	GLU	CB-CG	-14.59	1.08	1.52
2	D	26	GLU	CA-C	14.56	1.71	1.52
1	C	44	PRO	C-N	-14.55	1.11	1.33
1	A	42	TYR	CA-C	14.54	1.72	1.52
1	A	29	LEU	N-CA	14.54	1.63	1.46
1	A	16	LYS	C-N	14.51	1.52	1.33
2	D	79	ASP	CA-CB	14.51	1.73	1.53
2	B	49	SER	N-CA	14.51	1.67	1.46
1	C	106	LEU	CA-C	-14.51	1.33	1.52
2	B	80	ASN	CG-OD1	14.50	1.51	1.23
2	B	49	SER	CB-OG	14.50	1.71	1.42
2	B	94	ASP	CG-OD2	-14.47	0.97	1.25
2	D	121	GLU	CB-CG	-14.45	1.09	1.52
1	C	139	LYS	CD-CE	14.43	1.95	1.52
1	A	137	THR	CB-OG1	14.39	1.66	1.43
1	C	23	GLU	CA-C	14.38	1.71	1.52
2	B	42	PHE	CG-CD1	14.37	1.69	1.38
1	C	26	ALA	C-N	14.35	1.53	1.33
2	D	71	PHE	N-CA	14.35	1.63	1.46
2	B	59	LYS	CE-NZ	14.34	1.92	1.49
1	A	99	LYS	CB-CG	-14.31	1.09	1.52
1	A	4	PRO	CA-CB	14.31	1.73	1.53
1	A	8	THR	C-N	14.28	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	42	PHE	CG-CD1	14.27	1.68	1.38
1	C	41	THR	C-O	14.26	1.42	1.24
1	A	5	ALA	CA-CB	14.25	1.77	1.53
2	B	125	PRO	N-CD	14.25	1.67	1.47
2	B	134	VAL	N-CA	-14.24	1.29	1.46
1	C	29	LEU	CA-C	-14.24	1.34	1.52
1	A	67	THR	C-O	14.22	1.40	1.24
1	C	7	LYS	CG-CD	14.22	1.95	1.52
1	A	99	LYS	CD-CE	14.22	1.95	1.52
2	B	142	ALA	C-N	-14.16	1.15	1.33
2	D	121	GLU	CD-OE1	14.15	1.52	1.25
1	C	11	LYS	CE-NZ	14.15	1.91	1.49
1	C	50	HIS	CA-C	14.14	1.71	1.52
1	C	74	ASP	CG-OD1	14.12	1.52	1.25
2	D	125	PRO	N-CD	14.10	1.67	1.47
1	A	76	MET	SD-CE	-14.09	1.44	1.79
1	A	17	VAL	CA-CB	-14.07	1.38	1.54
1	C	37	PRO	N-CD	-14.07	1.28	1.47
2	B	113	VAL	C-O	14.03	1.42	1.24
2	B	104	ARG	CD-NE	13.98	1.65	1.46
2	D	144	LYS	CD-CE	-13.95	1.10	1.52
2	D	66	LYS	CB-CG	-13.94	1.10	1.52
2	D	137	VAL	CA-CB	13.94	1.73	1.54
1	A	104	CYS	N-CA	13.93	1.64	1.46
1	A	99	LYS	CA-C	-13.93	1.33	1.52
2	B	40	ARG	C-N	-13.87	1.13	1.33
1	C	7	LYS	C-N	13.83	1.51	1.33
1	C	16	LYS	CB-CG	13.82	1.94	1.52
1	A	106	LEU	CA-C	-13.79	1.33	1.52
2	B	43	GLU	CD-OE2	13.79	1.51	1.25
1	C	18	GLY	C-O	13.78	1.42	1.23
2	B	74	GLY	CA-C	-13.78	1.32	1.51
1	A	60	LYS	CD-CE	13.77	1.93	1.52
1	A	85	ASP	N-CA	13.77	1.64	1.46
2	D	4	THR	N-CA	-13.76	1.24	1.46
2	B	8	LYS	CA-CB	13.75	1.74	1.53
1	A	64	ASP	CG-OD1	13.73	1.51	1.25
1	A	58	HIS	CB-CG	13.69	1.69	1.50
1	A	79	ALA	CA-C	13.63	1.70	1.52
1	A	86	LEU	CB-CG	-13.61	1.26	1.53
2	B	61	LYS	CG-CD	13.61	1.93	1.52
2	D	13	ALA	C-N	13.61	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	ALA	C-N	-13.61	1.17	1.33
2	B	79	ASP	CB-CG	-13.58	1.18	1.52
2	B	22	GLU	CG-CD	13.53	1.85	1.52
2	B	73	ASP	C-O	13.50	1.40	1.24
1	A	58	HIS	CE1-NE2	-13.50	1.19	1.32
1	C	58	HIS	ND1-CE1	13.44	1.46	1.32
2	D	143	HIS	CG-ND1	-13.44	1.23	1.38
1	A	76	MET	CB-CG	-13.43	1.12	1.52
1	C	72	HIS	N-CA	-13.42	1.28	1.46
2	D	63	HIS	CB-CG	13.39	1.69	1.50
1	C	137	THR	CB-OG1	-13.39	1.22	1.43
2	D	80	ASN	C-O	-13.39	1.07	1.24
2	D	44	SER	CA-C	-13.36	1.34	1.52
1	C	115	ALA	N-CA	-13.36	1.29	1.46
2	B	101	GLU	C-N	13.33	1.52	1.34
1	C	112	HIS	CB-CG	-13.32	1.31	1.50
1	A	56	LYS	CA-C	-13.30	1.34	1.52
1	C	50	HIS	CB-CG	-13.30	1.31	1.50
1	C	38	THR	CA-C	-13.29	1.35	1.52
1	C	89	HIS	CE1-NE2	-13.28	1.19	1.32
1	A	16	LYS	CD-CE	13.28	1.92	1.52
2	D	63	HIS	CE1-NE2	-13.26	1.19	1.32
1	C	58	HIS	CA-C	13.26	1.69	1.52
1	A	78	ASN	C-O	13.25	1.39	1.24
2	D	12	THR	C-O	13.25	1.39	1.24
1	A	8	THR	CA-C	-13.24	1.35	1.52
2	D	77	HIS	CA-CB	13.21	1.75	1.53
1	A	10	VAL	CA-C	13.19	1.69	1.52
1	A	77	PRO	CA-CB	13.18	1.72	1.53
1	A	127	LYS	C-N	-13.17	1.16	1.33
2	B	98	VAL	CA-C	13.16	1.69	1.52
2	B	126	VAL	C-O	13.15	1.41	1.24
2	D	144	LYS	CA-CB	-13.14	1.30	1.53
2	B	132	LYS	CA-CB	-13.14	1.32	1.53
1	A	120	ALA	C-N	-13.13	1.17	1.33
2	B	12	THR	CB-OG1	-13.11	1.22	1.43
2	B	17	LYS	C-O	13.11	1.42	1.23
2	B	11	VAL	CA-CB	-13.10	1.39	1.54
1	C	131	SER	N-CA	13.10	1.63	1.46
2	B	132	LYS	CE-NZ	13.10	1.88	1.49
2	D	85	PHE	N-CA	13.10	1.63	1.46
2	B	54	VAL	CA-CB	13.08	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	VAL	CA-C	-13.05	1.38	1.52
1	A	113	LEU	CA-CB	-13.04	1.38	1.53
2	B	95	LYS	CA-CB	13.04	1.72	1.54
2	D	43	GLU	C-O	-13.02	1.07	1.24
1	A	14	TRP	CD2-CE2	13.01	1.63	1.41
2	D	54	VAL	N-CA	13.00	1.61	1.46
1	A	21	ALA	C-O	-12.99	1.07	1.24
2	D	84	THR	CB-OG1	-12.99	1.23	1.43
1	C	14	TRP	CZ3-CH2	12.99	1.73	1.40
2	B	10	ALA	N-CA	-12.98	1.29	1.46
2	D	126	VAL	C-N	12.97	1.50	1.33
2	B	108	ASN	CB-CG	12.97	1.84	1.52
1	C	23	GLU	N-CA	-12.94	1.30	1.46
2	D	116	HIS	ND1-CE1	12.94	1.45	1.32
1	C	90	LYS	CD-CE	12.93	1.91	1.52
2	D	117	HIS	CD2-NE2	-12.92	1.23	1.37
2	B	69	GLY	N-CA	-12.87	1.29	1.45
1	A	15	GLY	CA-C	12.85	1.70	1.51
2	B	21	ASP	CB-CG	12.84	1.84	1.52
1	C	63	ALA	CA-C	-12.83	1.36	1.52
2	D	9	SER	CB-OG	-12.82	1.16	1.42
2	D	121	GLU	N-CA	-12.82	1.29	1.46
2	D	84	THR	CA-C	12.79	1.68	1.52
1	A	92	ARG	CA-C	-12.79	1.37	1.53
1	A	41	THR	CA-C	-12.79	1.35	1.52
2	D	40	ARG	NE-CZ	12.78	1.47	1.33
1	A	60	LYS	C-N	12.77	1.51	1.33
1	C	109	LEU	C-N	12.76	1.49	1.33
1	C	48	LEU	CA-C	-12.73	1.32	1.52
1	A	132	VAL	CA-CB	-12.72	1.38	1.54
1	A	141	ARG	NE-CZ	12.72	1.47	1.33
2	D	48	LEU	CA-C	12.69	1.69	1.52
1	C	78	ASN	C-N	12.69	1.50	1.33
1	C	88	ALA	CA-C	12.69	1.68	1.52
2	B	72	SER	N-CA	12.69	1.61	1.46
2	B	75	LEU	CB-CG	-12.69	1.28	1.53
1	C	103	HIS	ND1-CE1	12.68	1.45	1.32
2	D	40	ARG	CZ-NH1	-12.68	1.15	1.32
2	D	40	ARG	CD-NE	-12.68	1.28	1.46
2	B	73	ASP	CG-OD2	-12.67	1.01	1.25
1	C	113	LEU	CA-CB	-12.66	1.33	1.53
1	A	40	LYS	CA-CB	12.64	1.75	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	22	GLU	N-CA	12.63	1.61	1.46
1	C	87	HIS	ND1-CE1	12.62	1.45	1.32
2	D	67	VAL	CA-C	-12.61	1.34	1.52
1	C	12	ALA	N-CA	-12.59	1.31	1.46
2	D	78	LEU	C-N	12.59	1.50	1.33
1	A	7	LYS	N-CA	12.58	1.62	1.46
2	D	70	ALA	C-O	12.57	1.39	1.24
2	D	58	PRO	C-N	-12.55	1.16	1.34
1	C	90	LYS	CG-CD	12.54	1.90	1.52
1	A	68	ASN	C-O	12.53	1.39	1.24
2	B	7	GLU	N-CA	12.52	1.62	1.46
2	D	108	ASN	CB-CG	12.49	1.83	1.52
1	A	72	HIS	CB-CG	-12.46	1.32	1.50
1	A	92	ARG	CZ-NH1	12.46	1.50	1.32
1	A	96	VAL	CB-CG1	-12.45	1.11	1.52
1	C	55	VAL	N-CA	12.45	1.61	1.46
1	C	114	PRO	C-O	12.44	1.38	1.24
1	C	2	LEU	CA-CB	-12.43	1.37	1.52
1	A	60	LYS	CA-C	-12.43	1.36	1.52
1	C	118	THR	CB-CG2	-12.41	1.11	1.52
1	C	58	HIS	CG-CD2	-12.40	1.22	1.35
1	C	75	ASP	C-N	12.40	1.59	1.33
1	C	46	PHE	C-N	12.39	1.54	1.33
1	A	46	PHE	CG-CD2	-12.39	1.12	1.38
1	A	64	ASP	C-N	12.38	1.50	1.34
2	B	92	HIS	CD2-NE2	-12.38	1.24	1.37
2	D	6	GLU	CA-CB	12.36	1.72	1.53
2	B	45	PHE	CE1-CZ	-12.35	1.01	1.38
2	D	95	LYS	CA-C	-12.35	1.37	1.53
1	A	16	LYS	C-O	-12.34	1.08	1.24
2	D	48	LEU	CA-CB	-12.34	1.34	1.53
2	D	54	VAL	C-O	12.32	1.38	1.24
2	D	82	LYS	CG-CD	12.32	1.89	1.52
2	D	66	LYS	C-N	12.32	1.48	1.33
2	B	123	THR	CA-C	12.31	1.70	1.53
2	D	82	LYS	C-N	12.30	1.53	1.33
2	D	46	GLY	C-O	12.29	1.40	1.23
2	B	80	ASN	CA-CB	-12.29	1.36	1.53
2	B	13	ALA	C-N	12.28	1.49	1.33
2	D	49	SER	C-O	12.24	1.40	1.24
1	A	49	SER	N-CA	12.22	1.61	1.45
2	B	41	PHE	C-O	-12.21	1.07	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	VAL	CA-CB	-12.19	1.37	1.54
1	A	48	LEU	CA-CB	12.18	1.70	1.53
1	A	14	TRP	CG-CD1	12.16	1.67	1.36
2	D	48	LEU	C-N	12.16	1.51	1.33
2	B	74	GLY	N-CA	-12.16	1.27	1.45
1	A	26	ALA	C-N	12.16	1.49	1.33
2	B	116	HIS	CG-ND1	12.16	1.51	1.38
2	B	134	VAL	C-O	12.15	1.37	1.24
1	C	48	LEU	N-CA	12.14	1.59	1.46
1	C	52	SER	N-CA	12.13	1.61	1.46
2	D	36	PRO	N-CD	-12.12	1.30	1.47
1	C	43	PHE	N-CA	12.12	1.59	1.46
1	C	17	VAL	C-O	12.11	1.38	1.24
1	C	73	VAL	CA-C	12.10	1.69	1.52
1	A	105	LEU	CB-CG	-12.09	1.29	1.53
1	A	132	VAL	C-O	12.09	1.38	1.24
2	D	12	THR	CA-C	-12.07	1.37	1.52
1	A	3	SER	N-CA	12.07	1.63	1.46
1	C	22	GLY	C-O	12.06	1.38	1.23
2	B	92	HIS	CG-ND1	12.06	1.51	1.38
2	B	95	LYS	C-N	12.06	1.51	1.33
2	B	144	LYS	CA-C	-12.04	1.35	1.52
2	B	44	SER	CB-OG	-12.03	1.18	1.42
1	C	14	TRP	CD2-CE3	-12.03	1.21	1.40
1	C	133	SER	C-N	-12.03	1.18	1.33
2	D	59	LYS	CD-CE	12.00	1.88	1.52
1	C	17	VAL	C-N	11.99	1.51	1.33
2	B	20	VAL	C-O	11.98	1.39	1.24
2	B	63	HIS	CE1-NE2	-11.96	1.20	1.32
2	B	53	ALA	C-N	11.96	1.48	1.33
1	A	61	LYS	CA-C	11.94	1.69	1.52
1	C	131	SER	CA-CB	11.94	1.73	1.53
2	B	1	VAL	N-CA	11.93	1.69	1.46
1	A	50	HIS	CB-CG	-11.90	1.33	1.50
1	C	132	VAL	CA-CB	-11.90	1.40	1.54
2	D	7	GLU	CB-CG	11.87	1.88	1.52
1	A	60	LYS	C-O	-11.86	1.10	1.24
2	D	64	GLY	C-N	11.86	1.50	1.34
2	B	40	ARG	CZ-NH1	-11.86	1.16	1.32
2	D	126	VAL	C-O	-11.84	1.10	1.24
2	D	126	VAL	CA-C	11.84	1.68	1.52
2	B	1	VAL	CA-CB	11.83	1.86	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	116	HIS	CG-ND1	-11.81	1.25	1.38
2	D	30	ARG	C-N	-11.80	1.19	1.33
1	C	84	SER	CB-OG	-11.80	1.18	1.42
1	A	57	GLY	CA-C	11.80	1.65	1.52
1	C	14	TRP	NE1-CE2	-11.78	1.24	1.37
2	B	47	ASP	C-N	11.78	1.49	1.33
2	B	90	GLU	C-N	11.77	1.48	1.33
2	D	13	ALA	C-O	-11.77	1.10	1.24
1	A	72	HIS	CA-C	-11.76	1.36	1.52
1	C	122	HIS	CD2-NE2	11.74	1.50	1.37
2	D	36	PRO	N-CA	11.74	1.63	1.47
1	A	22	GLY	C-N	11.73	1.49	1.33
1	C	65	ALA	C-N	11.72	1.49	1.33
1	C	47	ASP	CA-C	11.71	1.68	1.52
2	B	123	THR	C-N	-11.71	1.19	1.33
1	A	26	ALA	CA-C	11.70	1.68	1.52
1	C	139	LYS	CE-NZ	11.70	1.84	1.49
2	B	121	GLU	N-CA	-11.69	1.30	1.46
2	D	58	PRO	CA-C	11.69	1.69	1.52
1	A	63	ALA	CA-C	-11.68	1.36	1.52
2	D	79	ASP	CB-CG	-11.65	1.23	1.52
2	D	131	GLN	C-O	-11.64	1.10	1.24
2	B	33	VAL	CA-C	11.63	1.67	1.52
2	D	14	LEU	CA-CB	11.62	1.72	1.53
1	A	14	TRP	CE2-CZ2	-11.59	1.15	1.39
2	B	69	GLY	CA-C	11.57	1.65	1.52
1	C	75	ASP	N-CA	11.55	1.71	1.46
1	C	14	TRP	C-O	11.53	1.38	1.24
1	C	90	LYS	N-CA	-11.52	1.31	1.46
1	C	12	ALA	C-O	11.52	1.37	1.24
2	B	46	GLY	CA-C	11.51	1.68	1.51
2	B	77	HIS	CB-CG	11.51	1.66	1.50
2	B	94	ASP	C-O	11.51	1.39	1.24
2	B	73	ASP	CG-OD1	11.50	1.47	1.25
1	C	57	GLY	C-O	11.50	1.37	1.23
1	A	62	VAL	N-CA	11.49	1.60	1.46
2	B	83	GLY	N-CA	11.46	1.59	1.45
2	D	10	ALA	N-CA	11.45	1.60	1.46
1	A	8	THR	CA-CB	11.45	1.71	1.53
2	D	78	LEU	CA-C	-11.44	1.37	1.52
1	C	50	HIS	CA-CB	11.43	1.72	1.53
1	A	14	TRP	CZ2-CH2	-11.40	1.15	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	121	GLU	CA-C	11.39	1.68	1.52
1	C	119	PRO	N-CD	11.38	1.63	1.47
1	C	118	THR	C-N	-11.37	1.07	1.33
2	D	139	ASN	CG-ND2	11.36	1.57	1.33
1	A	87	HIS	CG-ND1	11.35	1.50	1.38
2	B	13	ALA	N-CA	-11.33	1.32	1.46
2	D	7	GLU	C-N	-11.32	1.18	1.34
2	D	7	GLU	CD-OE1	11.32	1.46	1.25
2	D	104	ARG	CZ-NH1	11.31	1.48	1.32
2	D	143	HIS	CB-CG	-11.31	1.34	1.50
1	C	77	PRO	CA-C	-11.31	1.35	1.52
2	D	86	ALA	N-CA	11.31	1.60	1.46
2	B	12	THR	CA-CB	11.30	1.70	1.53
1	A	89	HIS	ND1-CE1	11.28	1.43	1.32
1	A	74	ASP	CB-CG	11.28	1.80	1.52
2	B	48	LEU	N-CA	11.27	1.59	1.46
2	D	84	THR	N-CA	-11.25	1.33	1.46
2	D	4	THR	C-O	11.25	1.41	1.24
2	D	97	HIS	CB-CG	11.25	1.65	1.50
1	A	72	HIS	CG-CD2	11.24	1.48	1.35
2	D	20	VAL	CB-CG1	-11.24	1.15	1.52
1	A	1	VAL	CA-CB	11.22	1.84	1.54
1	A	3	SER	CA-C	-11.19	1.38	1.52
2	B	67	VAL	N-CA	11.19	1.59	1.46
1	C	47	ASP	CG-OD1	-11.19	1.04	1.25
2	B	93	CYS	C-O	-11.18	1.10	1.24
1	C	38	THR	CB-OG1	11.17	1.61	1.43
1	C	50	HIS	CD2-NE2	11.17	1.50	1.37
1	A	139	LYS	N-CA	11.14	1.59	1.46
2	B	23	VAL	CA-C	11.13	1.67	1.52
2	B	95	LYS	C-O	-11.13	1.10	1.23
2	B	92	HIS	CA-C	11.12	1.68	1.52
2	D	125	PRO	N-CA	-11.11	1.32	1.47
1	A	8	THR	CB-OG1	-11.11	1.25	1.43
1	A	69	ALA	C-O	-11.10	1.09	1.24
2	D	43	GLU	N-CA	11.09	1.61	1.46
1	C	5	ALA	CA-C	11.09	1.66	1.52
1	C	44	PRO	CA-CB	11.09	1.72	1.54
2	D	25	GLY	CA-C	-11.09	1.39	1.52
2	D	6	GLU	N-CA	-11.08	1.31	1.46
1	C	12	ALA	CA-C	-11.06	1.38	1.52
2	B	21	ASP	CG-OD2	11.05	1.46	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	ASP	N-CA	11.05	1.60	1.46
1	A	90	LYS	CG-CD	-11.04	1.19	1.52
1	A	5	ALA	CA-C	11.04	1.67	1.52
2	B	73	ASP	N-CA	11.01	1.59	1.46
2	B	3	LEU	N-CA	10.99	1.59	1.46
1	C	95	PRO	N-CA	10.98	1.61	1.47
1	A	54	GLN	CA-C	10.97	1.67	1.52
2	D	47	ASP	C-N	-10.96	1.19	1.33
1	C	115	ALA	CA-CB	10.95	1.71	1.53
2	B	69	GLY	C-O	-10.94	1.10	1.23
2	D	93	CYS	N-CA	10.94	1.59	1.46
1	C	18	GLY	CA-C	-10.93	1.36	1.51
1	C	122	HIS	CG-CD2	10.92	1.47	1.35
2	D	112	CYS	C-O	-10.92	1.11	1.24
2	B	8	LYS	N-CA	-10.92	1.33	1.46
2	D	146	HIS	CG-CD2	-10.92	1.23	1.35
1	C	45	HIS	CG-ND1	10.91	1.50	1.38
1	C	33	PHE	CA-C	-10.87	1.38	1.52
1	C	48	LEU	C-O	10.87	1.40	1.24
1	A	12	ALA	N-CA	-10.86	1.32	1.46
2	D	60	VAL	C-N	10.86	1.48	1.33
1	A	72	HIS	CE1-NE2	10.85	1.43	1.32
1	C	68	ASN	N-CA	-10.83	1.33	1.46
2	D	15	TRP	NE1-CE2	10.81	1.49	1.37
1	C	74	ASP	N-CA	10.80	1.60	1.46
1	A	120	ALA	N-CA	-10.80	1.33	1.46
2	B	13	ALA	CA-C	-10.79	1.39	1.52
2	B	43	GLU	C-N	10.78	1.46	1.33
2	D	18	VAL	C-N	-10.78	1.18	1.33
2	B	124	PRO	C-O	10.78	1.36	1.24
1	C	99	LYS	C-O	-10.78	1.11	1.24
1	C	1	VAL	CA-CB	-10.75	1.25	1.54
2	B	80	ASN	C-O	-10.74	1.08	1.23
1	A	56	LYS	CD-CE	10.73	1.84	1.52
1	C	130	ALA	C-O	10.73	1.36	1.24
1	A	106	LEU	C-O	10.70	1.37	1.24
2	D	95	LYS	N-CA	10.70	1.59	1.46
1	A	33	PHE	C-N	10.68	1.49	1.33
2	B	54	VAL	C-O	10.68	1.36	1.24
1	C	116	GLU	CD-OE2	10.66	1.45	1.25
1	A	90	LYS	CD-CE	10.64	1.84	1.52
1	A	47	ASP	CA-CB	10.63	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	TRP	NE1-CE2	-10.62	1.25	1.37
2	B	143	HIS	CA-CB	-10.62	1.36	1.53
2	B	39	GLN	N-CA	10.62	1.59	1.46
1	C	61	LYS	C-N	10.61	1.47	1.33
2	B	35	TYR	C-N	-10.59	1.22	1.34
2	B	44	SER	N-CA	10.59	1.58	1.46
2	D	1	VAL	CB-CG2	-10.58	1.17	1.52
2	B	66	LYS	CE-NZ	10.58	1.81	1.49
2	D	101	GLU	CD-OE2	10.57	1.45	1.25
1	C	72	HIS	CE1-NE2	10.56	1.43	1.32
2	B	53	ALA	CA-CB	-10.56	1.36	1.53
2	D	91	LEU	C-N	10.56	1.49	1.33
1	A	9	ASN	CA-C	10.56	1.66	1.52
2	D	76	ALA	CA-CB	-10.54	1.35	1.53
1	A	76	MET	N-CA	10.53	1.60	1.46
2	D	21	ASP	CB-CG	10.53	1.78	1.52
2	D	97	HIS	C-N	10.53	1.47	1.33
1	A	80	LEU	N-CA	10.50	1.59	1.46
2	B	73	ASP	CA-CB	10.49	1.69	1.53
2	D	20	VAL	CB-CG2	-10.49	1.18	1.52
1	C	85	ASP	CG-OD1	-10.48	1.05	1.25
1	A	37	PRO	N-CA	10.47	1.61	1.47
1	C	113	LEU	CA-C	10.46	1.66	1.52
2	D	77	HIS	N-CA	-10.46	1.32	1.46
2	B	79	ASP	N-CA	10.44	1.59	1.46
2	B	34	VAL	N-CA	10.43	1.59	1.46
2	D	44	SER	CA-CB	-10.42	1.34	1.53
2	D	75	LEU	CA-CB	10.41	1.69	1.53
2	B	64	GLY	C-O	-10.40	1.11	1.23
1	A	122	HIS	CD2-NE2	10.40	1.49	1.37
1	C	46	PHE	CA-C	-10.39	1.38	1.53
2	B	3	LEU	CA-CB	10.37	1.77	1.53
1	A	24	TYR	CE1-CZ	-10.36	1.13	1.38
1	A	108	THR	CA-CB	10.34	1.69	1.53
1	C	83	LEU	C-O	10.33	1.37	1.24
1	A	45	HIS	CG-ND1	10.33	1.49	1.38
1	C	26	ALA	C-O	-10.32	1.12	1.24
2	D	40	ARG	CB-CG	-10.32	1.21	1.52
2	D	97	HIS	CD2-NE2	10.31	1.49	1.37
2	B	112	CYS	CA-CB	-10.30	1.37	1.53
1	C	7	LYS	CD-CE	-10.30	1.21	1.52
1	C	24	TYR	C-O	-10.29	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	86	ALA	CA-C	-10.28	1.39	1.52
1	C	40	LYS	N-CA	10.28	1.60	1.46
2	D	112	CYS	CA-C	10.28	1.66	1.52
1	A	96	VAL	CA-CB	10.28	1.69	1.54
2	B	52	ASP	CB-CG	10.27	1.77	1.52
2	D	40	ARG	CZ-NH2	10.27	1.46	1.33
1	A	49	SER	CA-CB	-10.25	1.37	1.53
1	C	106	LEU	N-CA	10.25	1.58	1.46
2	D	45	PHE	C-O	10.25	1.37	1.24
2	B	59	LYS	CA-CB	-10.23	1.36	1.53
1	C	43	PHE	C-N	10.23	1.42	1.33
1	A	68	ASN	C-N	10.22	1.48	1.33
2	D	140	ALA	C-N	-10.22	1.20	1.33
1	C	68	ASN	CG-ND2	10.22	1.54	1.33
2	B	28	LEU	CB-CG	10.20	1.73	1.53
1	C	73	VAL	N-CA	-10.18	1.33	1.46
2	D	44	SER	C-N	10.18	1.49	1.33
1	C	110	ALA	C-O	10.18	1.36	1.24
2	B	51	PRO	N-CD	10.17	1.61	1.47
2	D	136	GLY	N-CA	-10.16	1.30	1.45
2	D	58	PRO	CB-CG	10.15	2.00	1.49
1	A	28	ALA	C-O	-10.15	1.12	1.24
2	D	115	ALA	C-O	-10.14	1.12	1.24
2	D	22	GLU	CD-OE1	10.11	1.44	1.25
2	B	117	HIS	CB-CG	-10.11	1.35	1.50
2	D	80	ASN	CB-CG	-10.11	1.26	1.52
2	D	14	LEU	N-CA	-10.11	1.33	1.46
2	B	112	CYS	C-N	-10.10	1.21	1.33
2	D	41	PHE	CE1-CZ	-10.10	1.08	1.38
2	D	131	GLN	CG-CD	10.10	1.77	1.52
2	D	77	HIS	CA-C	10.09	1.66	1.52
1	A	79	ALA	CA-CB	-10.07	1.37	1.53
2	D	68	LEU	CB-CG	-10.06	1.33	1.53
2	B	124	PRO	C-N	-10.06	1.20	1.34
1	A	19	ALA	CA-C	10.05	1.66	1.52
1	A	114	PRO	N-CA	10.05	1.60	1.47
1	C	99	LYS	CG-CD	10.05	1.82	1.52
1	C	87	HIS	CG-CD2	10.04	1.46	1.35
1	A	131	SER	CB-OG	-10.04	1.22	1.42
1	C	84	SER	C-N	10.03	1.47	1.33
1	A	11	LYS	N-CA	10.01	1.59	1.46
1	C	17	VAL	CA-C	-10.01	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	28	LEU	CA-C	-9.99	1.39	1.52
1	C	52	SER	C-O	9.99	1.36	1.23
2	B	52	ASP	CG-OD1	-9.98	1.06	1.25
2	D	2	HIS	CA-C	9.98	1.65	1.53
2	D	15	TRP	CD2-CE2	9.97	1.58	1.41
1	C	121	VAL	CA-CB	-9.97	1.42	1.54
1	C	78	ASN	CB-CG	9.96	1.76	1.52
2	D	92	HIS	ND1-CE1	9.96	1.42	1.32
1	A	40	LYS	C-O	-9.96	1.10	1.24
1	A	129	LEU	CA-C	-9.95	1.38	1.52
1	A	14	TRP	CA-C	9.95	1.66	1.52
1	C	76	MET	CG-SD	9.95	2.05	1.80
2	D	105	LEU	CA-CB	-9.95	1.38	1.53
2	B	123	THR	C-O	-9.94	1.11	1.23
1	A	20	HIS	CA-CB	-9.94	1.37	1.53
2	B	62	ALA	C-O	-9.91	1.12	1.24
1	A	105	LEU	CG-CD2	-9.91	1.19	1.52
2	B	84	THR	CB-OG1	9.90	1.59	1.43
1	C	78	ASN	CA-CB	9.89	1.70	1.53
2	B	48	LEU	CA-CB	-9.89	1.39	1.53
2	D	94	ASP	CG-OD1	-9.89	1.06	1.25
1	C	89	HIS	CD2-NE2	9.88	1.48	1.37
1	C	50	HIS	CG-CD2	-9.88	1.25	1.35
2	D	51	PRO	C-O	9.86	1.37	1.24
1	A	84	SER	CB-OG	-9.86	1.22	1.42
1	C	7	LYS	CE-NZ	-9.84	1.19	1.49
1	C	82	ALA	CA-C	-9.82	1.39	1.52
1	A	78	ASN	CG-ND2	-9.82	1.12	1.33
2	D	8	LYS	CG-CD	-9.82	1.23	1.52
2	D	11	VAL	N-CA	9.82	1.58	1.46
1	A	71	ALA	CA-CB	-9.81	1.37	1.53
2	B	146	HIS	N-CA	9.81	1.64	1.46
2	D	90	GLU	C-O	-9.81	1.12	1.24
2	D	51	PRO	C-N	9.80	1.47	1.33
1	A	9	ASN	C-O	-9.78	1.12	1.24
1	A	116	GLU	CD-OE2	9.78	1.44	1.25
1	A	35	SER	N-CA	-9.76	1.33	1.46
2	B	6	GLU	C-N	-9.76	1.20	1.33
1	A	69	ALA	C-N	9.75	1.45	1.33
2	B	76	ALA	N-CA	-9.75	1.33	1.46
1	A	70	VAL	N-CA	9.72	1.59	1.46
2	B	3	LEU	CA-C	9.72	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	105	LEU	N-CA	-9.71	1.34	1.46
2	D	146	HIS	CA-CB	9.71	1.72	1.53
1	C	120	ALA	C-O	9.71	1.35	1.24
2	B	17	LYS	CA-C	-9.70	1.39	1.52
1	C	16	LYS	CG-CD	9.70	1.81	1.52
2	B	84	THR	C-O	-9.69	1.12	1.24
1	C	14	TRP	CD2-CE2	9.69	1.57	1.41
1	A	44	PRO	N-CD	-9.68	1.34	1.47
1	A	122	HIS	CG-ND1	9.65	1.48	1.38
2	B	144	LYS	C-O	9.64	1.37	1.23
2	B	97	HIS	CB-CG	9.63	1.63	1.50
1	A	5	ALA	N-CA	-9.62	1.33	1.46
2	D	32	LEU	C-O	9.62	1.36	1.24
2	D	74	GLY	C-N	9.62	1.46	1.33
2	D	110	LEU	CA-CB	-9.62	1.38	1.53
1	C	3	SER	C-N	9.61	1.45	1.34
2	B	63	HIS	C-N	-9.59	1.21	1.33
2	D	47	ASP	CB-CG	9.59	1.76	1.52
1	C	61	LYS	CD-CE	9.58	1.81	1.52
2	B	83	GLY	CA-C	-9.57	1.41	1.52
2	D	59	LYS	N-CA	-9.57	1.34	1.46
2	D	86	ALA	CA-C	9.55	1.65	1.52
1	A	71	ALA	N-CA	9.54	1.58	1.46
1	C	30	GLU	N-CA	-9.53	1.35	1.46
2	D	111	VAL	C-N	9.52	1.45	1.33
2	D	23	VAL	C-N	-9.52	1.22	1.33
2	B	117	HIS	CA-C	-9.50	1.40	1.52
2	D	31	LEU	C-N	9.48	1.46	1.34
1	A	60	LYS	CA-CB	9.48	1.68	1.53
2	D	52	ASP	CB-CG	9.47	1.75	1.52
2	D	125	PRO	C-N	9.46	1.45	1.33
1	C	95	PRO	CA-C	-9.45	1.34	1.52
2	B	142	ALA	C-O	9.45	1.36	1.24
1	C	116	GLU	C-N	-9.45	1.22	1.33
2	D	86	ALA	CA-CB	9.45	1.68	1.53
1	C	31	ARG	CD-NE	9.44	1.59	1.46
1	C	118	THR	CA-C	9.44	1.64	1.52
1	A	41	THR	C-O	9.43	1.35	1.24
1	A	140	TYR	N-CA	-9.43	1.34	1.46
1	C	64	ASP	CG-OD2	-9.43	1.07	1.25
1	C	45	HIS	CA-C	9.42	1.65	1.52
2	B	80	ASN	CB-CG	9.41	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	LYS	CB-CG	-9.41	1.24	1.52
1	C	135	VAL	C-N	9.39	1.46	1.33
1	C	17	VAL	CA-CB	9.38	1.67	1.54
1	A	46	PHE	N-CA	-9.37	1.35	1.45
2	B	90	GLU	N-CA	-9.36	1.34	1.46
2	D	73	ASP	CB-CG	-9.36	1.28	1.52
2	B	30	ARG	CA-C	9.36	1.65	1.52
2	B	13	ALA	CA-CB	9.36	1.67	1.53
2	B	145	TYR	C-O	9.35	1.35	1.23
1	A	64	ASP	C-O	-9.35	1.12	1.24
2	D	144	LYS	CA-C	-9.35	1.39	1.52
1	C	135	VAL	CA-C	9.33	1.63	1.52
2	D	21	ASP	N-CA	9.33	1.57	1.46
1	A	112	HIS	CE1-NE2	9.33	1.41	1.32
1	A	81	SER	C-O	9.32	1.36	1.24
1	A	119	PRO	CA-C	-9.32	1.39	1.52
1	C	41	THR	N-CA	9.32	1.58	1.46
2	B	132	LYS	C-N	9.32	1.45	1.33
2	D	46	GLY	N-CA	-9.31	1.31	1.45
1	A	77	PRO	N-CA	-9.31	1.35	1.47
1	A	115	ALA	C-O	-9.31	1.12	1.24
1	A	86	LEU	C-N	9.30	1.47	1.33
2	D	39	GLN	CD-OE1	9.30	1.41	1.23
1	A	44	PRO	CA-CB	-9.29	1.37	1.54
1	C	4	PRO	C-N	-9.29	1.22	1.33
1	A	20	HIS	CB-CG	-9.29	1.37	1.50
1	A	90	LYS	CA-CB	9.27	1.69	1.53
1	C	113	LEU	CG-CD2	-9.27	1.22	1.52
1	A	20	HIS	C-N	-9.25	1.20	1.33
1	A	44	PRO	C-N	-9.25	1.19	1.33
2	B	78	LEU	CA-C	9.25	1.65	1.52
1	C	28	ALA	N-CA	9.25	1.57	1.46
1	C	27	GLU	C-N	9.25	1.46	1.33
1	A	78	ASN	N-CA	-9.24	1.34	1.46
2	D	10	ALA	CA-CB	-9.24	1.38	1.53
1	C	92	ARG	C-N	9.24	1.46	1.33
1	A	114	PRO	C-O	-9.23	1.12	1.24
2	B	70	ALA	N-CA	-9.22	1.35	1.46
1	A	95	PRO	C-O	9.21	1.35	1.24
2	B	79	ASP	C-N	9.20	1.46	1.33
1	C	35	SER	C-N	9.20	1.46	1.33
2	D	3	LEU	CA-C	9.20	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	LEU	N-CA	9.20	1.57	1.46
2	D	104	ARG	CA-C	9.20	1.64	1.52
2	D	145	TYR	N-CA	-9.20	1.34	1.46
1	C	130	ALA	CA-CB	-9.17	1.39	1.53
2	D	103	PHE	CA-C	9.17	1.64	1.52
1	A	114	PRO	CA-C	9.17	1.66	1.52
1	C	59	GLY	N-CA	-9.15	1.33	1.45
1	A	112	HIS	C-N	-9.15	1.22	1.33
2	D	3	LEU	C-N	9.14	1.52	1.33
2	B	120	LYS	C-N	-9.13	1.21	1.33
1	A	12	ALA	CA-C	-9.12	1.41	1.52
2	D	54	VAL	CA-C	-9.10	1.41	1.52
2	B	15	TRP	NE1-CE2	9.09	1.47	1.37
1	C	51	GLY	N-CA	-9.08	1.31	1.45
1	C	98	PHE	CA-C	9.08	1.65	1.52
2	D	88	LEU	C-N	9.06	1.44	1.33
1	C	4	PRO	CA-C	9.05	1.65	1.52
1	A	141	ARG	CB-CG	9.05	1.79	1.52
2	B	136	GLY	N-CA	9.05	1.57	1.45
1	A	34	LEU	CB-CG	-9.05	1.35	1.53
2	D	47	ASP	C-O	9.04	1.35	1.24
2	B	126	VAL	C-N	-9.04	1.21	1.33
1	A	113	LEU	CB-CG	9.03	1.71	1.53
1	C	94	ASP	CG-OD1	-9.03	1.08	1.25
1	C	128	PHE	C-O	9.02	1.34	1.24
1	C	19	ALA	N-CA	-9.01	1.34	1.46
2	D	13	ALA	CA-C	9.01	1.64	1.52
2	D	55	MET	CB-CG	-9.00	1.25	1.52
1	C	85	ASP	C-N	9.00	1.45	1.33
1	C	103	HIS	CA-C	-8.99	1.41	1.52
2	D	51	PRO	CA-C	-8.99	1.39	1.52
1	A	110	ALA	CA-C	-8.98	1.40	1.52
2	B	84	THR	C-N	8.98	1.47	1.33
2	D	52	ASP	C-N	-8.98	1.23	1.33
1	C	46	PHE	CA-CB	8.98	1.68	1.53
2	D	1	VAL	C-N	-8.97	1.18	1.33
1	A	74	ASP	C-O	8.96	1.35	1.24
2	D	8	LYS	CB-CG	8.95	1.79	1.52
2	D	119	GLY	C-N	8.95	1.45	1.33
1	C	14	TRP	CZ2-CH2	-8.94	1.20	1.37
1	A	141	ARG	CA-CB	-8.93	1.35	1.53
2	B	23	VAL	C-O	8.91	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	PHE	C-N	-8.91	1.21	1.33
2	B	63	HIS	CG-CD2	8.91	1.45	1.35
2	B	121	GLU	CA-CB	8.90	1.68	1.53
1	C	86	LEU	C-O	-8.90	1.13	1.24
2	B	40	ARG	CA-C	8.89	1.65	1.52
2	D	16	GLY	C-O	8.89	1.36	1.24
2	B	129	ALA	C-O	8.87	1.34	1.24
1	C	38	THR	N-CA	8.87	1.57	1.46
1	A	64	ASP	N-CA	-8.86	1.34	1.46
1	C	59	GLY	C-O	8.86	1.35	1.23
1	C	138	SER	CA-C	8.85	1.64	1.52
2	D	146	HIS	N-CA	8.85	1.63	1.46
1	A	14	TRP	CB-CG	-8.84	1.22	1.50
2	B	7	GLU	CA-C	8.83	1.64	1.52
2	D	16	GLY	CA-C	-8.83	1.39	1.51
2	B	72	SER	C-O	8.82	1.34	1.24
2	B	104	ARG	CA-CB	8.82	1.68	1.53
2	D	89	SER	C-N	8.81	1.45	1.33
2	B	123	THR	CB-OG1	-8.81	1.29	1.43
1	A	89	HIS	CD2-NE2	-8.80	1.28	1.37
2	B	8	LYS	CG-CD	8.79	1.78	1.52
2	B	19	ASN	CG-OD1	-8.79	1.06	1.23
2	B	121	GLU	CA-C	8.79	1.65	1.52
1	C	29	LEU	CA-CB	8.79	1.67	1.53
2	D	5	PRO	CB-CG	-8.79	1.05	1.49
2	D	133	VAL	C-N	-8.79	1.23	1.33
2	B	16	GLY	N-CA	8.78	1.58	1.45
1	C	25	GLY	N-CA	-8.78	1.33	1.45
1	A	5	ALA	C-N	8.77	1.44	1.33
1	A	23	GLU	CD-OE2	8.76	1.42	1.25
2	D	119	GLY	CA-C	8.76	1.63	1.52
1	A	101	LEU	C-N	8.75	1.45	1.33
2	D	4	THR	CB-CG2	-8.75	1.23	1.52
1	A	46	PHE	CB-CG	-8.74	1.30	1.50
1	C	124	SER	C-N	-8.74	1.22	1.34
2	D	31	LEU	C-O	-8.74	1.13	1.24
1	C	54	GLN	C-N	8.73	1.44	1.33
1	C	31	ARG	CA-C	8.72	1.63	1.52
1	C	54	GLN	N-CA	8.72	1.56	1.46
1	C	111	ALA	CA-C	8.72	1.64	1.52
1	A	46	PHE	C-N	8.72	1.46	1.33
1	A	85	ASP	C-O	-8.71	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97	ASN	CA-CB	-8.70	1.38	1.53
2	B	117	HIS	CA-CB	8.68	1.67	1.53
1	C	14	TRP	C-N	-8.66	1.20	1.33
1	C	29	LEU	N-CA	8.64	1.56	1.46
1	C	20	HIS	CA-CB	-8.62	1.38	1.53
2	D	63	HIS	CG-ND1	-8.62	1.28	1.38
1	C	139	LYS	CA-C	8.61	1.64	1.52
2	B	49	SER	CA-CB	8.60	1.83	1.54
2	D	75	LEU	CG-CD2	-8.59	1.24	1.52
1	A	85	ASP	C-N	8.58	1.45	1.33
2	B	61	LYS	CE-NZ	8.58	1.75	1.49
2	D	55	MET	CA-CB	8.58	1.67	1.53
2	D	68	LEU	CG-CD1	-8.58	1.24	1.52
1	A	88	ALA	N-CA	8.57	1.56	1.46
1	C	81	SER	CA-CB	8.57	1.66	1.53
2	B	23	VAL	C-N	-8.57	1.23	1.33
1	C	86	LEU	N-CA	-8.57	1.35	1.46
1	A	137	THR	C-N	-8.56	1.22	1.34
1	A	53	ALA	CA-CB	8.56	1.68	1.53
1	C	122	HIS	CA-CB	-8.56	1.40	1.53
1	A	76	MET	CG-SD	8.55	2.02	1.80
2	B	120	LYS	CA-CB	8.55	1.68	1.53
1	A	48	LEU	N-CA	-8.55	1.36	1.46
1	C	141	ARG	CZ-NH2	8.55	1.44	1.33
1	C	70	VAL	CA-CB	-8.54	1.45	1.54
1	A	33	PHE	CE2-CZ	-8.54	1.13	1.38
1	C	2	LEU	C-O	8.53	1.34	1.23
2	B	44	SER	CA-CB	-8.52	1.40	1.53
1	C	89	HIS	C-N	-8.52	1.21	1.33
2	D	138	ALA	C-O	-8.51	1.14	1.24
2	B	16	GLY	CA-C	-8.49	1.40	1.51
2	D	61	LYS	CE-NZ	-8.49	1.23	1.49
1	A	107	VAL	N-CA	-8.48	1.36	1.46
1	A	1	VAL	CB-CG2	-8.48	1.24	1.52
1	A	84	SER	C-O	-8.48	1.13	1.24
2	D	124	PRO	CA-C	-8.48	1.44	1.52
2	B	63	HIS	CA-CB	-8.47	1.39	1.53
1	C	113	LEU	C-N	-8.46	1.23	1.34
1	A	123	ALA	C-O	8.46	1.33	1.24
2	B	1	VAL	CB-CG2	-8.46	1.24	1.52
1	C	13	ALA	C-O	8.45	1.33	1.24
1	A	61	LYS	CE-NZ	8.45	1.74	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	LEU	CG-CD2	-8.45	1.24	1.52
2	D	130	TYR	CE1-CZ	8.45	1.58	1.38
2	D	37	TRP	N-CA	-8.44	1.34	1.46
1	C	101	LEU	CA-C	8.44	1.64	1.52
1	A	36	PHE	C-O	8.44	1.34	1.24
1	C	46	PHE	N-CA	-8.43	1.35	1.45
1	C	134	THR	C-O	8.43	1.33	1.24
1	C	95	PRO	C-O	8.41	1.36	1.24
1	A	52	SER	C-N	8.40	1.46	1.33
1	A	140	TYR	C-N	-8.40	1.21	1.33
2	D	39	GLN	C-N	8.40	1.45	1.34
1	A	68	ASN	CA-C	-8.39	1.41	1.52
1	C	114	PRO	N-CD	8.38	1.59	1.47
2	D	92	HIS	N-CA	8.38	1.57	1.46
2	B	19	ASN	CA-CB	8.38	1.63	1.53
1	C	110	ALA	C-N	8.37	1.45	1.33
2	D	104	ARG	CZ-NH2	-8.36	1.22	1.33
2	D	72	SER	C-O	8.36	1.34	1.24
1	A	10	VAL	CA-CB	-8.36	1.44	1.54
1	A	141	ARG	N-CA	8.34	1.62	1.46
1	A	21	ALA	N-CA	8.34	1.56	1.46
2	D	123	THR	CB-CG2	8.34	1.80	1.52
2	D	18	VAL	CB-CG2	8.33	1.80	1.52
2	B	7	GLU	CB-CG	8.33	1.77	1.52
1	C	2	LEU	CG-CD1	-8.32	1.25	1.52
2	D	146	HIS	C-OXT	8.32	1.40	1.23
1	C	127	LYS	C-N	-8.32	1.22	1.33
2	D	81	LEU	CG-CD1	-8.32	1.25	1.52
1	A	72	HIS	N-CA	-8.31	1.35	1.46
2	B	43	GLU	N-CA	8.29	1.56	1.46
2	B	66	LYS	CA-CB	8.29	1.66	1.53
2	B	57	ASN	CG-OD1	-8.29	1.07	1.23
1	A	24	TYR	CB-CG	8.29	1.69	1.51
2	B	89	SER	CB-OG	8.29	1.58	1.42
1	A	92	ARG	CD-NE	-8.28	1.34	1.46
2	D	102	ASN	N-CA	8.27	1.56	1.46
2	B	93	CYS	CA-C	8.26	1.63	1.52
1	C	14	TRP	CG-CD1	8.25	1.57	1.36
1	C	18	GLY	N-CA	8.25	1.57	1.45
2	D	61	LYS	CG-CD	-8.25	1.27	1.52
2	D	115	ALA	N-CA	8.25	1.56	1.46
1	A	9	ASN	N-CA	-8.25	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	45	PHE	CA-C	-8.25	1.41	1.52
1	C	112	HIS	ND1-CE1	-8.24	1.24	1.32
2	B	84	THR	CB-CG2	-8.22	1.25	1.52
1	A	109	LEU	CG-CD2	-8.22	1.25	1.52
2	B	143	HIS	N-CA	8.22	1.56	1.46
1	C	47	ASP	CB-CG	8.21	1.72	1.52
2	D	28	LEU	CA-C	-8.19	1.42	1.52
2	D	102	ASN	CA-CB	-8.19	1.39	1.53
2	B	14	LEU	C-O	-8.18	1.14	1.24
2	B	72	SER	C-N	-8.18	1.23	1.33
2	D	111	VAL	N-CA	8.18	1.56	1.46
1	A	112	HIS	CA-CB	8.16	1.66	1.54
1	C	88	ALA	N-CA	-8.15	1.36	1.46
2	D	44	SER	CB-OG	-8.15	1.25	1.42
1	A	59	GLY	N-CA	8.15	1.56	1.45
1	C	90	LYS	CA-C	8.14	1.63	1.52
1	A	39	THR	C-N	-8.13	1.21	1.33
1	C	24	TYR	CZ-OH	8.12	1.55	1.38
2	D	49	SER	N-CA	8.12	1.56	1.46
2	D	58	PRO	CA-CB	8.12	1.65	1.53
1	C	105	LEU	CG-CD1	8.12	1.79	1.52
1	A	115	ALA	N-CA	8.11	1.56	1.46
1	A	117	PHE	CA-C	8.10	1.63	1.52
2	D	28	LEU	C-N	8.10	1.45	1.33
2	D	51	PRO	N-CD	8.10	1.59	1.47
2	D	19	ASN	CB-CG	8.09	1.72	1.52
1	A	48	LEU	CG-CD2	-8.09	1.25	1.52
2	D	72	SER	CA-CB	8.08	1.67	1.53
1	A	105	LEU	CA-CB	8.07	1.66	1.53
1	C	45	HIS	CB-CG	8.07	1.61	1.50
2	B	50	THR	C-O	8.07	1.31	1.24
1	A	140	TYR	CZ-OH	-8.07	1.21	1.38
1	A	28	ALA	C-N	8.07	1.44	1.33
2	D	5	PRO	C-O	-8.06	1.15	1.23
2	B	45	PHE	CD1-CE1	8.06	1.62	1.38
1	A	34	LEU	CA-CB	-8.05	1.40	1.53
1	A	93	VAL	C-O	8.05	1.33	1.24
2	B	65	LYS	N-CA	-8.05	1.36	1.46
2	B	60	VAL	CA-C	-8.04	1.42	1.52
1	C	79	ALA	CA-C	8.03	1.63	1.52
2	B	42	PHE	C-N	-8.02	1.22	1.33
1	A	125	LEU	CA-C	-8.01	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	GLU	CA-C	8.01	1.62	1.52
2	B	19	ASN	C-N	-8.00	1.24	1.34
2	D	17	LYS	N-CA	-8.00	1.35	1.46
2	D	98	VAL	CA-C	8.00	1.62	1.52
1	C	24	TYR	CA-C	8.00	1.63	1.52
2	D	30	ARG	CZ-NH2	7.99	1.43	1.33
1	C	53	ALA	CA-CB	-7.99	1.40	1.53
2	B	145	TYR	CD2-CE2	7.98	1.62	1.38
1	C	80	LEU	CA-C	7.98	1.64	1.52
1	C	50	HIS	C-N	-7.98	1.22	1.33
2	B	7	GLU	C-N	-7.98	1.24	1.33
1	C	85	ASP	CA-C	-7.97	1.42	1.52
1	C	140	TYR	CG-CD1	-7.97	1.22	1.39
1	A	111	ALA	N-CA	-7.97	1.36	1.46
2	D	37	TRP	CE2-CZ2	7.96	1.56	1.39
2	B	114	LEU	CA-CB	-7.96	1.41	1.53
2	B	68	LEU	C-O	7.96	1.33	1.24
2	B	119	GLY	C-O	7.95	1.34	1.24
1	A	39	THR	C-O	-7.95	1.13	1.24
2	B	73	ASP	CB-CG	7.94	1.72	1.52
1	A	126	ASP	CA-C	-7.93	1.42	1.52
2	B	77	HIS	CA-CB	-7.93	1.39	1.53
2	B	144	LYS	C-N	-7.92	1.23	1.33
2	D	6	GLU	C-N	-7.92	1.22	1.33
2	B	2	HIS	N-CA	7.91	1.55	1.46
1	A	128	PHE	CG-CD2	-7.91	1.22	1.38
2	B	104	ARG	CG-CD	7.90	1.76	1.52
2	B	126	VAL	CA-CB	7.90	1.65	1.54
1	C	3	SER	CA-CB	-7.90	1.41	1.53
1	A	80	LEU	C-N	7.89	1.44	1.33
1	C	128	PHE	CG-CD2	-7.88	1.22	1.38
1	C	140	TYR	C-O	7.88	1.33	1.24
1	C	112	HIS	C-N	-7.87	1.17	1.33
2	B	85	PHE	N-CA	7.87	1.56	1.46
2	B	145	TYR	CE1-CZ	7.86	1.57	1.38
2	B	119	GLY	C-N	-7.86	1.22	1.33
2	B	136	GLY	C-N	7.85	1.43	1.33
2	B	26	GLU	CA-CB	-7.84	1.41	1.53
2	B	32	LEU	CG-CD1	-7.84	1.26	1.52
2	B	71	PHE	CA-C	7.84	1.62	1.52
1	C	89	HIS	ND1-CE1	-7.84	1.24	1.32
1	C	56	LYS	CE-NZ	7.84	1.72	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	124	SER	CA-C	7.84	1.62	1.52
1	C	25	GLY	CA-C	-7.83	1.42	1.52
1	A	6	ASP	CA-CB	-7.82	1.41	1.53
1	A	111	ALA	CA-C	7.82	1.62	1.52
2	B	20	VAL	N-CA	7.82	1.56	1.46
2	B	103	PHE	CA-C	7.82	1.62	1.52
2	B	118	PHE	CA-CB	-7.80	1.40	1.53
2	B	118	PHE	CG-CD2	7.80	1.55	1.38
1	A	74	ASP	CA-C	7.80	1.63	1.52
2	D	54	VAL	CB-CG2	-7.80	1.26	1.52
1	C	94	ASP	N-CA	-7.80	1.35	1.45
2	D	82	LYS	CB-CG	-7.79	1.29	1.52
2	D	63	HIS	CG-CD2	7.79	1.44	1.35
1	C	90	LYS	C-N	7.79	1.44	1.33
1	C	45	HIS	CD2-NE2	-7.78	1.29	1.37
1	C	81	SER	N-CA	7.78	1.55	1.46
1	C	136	LEU	C-O	7.78	1.34	1.24
1	C	46	PHE	C-O	7.77	1.33	1.23
1	A	91	LEU	CA-CB	7.76	1.66	1.53
2	B	140	ALA	C-O	7.76	1.34	1.24
2	D	131	GLN	CA-C	-7.76	1.42	1.52
1	A	33	PHE	CG-CD2	7.75	1.55	1.38
2	D	118	PHE	C-O	7.75	1.34	1.24
1	A	98	PHE	CA-C	7.74	1.62	1.52
2	B	19	ASN	CG-ND2	7.74	1.49	1.33
1	A	92	ARG	CA-CB	7.74	1.65	1.53
1	C	85	ASP	C-O	-7.74	1.15	1.24
2	D	141	LEU	CG-CD2	7.73	1.78	1.52
2	B	102	ASN	CA-C	-7.72	1.42	1.52
1	C	2	LEU	N-CA	-7.72	1.36	1.46
1	A	87	HIS	CB-CG	7.71	1.60	1.50
2	B	108	ASN	CA-C	7.71	1.63	1.52
2	D	143	HIS	C-N	-7.70	1.23	1.33
1	A	94	ASP	C-O	-7.70	1.14	1.23
1	A	21	ALA	CA-CB	-7.70	1.40	1.53
1	C	12	ALA	CA-CB	-7.69	1.41	1.53
1	A	45	HIS	CA-CB	-7.69	1.40	1.53
2	B	58	PRO	CA-CB	7.69	1.65	1.53
2	B	99	ASP	CA-C	7.69	1.61	1.52
1	A	92	ARG	N-CA	7.69	1.57	1.46
1	C	75	ASP	CA-CB	7.68	1.61	1.53
2	B	22	GLU	CA-C	7.68	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	99	LYS	C-N	7.66	1.43	1.33
1	C	128	PHE	CB-CG	7.66	1.68	1.50
2	B	14	LEU	C-N	7.66	1.44	1.34
1	C	69	ALA	CA-C	7.65	1.62	1.52
2	D	116	HIS	C-O	7.62	1.32	1.24
1	C	7	LYS	C-O	-7.62	1.15	1.24
2	D	27	ALA	N-CA	7.61	1.55	1.46
2	B	14	LEU	CA-CB	7.61	1.65	1.53
2	D	12	THR	C-N	-7.60	1.24	1.33
2	B	6	GLU	CA-CB	7.60	1.65	1.53
1	C	56	LYS	C-N	7.59	1.42	1.33
1	C	139	LYS	CG-CD	-7.59	1.29	1.52
1	A	11	LYS	CA-CB	-7.59	1.40	1.53
2	D	120	LYS	CA-CB	7.59	1.65	1.53
2	B	67	VAL	C-O	7.58	1.33	1.24
1	A	79	ALA	C-N	-7.58	1.22	1.33
2	B	140	ALA	CA-CB	7.58	1.65	1.53
2	D	54	VAL	C-N	7.57	1.45	1.33
1	A	14	TRP	CD1-NE1	7.57	1.53	1.37
2	D	45	PHE	CG-CD2	-7.57	1.23	1.38
1	C	60	LYS	CA-C	-7.57	1.43	1.52
1	C	54	GLN	CA-CB	-7.56	1.41	1.53
1	A	63	ALA	N-CA	7.55	1.56	1.46
2	B	28	LEU	C-N	7.55	1.43	1.33
2	B	102	ASN	CG-ND2	7.55	1.49	1.33
1	C	45	HIS	CE1-NE2	7.54	1.40	1.32
1	C	10	VAL	C-O	-7.53	1.15	1.24
1	C	129	LEU	CA-CB	-7.53	1.40	1.53
2	B	68	LEU	CG-CD2	-7.52	1.27	1.52
1	A	90	LYS	C-O	-7.51	1.14	1.23
1	A	97	ASN	CA-C	7.51	1.62	1.52
1	A	34	LEU	C-N	7.50	1.45	1.33
2	B	127	GLN	CA-C	-7.50	1.42	1.52
1	C	100	LEU	N-CA	7.49	1.55	1.46
1	C	135	VAL	N-CA	7.49	1.55	1.46
1	A	8	THR	CB-CG2	-7.49	1.27	1.52
2	D	32	LEU	CG-CD2	-7.49	1.27	1.52
1	A	12	ALA	CA-CB	7.48	1.65	1.53
1	A	18	GLY	C-O	7.48	1.34	1.23
1	A	86	LEU	N-CA	-7.47	1.37	1.46
2	D	5	PRO	N-CD	7.46	1.58	1.47
2	D	53	ALA	N-CA	-7.46	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	60	VAL	C-N	7.45	1.44	1.34
2	D	15	TRP	CZ2-CH2	-7.45	1.23	1.37
2	B	14	LEU	CA-C	-7.45	1.43	1.52
2	B	87	THR	CB-OG1	-7.45	1.31	1.43
2	D	51	PRO	N-CA	-7.44	1.37	1.47
1	C	41	THR	CA-C	-7.44	1.42	1.52
2	D	45	PHE	CD1-CE1	7.43	1.60	1.38
2	D	20	VAL	C-N	7.43	1.43	1.33
2	D	92	HIS	CB-CG	7.43	1.60	1.50
2	B	59	LYS	C-N	-7.43	1.23	1.33
2	B	118	PHE	CD2-CE2	-7.42	1.16	1.38
1	A	48	LEU	C-N	7.42	1.43	1.33
1	A	89	HIS	CA-C	-7.42	1.42	1.52
2	D	72	SER	N-CA	-7.42	1.36	1.46
2	B	64	GLY	CA-C	-7.41	1.43	1.52
1	A	50	HIS	ND1-CE1	7.40	1.40	1.32
1	C	43	PHE	CA-CB	7.40	1.61	1.53
2	D	140	ALA	N-CA	7.40	1.55	1.46
1	C	115	ALA	C-O	7.40	1.33	1.24
1	C	122	HIS	N-CA	7.39	1.55	1.46
1	C	44	PRO	N-CA	7.38	1.55	1.47
1	A	112	HIS	C-O	7.38	1.33	1.24
2	D	132	LYS	C-O	-7.36	1.14	1.24
1	A	72	HIS	ND1-CE1	7.36	1.40	1.32
2	B	109	VAL	C-O	7.35	1.33	1.24
1	C	16	LYS	CE-NZ	7.34	1.71	1.49
1	C	103	HIS	CD2-NE2	7.34	1.46	1.37
2	D	35	TYR	CG-CD2	-7.33	1.24	1.39
1	C	35	SER	C-O	-7.33	1.14	1.24
2	D	56	GLY	C-N	7.33	1.45	1.33
2	B	50	THR	CA-C	7.32	1.59	1.52
2	D	11	VAL	CB-CG1	-7.32	1.28	1.52
1	C	134	THR	CB-OG1	-7.32	1.32	1.43
2	B	146	HIS	CA-C	-7.31	1.37	1.52
2	B	100	PRO	C-O	7.31	1.34	1.24
2	B	94	ASP	CB-CG	7.31	1.70	1.52
1	A	116	GLU	N-CA	7.30	1.55	1.46
1	C	126	ASP	CB-CG	7.30	1.70	1.52
2	B	90	GLU	CB-CG	-7.29	1.30	1.52
1	A	36	PHE	CG-CD2	7.29	1.54	1.38
1	A	13	ALA	N-CA	-7.28	1.37	1.46
1	C	113	LEU	CB-CG	-7.27	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	PRO	CA-CB	7.27	1.64	1.53
1	A	109	LEU	CA-C	7.27	1.62	1.52
2	B	63	HIS	CA-C	7.27	1.62	1.52
1	A	111	ALA	C-O	-7.26	1.15	1.24
2	B	41	PHE	CG-CD2	7.26	1.54	1.38
1	A	76	MET	CA-CB	7.25	1.64	1.53
2	D	108	ASN	C-O	7.25	1.32	1.24
2	B	48	LEU	C-O	-7.25	1.14	1.24
2	B	52	ASP	CG-OD2	7.25	1.39	1.25
1	C	72	HIS	CD2-NE2	7.24	1.45	1.37
1	C	100	LEU	CB-CG	-7.23	1.39	1.53
1	C	117	PHE	CD1-CE1	7.22	1.60	1.38
2	D	116	HIS	CG-CD2	-7.21	1.27	1.35
2	B	117	HIS	N-CA	-7.21	1.37	1.46
1	C	80	LEU	C-N	7.21	1.43	1.33
1	C	19	ALA	CA-CB	-7.21	1.40	1.53
2	B	105	LEU	CA-CB	-7.20	1.42	1.53
2	B	16	GLY	C-N	-7.20	1.23	1.33
1	C	39	THR	C-N	-7.20	1.24	1.33
2	D	32	LEU	CA-C	-7.20	1.43	1.52
1	A	27	GLU	CG-CD	7.18	1.70	1.52
2	D	112	CYS	N-CA	-7.16	1.37	1.46
2	B	106	LEU	CG-CD2	-7.16	1.28	1.52
2	D	15	TRP	N-CA	7.15	1.55	1.46
2	D	114	LEU	C-O	-7.15	1.15	1.24
2	B	94	ASP	CG-OD1	-7.14	1.11	1.25
1	C	110	ALA	N-CA	7.14	1.54	1.46
1	C	65	ALA	CA-C	7.14	1.62	1.52
1	C	6	ASP	CG-OD1	7.13	1.39	1.25
2	B	85	PHE	CA-C	-7.13	1.43	1.52
1	C	36	PHE	CA-C	7.12	1.61	1.52
2	B	4	THR	C-N	7.12	1.42	1.34
1	A	33	PHE	CG-CD1	-7.12	1.24	1.38
2	B	95	LYS	N-CA	-7.11	1.36	1.45
1	A	97	ASN	CG-ND2	7.11	1.48	1.33
1	A	134	THR	N-CA	-7.10	1.37	1.46
2	B	35	TYR	CA-C	7.10	1.61	1.52
1	A	73	VAL	C-N	7.09	1.43	1.33
1	A	113	LEU	N-CA	7.09	1.53	1.46
1	C	58	HIS	CE1-NE2	7.09	1.39	1.32
2	B	78	LEU	CB-CG	7.09	1.67	1.53
2	B	91	LEU	CG-CD2	-7.09	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	48	LEU	CB-CG	-7.08	1.39	1.53
1	A	82	ALA	N-CA	-7.06	1.38	1.46
2	D	127	GLN	CA-C	-7.06	1.42	1.52
2	B	68	LEU	CA-CB	-7.05	1.42	1.53
1	A	2	LEU	CB-CG	-7.05	1.39	1.53
2	B	130	TYR	CD2-CE2	7.05	1.59	1.38
1	A	51	GLY	C-O	-7.05	1.14	1.23
1	C	132	VAL	C-N	7.05	1.42	1.33
2	D	96	LEU	C-N	-7.04	1.23	1.33
2	B	86	ALA	N-CA	7.04	1.54	1.46
1	A	24	TYR	CE2-CZ	7.03	1.55	1.38
2	D	94	ASP	C-O	-7.03	1.15	1.24
2	B	96	LEU	C-O	-7.03	1.14	1.24
1	A	44	PRO	C-O	-7.03	1.15	1.24
1	C	141	ARG	CA-C	7.02	1.67	1.52
2	D	7	GLU	CD-OE2	7.02	1.38	1.25
1	A	23	GLU	CA-C	7.02	1.62	1.52
2	D	41	PHE	C-N	-7.02	1.22	1.33
2	D	139	ASN	C-N	7.01	1.43	1.33
2	D	48	LEU	CG-CD1	7.01	1.75	1.52
1	C	50	HIS	C-O	-7.01	1.15	1.23
2	D	95	LYS	C-O	-7.00	1.15	1.23
1	A	25	GLY	CA-C	-7.00	1.42	1.51
2	B	113	VAL	CA-C	-7.00	1.42	1.52
2	D	122	PHE	CA-CB	-6.99	1.43	1.52
1	C	110	ALA	CA-C	-6.98	1.43	1.52
1	A	83	LEU	N-CA	6.97	1.55	1.46
1	C	9	ASN	CG-ND2	-6.96	1.18	1.33
2	D	137	VAL	CA-C	-6.96	1.42	1.52
2	D	101	GLU	N-CA	-6.95	1.37	1.46
1	C	36	PHE	CG-CD2	6.95	1.53	1.38
2	B	139	ASN	CA-CB	6.94	1.65	1.53
2	B	46	GLY	N-CA	-6.93	1.35	1.45
2	B	57	ASN	CA-C	-6.93	1.44	1.52
1	C	11	LYS	CD-CE	-6.93	1.31	1.52
1	C	113	LEU	CG-CD1	6.93	1.75	1.52
1	A	76	MET	CA-C	6.93	1.61	1.52
2	B	32	LEU	N-CA	-6.92	1.36	1.46
2	B	57	ASN	C-O	6.92	1.33	1.24
2	D	33	VAL	C-O	-6.92	1.16	1.24
1	C	62	VAL	C-N	6.92	1.42	1.33
2	D	99	ASP	C-N	-6.92	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	VAL	C-O	-6.91	1.16	1.24
1	C	57	GLY	N-CA	-6.90	1.37	1.45
2	D	52	ASP	CA-C	6.90	1.61	1.52
2	D	68	LEU	C-N	6.90	1.43	1.33
2	B	50	THR	CB-CG2	6.90	1.75	1.52
2	D	134	VAL	CA-C	6.90	1.62	1.52
1	C	20	HIS	CA-C	6.90	1.62	1.52
1	C	91	LEU	CB-CG	-6.90	1.39	1.53
1	C	89	HIS	CA-C	-6.89	1.43	1.52
1	A	24	TYR	CA-CB	6.89	1.64	1.53
2	D	18	VAL	CB-CG1	-6.89	1.29	1.52
1	A	32	MET	C-N	-6.88	1.24	1.34
2	B	55	MET	SD-CE	-6.88	1.62	1.79
1	A	59	GLY	C-O	6.88	1.32	1.23
2	B	29	GLY	N-CA	-6.88	1.37	1.45
1	C	132	VAL	C-O	6.88	1.31	1.24
1	C	71	ALA	C-O	6.88	1.32	1.24
1	A	124	SER	N-CA	-6.87	1.38	1.46
1	C	99	LYS	CA-CB	6.87	1.64	1.53
2	B	59	LYS	N-CA	6.87	1.55	1.46
2	D	61	LYS	CD-CE	6.87	1.73	1.52
2	D	42	PHE	CA-CB	-6.86	1.44	1.53
2	B	26	GLU	CB-CG	6.86	1.73	1.52
1	C	116	GLU	N-CA	6.86	1.55	1.46
2	D	55	MET	SD-CE	-6.86	1.62	1.79
1	A	11	LYS	CG-CD	-6.85	1.31	1.52
2	D	91	LEU	N-CA	-6.84	1.38	1.46
2	B	127	GLN	C-N	6.84	1.43	1.33
2	B	22	GLU	CB-CG	-6.84	1.31	1.52
1	A	126	ASP	C-N	6.83	1.42	1.33
1	C	3	SER	CA-C	-6.82	1.44	1.52
1	C	63	ALA	N-CA	6.82	1.54	1.46
2	D	93	CYS	CA-C	6.82	1.61	1.52
2	B	133	VAL	C-O	6.81	1.32	1.24
1	C	24	TYR	CG-CD1	6.81	1.53	1.39
1	A	11	LYS	C-O	6.80	1.32	1.24
2	B	82	LYS	CG-CD	6.80	1.72	1.52
2	D	106	LEU	CA-C	-6.80	1.43	1.52
2	B	118	PHE	CB-CG	-6.79	1.35	1.50
1	A	63	ALA	C-O	6.79	1.32	1.24
1	C	58	HIS	CA-CB	-6.78	1.42	1.53
2	B	140	ALA	C-N	-6.78	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	LYS	CE-NZ	6.77	1.69	1.49
1	C	62	VAL	CA-CB	6.76	1.62	1.54
2	D	17	LYS	CB-CG	-6.76	1.32	1.52
1	C	5	ALA	C-O	-6.75	1.16	1.24
1	C	56	LYS	N-CA	-6.75	1.38	1.46
1	A	118	THR	CA-C	-6.75	1.44	1.52
2	B	111	VAL	C-O	6.75	1.31	1.24
2	B	15	TRP	CA-CB	-6.75	1.42	1.53
2	D	61	LYS	CA-C	-6.74	1.43	1.52
1	C	137	THR	C-O	-6.73	1.14	1.24
1	C	109	LEU	N-CA	6.72	1.54	1.46
2	B	120	LYS	CB-CG	-6.72	1.32	1.52
1	A	73	VAL	N-CA	6.72	1.54	1.46
2	D	7	GLU	N-CA	6.72	1.54	1.46
1	A	90	LYS	CB-CG	6.71	1.72	1.52
1	C	26	ALA	N-CA	-6.71	1.38	1.46
2	D	82	LYS	CA-C	-6.70	1.43	1.52
1	A	7	LYS	C-O	-6.70	1.15	1.24
1	C	46	PHE	CB-CG	-6.70	1.35	1.50
1	C	48	LEU	CG-CD2	6.70	1.74	1.52
2	B	138	ALA	CA-C	-6.70	1.44	1.52
2	D	75	LEU	C-O	-6.70	1.16	1.24
2	D	113	VAL	CB-CG2	6.70	1.74	1.52
2	B	101	GLU	CA-CB	-6.69	1.42	1.53
1	A	135	VAL	C-O	6.69	1.33	1.24
2	B	14	LEU	CG-CD1	-6.69	1.30	1.52
2	B	116	HIS	CB-CG	-6.69	1.40	1.50
1	A	50	HIS	CD2-NE2	6.69	1.45	1.37
2	D	7	GLU	CG-CD	-6.69	1.35	1.52
1	C	102	SER	C-O	6.68	1.32	1.24
1	A	66	LEU	C-N	-6.68	1.25	1.33
2	B	9	SER	C-O	-6.68	1.15	1.24
2	B	4	THR	N-CA	6.68	1.55	1.46
2	B	22	GLU	C-O	-6.67	1.16	1.24
1	C	74	ASP	CB-CG	-6.67	1.35	1.52
2	B	103	PHE	CE1-CZ	-6.66	1.18	1.38
1	C	20	HIS	N-CA	6.65	1.54	1.46
2	D	137	VAL	C-O	-6.65	1.15	1.24
2	D	4	THR	CA-C	6.65	1.61	1.52
1	A	140	TYR	CE1-CZ	-6.64	1.22	1.38
2	B	102	ASN	C-O	6.64	1.32	1.24
1	C	83	LEU	C-N	-6.64	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	PHE	CE1-CZ	-6.63	1.18	1.38
2	D	120	LYS	CA-C	-6.63	1.41	1.52
1	C	80	LEU	CB-CG	6.63	1.66	1.53
2	D	17	LYS	CA-C	-6.63	1.43	1.52
1	A	96	VAL	C-N	6.62	1.43	1.33
1	A	108	THR	CA-C	-6.62	1.44	1.52
2	D	17	LYS	CA-CB	6.62	1.64	1.53
1	A	33	PHE	CD2-CE2	6.62	1.58	1.38
2	D	101	GLU	CB-CG	6.62	1.72	1.52
1	C	129	LEU	C-O	6.61	1.32	1.24
2	B	57	ASN	N-CA	-6.61	1.35	1.46
2	B	75	LEU	N-CA	-6.61	1.37	1.46
1	C	22	GLY	C-N	6.60	1.42	1.33
1	A	24	TYR	C-O	6.60	1.31	1.24
1	C	51	GLY	CA-C	-6.60	1.42	1.51
2	D	26	GLU	N-CA	-6.60	1.38	1.46
1	A	131	SER	C-N	-6.60	1.25	1.33
1	C	37	PRO	CA-C	6.60	1.63	1.52
1	A	63	ALA	C-N	6.59	1.43	1.33
1	A	139	LYS	C-O	-6.59	1.15	1.24
1	C	68	ASN	C-N	-6.59	1.25	1.33
2	B	19	ASN	N-CA	6.59	1.54	1.46
1	C	112	HIS	CE1-NE2	6.58	1.39	1.32
1	A	26	ALA	C-O	-6.57	1.16	1.24
1	C	109	LEU	C-O	-6.57	1.16	1.24
2	D	70	ALA	CA-C	-6.57	1.44	1.52
2	D	96	LEU	CA-C	6.57	1.61	1.52
1	A	131	SER	CA-CB	6.57	1.64	1.53
2	D	135	ALA	CA-CB	-6.57	1.43	1.53
1	A	3	SER	C-O	6.57	1.32	1.24
1	A	89	HIS	CE1-NE2	6.57	1.39	1.32
1	C	76	MET	SD-CE	-6.56	1.63	1.79
2	D	75	LEU	CB-CG	-6.56	1.40	1.53
1	C	23	GLU	CA-CB	6.56	1.63	1.53
1	C	2	LEU	C-N	-6.55	1.20	1.33
1	A	8	THR	C-O	-6.55	1.16	1.24
1	A	56	LYS	N-CA	-6.55	1.37	1.46
1	A	124	SER	CA-C	6.55	1.61	1.52
1	A	3	SER	CB-OG	-6.55	1.29	1.42
1	C	2	LEU	CB-CG	6.55	1.66	1.53
1	A	131	SER	C-O	6.55	1.32	1.24
1	C	48	LEU	C-N	6.55	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	SER	CA-CB	-6.55	1.43	1.53
1	C	109	LEU	CA-C	-6.55	1.44	1.52
1	C	101	LEU	CB-CG	-6.54	1.40	1.53
1	A	109	LEU	CG-CD1	-6.54	1.30	1.52
2	D	32	LEU	N-CA	-6.54	1.38	1.46
1	A	20	HIS	C-O	6.54	1.32	1.24
1	A	38	THR	CB-OG1	-6.53	1.33	1.43
1	A	138	SER	CA-C	6.53	1.61	1.52
1	A	96	VAL	CA-C	-6.52	1.43	1.52
2	D	50	THR	CB-OG1	6.52	1.54	1.43
1	A	11	LYS	CB-CG	-6.52	1.32	1.52
2	B	105	LEU	CB-CG	6.51	1.66	1.53
2	D	75	LEU	CA-C	-6.51	1.44	1.52
1	A	31	ARG	CA-C	6.51	1.61	1.52
2	D	62	ALA	C-O	-6.51	1.16	1.24
1	C	141	ARG	NE-CZ	6.51	1.40	1.33
2	B	87	THR	C-N	6.50	1.42	1.34
2	D	139	ASN	C-O	6.50	1.31	1.24
1	A	90	LYS	CA-C	-6.49	1.47	1.52
2	B	42	PHE	CE1-CZ	-6.49	1.19	1.38
2	D	14	LEU	CG-CD2	-6.49	1.31	1.52
2	B	58	PRO	CB-CG	-6.48	1.17	1.49
2	B	125	PRO	C-N	-6.48	1.25	1.33
1	C	43	PHE	CG-CD2	6.48	1.52	1.38
1	A	53	ALA	C-N	6.48	1.43	1.33
2	B	81	LEU	C-O	-6.48	1.16	1.24
2	D	23	VAL	CA-CB	6.47	1.61	1.54
2	B	30	ARG	NE-CZ	-6.47	1.25	1.33
1	C	140	TYR	CE2-CZ	-6.46	1.22	1.38
1	C	85	ASP	CG-OD2	6.46	1.37	1.25
1	A	11	LYS	CA-C	6.46	1.61	1.52
1	A	72	HIS	C-N	6.44	1.42	1.34
2	D	33	VAL	N-CA	6.44	1.54	1.46
1	C	116	GLU	CD-OE1	-6.44	1.13	1.25
1	A	63	ALA	CA-CB	6.43	1.64	1.53
1	C	80	LEU	N-CA	6.43	1.53	1.46
1	C	128	PHE	CD2-CE2	6.43	1.57	1.38
2	D	71	PHE	C-O	-6.43	1.16	1.24
2	B	135	ALA	CA-CB	-6.43	1.43	1.53
2	D	82	LYS	CA-CB	6.43	1.63	1.53
2	D	88	LEU	CA-C	6.43	1.61	1.52
2	B	103	PHE	CA-CB	-6.42	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	ALA	CA-C	6.42	1.61	1.52
1	C	44	PRO	CA-C	6.42	1.59	1.52
1	C	104	CYS	N-CA	6.41	1.54	1.46
1	C	105	LEU	C-N	-6.41	1.25	1.33
2	B	116	HIS	N-CA	6.40	1.54	1.46
2	B	107	GLY	C-O	6.39	1.31	1.23
2	B	7	GLU	CD-OE2	6.37	1.37	1.25
1	A	103	HIS	C-N	6.37	1.42	1.33
1	A	55	VAL	C-N	6.37	1.42	1.33
1	C	129	LEU	N-CA	6.36	1.54	1.46
1	C	86	LEU	C-N	6.36	1.43	1.33
2	D	56	GLY	C-O	6.35	1.31	1.23
1	A	58	HIS	CD2-NE2	-6.35	1.30	1.37
2	B	43	GLU	CA-C	6.34	1.62	1.52
1	A	69	ALA	CA-C	6.34	1.61	1.52
2	B	101	GLU	C-O	-6.34	1.16	1.24
2	B	63	HIS	C-O	6.33	1.32	1.24
2	B	5	PRO	CA-CB	-6.33	1.44	1.53
1	A	116	GLU	CA-CB	6.32	1.64	1.53
1	A	57	GLY	C-N	-6.31	1.25	1.33
2	B	108	ASN	CG-OD1	6.31	1.35	1.23
2	B	121	GLU	CD-OE2	-6.31	1.13	1.25
2	D	1	VAL	CB-CG1	6.31	1.73	1.52
1	A	75	ASP	C-O	6.31	1.33	1.23
1	C	9	ASN	CA-C	-6.31	1.44	1.52
1	A	23	GLU	CA-CB	6.30	1.63	1.53
1	C	45	HIS	N-CA	6.30	1.54	1.46
2	D	123	THR	CA-C	-6.30	1.44	1.52
2	B	28	LEU	N-CA	-6.30	1.38	1.46
2	D	12	THR	CB-OG1	6.30	1.53	1.43
2	D	79	ASP	C-N	6.29	1.42	1.33
2	D	69	GLY	C-O	-6.29	1.16	1.23
1	C	58	HIS	C-N	-6.29	1.25	1.33
2	D	143	HIS	CA-C	6.29	1.61	1.52
2	B	116	HIS	CA-CB	-6.29	1.43	1.53
1	C	124	SER	N-CA	6.28	1.54	1.46
2	B	142	ALA	N-CA	-6.28	1.37	1.46
1	C	61	LYS	CB-CG	-6.28	1.33	1.52
2	D	145	TYR	CE2-CZ	-6.28	1.23	1.38
2	D	50	THR	C-N	-6.28	1.25	1.33
2	D	15	TRP	CG-CD2	6.27	1.55	1.43
1	A	83	LEU	CA-C	-6.27	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	140	ALA	CA-CB	-6.27	1.43	1.53
1	A	37	PRO	CA-C	-6.27	1.41	1.52
2	D	66	LYS	CA-CB	-6.26	1.43	1.53
1	A	138	SER	C-O	-6.26	1.16	1.24
1	A	65	ALA	CA-C	6.25	1.61	1.52
1	A	136	LEU	C-O	6.25	1.31	1.24
2	B	13	ALA	C-O	-6.24	1.17	1.24
2	D	132	LYS	CD-CE	6.24	1.71	1.52
2	B	105	LEU	CA-C	6.24	1.60	1.52
1	C	109	LEU	CG-CD2	-6.24	1.31	1.52
2	B	103	PHE	N-CA	-6.24	1.39	1.46
1	C	17	VAL	CB-CG1	-6.24	1.31	1.52
2	D	131	GLN	C-N	6.24	1.42	1.34
1	A	91	LEU	CG-CD1	-6.23	1.31	1.52
1	C	138	SER	CB-OG	-6.23	1.29	1.42
1	A	58	HIS	C-N	-6.22	1.25	1.33
1	C	122	HIS	CB-CG	-6.21	1.41	1.50
1	C	46	PHE	CE2-CZ	6.21	1.57	1.38
2	D	57	ASN	CG-ND2	-6.20	1.20	1.33
2	D	74	GLY	N-CA	-6.20	1.37	1.45
2	D	41	PHE	CB-CG	6.20	1.64	1.50
2	D	42	PHE	CE1-CZ	-6.20	1.20	1.38
1	A	105	LEU	C-O	-6.19	1.16	1.24
2	B	48	LEU	CG-CD2	-6.19	1.32	1.52
2	B	24	GLY	N-CA	-6.19	1.38	1.45
2	B	17	LYS	CG-CD	-6.19	1.33	1.52
2	B	113	VAL	CA-CB	6.18	1.63	1.54
2	B	104	ARG	CA-C	-6.18	1.44	1.52
1	A	122	HIS	CB-CG	-6.17	1.41	1.50
1	A	1	VAL	CB-CG1	-6.17	1.32	1.52
2	D	102	ASN	CG-OD1	-6.17	1.11	1.23
2	B	108	ASN	CG-ND2	-6.17	1.20	1.33
2	D	23	VAL	N-CA	6.16	1.53	1.46
1	A	98	PHE	C-O	6.16	1.31	1.24
1	A	94	ASP	C-N	-6.16	1.26	1.34
2	B	45	PHE	CB-CG	6.15	1.64	1.50
2	B	122	PHE	CA-C	6.15	1.60	1.53
1	A	102	SER	C-O	6.15	1.31	1.24
1	C	89	HIS	CG-CD2	-6.14	1.29	1.35
1	C	139	LYS	N-CA	6.14	1.53	1.46
2	D	102	ASN	CG-ND2	6.14	1.46	1.33
2	D	52	ASP	CG-OD1	-6.14	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	PHE	CA-CB	-6.13	1.43	1.53
2	B	131	GLN	CD-NE2	-6.13	1.20	1.33
1	A	16	LYS	N-CA	6.13	1.54	1.46
1	A	103	HIS	CA-CB	-6.13	1.44	1.53
2	B	63	HIS	CD2-NE2	6.12	1.44	1.37
1	C	124	SER	CA-CB	6.12	1.63	1.53
2	D	88	LEU	N-CA	-6.12	1.38	1.46
1	C	112	HIS	C-O	6.12	1.31	1.24
2	B	96	LEU	N-CA	-6.11	1.38	1.46
2	D	92	HIS	CE1-NE2	-6.11	1.26	1.32
2	B	129	ALA	CA-CB	-6.10	1.43	1.53
1	C	62	VAL	C-O	-6.10	1.17	1.24
2	B	131	GLN	N-CA	-6.10	1.39	1.46
1	A	30	GLU	C-O	-6.09	1.17	1.24
2	D	62	ALA	N-CA	6.09	1.53	1.46
2	B	3	LEU	CG-CD1	-6.09	1.32	1.52
2	D	24	GLY	CA-C	-6.09	1.45	1.52
1	A	109	LEU	CA-CB	-6.08	1.43	1.53
2	B	79	ASP	CA-C	6.08	1.60	1.52
1	C	67	THR	N-CA	6.08	1.53	1.46
1	A	91	LEU	N-CA	-6.07	1.38	1.46
1	A	137	THR	CA-C	-6.07	1.43	1.52
1	C	116	GLU	CA-CB	6.07	1.64	1.53
1	C	81	SER	CB-OG	6.06	1.54	1.42
2	D	68	LEU	CG-CD2	-6.06	1.32	1.52
2	D	131	GLN	CD-NE2	-6.06	1.20	1.33
2	D	42	PHE	C-O	6.05	1.32	1.23
1	C	132	VAL	CB-CG2	6.05	1.72	1.52
2	B	92	HIS	CE1-NE2	-6.04	1.26	1.32
1	A	48	LEU	C-O	-6.04	1.14	1.23
2	B	53	ALA	C-O	-6.04	1.17	1.24
2	B	25	GLY	CA-C	6.04	1.58	1.51
2	D	104	ARG	CG-CD	6.04	1.70	1.52
1	C	120	ALA	N-CA	-6.03	1.39	1.46
1	A	140	TYR	CG-CD1	6.03	1.52	1.39
1	A	66	LEU	C-O	6.03	1.31	1.24
2	D	65	LYS	N-CA	6.02	1.54	1.46
2	D	67	VAL	N-CA	6.01	1.54	1.46
1	C	4	PRO	C-O	-6.01	1.17	1.24
1	C	103	HIS	CG-CD2	-5.99	1.29	1.35
1	C	31	ARG	CZ-NH2	-5.99	1.25	1.33
1	A	130	ALA	C-N	5.99	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	128	PHE	N-CA	-5.99	1.39	1.46
2	B	42	PHE	CB-CG	-5.98	1.36	1.50
2	B	19	ASN	CA-C	5.98	1.60	1.52
1	C	85	ASP	CA-CB	-5.98	1.44	1.53
2	B	104	ARG	C-N	5.98	1.41	1.33
1	A	48	LEU	CG-CD1	5.97	1.72	1.52
1	A	121	VAL	C-N	-5.96	1.25	1.33
1	A	75	ASP	N-CA	5.96	1.57	1.47
2	D	41	PHE	CG-CD2	-5.96	1.26	1.38
1	A	50	HIS	CE1-NE2	5.95	1.38	1.32
2	D	65	LYS	CA-CB	5.95	1.63	1.53
1	A	110	ALA	C-N	5.95	1.41	1.33
1	A	45	HIS	CB-CG	5.94	1.58	1.50
1	C	13	ALA	CA-C	-5.94	1.45	1.52
1	A	102	SER	CA-C	5.94	1.60	1.52
2	B	6	GLU	N-CA	-5.93	1.38	1.46
1	C	60	LYS	CD-CE	-5.93	1.34	1.52
2	B	141	LEU	CA-C	-5.91	1.45	1.52
2	D	38	THR	CA-C	5.91	1.60	1.52
1	C	64	ASP	CG-OD1	-5.91	1.14	1.25
1	C	35	SER	CA-C	-5.90	1.44	1.52
1	C	66	LEU	CG-CD1	-5.90	1.33	1.52
2	B	119	GLY	CA-C	-5.90	1.43	1.52
2	B	26	GLU	C-N	-5.90	1.25	1.33
2	D	130	TYR	CD1-CE1	5.90	1.56	1.38
2	D	44	SER	N-CA	5.90	1.54	1.46
2	B	122	PHE	C-N	-5.89	1.24	1.33
1	C	93	VAL	CA-CB	5.89	1.61	1.54
2	D	76	ALA	C-N	5.89	1.42	1.33
2	B	65	LYS	C-O	-5.89	1.17	1.24
2	B	81	LEU	CA-CB	-5.88	1.44	1.53
2	B	61	LYS	CD-CE	5.88	1.70	1.52
1	C	27	GLU	N-CA	5.87	1.53	1.46
1	C	91	LEU	C-O	-5.87	1.17	1.24
1	A	62	VAL	C-O	-5.87	1.17	1.24
2	D	104	ARG	CA-CB	5.86	1.62	1.53
1	C	28	ALA	CA-CB	-5.86	1.44	1.53
2	D	42	PHE	CE2-CZ	5.86	1.56	1.38
2	D	55	MET	C-O	-5.85	1.16	1.24
1	C	49	SER	N-CA	5.84	1.53	1.45
2	D	38	THR	C-N	5.83	1.42	1.33
1	C	106	LEU	CB-CG	-5.83	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	PHE	CD2-CE2	5.83	1.56	1.38
1	A	92	ARG	CB-CG	-5.83	1.34	1.52
1	A	114	PRO	N-CD	-5.83	1.39	1.47
1	C	24	TYR	CD2-CE2	5.82	1.56	1.38
2	B	18	VAL	CB-CG2	5.82	1.71	1.52
2	D	108	ASN	CG-OD1	5.82	1.34	1.23
2	D	15	TRP	CZ3-CH2	5.82	1.54	1.40
2	D	140	ALA	CA-C	5.82	1.60	1.52
1	C	137	THR	CA-CB	5.81	1.63	1.53
2	D	99	ASP	CB-CG	5.81	1.66	1.52
2	D	143	HIS	CD2-NE2	-5.81	1.31	1.37
2	D	64	GLY	CA-C	5.80	1.58	1.51
1	A	1	VAL	CA-C	5.80	1.65	1.52
1	A	136	LEU	C-N	-5.80	1.25	1.33
2	D	125	PRO	CG-CD	-5.79	1.31	1.50
1	A	54	GLN	CD-NE2	5.78	1.45	1.33
1	C	64	ASP	CB-CG	5.78	1.66	1.52
1	C	76	MET	CA-CB	5.78	1.62	1.53
1	C	135	VAL	CA-CB	5.78	1.60	1.54
2	D	101	GLU	C-O	5.78	1.31	1.24
2	D	93	CYS	CB-SG	5.77	2.00	1.81
2	B	29	GLY	CA-C	5.77	1.58	1.52
2	B	92	HIS	CA-CB	5.77	1.63	1.53
1	A	127	LYS	N-CA	-5.76	1.39	1.46
2	D	1	VAL	CA-CB	5.76	1.70	1.54
2	D	3	LEU	CB-CG	5.76	1.65	1.53
2	B	51	PRO	C-N	5.76	1.41	1.33
2	D	120	LYS	C-O	5.75	1.31	1.24
2	B	82	LYS	C-N	5.75	1.40	1.33
2	D	30	ARG	CA-CB	5.75	1.62	1.53
2	B	109	VAL	CA-C	-5.75	1.44	1.52
2	B	120	LYS	CE-NZ	-5.75	1.32	1.49
1	C	134	THR	C-N	-5.75	1.26	1.33
2	D	32	LEU	C-N	5.75	1.40	1.33
1	A	103	HIS	CE1-NE2	5.74	1.38	1.32
2	B	32	LEU	CA-CB	5.73	1.63	1.53
2	D	102	ASN	C-N	-5.73	1.26	1.33
2	D	16	GLY	N-CA	5.73	1.53	1.45
2	B	94	ASP	CA-C	-5.73	1.44	1.52
2	D	17	LYS	C-O	5.73	1.31	1.24
2	B	136	GLY	CA-C	-5.73	1.45	1.52
2	B	17	LYS	CD-CE	5.72	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	TYR	CA-CB	-5.72	1.44	1.53
1	A	65	ALA	CA-CB	5.71	1.62	1.53
2	D	77	HIS	CG-CD2	5.71	1.42	1.35
2	D	88	LEU	CG-CD2	-5.71	1.33	1.52
2	D	122	PHE	CG-CD1	-5.71	1.26	1.38
2	B	8	LYS	CD-CE	-5.71	1.35	1.52
2	D	139	ASN	CB-CG	-5.71	1.37	1.52
1	C	77	PRO	CA-CB	5.71	1.62	1.53
2	D	146	HIS	CB-CG	-5.70	1.42	1.50
2	D	97	HIS	N-CA	5.69	1.53	1.46
2	B	64	GLY	N-CA	5.68	1.53	1.45
2	B	71	PHE	C-O	-5.67	1.17	1.24
1	C	97	ASN	C-O	5.67	1.31	1.24
1	C	108	THR	CA-CB	5.66	1.62	1.53
2	B	77	HIS	C-N	-5.66	1.25	1.33
1	A	135	VAL	CA-CB	5.66	1.62	1.54
1	C	137	THR	N-CA	5.66	1.53	1.46
1	A	53	ALA	N-CA	-5.65	1.38	1.46
2	B	65	LYS	C-N	-5.65	1.25	1.33
1	A	138	SER	CB-OG	-5.65	1.30	1.42
1	C	131	SER	C-N	-5.64	1.26	1.33
1	C	21	ALA	C-O	5.64	1.31	1.24
1	A	131	SER	CA-C	5.63	1.60	1.52
1	A	47	ASP	CG-OD1	-5.63	1.14	1.25
1	C	8	THR	CB-CG2	-5.63	1.33	1.52
2	D	122	PHE	CG-CD2	5.62	1.50	1.38
2	D	11	VAL	C-O	-5.62	1.17	1.24
1	C	106	LEU	C-N	-5.62	1.25	1.33
2	D	114	LEU	CA-CB	-5.61	1.44	1.53
2	D	144	LYS	C-O	5.61	1.31	1.24
1	C	24	TYR	CE1-CZ	-5.61	1.24	1.38
1	A	68	ASN	CG-OD1	-5.60	1.12	1.23
2	D	91	LEU	CG-CD1	5.60	1.71	1.52
1	A	6	ASP	C-O	5.60	1.30	1.24
1	A	104	CYS	C-N	-5.60	1.25	1.33
2	D	72	SER	C-N	5.60	1.41	1.33
1	C	126	ASP	CG-OD1	-5.59	1.14	1.25
1	C	74	ASP	CG-OD2	-5.59	1.14	1.25
1	A	33	PHE	N-CA	5.58	1.53	1.46
1	A	112	HIS	CB-CG	-5.58	1.42	1.50
1	A	60	LYS	CB-CG	-5.58	1.35	1.52
1	A	81	SER	C-N	-5.57	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	ARG	CA-C	5.57	1.60	1.53
1	A	26	ALA	CA-CB	-5.56	1.44	1.53
2	B	21	ASP	C-O	5.56	1.31	1.24
1	A	127	LYS	C-O	5.55	1.30	1.24
2	B	140	ALA	N-CA	-5.55	1.39	1.46
1	A	16	LYS	CB-CG	5.55	1.69	1.52
2	D	120	LYS	CB-CG	-5.55	1.35	1.52
2	D	130	TYR	CA-CB	-5.55	1.44	1.53
1	A	118	THR	CB-OG1	-5.55	1.34	1.43
1	C	94	ASP	CA-CB	5.55	1.61	1.53
2	B	9	SER	C-N	5.54	1.42	1.33
1	C	42	TYR	CG-CD1	5.54	1.50	1.39
1	C	42	TYR	N-CA	-5.54	1.38	1.46
1	A	50	HIS	CA-C	-5.54	1.45	1.52
1	C	106	LEU	CA-CB	5.53	1.62	1.53
1	C	112	HIS	CA-C	-5.53	1.45	1.52
2	B	36	PRO	C-O	5.53	1.32	1.24
1	C	97	ASN	N-CA	-5.53	1.39	1.46
2	D	26	GLU	C-N	-5.53	1.26	1.33
1	A	85	ASP	CA-C	-5.52	1.45	1.52
2	D	35	TYR	CA-C	5.52	1.58	1.52
2	B	83	GLY	C-O	5.52	1.30	1.23
2	B	130	TYR	C-O	-5.52	1.16	1.24
2	D	51	PRO	CG-CD	5.52	1.69	1.50
1	C	64	ASP	CA-C	-5.52	1.45	1.52
2	D	119	GLY	C-O	-5.52	1.17	1.24
1	C	107	VAL	CA-C	5.51	1.59	1.52
2	D	94	ASP	CB-CG	5.51	1.65	1.52
1	A	43	PHE	CG-CD2	-5.50	1.27	1.38
2	B	118	PHE	N-CA	-5.50	1.38	1.46
2	D	26	GLU	CA-CB	5.49	1.62	1.53
1	A	40	LYS	C-N	5.49	1.41	1.34
1	A	126	ASP	CG-OD2	-5.49	1.15	1.25
2	D	144	LYS	CB-CG	5.49	1.69	1.52
1	A	67	THR	CA-C	5.49	1.60	1.52
1	A	38	THR	C-N	5.48	1.41	1.33
1	C	37	PRO	C-N	-5.48	1.26	1.33
1	A	99	LYS	CA-CB	5.47	1.62	1.53
2	D	25	GLY	N-CA	5.47	1.52	1.45
1	A	30	GLU	CB-CG	-5.47	1.36	1.52
2	B	85	PHE	C-N	-5.46	1.27	1.33
1	A	129	LEU	CG-CD2	5.45	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ALA	CA-CB	-5.45	1.44	1.53
2	B	106	LEU	N-CA	5.45	1.53	1.46
1	A	18	GLY	C-N	-5.44	1.26	1.33
1	A	13	ALA	C-O	-5.43	1.17	1.24
1	A	46	PHE	CE1-CZ	5.43	1.54	1.38
2	B	78	LEU	C-N	5.43	1.42	1.33
1	C	103	HIS	C-O	5.43	1.30	1.24
2	D	52	ASP	C-O	-5.42	1.17	1.24
2	D	115	ALA	CA-CB	5.42	1.61	1.53
2	D	144	LYS	CG-CD	-5.42	1.36	1.52
1	A	40	LYS	CD-CE	-5.42	1.36	1.52
2	B	7	GLU	CG-CD	-5.42	1.38	1.52
2	B	57	ASN	CA-CB	-5.42	1.44	1.52
2	D	83	GLY	CA-C	-5.42	1.41	1.51
1	A	82	ALA	CA-C	-5.41	1.46	1.52
2	D	78	LEU	CG-CD1	5.41	1.70	1.52
2	D	123	THR	N-CA	5.40	1.53	1.45
1	A	76	MET	C-N	-5.40	1.21	1.33
1	A	87	HIS	N-CA	5.39	1.53	1.46
1	A	129	LEU	CG-CD1	-5.39	1.34	1.52
2	B	124	PRO	CA-C	-5.39	1.47	1.52
1	C	45	HIS	CA-CB	-5.39	1.44	1.53
2	B	26	GLU	CG-CD	-5.39	1.38	1.52
2	B	17	LYS	N-CA	-5.38	1.39	1.46
1	C	8	THR	C-N	5.38	1.41	1.33
1	A	39	THR	CA-CB	-5.38	1.43	1.53
1	A	123	ALA	C-N	5.38	1.41	1.33
2	B	123	THR	CA-CB	-5.38	1.45	1.53
1	A	133	SER	C-N	-5.37	1.26	1.33
1	A	140	TYR	C-O	5.37	1.30	1.24
2	D	103	PHE	CA-CB	-5.36	1.45	1.53
2	D	97	HIS	CE1-NE2	-5.36	1.27	1.32
1	A	6	ASP	C-N	5.36	1.41	1.34
1	A	101	LEU	C-O	5.35	1.30	1.24
2	B	139	ASN	N-CA	5.35	1.53	1.46
1	A	137	THR	C-O	5.35	1.31	1.24
2	D	23	VAL	CB-CG1	-5.35	1.34	1.52
2	B	48	LEU	C-N	-5.34	1.26	1.33
2	D	22	GLU	C-O	-5.34	1.17	1.24
2	D	24	GLY	C-O	5.34	1.30	1.23
2	D	85	PHE	CA-C	5.33	1.60	1.52
1	C	83	LEU	CA-CB	5.33	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	71	PHE	CG-CD2	5.32	1.50	1.38
1	A	10	VAL	CB-CG2	-5.32	1.35	1.52
1	C	75	ASP	CG-OD2	5.32	1.35	1.25
2	D	118	PHE	CD2-CE2	5.30	1.54	1.38
1	C	94	ASP	CG-OD2	5.30	1.35	1.25
2	D	145	TYR	C-N	-5.30	1.25	1.33
2	B	62	ALA	CA-C	5.29	1.59	1.52
1	A	7	LYS	CG-CD	5.29	1.68	1.52
2	B	134	VAL	C-N	5.29	1.40	1.33
1	A	55	VAL	CA-CB	5.29	1.60	1.54
2	D	11	VAL	CB-CG2	5.28	1.70	1.52
2	B	19	ASN	C-O	5.27	1.30	1.24
1	C	89	HIS	CB-CG	5.27	1.57	1.50
1	C	80	LEU	CA-CB	-5.27	1.45	1.53
1	A	108	THR	C-N	5.26	1.40	1.33
2	B	70	ALA	CA-CB	-5.26	1.45	1.53
1	C	136	LEU	CA-CB	-5.26	1.43	1.53
1	C	96	VAL	C-O	5.25	1.30	1.24
1	C	134	THR	N-CA	5.25	1.52	1.46
2	D	144	LYS	N-CA	5.25	1.53	1.46
1	A	38	THR	C-O	-5.25	1.17	1.24
1	C	140	TYR	CA-CB	5.25	1.61	1.53
2	D	3	LEU	CG-CD2	-5.24	1.35	1.52
1	C	119	PRO	CA-CB	-5.24	1.46	1.53
2	D	62	ALA	C-N	5.23	1.41	1.33
2	D	81	LEU	CA-C	5.23	1.59	1.52
1	C	13	ALA	CA-CB	-5.23	1.45	1.53
1	C	117	PHE	N-CA	5.23	1.53	1.46
1	A	91	LEU	CA-C	5.22	1.59	1.52
1	C	16	LYS	C-N	5.22	1.40	1.33
1	A	107	VAL	CA-C	-5.22	1.46	1.52
1	A	75	ASP	CA-C	5.21	1.61	1.53
2	D	64	GLY	C-O	-5.20	1.16	1.23
2	B	110	LEU	CB-CG	5.20	1.63	1.53
2	D	122	PHE	N-CA	5.19	1.53	1.46
1	A	39	THR	CB-OG1	5.19	1.52	1.43
2	D	27	ALA	CA-CB	-5.19	1.45	1.53
1	A	83	LEU	CG-CD2	5.19	1.69	1.52
1	A	45	HIS	CD2-NE2	-5.18	1.32	1.37
1	A	118	THR	CA-CB	-5.17	1.46	1.53
1	A	116	GLU	CA-C	5.17	1.59	1.52
2	B	134	VAL	CA-CB	-5.17	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	LYS	CA-CB	5.17	1.61	1.53
2	D	31	LEU	CA-CB	5.16	1.61	1.53
1	A	95	PRO	CA-CB	-5.15	1.46	1.53
2	B	25	GLY	C-N	-5.15	1.27	1.33
1	A	49	SER	C-O	5.13	1.30	1.23
1	A	41	THR	CA-CB	5.12	1.61	1.53
1	C	20	HIS	CG-CD2	-5.12	1.30	1.35
2	B	55	MET	CA-CB	5.12	1.61	1.53
1	A	141	ARG	CZ-NH2	5.12	1.40	1.33
2	B	67	VAL	CA-C	-5.11	1.46	1.52
1	A	84	SER	CA-C	5.11	1.59	1.52
1	A	68	ASN	N-CA	5.11	1.52	1.46
2	D	9	SER	N-CA	-5.10	1.39	1.46
1	C	20	HIS	C-O	5.10	1.30	1.24
2	D	81	LEU	CA-CB	-5.09	1.45	1.53
1	A	59	GLY	C-N	5.09	1.40	1.33
1	A	9	ASN	CG-ND2	-5.09	1.22	1.33
2	B	122	PHE	CA-CB	5.09	1.59	1.52
2	D	28	LEU	CB-CG	5.09	1.63	1.53
1	C	22	GLY	N-CA	-5.09	1.39	1.45
1	C	27	GLU	C-O	5.09	1.30	1.24
2	D	141	LEU	N-CA	-5.09	1.40	1.46
1	A	61	LYS	CA-CB	5.08	1.62	1.53
1	A	92	ARG	C-N	-5.08	1.27	1.33
2	D	141	LEU	CA-CB	5.08	1.61	1.53
2	B	67	VAL	C-N	-5.08	1.27	1.33
1	C	96	VAL	CB-CG2	-5.08	1.35	1.52
2	D	103	PHE	C-O	5.08	1.29	1.24
1	C	60	LYS	CA-CB	5.07	1.61	1.53
2	D	10	ALA	C-O	5.07	1.30	1.24
1	C	134	THR	CA-CB	5.07	1.61	1.53
1	A	92	ARG	C-O	5.06	1.30	1.23
2	B	17	LYS	CB-CG	5.06	1.67	1.52
2	B	31	LEU	N-CA	-5.06	1.40	1.46
1	C	141	ARG	CZ-NH1	-5.06	1.25	1.32
1	C	28	ALA	C-O	-5.06	1.18	1.24
1	C	126	ASP	CA-C	-5.06	1.46	1.52
2	D	86	ALA	C-N	-5.05	1.27	1.33
1	A	138	SER	C-N	-5.05	1.27	1.33
1	A	141	ARG	CA-C	5.05	1.63	1.52
2	B	96	LEU	CB-CG	5.05	1.63	1.53
2	D	35	TYR	N-CA	5.05	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	HIS	C-O	-5.05	1.17	1.24
2	B	73	ASP	C-N	5.05	1.40	1.33
2	D	37	TRP	C-O	5.05	1.30	1.24
2	B	134	VAL	CA-C	-5.05	1.46	1.52
1	A	82	ALA	C-N	5.04	1.41	1.33
2	D	40	ARG	CA-C	-5.04	1.45	1.52
2	D	99	ASP	N-CA	5.04	1.52	1.46
1	A	43	PHE	CG-CD1	5.04	1.49	1.38
2	B	98	VAL	N-CA	5.03	1.52	1.46
1	A	83	LEU	C-O	5.03	1.30	1.24
1	C	140	TYR	CG-CD2	5.02	1.49	1.39
2	B	15	TRP	CD2-CE2	5.02	1.49	1.41
1	C	117	PHE	CG-CD1	5.01	1.49	1.38
1	C	50	HIS	ND1-CE1	-5.01	1.27	1.32
2	D	22	GLU	C-N	-5.01	1.27	1.33
1	C	9	ASN	N-CA	5.00	1.52	1.46
2	B	145	TYR	CB-CG	5.00	1.62	1.51

All (2460) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ARG	NE-CZ-NH2	-90.86	37.43	119.20
2	D	80	ASN	CA-CB-CG	63.24	175.84	112.60
2	B	139	ASN	OD1-CG-ND2	-59.66	62.94	122.60
1	A	92	ARG	CD-NE-CZ	-52.47	50.94	124.40
2	B	143	HIS	ND1-CG-CD2	48.68	154.78	106.10
2	D	104	ARG	NE-CZ-NH2	-47.07	76.84	119.20
2	D	19	ASN	OD1-CG-ND2	-43.89	78.71	122.60
2	D	3	LEU	O-C-N	-42.00	76.00	122.20
2	B	108	ASN	OD1-CG-ND2	41.66	164.26	122.60
1	A	75	ASP	CA-CB-CG	-40.07	72.53	112.60
2	D	26	GLU	CB-CG-CD	-39.15	46.05	112.60
2	B	44	SER	O-C-N	-38.06	81.36	122.08
2	B	104	ARG	CD-NE-CZ	-37.76	71.54	124.40
1	A	78	ASN	OD1-CG-ND2	-37.64	84.96	122.60
2	D	2	HIS	CE1-NE2-CD2	36.24	145.24	109.00
2	D	146	HIS	CE1-NE2-CD2	-35.89	73.11	109.00
1	C	92	ARG	CD-NE-CZ	-35.02	75.38	124.40
1	A	72	HIS	ND1-CG-CD2	-34.04	72.06	106.10
2	B	26	GLU	CB-CG-CD	33.95	170.31	112.60
2	D	6	GLU	OE1-CD-OE2	-32.98	43.74	122.90
1	A	17	VAL	O-C-N	32.49	153.75	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	146	HIS	ND1-CG-CD2	-32.46	73.64	106.10
2	D	47	ASP	O-C-N	32.06	163.93	123.21
2	D	46	GLY	CA-C-N	-31.97	76.58	122.93
2	D	46	GLY	C-N-CA	-31.97	76.58	122.93
2	B	5	PRO	N-CA-CB	31.96	139.23	103.44
2	D	17	LYS	CA-C-O	31.82	156.50	119.27
2	D	80	ASN	OD1-CG-ND2	31.80	154.40	122.60
2	D	146	HIS	CG-CD2-NE2	31.04	138.24	107.20
2	D	58	PRO	N-CD-CG	-30.98	56.72	103.20
1	A	92	ARG	NE-CZ-NH2	-30.54	91.72	119.20
2	D	104	ARG	NE-CZ-NH1	-30.42	91.08	121.50
2	B	146	HIS	CB-CG-CD2	-30.10	92.07	131.20
1	A	92	ARG	CG-CD-NE	-29.83	46.37	112.00
2	B	146	HIS	ND1-CE1-NE2	-29.33	79.07	108.40
1	C	92	ARG	NE-CZ-NH1	-29.31	92.19	121.50
2	B	1	VAL	CA-C-N	-29.30	81.69	123.00
2	B	1	VAL	C-N-CA	-29.30	81.69	123.00
1	A	138	SER	CA-CB-OG	-29.22	52.65	111.10
2	B	143	HIS	CG-ND1-CE1	-29.20	59.66	109.30
2	D	73	ASP	CA-CB-CG	-29.10	83.50	112.60
1	A	72	HIS	CA-CB-CG	-28.79	85.01	113.80
1	C	138	SER	CA-CB-OG	-28.68	53.75	111.10
1	A	89	HIS	CE1-NE2-CD2	28.38	137.38	109.00
2	B	26	GLU	CG-CD-OE2	-28.31	53.28	118.40
2	D	2	HIS	CB-CG-CD2	28.30	167.99	131.20
2	D	55	MET	O-C-N	27.47	160.37	122.46
2	B	117	HIS	CG-CD2-NE2	-27.40	79.80	107.20
1	C	22	GLY	O-C-N	-27.32	95.95	122.18
2	D	77	HIS	CG-CD2-NE2	-27.31	79.89	107.20
2	B	12	THR	OG1-CB-CG2	27.26	163.82	109.30
2	D	104	ARG	CD-NE-CZ	-27.17	86.37	124.40
1	C	12	ALA	CA-C-O	26.80	150.55	121.07
2	D	47	ASP	N-CA-CB	-26.61	67.84	110.69
2	D	4	THR	CA-C-O	-26.59	95.47	120.19
2	D	20	VAL	CA-C-O	26.57	149.04	121.41
1	C	38	THR	OG1-CB-CG2	-26.56	56.18	109.30
1	C	72	HIS	ND1-CE1-NE2	26.49	134.89	108.40
1	C	45	HIS	ND1-CE1-NE2	26.20	134.60	108.40
1	C	1	VAL	CG1-CB-CG2	-26.02	53.57	110.80
2	D	21	ASP	N-CA-C	26.00	142.79	111.33
1	C	50	HIS	CG-CD2-NE2	25.93	133.13	107.20
2	D	43	GLU	CA-CB-CG	25.88	165.87	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	LEU	O-C-N	25.88	152.89	123.13
2	D	97	HIS	CE1-NE2-CD2	25.71	134.71	109.00
2	D	6	GLU	O-C-N	25.56	158.66	122.36
1	A	89	HIS	ND1-CE1-NE2	-25.56	82.84	108.40
1	C	89	HIS	ND1-CE1-NE2	25.50	133.91	108.40
2	B	49	SER	O-C-N	-25.47	88.45	122.83
2	B	26	GLU	OE1-CD-OE2	-25.29	62.20	122.90
2	B	20	VAL	O-C-N	-25.18	96.44	121.87
2	D	17	LYS	O-C-N	-25.15	88.00	122.46
1	A	92	ARG	NH1-CZ-NH2	25.03	151.84	119.30
1	C	1	VAL	N-CA-CB	-24.99	69.02	111.50
2	D	47	ASP	N-CA-C	-24.74	69.75	109.59
1	A	20	HIS	ND1-CE1-NE2	24.68	133.08	108.40
2	B	146	HIS	CG-CD2-NE2	-24.65	82.55	107.20
2	D	57	ASN	CA-C-O	24.54	143.56	119.51
2	B	49	SER	CA-C-N	24.34	157.11	122.07
2	B	49	SER	C-N-CA	24.34	157.11	122.07
2	B	77	HIS	CG-CD2-NE2	-24.29	82.91	107.20
2	D	18	VAL	O-C-N	24.10	149.56	122.81
2	B	2	HIS	ND1-CE1-NE2	24.02	132.43	108.40
2	D	77	HIS	CE1-NE2-CD2	23.89	132.89	109.00
2	B	73	ASP	O-C-N	-23.89	96.80	122.12
2	B	53	ALA	CA-C-O	23.66	145.63	120.55
2	D	20	VAL	CG1-CB-CG2	23.65	162.83	110.80
2	D	146	HIS	ND1-CE1-NE2	23.62	132.02	108.40
2	B	144	LYS	CG-CD-CE	23.60	165.57	111.30
1	A	4	PRO	CB-CA-C	-23.50	80.99	109.89
2	D	2	HIS	CA-C-O	-23.49	95.47	120.84
2	D	2	HIS	ND1-CE1-NE2	-23.37	85.03	108.40
2	D	78	LEU	CA-C-O	23.25	153.76	120.51
2	B	101	GLU	OE1-CD-OE2	23.17	178.51	122.90
2	D	56	GLY	O-C-N	-23.01	93.29	122.29
2	D	20	VAL	CA-CB-CG2	-22.86	71.55	110.40
1	C	50	HIS	CE1-NE2-CD2	-22.68	86.31	109.00
1	A	62	VAL	O-C-N	22.62	145.12	121.83
1	C	1	VAL	CA-CB-CG1	-22.57	72.03	110.40
2	D	77	HIS	ND1-CG-CD2	22.55	128.65	106.10
1	C	2	LEU	CA-C-O	-22.44	96.74	120.98
2	D	5	PRO	N-CA-CB	-22.31	76.49	102.60
2	D	26	GLU	CG-CD-OE1	-22.26	67.20	118.40
1	C	72	HIS	N-CA-C	22.15	139.60	113.02
2	B	143	HIS	CB-CG-ND1	-22.02	89.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	63	HIS	CG-CD2-NE2	-21.75	85.44	107.20
2	B	117	HIS	CB-CG-ND1	-21.71	90.13	122.70
2	D	97	HIS	CG-CD2-NE2	-21.68	85.52	107.20
1	A	92	ARG	NE-CZ-NH1	-21.64	99.86	121.50
1	A	72	HIS	CG-CD2-NE2	21.63	128.83	107.20
1	A	22	GLY	O-C-N	-21.59	94.63	122.70
2	D	73	ASP	OD1-CG-OD2	-21.57	71.12	122.90
2	B	22	GLU	OE1-CD-OE2	-21.54	71.20	122.90
2	D	55	MET	CA-C-N	-21.52	78.33	122.66
2	D	55	MET	C-N-CA	-21.52	78.33	122.66
1	A	73	VAL	CA-C-O	21.48	143.39	121.05
2	B	43	GLU	CG-CD-OE2	-21.38	69.22	118.40
2	B	64	GLY	CA-C-O	21.30	142.69	120.75
1	A	58	HIS	O-C-N	21.28	146.41	122.15
2	B	108	ASN	CB-CG-ND2	-21.25	84.52	116.40
2	B	145	TYR	CA-C-O	-21.20	99.75	120.95
1	A	137	THR	CA-CB-OG1	-21.15	77.88	109.60
1	C	70	VAL	O-C-N	21.02	142.96	121.94
1	A	12	ALA	O-C-N	-20.96	96.83	122.19
1	A	16	LYS	CG-CD-CE	-20.86	63.33	111.30
1	C	16	LYS	N-CA-CB	20.85	142.40	110.30
1	C	71	ALA	O-C-N	-20.82	99.80	122.08
2	D	24	GLY	O-C-N	-20.71	102.30	122.18
2	D	3	LEU	CA-C-O	-20.58	98.05	120.89
1	C	72	HIS	ND1-CG-CD2	-20.56	85.54	106.10
1	C	70	VAL	CA-C-O	-20.49	99.96	121.27
2	B	65	LYS	CG-CD-CE	-20.40	64.38	111.30
1	A	75	ASP	OD1-CG-OD2	-20.38	73.99	122.90
2	B	22	GLU	CB-CG-CD	20.25	147.02	112.60
1	C	25	GLY	O-C-N	-20.22	100.81	122.24
2	B	2	HIS	CB-CA-C	-20.16	76.70	110.16
2	D	40	ARG	NE-CZ-NH2	-20.16	101.06	119.20
2	D	44	SER	O-C-N	-20.08	94.75	122.46
2	D	97	HIS	ND1-CE1-NE2	-20.00	88.40	108.40
1	C	12	ALA	N-CA-C	19.96	135.37	111.02
1	C	78	ASN	CA-C-O	19.92	149.00	120.51
1	C	50	HIS	CB-CG-CD2	19.83	156.98	131.20
1	C	1	VAL	CA-CB-CG2	-19.80	76.74	110.40
1	C	14	TRP	O-C-N	-19.80	95.90	122.43
1	A	2	LEU	CA-C-O	-19.75	98.31	120.43
1	A	8	THR	CA-C-O	19.69	141.42	120.55
2	D	63	HIS	CA-CB-CG	19.66	133.46	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ALA	CA-C-O	19.56	141.83	120.90
1	C	56	LYS	CG-CD-CE	-19.54	66.36	111.30
2	B	2	HIS	CA-CB-CG	19.53	133.33	113.80
1	C	15	GLY	CA-C-N	19.49	153.81	120.68
1	C	15	GLY	C-N-CA	19.49	153.81	120.68
2	D	45	PHE	CA-C-O	-19.46	96.02	119.18
2	D	92	HIS	ND1-CE1-NE2	19.46	127.86	108.40
1	C	114	PRO	CB-CA-C	19.41	140.45	112.11
2	D	57	ASN	O-C-N	-19.35	104.47	121.31
2	D	108	ASN	OD1-CG-ND2	19.33	141.93	122.60
1	A	18	GLY	O-C-N	19.31	147.81	122.70
2	B	8	LYS	O-C-N	-19.25	102.07	122.09
2	B	134	VAL	N-CA-CB	19.21	135.16	110.57
2	D	59	LYS	O-C-N	19.20	145.89	122.27
2	D	90	GLU	CG-CD-OE1	-19.20	74.24	118.40
2	D	92	HIS	CE1-NE2-CD2	-19.14	89.86	109.00
2	B	74	GLY	O-C-N	-18.99	98.02	122.70
2	D	26	GLU	CG-CD-OE2	-18.98	74.76	118.40
2	D	146	HIS	CB-CG-CD2	18.97	155.87	131.20
1	A	57	GLY	O-C-N	18.96	140.56	122.17
2	D	2	HIS	CB-CG-ND1	-18.91	94.33	122.70
2	B	40	ARG	NH1-CZ-NH2	18.89	143.86	119.30
2	B	30	ARG	NE-CZ-NH2	18.87	136.18	119.20
1	A	49	SER	CB-CA-C	18.75	143.95	109.46
2	D	73	ASP	CA-C-O	18.72	147.28	120.51
2	D	79	ASP	CB-CA-C	-18.68	80.94	111.02
2	D	76	ALA	O-C-N	-18.66	97.77	122.59
1	C	46	PHE	O-C-N	-18.64	102.07	122.94
1	A	74	ASP	CA-C-O	-18.63	96.46	119.38
1	A	7	LYS	N-CA-C	18.58	133.07	111.71
2	B	40	ARG	NE-CZ-NH2	-18.54	102.52	119.20
1	C	74	ASP	CA-CB-CG	18.52	131.12	112.60
2	B	101	GLU	CG-CD-OE2	-18.51	75.82	118.40
2	B	117	HIS	ND1-CG-CD2	18.51	124.61	106.10
1	A	45	HIS	CA-CB-CG	18.43	132.23	113.80
1	C	7	LYS	CA-C-O	18.42	141.55	120.92
1	C	58	HIS	CE1-NE2-CD2	-18.40	90.60	109.00
2	B	44	SER	CA-CB-OG	18.20	147.51	111.10
2	B	146	HIS	ND1-CG-CD2	-18.20	87.90	106.10
1	C	45	HIS	CA-CB-CG	18.19	131.99	113.80
2	B	49	SER	CB-CA-C	-18.18	84.79	111.70
2	D	18	VAL	CA-C-O	-18.18	100.12	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	VAL	O-C-N	-18.16	104.09	121.89
1	C	20	HIS	CB-CG-ND1	-18.16	95.46	122.70
2	D	8	LYS	CA-CB-CG	-18.10	77.90	114.10
1	C	116	GLU	CB-CG-CD	-18.08	81.86	112.60
2	B	56	GLY	O-C-N	-18.08	99.20	122.70
2	D	3	LEU	N-CA-C	-18.07	82.71	109.63
2	D	43	GLU	O-C-N	18.06	147.38	122.46
2	B	104	ARG	NE-CZ-NH2	-18.03	102.98	119.20
2	D	20	VAL	O-C-N	-18.01	102.51	121.96
1	C	141	ARG	NE-CZ-NH2	-18.00	103.00	119.20
1	A	75	ASP	CB-CA-C	-17.98	85.88	111.95
2	D	77	HIS	ND1-CE1-NE2	-17.96	90.44	108.40
1	C	14	TRP	CA-C-N	17.95	156.60	121.41
1	C	14	TRP	C-N-CA	17.95	156.60	121.41
2	D	76	ALA	N-CA-CB	-17.91	80.22	110.49
1	A	19	ALA	N-CA-C	-17.81	89.91	112.88
2	D	72	SER	N-CA-CB	17.71	140.43	110.49
2	D	77	HIS	CA-C-O	17.67	145.78	120.51
2	B	77	HIS	ND1-CE1-NE2	17.66	126.06	108.40
1	A	110	ALA	O-C-N	-17.58	101.65	122.22
2	B	45	PHE	CG-CD2-CE2	17.55	150.53	120.70
1	C	73	VAL	O-C-N	17.54	139.62	121.90
1	C	72	HIS	CE1-NE2-CD2	-17.54	91.46	109.00
1	C	86	LEU	CA-C-O	17.52	139.12	120.55
1	C	10	VAL	O-C-N	17.51	139.86	121.83
1	C	23	GLU	CG-CD-OE1	-17.48	78.20	118.40
1	A	21	ALA	CA-C-O	-17.48	95.52	120.51
2	D	5	PRO	CB-CA-C	-17.46	86.78	110.52
1	A	12	ALA	CB-CA-C	-17.43	80.66	110.64
2	D	6	GLU	CA-C-O	-17.39	99.25	119.60
2	B	139	ASN	CB-CG-OD1	17.37	155.55	120.80
2	D	73	ASP	O-C-N	-17.35	99.51	122.59
2	B	77	HIS	CB-CG-CD2	-17.30	108.71	131.20
2	D	2	HIS	O-C-N	17.29	144.14	122.87
1	A	65	ALA	O-C-N	17.28	142.44	122.22
2	D	63	HIS	ND1-CG-CD2	17.26	123.36	106.10
2	D	58	PRO	CA-CB-CG	-17.25	71.72	104.50
2	D	93	CYS	O-C-N	17.25	142.12	122.11
1	A	75	ASP	CB-CG-OD2	-17.20	78.85	118.40
2	B	74	GLY	CA-C-O	17.19	150.49	120.57
2	D	92	HIS	CG-CD2-NE2	17.18	124.38	107.20
1	C	49	SER	CA-C-O	17.17	140.28	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	82	LYS	CD-CE-NZ	-17.15	57.02	111.90
2	D	8	LYS	O-C-N	-17.09	101.25	122.27
2	D	52	ASP	CA-C-O	-17.05	101.31	120.24
2	D	26	GLU	OE1-CD-OE2	-17.05	81.99	122.90
2	D	79	ASP	OD1-CG-OD2	-17.01	82.07	122.90
2	D	89	SER	CA-C-O	16.98	139.75	121.07
1	C	12	ALA	O-C-N	-16.97	103.92	122.08
2	D	47	ASP	CA-CB-CG	-16.97	95.63	112.60
2	D	41	PHE	O-C-N	16.90	146.41	122.41
2	D	73	ASP	CB-CG-OD1	16.89	157.24	118.40
1	C	22	GLY	CA-C-N	16.77	142.24	120.44
1	C	22	GLY	C-N-CA	16.77	142.24	120.44
1	C	114	PRO	N-CA-C	-16.75	91.63	113.57
2	B	50	THR	N-CA-C	16.71	127.36	108.14
2	B	41	PHE	O-C-N	16.69	144.28	122.42
2	D	4	THR	CA-C-N	-16.68	103.81	120.83
2	D	4	THR	C-N-CA	-16.68	103.81	120.83
2	B	48	LEU	CA-C-N	-16.68	100.19	123.20
2	B	48	LEU	C-N-CA	-16.68	100.19	123.20
2	D	80	ASN	CB-CG-ND2	-16.61	91.49	116.40
2	D	53	ALA	CA-C-O	16.60	139.33	121.07
1	C	53	ALA	O-C-N	16.54	141.13	122.11
1	C	131	SER	CA-C-O	-16.52	100.97	119.97
2	D	46	GLY	O-C-N	16.52	144.17	122.70
2	D	46	GLY	CA-C-O	-16.51	91.84	120.57
1	C	112	HIS	ND1-CG-CD2	-16.44	89.66	106.10
1	C	82	ALA	CA-C-O	16.32	138.54	120.10
2	D	101	GLU	CG-CD-OE2	-16.32	80.88	118.40
1	C	30	GLU	OE1-CD-OE2	16.31	162.05	122.90
1	C	46	PHE	CE1-CZ-CE2	-16.30	90.65	120.00
1	A	60	LYS	CA-C-O	16.25	137.78	120.55
2	D	47	ASP	CB-CA-C	-16.17	80.28	109.38
2	D	131	GLN	OE1-CD-NE2	16.13	138.73	122.60
1	C	113	LEU	CA-C-O	-16.12	98.07	120.16
1	C	128	PHE	CD1-CG-CD2	16.07	142.71	118.60
1	C	63	ALA	O-C-N	-16.06	105.53	122.07
1	A	112	HIS	CA-C-O	-16.05	101.39	119.05
2	B	43	GLU	OE1-CD-OE2	15.99	161.28	122.90
1	C	29	LEU	O-C-N	-15.99	105.17	122.12
2	D	11	VAL	O-C-N	15.96	138.50	121.90
1	A	49	SER	CA-C-N	-15.93	94.82	122.07
1	A	49	SER	C-N-CA	-15.93	94.82	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	ALA	N-CA-C	15.91	128.10	111.07
2	B	87	THR	OG1-CB-CG2	-15.88	77.55	109.30
2	D	52	ASP	CA-CB-CG	15.86	128.46	112.60
2	B	22	GLU	CG-CD-OE2	-15.81	82.03	118.40
1	C	73	VAL	CG1-CB-CG2	15.80	145.55	110.80
2	B	1	VAL	CG1-CB-CG2	15.75	145.45	110.80
1	C	48	LEU	O-C-N	-15.74	100.97	122.06
1	A	1	VAL	CA-C-N	-15.71	101.08	122.30
1	A	1	VAL	C-N-CA	-15.71	101.08	122.30
2	D	50	THR	N-CA-CB	-15.69	82.45	110.37
1	A	110	ALA	CA-C-N	15.68	141.29	120.28
1	A	110	ALA	C-N-CA	15.68	141.29	120.28
2	B	60	VAL	CA-C-O	15.65	140.34	120.78
2	D	116	HIS	ND1-CG-CD2	15.64	121.74	106.10
2	B	45	PHE	CZ-CE2-CD2	-15.60	91.92	120.00
2	B	50	THR	CA-CB-CG2	15.59	137.00	110.50
2	D	117	HIS	ND1-CG-CD2	-15.58	90.52	106.10
1	C	14	TRP	CG-CD1-NE1	-15.55	89.98	110.20
1	A	90	LYS	N-CA-C	15.55	133.43	112.13
1	C	56	LYS	O-C-N	-15.51	105.68	122.12
1	A	47	ASP	O-C-N	15.50	141.53	122.93
2	B	4	THR	CA-C-N	15.49	135.74	118.85
2	B	4	THR	C-N-CA	15.49	135.74	118.85
1	A	61	LYS	O-C-N	15.49	143.19	122.43
1	C	116	GLU	CG-CD-OE2	-15.48	82.78	118.40
1	A	112	HIS	CE1-NE2-CD2	-15.44	93.56	109.00
1	A	50	HIS	N-CA-CB	-15.41	85.29	110.41
2	D	45	PHE	O-C-N	15.38	144.26	122.41
2	D	41	PHE	CA-C-O	-15.37	100.90	119.18
2	D	78	LEU	N-CA-C	15.32	143.43	110.80
1	A	11	LYS	CA-C-N	-15.31	98.80	122.37
1	A	11	LYS	C-N-CA	-15.31	98.80	122.37
1	C	46	PHE	CZ-CE2-CD2	15.30	147.54	120.00
2	B	9	SER	CA-CB-OG	-15.30	80.51	111.10
1	C	64	ASP	CA-CB-CG	15.29	127.89	112.60
1	C	48	LEU	CA-C-N	15.27	144.92	120.94
1	C	48	LEU	C-N-CA	15.27	144.92	120.94
1	C	112	HIS	CG-CD2-NE2	15.23	122.43	107.20
2	D	92	HIS	CB-CG-CD2	15.19	150.95	131.20
2	D	65	LYS	CG-CD-CE	-15.16	76.43	111.30
1	A	88	ALA	O-C-N	15.13	138.43	122.09
2	D	13	ALA	N-CA-CB	15.11	132.46	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	95	LYS	CA-C-O	15.10	139.19	120.31
2	D	110	LEU	CA-C-O	15.07	137.02	120.90
1	C	138	SER	CA-C-O	-15.06	103.08	120.10
2	D	72	SER	CA-C-O	15.04	142.02	120.51
2	D	82	LYS	O-C-N	-15.03	106.18	122.12
1	C	16	LYS	CB-CG-CD	-15.00	76.80	111.30
2	B	1	VAL	CA-C-O	-14.99	95.31	120.80
2	D	54	VAL	O-C-N	-14.99	107.33	121.87
1	A	1	VAL	CA-CB-CG2	-14.98	84.94	110.40
2	D	12	THR	CA-CB-OG1	-14.97	87.15	109.60
1	A	75	ASP	CB-CG-OD1	14.94	152.77	118.40
2	B	50	THR	CA-C-O	-14.93	107.72	120.71
2	B	2	HIS	CE1-NE2-CD2	-14.90	94.10	109.00
2	B	4	THR	CA-CB-CG2	14.90	135.83	110.50
1	C	113	LEU	CA-C-N	14.89	134.97	119.19
1	C	113	LEU	C-N-CA	14.89	134.97	119.19
2	D	12	THR	O-C-N	-14.89	105.18	122.15
1	A	23	GLU	CG-CD-OE1	-14.88	84.19	118.40
1	C	26	ALA	CA-C-O	14.88	136.82	120.90
2	D	85	PHE	CA-CB-CG	-14.87	98.93	113.80
1	A	126	ASP	O-C-N	-14.87	106.75	122.07
2	B	146	HIS	CB-CG-ND1	-14.84	100.45	122.70
1	A	6	ASP	O-C-N	14.82	137.51	122.09
1	C	103	HIS	ND1-CE1-NE2	14.80	123.20	108.40
2	D	139	ASN	CB-CG-OD1	-14.78	91.23	120.80
1	C	89	HIS	CE1-NE2-CD2	-14.75	94.25	109.00
2	D	66	LYS	CA-CB-CG	14.70	143.51	114.10
2	D	79	ASP	N-CA-CB	-14.70	87.40	110.92
2	D	50	THR	CB-CA-C	-14.70	81.22	110.17
1	A	110	ALA	CA-C-O	14.69	136.69	120.10
2	D	1	VAL	O-C-N	14.66	146.46	123.00
2	B	43	GLU	O-C-N	-14.65	103.49	122.39
2	B	58	PRO	N-CD-CG	-14.65	81.22	103.20
1	C	16	LYS	N-CA-C	-14.65	93.78	112.23
1	C	19	ALA	O-C-N	-14.64	102.16	122.37
2	D	60	VAL	CB-CA-C	14.63	130.09	111.81
2	B	49	SER	CA-C-O	-14.59	92.07	120.96
1	C	52	SER	O-C-N	-14.58	103.09	123.07
1	A	50	HIS	CG-CD2-NE2	-14.58	92.62	107.20
2	D	82	LYS	CG-CD-CE	-14.57	77.80	111.30
2	D	120	LYS	O-C-N	-14.54	103.76	122.37
1	A	72	HIS	CE1-NE2-CD2	-14.54	94.46	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ALA	CA-C-O	14.51	136.06	120.82
1	A	78	ASN	CB-CG-ND2	14.50	138.16	116.40
2	D	43	GLU	OE1-CD-OE2	-14.49	88.12	122.90
2	B	144	LYS	CA-C-N	14.45	144.11	121.56
2	B	144	LYS	C-N-CA	14.45	144.11	121.56
2	D	58	PRO	CB-CG-CD	14.46	152.35	106.10
2	B	121	GLU	CG-CD-OE2	-14.44	85.18	118.40
1	A	52	SER	CA-C-O	14.35	136.93	121.44
2	D	6	GLU	N-CA-C	-14.30	94.16	112.90
2	B	146	HIS	CA-CB-CG	-14.30	99.50	113.80
1	C	77	PRO	N-CA-C	14.29	135.04	113.75
1	A	54	GLN	OE1-CD-NE2	-14.29	108.31	122.60
1	A	21	ALA	CA-C-N	-14.25	93.47	121.41
1	A	21	ALA	C-N-CA	-14.25	93.47	121.41
2	B	125	PRO	N-CA-CB	14.23	118.99	103.33
2	D	143	HIS	CG-CD2-NE2	-14.21	92.99	107.20
2	B	145	TYR	N-CA-CB	14.19	131.06	109.34
2	D	101	GLU	OE1-CD-OE2	14.19	156.95	122.90
1	C	56	LYS	CA-C-O	14.17	135.57	120.55
2	D	71	PHE	CG-CD2-CE2	-14.17	96.61	120.70
1	C	71	ALA	CB-CA-C	14.11	133.35	110.92
2	B	43	GLU	N-CA-CB	-14.10	90.03	110.47
1	C	23	GLU	OE1-CD-OE2	-14.10	89.06	122.90
2	D	52	ASP	N-CA-CB	-14.10	89.20	110.20
2	B	87	THR	CA-CB-OG1	-14.09	88.47	109.60
1	C	14	TRP	CE3-CZ3-CH2	-13.98	102.92	121.10
1	A	41	THR	O-C-N	-13.94	105.91	122.22
2	B	53	ALA	O-C-N	-13.93	107.36	122.12
2	B	15	TRP	O-C-N	13.93	138.51	122.22
2	B	79	ASP	N-CA-C	-13.91	95.98	113.23
2	B	139	ASN	CA-CB-CG	-13.91	98.69	112.60
1	C	74	ASP	OD1-CG-OD2	-13.90	89.55	122.90
2	D	65	LYS	CB-CG-CD	-13.89	79.34	111.30
1	A	17	VAL	N-CA-CB	13.88	126.79	110.55
2	D	79	ASP	CA-C-N	-13.88	95.03	121.54
2	D	79	ASP	C-N-CA	-13.88	95.03	121.54
2	D	55	MET	CA-C-O	-13.88	102.10	119.31
2	B	144	LYS	O-C-N	-13.87	105.00	122.34
2	B	42	PHE	CD1-CE1-CZ	13.86	144.95	120.00
1	A	81	SER	CA-CB-OG	-13.85	83.40	111.10
1	C	58	HIS	CG-CD2-NE2	13.84	121.04	107.20
2	D	143	HIS	CB-CG-CD2	-13.81	113.25	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	GLU	CA-C-O	-13.81	104.92	120.24
2	B	2	HIS	CG-ND1-CE1	-13.78	85.88	109.30
2	B	60	VAL	O-C-N	-13.77	105.35	122.57
2	B	17	LYS	O-C-N	-13.77	105.12	122.34
2	D	30	ARG	NE-CZ-NH1	13.76	135.26	121.50
2	D	24	GLY	CA-C-N	13.75	135.25	119.98
2	D	24	GLY	C-N-CA	13.75	135.25	119.98
1	A	25	GLY	O-C-N	-13.72	104.87	122.70
1	C	114	PRO	O-C-N	-13.71	103.75	122.27
1	C	71	ALA	CA-C-N	13.70	146.12	122.56
1	C	71	ALA	C-N-CA	13.70	146.12	122.56
1	C	84	SER	CA-CB-OG	-13.69	83.72	111.10
2	B	143	HIS	CB-CG-CD2	-13.66	113.44	131.20
2	B	44	SER	CB-CA-C	13.66	132.63	110.92
1	C	45	HIS	CG-ND1-CE1	-13.65	86.09	109.30
1	C	69	ALA	O-C-N	13.65	136.13	122.07
2	B	68	LEU	CD1-CG-CD2	13.64	140.82	110.80
1	C	72	HIS	CA-C-O	13.64	135.94	119.43
1	A	90	LYS	CD-CE-NZ	-13.62	68.30	111.90
1	A	81	SER	N-CA-CB	-13.61	87.80	110.39
1	C	45	HIS	CE1-NE2-CD2	-13.61	95.39	109.00
2	B	40	ARG	CA-C-O	-13.61	103.02	119.49
2	B	82	LYS	N-CA-CB	-13.61	89.19	110.28
2	B	57	ASN	O-C-N	-13.60	106.26	121.36
2	D	90	GLU	CB-CG-CD	-13.60	89.48	112.60
2	D	92	HIS	N-CA-C	-13.57	96.76	113.18
1	C	23	GLU	CG-CD-OE2	-13.57	87.19	118.40
2	B	143	HIS	CE1-NE2-CD2	-13.57	95.43	109.00
2	B	79	ASP	O-C-N	-13.54	103.90	122.46
2	B	44	SER	CA-C-O	-13.54	106.18	121.07
2	B	5	PRO	CA-N-CD	-13.48	93.13	112.00
1	C	58	HIS	ND1-CE1-NE2	13.48	121.88	108.40
1	C	41	THR	O-C-N	-13.46	103.89	122.46
2	B	143	HIS	ND1-CE1-NE2	13.45	121.85	108.40
2	D	6	GLU	CG-CD-OE2	-13.43	87.51	118.40
2	D	7	GLU	O-C-N	13.41	139.67	122.23
1	A	50	HIS	CA-C-N	13.39	150.51	121.18
1	A	50	HIS	C-N-CA	13.39	150.51	121.18
1	C	138	SER	O-C-N	13.39	137.89	122.22
1	C	131	SER	O-C-N	13.39	138.74	122.27
2	D	66	LYS	N-CA-C	-13.37	96.40	110.97
1	C	89	HIS	CB-CG-CD2	-13.35	113.85	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	80	ASN	CB-CG-ND2	-13.35	96.38	116.40
2	B	50	THR	N-CA-CB	-13.34	94.41	111.35
2	B	94	ASP	OD1-CG-OD2	13.29	154.79	122.90
2	D	41	PHE	CG-CD1-CE1	-13.27	98.15	120.70
2	D	97	HIS	ND1-CG-CD2	13.27	119.37	106.10
1	A	36	PHE	O-C-N	13.23	133.36	121.32
1	A	81	SER	CA-C-N	13.21	138.09	120.65
1	A	81	SER	C-N-CA	13.21	138.09	120.65
2	D	16	GLY	CA-C-N	13.21	144.90	121.66
2	D	16	GLY	C-N-CA	13.21	144.90	121.66
2	B	81	LEU	N-CA-CB	-13.20	90.71	110.12
2	B	111	VAL	O-C-N	-13.20	108.74	121.94
2	D	71	PHE	CD1-CG-CD2	13.18	138.37	118.60
1	C	49	SER	N-CA-C	-13.18	91.91	110.50
1	C	47	ASP	CA-CB-CG	-13.18	99.42	112.60
1	A	131	SER	O-C-N	13.17	139.35	122.23
1	C	50	HIS	ND1-CE1-NE2	13.12	121.52	108.40
1	A	6	ASP	CA-C-N	-13.10	101.41	120.28
1	A	6	ASP	C-N-CA	-13.10	101.41	120.28
1	C	38	THR	CA-CB-OG1	-13.08	89.98	109.60
2	D	77	HIS	CB-CA-C	-13.08	84.39	110.42
1	A	3	SER	CA-C-N	-13.06	105.24	121.04
1	A	3	SER	C-N-CA	-13.06	105.24	121.04
2	D	117	HIS	ND1-CE1-NE2	13.06	121.46	108.40
2	B	90	GLU	N-CA-C	13.03	138.56	110.80
1	C	84	SER	N-CA-CB	13.03	129.28	110.12
2	D	91	LEU	N-CA-C	13.03	125.48	111.28
2	D	9	SER	O-C-N	13.01	139.76	122.33
2	B	4	THR	N-CA-CB	-13.01	87.22	110.37
1	A	60	LYS	N-CA-C	13.00	125.45	111.28
2	D	13	ALA	CA-C-O	12.99	134.81	120.90
1	C	51	GLY	CA-C-O	12.97	133.98	119.06
2	D	73	ASP	N-CA-C	12.97	138.43	110.80
1	C	105	LEU	CD1-CG-CD2	-12.95	82.32	110.80
2	D	49	SER	CA-C-N	-12.93	90.25	121.80
2	D	49	SER	C-N-CA	-12.93	90.25	121.80
1	C	29	LEU	CA-C-O	12.92	134.25	120.55
1	A	3	SER	O-C-N	-12.92	106.46	121.32
1	C	4	PRO	O-C-N	12.91	138.37	122.23
2	D	21	ASP	O-C-N	-12.90	108.45	122.12
2	D	137	VAL	O-C-N	-12.86	107.27	121.80
1	C	78	ASN	O-C-N	-12.84	105.51	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH2	-12.83	107.66	119.20
1	C	54	GLN	O-C-N	12.82	135.71	122.12
2	B	35	TYR	O-C-N	12.81	132.74	121.34
2	D	143	HIS	O-C-N	12.81	135.70	122.12
2	B	26	GLU	O-C-N	12.80	135.25	122.07
1	C	82	ALA	O-C-N	-12.78	107.27	122.22
2	D	78	LEU	CA-C-N	-12.76	102.38	122.67
2	D	78	LEU	C-N-CA	-12.76	102.38	122.67
1	A	56	LYS	CA-C-O	12.74	138.73	120.51
2	D	91	LEU	CA-C-O	12.74	134.05	120.55
2	D	94	ASP	OD1-CG-OD2	12.74	153.47	122.90
2	D	143	HIS	ND1-CG-CD2	12.73	118.83	106.10
1	A	87	HIS	CA-CB-CG	-12.72	101.08	113.80
1	C	75	ASP	CB-CG-OD2	-12.71	89.17	118.40
2	B	65	LYS	CD-CE-NZ	-12.70	71.25	111.90
2	B	19	ASN	CB-CG-ND2	-12.69	97.37	116.40
1	C	3	SER	O-C-N	-12.69	106.73	121.32
1	A	103	HIS	ND1-CE1-NE2	12.68	121.08	108.40
1	A	141	ARG	CD-NE-CZ	-12.66	106.67	124.40
1	C	73	VAL	CA-CB-CG1	-12.65	88.89	110.40
1	A	20	HIS	CG-CD2-NE2	-12.65	94.55	107.20
2	B	64	GLY	O-C-N	-12.63	110.06	122.19
2	B	124	PRO	CA-C-N	12.63	133.07	119.05
2	B	124	PRO	C-N-CA	12.63	133.07	119.05
1	C	72	HIS	CG-CD2-NE2	12.62	119.82	107.20
1	A	72	HIS	ND1-CE1-NE2	-12.62	95.78	108.40
2	D	132	LYS	CD-CE-NZ	-12.60	71.58	111.90
2	B	59	LYS	CD-CE-NZ	-12.59	71.60	111.90
2	B	76	ALA	CA-C-O	12.59	134.51	119.28
2	D	73	ASP	CB-CG-OD2	-12.54	89.55	118.40
2	D	108	ASN	CB-CG-ND2	-12.54	97.59	116.40
2	D	101	GLU	CG-CD-OE1	-12.54	89.57	118.40
1	A	1	VAL	CG1-CB-CG2	12.52	138.34	110.80
2	D	2	HIS	N-CA-C	12.49	130.99	107.75
2	D	52	ASP	CB-CG-OD2	-12.47	89.71	118.40
1	A	10	VAL	O-C-N	12.47	134.13	121.91
2	D	40	ARG	N-CA-C	-12.46	97.38	111.71
2	B	2	HIS	CA-C-O	12.45	133.63	120.30
2	B	39	GLN	OE1-CD-NE2	12.42	135.02	122.60
1	A	85	ASP	CA-CB-CG	-12.42	100.18	112.60
1	A	126	ASP	CA-C-O	12.42	133.86	120.82
1	A	20	HIS	N-CA-C	-12.41	97.65	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASP	N-CA-C	12.39	127.85	112.23
1	C	75	ASP	OD1-CG-OD2	12.39	152.64	122.90
2	D	41	PHE	CD1-CE1-CZ	12.38	142.29	120.00
1	A	15	GLY	CA-C-O	-12.38	99.03	120.57
2	D	47	ASP	CA-C-N	-12.38	103.31	122.37
2	D	47	ASP	C-N-CA	-12.38	103.31	122.37
1	C	124	SER	O-C-N	12.32	136.19	122.15
2	D	3	LEU	N-CA-CB	12.31	131.21	109.18
1	C	50	HIS	CA-C-O	-12.30	106.90	120.92
2	B	26	GLU	CG-CD-OE1	-12.30	90.12	118.40
1	C	24	TYR	CE1-CZ-CE2	12.28	144.85	120.30
2	B	58	PRO	CB-CG-CD	12.26	145.32	106.10
2	D	118	PHE	CG-CD1-CE1	12.24	141.50	120.70
1	C	50	HIS	O-C-N	12.23	138.12	122.95
1	A	118	THR	CA-CB-OG1	12.23	127.94	109.60
2	D	117	HIS	CB-CG-CD2	12.21	147.08	131.20
2	D	126	VAL	O-C-N	12.21	134.41	121.83
1	C	58	HIS	O-C-N	12.18	134.61	122.07
2	D	37	TRP	CZ3-CH2-CZ2	12.17	137.32	121.50
2	B	2	HIS	ND1-CG-CD2	12.16	118.26	106.10
1	C	2	LEU	O-C-N	12.15	138.85	122.57
1	A	58	HIS	CA-C-N	-12.14	104.96	120.14
1	A	58	HIS	C-N-CA	-12.14	104.96	120.14
2	B	2	HIS	CB-CG-CD2	-12.14	115.41	131.20
2	B	50	THR	O-C-N	12.14	131.86	121.54
2	B	40	ARG	NE-CZ-NH1	-12.12	109.38	121.50
2	B	80	ASN	CA-C-O	-12.12	104.02	122.32
2	D	30	ARG	NH1-CZ-NH2	-12.12	103.55	119.30
2	B	138	ALA	CA-C-O	12.10	133.71	121.00
2	D	139	ASN	CA-C-O	12.10	133.25	120.42
2	B	84	THR	CA-C-O	12.10	135.17	121.02
1	C	25	GLY	CA-C-N	12.09	136.85	120.54
1	C	25	GLY	C-N-CA	12.09	136.85	120.54
2	D	8	LYS	CA-C-O	12.08	133.86	119.97
1	A	58	HIS	CA-CB-CG	-12.07	101.73	113.80
1	C	103	HIS	CE1-NE2-CD2	-12.07	96.93	109.00
1	A	103	HIS	CA-C-O	12.06	135.13	121.02
2	B	79	ASP	CA-CB-CG	-12.05	100.55	112.60
1	C	124	SER	CA-C-O	-12.03	107.67	120.42
1	C	75	ASP	CA-CB-CG	12.02	124.62	112.60
1	C	41	THR	N-CA-C	-12.02	98.59	113.01
2	B	72	SER	CB-CA-C	12.01	130.02	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASN	N-CA-CB	12.00	127.92	110.16
1	C	139	LYS	CD-CE-NZ	-11.98	73.58	111.90
2	B	17	LYS	CA-C-N	11.96	138.00	122.93
2	B	17	LYS	C-N-CA	11.96	138.00	122.93
2	B	121	GLU	CG-CD-OE1	-11.94	90.94	118.40
1	C	77	PRO	O-C-N	-11.94	108.51	122.24
2	D	42	PHE	CG-CD1-CE1	-11.94	100.41	120.70
1	A	19	ALA	O-C-N	-11.93	108.05	122.25
1	A	60	LYS	CD-CE-NZ	-11.93	73.74	111.90
2	D	9	SER	CA-C-N	-11.91	102.20	120.31
2	D	9	SER	C-N-CA	-11.91	102.20	120.31
2	D	1	VAL	CA-C-O	-11.91	100.55	120.80
2	D	43	GLU	CG-CD-OE2	11.91	145.80	118.40
1	C	69	ALA	CA-C-O	-11.90	108.33	120.82
2	B	43	GLU	CA-CB-CG	11.89	137.87	114.10
1	A	89	HIS	CG-CD2-NE2	-11.88	95.32	107.20
1	A	87	HIS	O-C-N	11.87	138.84	122.46
1	A	112	HIS	ND1-CE1-NE2	11.87	120.27	108.40
1	A	127	LYS	CB-CA-C	11.86	129.22	110.96
2	D	12	THR	CA-CB-CG2	-11.86	90.35	110.50
2	D	20	VAL	CB-CA-C	11.85	126.87	111.70
2	D	49	SER	CB-CA-C	-11.85	89.03	109.65
2	D	131	GLN	CA-C-O	11.84	133.10	120.55
2	D	1	VAL	CA-C-N	-11.84	106.40	122.85
2	D	1	VAL	C-N-CA	-11.84	106.40	122.85
1	C	49	SER	CB-CA-C	11.82	131.29	109.54
2	B	22	GLU	CG-CD-OE1	-11.82	91.22	118.40
2	D	83	GLY	O-C-N	-11.82	103.63	122.42
2	D	2	HIS	ND1-CG-CD2	-11.81	94.29	106.10
1	A	141	ARG	NE-CZ-NH2	-11.80	108.58	119.20
1	C	24	TYR	CG-CD1-CE1	-11.80	103.50	121.20
1	C	61	LYS	CD-CE-NZ	-11.79	74.17	111.90
2	B	5	PRO	O-C-N	11.79	136.97	122.23
1	C	46	PHE	CD1-CG-CD2	-11.78	100.92	118.60
1	A	33	PHE	CA-C-O	11.78	133.41	120.10
1	A	111	ALA	N-CA-CB	11.76	127.41	110.12
2	B	81	LEU	CB-CA-C	11.75	130.30	110.79
1	A	49	SER	CA-C-O	11.74	134.97	121.47
2	B	65	LYS	N-CA-C	11.74	124.07	111.28
2	B	77	HIS	CB-CG-ND1	11.73	140.29	122.70
2	D	58	PRO	CA-N-CD	-11.72	95.59	112.00
1	A	14	TRP	CA-CB-CG	-11.71	91.35	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	PHE	CG-CD1-CE1	-11.71	100.79	120.70
1	A	52	SER	O-C-N	-11.71	107.83	122.82
1	A	62	VAL	CA-C-N	-11.71	100.66	121.14
1	A	62	VAL	C-N-CA	-11.71	100.66	121.14
2	B	28	LEU	CA-C-O	11.70	134.71	121.02
1	C	50	HIS	ND1-CG-CD2	-11.69	94.41	106.10
2	B	127	GLN	CA-C-O	11.68	137.22	120.51
2	B	116	HIS	CG-CD2-NE2	11.68	118.88	107.20
1	C	14	TRP	CD2-CE2-CZ2	-11.67	110.73	122.40
2	B	6	GLU	CA-CB-CG	11.65	137.40	114.10
2	B	94	ASP	O-C-N	-11.64	106.73	122.33
2	B	12	THR	O-C-N	-11.63	110.09	122.07
2	B	41	PHE	CA-C-O	-11.62	105.90	119.15
1	C	115	ALA	O-C-N	-11.60	105.22	122.28
2	D	22	GLU	CG-CD-OE2	-11.60	91.72	118.40
1	A	3	SER	CA-C-O	11.59	136.04	120.16
2	D	12	THR	CA-C-N	11.59	136.18	120.54
2	D	12	THR	C-N-CA	11.59	136.18	120.54
2	D	16	GLY	O-C-N	-11.58	109.80	122.54
1	C	20	HIS	CG-ND1-CE1	-11.58	89.62	109.30
1	C	56	LYS	CD-CE-NZ	-11.58	74.85	111.90
1	A	59	GLY	O-C-N	-11.56	109.99	122.24
2	B	42	PHE	CB-CG-CD2	11.55	140.34	120.70
1	C	116	GLU	CB-CA-C	-11.55	89.56	109.65
1	A	96	VAL	CA-C-O	11.55	132.93	120.57
2	B	76	ALA	N-CA-C	11.54	127.47	113.16
1	A	128	PHE	CZ-CE2-CD2	-11.54	99.23	120.00
1	A	8	THR	N-CA-C	11.54	123.85	111.28
2	D	63	HIS	CB-CG-CD2	-11.54	116.20	131.20
1	A	36	PHE	CA-C-N	-11.53	107.91	119.56
1	A	36	PHE	C-N-CA	-11.53	107.91	119.56
2	B	77	HIS	N-CA-C	-11.53	96.60	110.44
2	D	53	ALA	N-CA-CB	11.53	127.34	109.82
2	B	134	VAL	O-C-N	-11.52	109.92	121.90
1	A	103	HIS	CE1-NE2-CD2	-11.52	97.48	109.00
2	D	8	LYS	N-CA-CB	-11.51	92.44	110.28
1	A	88	ALA	CA-C-O	-11.50	108.86	120.70
2	D	79	ASP	CB-CG-OD2	-11.45	92.06	118.40
1	A	71	ALA	CA-C-O	-11.45	108.28	120.42
2	B	12	THR	CA-C-O	11.44	132.83	120.82
1	A	141	ARG	NE-CZ-NH1	11.43	132.93	121.50
2	D	143	HIS	CA-C-O	-11.41	108.30	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	119	GLY	CA-C-O	11.40	135.81	121.67
2	D	121	GLU	CG-CD-OE2	-11.40	92.17	118.40
1	C	36	PHE	O-C-N	11.40	130.86	121.17
2	D	95	LYS	O-C-N	-11.39	106.92	122.30
1	A	50	HIS	CB-CG-CD2	-11.36	116.43	131.20
1	A	93	VAL	O-C-N	-11.32	110.33	122.67
2	D	64	GLY	CA-C-O	11.30	131.98	120.45
1	A	89	HIS	CA-C-O	11.30	132.49	119.27
2	B	5	PRO	CA-CB-CG	-11.30	83.03	104.50
2	D	40	ARG	O-C-N	-11.30	109.00	122.22
1	C	17	VAL	CA-C-O	11.29	134.90	120.78
2	B	55	MET	O-C-N	11.29	136.15	122.27
1	A	20	HIS	CG-ND1-CE1	-11.28	90.13	109.30
1	C	38	THR	CB-CA-C	11.27	129.50	110.79
1	A	71	ALA	O-C-N	-11.27	109.30	122.15
1	A	131	SER	CA-C-O	-11.25	107.75	120.24
1	C	23	GLU	CB-CG-CD	-11.25	93.48	112.60
1	A	141	ARG	CG-CD-NE	-11.23	87.28	112.00
1	C	72	HIS	CB-CG-CD2	11.23	145.80	131.20
1	A	26	ALA	N-CA-CB	11.23	126.67	109.94
2	D	20	VAL	N-CA-C	11.20	121.88	110.23
1	A	31	ARG	O-C-N	11.18	133.59	122.07
1	C	62	VAL	N-CA-C	11.18	122.02	110.62
2	B	95	LYS	CA-C-O	11.16	130.91	118.97
2	B	49	SER	N-CA-C	-11.16	92.80	108.54
1	C	81	SER	CA-CB-OG	-11.16	88.78	111.10
2	B	8	LYS	CB-CG-CD	11.15	136.95	111.30
1	C	81	SER	N-CA-CB	-11.15	93.84	110.01
2	D	63	HIS	O-C-N	11.15	136.73	122.23
1	A	46	PHE	CD1-CG-CD2	-11.15	101.88	118.60
2	B	47	ASP	CB-CA-C	-11.14	92.95	110.78
2	B	127	GLN	O-C-N	-11.13	107.79	122.59
2	D	6	GLU	CB-CA-C	-11.12	87.32	109.67
2	B	13	ALA	O-C-N	-11.11	110.62	122.07
1	C	72	HIS	O-C-N	-11.11	108.06	122.39
1	A	65	ALA	N-CA-C	11.10	124.48	111.71
1	C	111	ALA	CA-C-O	-11.10	108.78	120.55
1	A	54	GLN	CA-C-O	-11.10	107.92	120.24
2	B	57	ASN	CA-C-N	11.08	131.35	119.05
2	B	57	ASN	C-N-CA	11.08	131.35	119.05
1	C	30	GLU	CG-CD-OE1	-11.07	92.94	118.40
1	A	14	TRP	CD1-NE1-CE2	11.06	128.82	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	GLU	CG-CD-OE1	-11.06	92.96	118.40
1	A	112	HIS	CG-ND1-CE1	-11.06	90.50	109.30
1	C	11	LYS	CA-C-O	11.06	132.27	120.55
2	D	9	SER	CA-CB-OG	11.05	133.20	111.10
1	A	46	PHE	CE1-CZ-CE2	-11.04	100.12	120.00
1	C	107	VAL	CA-C-O	11.04	134.58	120.78
1	C	89	HIS	CG-ND1-CE1	-11.03	90.55	109.30
1	C	7	LYS	CD-CE-NZ	11.03	147.18	111.90
1	A	50	HIS	CB-CA-C	-11.02	90.66	109.51
2	B	142	ALA	O-C-N	11.02	138.52	122.43
1	A	141	ARG	CB-CA-C	11.01	131.01	110.10
1	C	112	HIS	CA-CB-CG	-10.99	102.81	113.80
2	D	102	ASN	CA-C-N	10.99	134.73	120.44
2	D	102	ASN	C-N-CA	10.99	134.73	120.44
1	C	35	SER	N-CA-C	10.98	126.06	112.23
2	D	2	HIS	CA-C-N	-10.97	99.56	122.82
2	D	2	HIS	C-N-CA	-10.97	99.56	122.82
2	B	96	LEU	N-CA-C	10.96	126.48	112.89
1	A	89	HIS	O-C-N	-10.95	107.46	122.46
2	D	43	GLU	CB-CA-C	-10.95	87.83	110.17
2	B	3	LEU	N-CA-CB	-10.95	91.78	110.83
2	B	3	LEU	CA-C-N	-10.93	95.13	121.80
2	B	3	LEU	C-N-CA	-10.93	95.13	121.80
1	C	87	HIS	O-C-N	10.93	136.97	122.33
1	A	61	LYS	CA-C-N	-10.92	104.91	120.42
1	A	61	LYS	C-N-CA	-10.92	104.91	120.42
1	C	45	HIS	CB-CG-ND1	-10.91	106.33	122.70
2	D	41	PHE	CA-C-N	-10.91	105.00	122.79
2	D	41	PHE	C-N-CA	-10.91	105.00	122.79
1	A	33	PHE	N-CA-C	10.90	124.25	111.71
1	A	28	ALA	CA-C-N	-10.90	106.27	120.44
1	A	28	ALA	C-N-CA	-10.90	106.27	120.44
1	C	109	LEU	CB-CA-C	10.88	128.23	110.92
2	D	65	LYS	CA-CB-CG	-10.88	92.33	114.10
2	D	67	VAL	N-CA-CB	-10.88	91.07	110.77
2	D	90	GLU	CA-C-N	-10.86	105.73	120.28
2	D	90	GLU	C-N-CA	-10.86	105.73	120.28
2	D	19	ASN	CB-CG-ND2	-10.85	100.13	116.40
2	D	7	GLU	CG-CD-OE2	10.83	143.31	118.40
1	C	90	LYS	CB-CG-CD	-10.82	86.42	111.30
1	A	13	ALA	O-C-N	10.82	136.29	122.23
2	B	99	ASP	N-CA-C	-10.82	93.60	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	LYS	N-CA-C	10.81	127.81	113.97
1	A	28	ALA	CA-C-O	10.81	132.46	120.90
1	A	122	HIS	CB-CA-C	10.81	131.92	110.42
2	B	80	ASN	CA-C-N	-10.80	105.80	120.28
2	B	80	ASN	C-N-CA	-10.80	105.80	120.28
2	D	92	HIS	CA-C-O	-10.81	105.28	119.11
2	D	39	GLN	CA-C-N	10.79	135.82	120.28
2	D	39	GLN	C-N-CA	10.79	135.82	120.28
1	C	14	TRP	CB-CG-CD1	-10.79	110.72	126.90
2	D	137	VAL	N-CA-C	10.78	124.57	111.09
1	C	89	HIS	ND1-CG-CD2	10.78	116.88	106.10
1	A	4	PRO	CA-C-O	10.78	130.56	118.38
1	A	22	GLY	CA-C-O	10.77	139.31	120.57
2	B	77	HIS	CE1-NE2-CD2	10.75	119.75	109.00
2	D	110	LEU	O-C-N	-10.75	110.91	122.09
1	C	56	LYS	CB-CG-CD	-10.74	86.59	111.30
2	D	89	SER	O-C-N	-10.74	110.58	122.08
2	B	85	PHE	CZ-CE2-CD2	10.73	139.32	120.00
1	A	112	HIS	CG-CD2-NE2	10.73	117.93	107.20
2	D	44	SER	N-CA-C	-10.72	100.14	113.01
2	B	117	HIS	CB-CG-CD2	10.71	145.12	131.20
1	C	50	HIS	CA-CB-CG	-10.71	103.09	113.80
2	D	80	ASN	CA-C-N	-10.71	105.08	120.29
2	D	80	ASN	C-N-CA	-10.71	105.08	120.29
2	B	97	HIS	ND1-CG-CD2	10.70	116.80	106.10
2	D	10	ALA	CB-CA-C	-10.70	90.12	110.67
1	A	26	ALA	CB-CA-C	-10.66	93.76	110.81
2	D	52	ASP	N-CA-C	-10.65	98.59	111.69
2	D	144	LYS	CG-CD-CE	10.65	135.79	111.30
2	D	63	HIS	CG-ND1-CE1	-10.64	91.20	109.30
2	D	10	ALA	N-CA-C	-10.64	99.48	111.82
2	D	78	LEU	CB-CG-CD2	10.64	142.62	110.70
1	A	7	LYS	CA-C-N	-10.63	106.03	120.28
1	A	7	LYS	C-N-CA	-10.63	106.03	120.28
2	B	76	ALA	CB-CA-C	-10.62	90.89	110.01
1	A	54	GLN	O-C-N	10.62	136.03	122.23
1	A	56	LYS	O-C-N	-10.60	108.49	122.59
2	D	3	LEU	CD1-CG-CD2	-10.58	87.52	110.80
1	C	21	ALA	CA-C-N	10.58	131.68	119.94
1	C	21	ALA	C-N-CA	10.58	131.68	119.94
2	D	72	SER	CA-CB-OG	-10.56	89.98	111.10
2	D	112	CYS	CA-C-O	10.56	132.20	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	LEU	CB-CA-C	-10.56	90.05	110.11
1	A	20	HIS	CB-CG-CD2	-10.55	117.48	131.20
1	C	14	TRP	CD1-NE1-CE2	10.55	127.89	108.90
2	D	17	LYS	CG-CD-CE	10.54	135.55	111.30
2	D	121	GLU	CG-CD-OE1	-10.54	94.16	118.40
1	A	50	HIS	O-C-N	-10.53	111.26	123.06
2	D	52	ASP	O-C-N	10.53	135.92	122.23
1	A	2	LEU	N-CA-CB	-10.52	92.49	110.17
2	B	87	THR	CB-CA-C	-10.52	90.47	110.67
1	A	49	SER	N-CA-C	-10.52	94.91	110.48
1	C	118	THR	N-CA-CB	-10.51	96.88	109.59
2	D	139	ASN	OD1-CG-ND2	10.51	133.11	122.60
2	B	80	ASN	CB-CG-OD1	-10.50	99.80	120.80
1	A	14	TRP	CG-CD1-NE1	-10.50	96.55	110.20
1	C	47	ASP	CA-C-O	-10.50	109.62	120.54
1	C	45	HIS	O-C-N	10.48	137.29	122.41
1	C	99	LYS	CA-C-O	10.48	131.66	120.55
1	A	120	ALA	N-CA-CB	10.48	125.66	110.16
2	D	117	HIS	O-C-N	-10.48	110.72	122.03
2	D	26	GLU	O-C-N	10.45	133.38	122.09
1	A	134	THR	O-C-N	-10.45	108.33	122.33
1	C	29	LEU	CA-C-N	10.44	135.30	120.79
1	C	29	LEU	C-N-CA	10.44	135.30	120.79
2	D	43	GLU	CB-CG-CD	-10.43	94.87	112.60
2	B	24	GLY	CA-C-O	10.42	132.25	121.00
2	D	84	THR	CA-C-O	-10.41	110.17	120.90
1	C	46	PHE	CB-CG-CD2	10.40	138.39	120.70
2	D	92	HIS	CA-CB-CG	-10.40	103.40	113.80
1	C	53	ALA	CB-CA-C	10.39	128.00	110.74
1	A	56	LYS	CB-CG-CD	-10.39	87.40	111.30
1	A	51	GLY	CA-C-N	-10.39	105.55	120.82
1	A	51	GLY	C-N-CA	-10.39	105.55	120.82
2	B	13	ALA	CA-C-O	10.38	131.72	120.82
1	C	84	SER	CB-CA-C	-10.37	93.58	110.79
1	C	118	THR	CA-CB-CG2	10.37	128.13	110.50
2	D	50	THR	CA-CB-OG1	10.37	125.15	109.60
1	C	49	SER	O-C-N	-10.36	110.63	122.86
1	C	90	LYS	N-CA-CB	10.36	128.00	110.49
2	D	42	PHE	CA-CB-CG	-10.35	103.45	113.80
1	A	58	HIS	CA-C-O	-10.35	109.45	120.42
2	B	102	ASN	CA-C-N	10.34	133.88	120.44
2	B	102	ASN	C-N-CA	10.34	133.88	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	PHE	CG-CD2-CE2	-10.33	103.14	120.70
1	C	112	HIS	CB-CG-CD2	10.31	144.61	131.20
2	D	104	ARG	CG-CD-NE	-10.31	89.31	112.00
1	C	90	LYS	CG-CD-CE	-10.31	87.59	111.30
1	A	106	LEU	O-C-N	-10.30	110.17	122.22
1	A	57	GLY	CA-C-O	-10.30	110.71	120.80
2	D	60	VAL	CA-C-O	10.30	132.31	121.29
1	C	14	TRP	NE1-CE2-CZ2	10.29	145.54	130.10
1	C	106	LEU	CA-C-N	10.29	140.50	121.97
1	C	106	LEU	C-N-CA	10.29	140.50	121.97
1	C	116	GLU	CG-CD-OE1	10.29	142.07	118.40
2	B	142	ALA	CA-C-O	-10.29	105.94	119.11
2	B	12	THR	CA-CB-OG1	-10.29	94.17	109.60
2	B	63	HIS	CA-CB-CG	10.29	124.09	113.80
1	A	15	GLY	N-CA-C	-10.28	88.81	113.18
2	B	18	VAL	CA-CB-CG2	-10.27	92.94	110.40
1	C	137	THR	OG1-CB-CG2	10.27	129.84	109.30
2	B	132	LYS	CD-CE-NZ	-10.26	79.06	111.90
2	B	85	PHE	CE1-CZ-CE2	-10.23	101.58	120.00
2	B	69	GLY	CA-C-O	10.20	131.25	120.75
1	C	61	LYS	O-C-N	10.20	132.93	122.12
2	B	99	ASP	CA-C-O	10.19	129.99	119.80
2	B	111	VAL	CA-C-N	10.19	133.94	120.28
2	B	111	VAL	C-N-CA	10.19	133.94	120.28
1	C	19	ALA	CA-C-O	10.19	131.61	119.28
2	D	120	LYS	CB-CG-CD	10.19	134.73	111.30
2	D	76	ALA	CA-C-O	-10.18	105.95	120.51
1	A	65	ALA	CA-C-N	-10.17	103.39	120.68
1	A	65	ALA	C-N-CA	-10.17	103.39	120.68
2	B	125	PRO	CA-N-CD	-10.17	97.77	112.00
1	C	74	ASP	CB-CG-OD2	10.15	141.74	118.40
1	C	112	HIS	O-C-N	-10.15	107.95	122.36
2	D	52	ASP	CB-CG-OD1	-10.15	95.06	118.40
1	A	92	ARG	O-C-N	-10.14	110.41	122.58
1	A	19	ALA	N-CA-CB	10.13	126.43	110.73
1	A	55	VAL	CA-C-O	10.12	131.90	121.17
1	C	44	PRO	N-CA-CB	-10.12	90.38	102.33
1	A	112	HIS	CB-CG-ND1	-10.11	107.53	122.70
2	D	20	VAL	CA-CB-CG1	-10.11	93.21	110.40
2	D	59	LYS	CA-C-N	-10.11	108.07	120.70
2	D	59	LYS	C-N-CA	-10.11	108.07	120.70
1	A	14	TRP	CH2-CZ2-CE2	10.10	130.63	117.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	SER	O-C-N	10.10	134.69	122.27
2	D	48	LEU	CA-C-N	-10.07	104.84	122.26
2	D	48	LEU	C-N-CA	-10.07	104.84	122.26
1	C	68	ASN	OD1-CG-ND2	-10.06	112.54	122.60
1	C	128	PHE	O-C-N	10.06	133.62	122.15
2	B	80	ASN	OD1-CG-ND2	10.06	132.66	122.60
2	D	51	PRO	CA-C-O	10.05	135.94	120.05
2	D	140	ALA	CA-C-O	-10.05	109.89	120.55
1	C	20	HIS	ND1-CG-CD2	10.05	116.15	106.10
1	A	74	ASP	N-CA-C	-10.04	100.29	112.54
2	D	6	GLU	CA-C-N	-10.03	103.43	120.58
2	D	6	GLU	C-N-CA	-10.03	103.43	120.58
1	C	20	HIS	ND1-CE1-NE2	-10.03	98.37	108.40
2	D	18	VAL	CA-CB-CG1	10.02	127.43	110.40
2	D	75	LEU	N-CA-C	9.99	122.17	111.28
2	B	145	TYR	CD1-CG-CD2	9.98	133.06	118.10
1	C	128	PHE	CA-C-O	-9.98	109.84	120.42
1	C	24	TYR	CA-C-O	9.96	131.56	120.90
1	C	46	PHE	CA-CB-CG	-9.96	103.84	113.80
1	C	110	ALA	O-C-N	-9.95	110.16	122.20
2	B	37	TRP	CH2-CZ2-CE2	-9.92	104.61	117.50
2	D	40	ARG	CA-CB-CG	9.91	133.93	114.10
1	A	21	ALA	CB-CA-C	9.90	130.13	110.42
2	B	11	VAL	O-C-N	9.89	132.12	121.94
2	D	97	HIS	CB-CG-CD2	-9.87	118.37	131.20
1	A	83	LEU	CD1-CG-CD2	-9.86	89.11	110.80
2	B	66	LYS	CG-CD-CE	-9.86	88.62	111.30
2	D	66	LYS	CG-CD-CE	-9.86	88.63	111.30
2	D	6	GLU	CB-CG-CD	9.85	129.35	112.60
1	C	8	THR	N-CA-C	9.84	122.91	111.11
1	A	92	ARG	CA-C-N	9.84	134.36	120.98
1	A	92	ARG	C-N-CA	9.84	134.36	120.98
1	A	75	ASP	N-CA-CB	-9.83	95.66	111.58
2	B	51	PRO	O-C-N	-9.82	109.01	122.27
2	B	38	THR	N-CA-CB	9.82	125.34	110.22
2	D	83	GLY	N-CA-C	-9.82	100.34	115.66
1	C	98	PHE	CZ-CE2-CD2	9.81	137.66	120.00
2	D	56	GLY	CA-C-O	9.81	132.91	119.28
1	C	117	PHE	CA-CB-CG	9.80	123.60	113.80
2	D	117	HIS	CG-ND1-CE1	-9.80	92.64	109.30
1	A	136	LEU	CD1-CG-CD2	9.78	132.31	110.80
1	A	79	ALA	O-C-N	9.76	132.47	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	GLU	CA-C-O	9.76	131.13	120.10
2	D	60	VAL	O-C-N	-9.76	111.88	121.94
2	D	67	VAL	CG1-CB-CG2	9.76	132.28	110.80
1	A	137	THR	N-CA-C	-9.75	100.92	112.92
1	A	89	HIS	N-CA-C	9.75	125.32	113.23
2	B	45	PHE	CE1-CZ-CE2	9.75	137.54	120.00
1	C	35	SER	CA-C-O	9.74	131.28	119.79
1	C	11	LYS	N-CA-C	9.74	121.89	111.28
2	D	6	GLU	N-CA-CB	9.74	124.93	110.33
2	B	8	LYS	CA-C-N	9.72	134.28	120.28
2	B	8	LYS	C-N-CA	9.72	134.28	120.28
2	D	37	TRP	CH2-CZ2-CE2	-9.71	104.88	117.50
1	C	45	HIS	CA-C-O	-9.71	107.63	119.18
1	C	116	GLU	CA-C-O	-9.70	108.09	119.15
1	A	45	HIS	CB-CG-ND1	-9.70	108.15	122.70
1	C	74	ASP	O-C-N	9.70	136.59	122.43
2	D	76	ALA	CB-CA-C	9.69	129.70	110.42
1	C	7	LYS	CB-CA-C	9.67	126.79	110.74
2	B	140	ALA	CA-C-N	9.67	133.23	120.28
2	B	140	ALA	C-N-CA	9.67	133.23	120.28
1	C	24	TYR	CD1-CG-CD2	9.66	132.59	118.10
2	D	93	CYS	CB-CA-C	9.65	126.78	110.86
1	A	47	ASP	CB-CG-OD2	-9.65	96.21	118.40
2	D	68	LEU	CA-C-O	9.64	131.26	119.31
1	A	25	GLY	CA-C-N	9.63	133.53	120.54
1	A	25	GLY	C-N-CA	9.63	133.53	120.54
2	D	94	ASP	CB-CG-OD1	-9.62	96.27	118.40
1	A	74	ASP	CA-CB-CG	-9.62	102.98	112.60
2	D	69	GLY	N-CA-C	9.61	124.56	112.83
2	B	41	PHE	CA-CB-CG	-9.60	104.20	113.80
2	B	99	ASP	O-C-N	-9.59	111.69	121.28
1	C	99	LYS	CG-CD-CE	-9.58	89.26	111.30
1	A	63	ALA	O-C-N	-9.58	109.24	122.46
1	A	71	ALA	N-CA-C	-9.57	100.92	111.36
2	D	93	CYS	N-CA-CB	-9.57	96.00	110.07
2	B	5	PRO	N-CA-C	-9.55	100.60	113.40
1	A	82	ALA	N-CA-CB	9.52	123.81	109.91
1	A	101	LEU	O-C-N	-9.52	110.56	122.27
1	C	58	HIS	CG-ND1-CE1	-9.52	93.11	109.30
2	B	2	HIS	N-CA-CB	-9.52	95.80	110.65
2	D	121	GLU	O-C-N	9.51	135.49	122.46
1	C	65	ALA	CA-C-O	9.51	130.85	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	HIS	CA-C-N	9.50	136.81	122.56
1	A	89	HIS	C-N-CA	9.50	136.81	122.56
2	B	47	ASP	N-CA-CB	-9.50	94.70	110.37
1	C	62	VAL	CA-C-O	9.49	130.82	120.95
2	B	114	LEU	CB-CA-C	9.49	125.99	110.81
1	A	51	GLY	O-C-N	9.48	134.97	122.35
1	C	50	HIS	CB-CG-ND1	-9.48	108.47	122.70
1	A	112	HIS	ND1-CG-CD2	9.47	115.58	106.10
1	A	125	LEU	CA-C-N	9.46	132.75	120.44
1	A	125	LEU	C-N-CA	9.46	132.75	120.44
2	B	97	HIS	CG-CD2-NE2	-9.46	97.74	107.20
2	D	90	GLU	CA-CB-CG	-9.46	95.18	114.10
2	D	95	LYS	CB-CG-CD	-9.46	89.54	111.30
2	D	100	PRO	CB-CA-C	9.46	128.06	112.26
1	C	103	HIS	CG-CD2-NE2	9.45	116.65	107.20
2	B	117	HIS	N-CA-C	9.45	122.44	111.11
2	B	43	GLU	CG-CD-OE1	-9.44	96.69	118.40
2	B	4	THR	O-C-N	-9.43	110.47	121.32
1	C	24	TYR	CZ-CE2-CD2	-9.43	102.62	119.60
2	B	95	LYS	N-CA-CB	-9.43	97.56	110.67
1	A	72	HIS	CB-CG-CD2	9.42	143.44	131.20
2	B	6	GLU	N-CA-C	-9.42	100.36	112.23
1	C	30	GLU	CG-CD-OE2	-9.42	96.74	118.40
1	C	55	VAL	N-CA-C	-9.41	101.21	110.72
1	A	46	PHE	CG-CD2-CE2	9.41	136.70	120.70
2	D	63	HIS	ND1-CE1-NE2	-9.41	98.99	108.40
2	B	50	THR	CA-CB-OG1	9.40	123.70	109.60
1	A	36	PHE	CA-CB-CG	9.40	123.20	113.80
2	D	84	THR	CA-CB-CG2	9.39	126.47	110.50
2	D	90	GLU	CG-CD-OE2	-9.39	96.79	118.40
1	A	11	LYS	N-CA-C	-9.39	101.08	112.54
2	D	47	ASP	OD1-CG-OD2	9.38	145.42	122.90
2	B	61	LYS	O-C-N	-9.38	111.25	122.22
2	B	58	PRO	O-C-N	9.37	133.48	122.23
2	D	143	HIS	CG-ND1-CE1	-9.37	93.37	109.30
1	C	79	ALA	CB-CA-C	-9.37	95.24	110.79
2	B	123	THR	O-C-N	9.36	132.26	121.31
2	D	52	ASP	OD1-CG-OD2	-9.36	100.44	122.90
2	D	126	VAL	CA-CB-CG2	-9.35	94.50	110.40
2	D	100	PRO	O-C-N	9.35	133.48	122.17
2	D	145	TYR	CB-CG-CD1	9.35	134.82	120.80
2	B	104	ARG	NH1-CZ-NH2	9.34	131.45	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	PRO	N-CA-C	-9.34	101.54	114.80
2	B	78	LEU	CA-C-O	-9.33	106.89	119.12
2	B	87	THR	CA-CB-CG2	-9.33	94.64	110.50
2	D	135	ALA	N-CA-C	-9.32	101.07	111.14
1	A	46	PHE	CB-CG-CD2	9.32	136.54	120.70
2	B	24	GLY	O-C-N	-9.32	113.23	122.18
1	C	107	VAL	O-C-N	-9.32	110.92	122.57
2	B	141	LEU	O-C-N	-9.31	112.25	122.12
2	B	45	PHE	O-C-N	-9.31	110.21	122.59
1	C	140	TYR	O-C-N	9.31	133.11	122.22
1	A	12	ALA	N-CA-CB	-9.31	95.62	110.98
2	D	19	ASN	CA-C-O	-9.31	107.20	120.51
1	C	43	PHE	CZ-CE2-CD2	9.30	136.74	120.00
1	A	116	GLU	CG-CD-OE1	9.29	139.76	118.40
2	D	67	VAL	CA-CB-CG1	-9.29	94.61	110.40
1	A	47	ASP	CA-CB-CG	-9.28	103.33	112.60
1	A	127	LYS	CG-CD-CE	-9.27	89.97	111.30
1	C	103	HIS	CG-ND1-CE1	-9.26	93.55	109.30
1	A	50	HIS	ND1-CG-CD2	-9.26	96.84	106.10
1	A	14	TRP	CA-C-N	-9.25	103.27	121.41
1	A	14	TRP	C-N-CA	-9.25	103.27	121.41
1	A	81	SER	O-C-N	-9.25	110.03	122.43
2	B	90	GLU	CA-C-O	9.24	133.73	120.51
2	B	131	GLN	CG-CD-NE2	9.24	130.27	116.40
2	B	23	VAL	CA-CB-CG2	-9.24	94.69	110.40
2	D	14	LEU	O-C-N	9.24	133.63	122.27
2	B	81	LEU	CA-C-N	-9.23	106.28	120.31
2	B	81	LEU	C-N-CA	-9.23	106.28	120.31
1	A	64	ASP	OD1-CG-OD2	9.22	145.02	122.90
1	A	82	ALA	CA-C-O	9.22	130.68	121.00
1	A	131	SER	CA-C-N	-9.22	107.83	120.46
1	A	131	SER	C-N-CA	-9.22	107.83	120.46
1	C	14	TRP	CH2-CZ2-CE2	9.22	129.48	117.50
2	B	48	LEU	CB-CA-C	9.22	125.86	111.02
1	A	17	VAL	CA-C-O	-9.21	111.40	121.17
2	D	106	LEU	CA-C-N	9.21	130.17	119.94
2	D	106	LEU	C-N-CA	9.21	130.17	119.94
2	D	130	TYR	CG-CD1-CE1	9.21	135.02	121.20
2	B	24	GLY	CA-C-N	9.21	130.39	119.99
2	B	24	GLY	C-N-CA	9.21	130.39	119.99
2	B	80	ASN	N-CA-C	-9.21	92.62	109.56
1	C	112	HIS	CA-C-N	9.21	144.26	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	HIS	C-N-CA	9.21	144.26	121.80
1	C	47	ASP	CA-C-N	-9.20	107.66	122.66
1	C	47	ASP	C-N-CA	-9.20	107.66	122.66
2	B	135	ALA	CA-C-N	9.20	130.15	119.94
2	B	135	ALA	C-N-CA	9.20	130.15	119.94
1	C	11	LYS	CA-CB-CG	9.20	132.50	114.10
1	C	18	GLY	CA-C-N	-9.20	105.74	122.38
1	C	18	GLY	C-N-CA	-9.20	105.74	122.38
2	D	30	ARG	CD-NE-CZ	9.20	137.27	124.40
2	D	51	PRO	O-C-N	-9.19	112.25	122.18
1	A	104	CYS	CA-C-O	-9.19	108.08	119.38
1	C	44	PRO	CA-C-O	-9.18	106.87	118.81
1	C	102	SER	CA-C-O	-9.18	110.69	120.42
2	B	26	GLU	CA-C-O	-9.17	111.19	120.82
2	D	2	HIS	CB-CA-C	9.16	126.69	111.31
2	D	102	ASN	CA-CB-CG	-9.16	103.44	112.60
2	D	103	PHE	CA-CB-CG	-9.15	104.64	113.80
2	D	51	PRO	N-CD-CG	-9.15	89.48	103.20
1	A	72	HIS	O-C-N	-9.14	109.61	121.95
1	A	65	ALA	CA-C-O	-9.13	109.78	120.10
2	B	94	ASP	CB-CG-OD1	-9.12	97.42	118.40
2	B	118	PHE	CE1-CZ-CE2	-9.12	103.59	120.00
1	A	64	ASP	CB-CG-OD1	-9.11	97.44	118.40
1	C	45	HIS	ND1-CG-CD2	9.11	115.21	106.10
2	B	46	GLY	O-C-N	9.11	134.54	122.70
1	A	114	PRO	N-CA-CB	-9.11	93.56	103.39
2	B	47	ASP	CA-CB-CG	-9.10	103.50	112.60
1	A	50	HIS	CA-CB-CG	-9.10	104.70	113.80
1	C	43	PHE	CA-C-N	-9.10	109.88	120.89
1	C	43	PHE	C-N-CA	-9.10	109.88	120.89
1	C	138	SER	N-CA-CB	-9.09	96.22	110.22
1	C	84	SER	CA-C-O	9.09	130.18	120.55
2	B	72	SER	N-CA-C	-9.08	99.94	111.02
2	B	139	ASN	CB-CA-C	-9.08	91.33	110.31
2	D	23	VAL	CA-C-N	9.08	130.02	119.94
2	D	23	VAL	C-N-CA	9.08	130.02	119.94
2	B	93	CYS	O-C-N	9.07	132.64	122.11
1	A	105	LEU	O-C-N	9.07	134.49	122.33
2	D	19	ASN	CB-CG-OD1	-9.07	102.65	120.80
1	C	5	ALA	N-CA-CB	9.06	123.14	109.91
2	B	49	SER	N-CA-CB	-9.06	94.30	110.60
2	B	81	LEU	CA-C-O	9.04	130.13	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	THR	CA-C-N	9.03	133.29	120.28
1	A	137	THR	C-N-CA	9.03	133.29	120.28
2	D	63	HIS	CB-CG-ND1	-9.02	109.17	122.70
1	C	78	ASN	N-CA-C	9.01	130.00	110.80
1	C	43	PHE	CG-CD2-CE2	-9.01	105.39	120.70
2	D	47	ASP	CB-CG-OD1	-9.01	97.68	118.40
1	C	53	ALA	CA-C-N	-9.01	108.21	120.28
1	C	53	ALA	C-N-CA	-9.01	108.21	120.28
2	D	117	HIS	CG-CD2-NE2	9.00	116.20	107.20
2	B	79	ASP	N-CA-CB	-8.98	96.43	110.44
1	C	15	GLY	O-C-N	-8.98	111.03	122.70
1	C	103	HIS	O-C-N	-8.98	112.60	122.12
1	C	17	VAL	CB-CA-C	8.97	126.01	111.29
2	B	32	LEU	CB-CG-CD1	8.97	137.61	110.70
1	A	77	PRO	CA-C-N	8.96	133.02	120.29
1	A	77	PRO	C-N-CA	8.96	133.02	120.29
2	D	42	PHE	CB-CG-CD1	-8.96	105.47	120.70
2	D	139	ASN	CA-CB-CG	8.96	121.56	112.60
2	B	2	HIS	CA-C-N	-8.95	109.51	122.94
2	B	2	HIS	C-N-CA	-8.95	109.51	122.94
2	D	53	ALA	CB-CA-C	-8.95	96.69	110.92
2	D	54	VAL	CA-CB-CG1	-8.94	95.21	110.40
2	B	42	PHE	CD1-CG-CD2	-8.93	105.20	118.60
1	C	10	VAL	CA-C-O	-8.93	111.39	120.85
1	A	138	SER	O-C-N	8.92	132.66	122.22
2	B	91	LEU	CA-C-N	-8.91	105.54	121.14
2	B	91	LEU	C-N-CA	-8.91	105.54	121.14
1	A	30	GLU	OE1-CD-OE2	8.90	144.27	122.90
2	D	146	HIS	N-CA-CB	-8.90	95.37	110.50
2	B	129	ALA	CA-C-O	-8.90	110.99	120.42
1	A	105	LEU	N-CA-CB	-8.89	96.61	110.30
2	B	145	TYR	CB-CG-CD2	-8.89	107.46	120.80
2	B	62	ALA	CA-C-N	-8.88	107.49	120.28
2	B	62	ALA	C-N-CA	-8.88	107.49	120.28
1	A	89	HIS	CG-ND1-CE1	8.88	124.40	109.30
2	D	118	PHE	CD1-CE1-CZ	-8.88	104.02	120.00
2	B	7	GLU	CB-CA-C	8.88	128.08	110.42
1	C	77	PRO	CA-C-O	8.87	134.83	119.84
1	C	46	PHE	CA-C-O	8.87	132.18	121.72
2	B	42	PHE	CE1-CZ-CE2	-8.86	104.05	120.00
1	A	52	SER	CB-CA-C	8.85	125.30	109.64
2	B	122	PHE	CA-CB-CG	-8.85	104.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	GLU	CB-CG-CD	-8.82	97.61	112.60
1	A	134	THR	N-CA-CB	-8.81	96.73	110.30
1	C	121	VAL	O-C-N	8.81	130.54	121.91
2	D	9	SER	CA-C-O	-8.80	109.40	119.79
1	A	109	LEU	O-C-N	8.80	131.45	122.12
2	B	46	GLY	CA-C-N	-8.80	111.40	122.84
2	B	46	GLY	C-N-CA	-8.80	111.40	122.84
1	A	33	PHE	CG-CD2-CE2	-8.80	105.74	120.70
2	B	1	VAL	CA-CB-CG1	-8.80	95.45	110.40
1	A	47	ASP	CA-C-O	-8.79	111.17	120.58
1	C	44	PRO	CA-N-CD	8.79	124.30	112.00
1	A	16	LYS	N-CA-CB	8.78	125.33	110.49
1	A	64	ASP	CA-C-N	-8.78	107.63	120.28
1	A	64	ASP	C-N-CA	-8.78	107.63	120.28
1	C	102	SER	N-CA-C	-8.78	101.79	111.36
2	B	112	CYS	N-CA-CB	8.78	123.02	110.12
1	A	78	ASN	O-C-N	-8.77	112.16	122.15
1	A	86	LEU	CA-C-N	-8.77	105.80	121.14
1	A	86	LEU	C-N-CA	-8.77	105.80	121.14
2	B	82	LYS	O-C-N	-8.77	111.49	122.27
1	A	133	SER	CA-C-O	-8.75	111.28	120.55
1	C	129	LEU	O-C-N	-8.75	111.51	122.27
1	A	77	PRO	O-C-N	-8.74	110.84	122.64
2	B	3	LEU	O-C-N	8.74	134.59	123.23
2	D	65	LYS	CD-CE-NZ	-8.74	83.93	111.90
1	A	117	PHE	CA-CB-CG	8.73	122.53	113.80
2	B	66	LYS	O-C-N	8.73	133.58	122.23
2	D	137	VAL	CB-CA-C	-8.73	98.11	112.26
1	C	107	VAL	N-CA-CB	8.71	125.61	111.23
2	D	122	PHE	CE1-CZ-CE2	8.71	135.68	120.00
2	D	74	GLY	CA-C-N	-8.71	108.61	120.28
2	D	74	GLY	C-N-CA	-8.71	108.61	120.28
2	D	45	PHE	CB-CG-CD2	8.69	135.48	120.70
1	C	3	SER	CA-C-N	8.69	128.32	118.85
1	C	3	SER	C-N-CA	8.69	128.32	118.85
2	D	39	GLN	OE1-CD-NE2	-8.69	113.91	122.60
1	A	19	ALA	CB-CA-C	-8.68	96.05	110.72
1	C	11	LYS	O-C-N	-8.68	112.92	122.12
1	A	86	LEU	CD1-CG-CD2	-8.67	91.73	110.80
1	C	115	ALA	CA-C-O	8.66	130.57	120.00
2	B	112	CYS	N-CA-C	-8.65	101.85	111.28
1	A	26	ALA	O-C-N	-8.65	113.09	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	37	TRP	CA-C-N	8.64	132.72	120.28
2	B	37	TRP	C-N-CA	8.64	132.72	120.28
2	D	64	GLY	N-CA-C	8.64	124.76	113.27
1	A	7	LYS	CD-CE-NZ	-8.63	84.29	111.90
1	A	26	ALA	N-CA-C	8.63	121.46	111.11
2	D	94	ASP	N-CA-CB	-8.63	97.01	110.30
1	A	77	PRO	CA-CB-CG	-8.62	88.11	104.50
1	A	135	VAL	CA-C-O	-8.62	110.94	120.25
2	B	6	GLU	OE1-CD-OE2	-8.62	102.21	122.90
2	D	63	HIS	CE1-NE2-CD2	8.62	117.62	109.00
2	B	140	ALA	O-C-N	-8.62	110.78	122.33
1	C	79	ALA	O-C-N	8.62	131.25	122.12
1	A	59	GLY	CA-C-O	8.61	129.70	120.40
1	C	86	LEU	N-CA-C	8.61	120.67	111.28
1	C	96	VAL	CA-CB-CG2	8.60	125.03	110.40
2	D	103	PHE	N-CA-CB	8.60	122.48	110.01
1	C	71	ALA	N-CA-C	-8.59	100.54	111.02
2	D	141	LEU	CD1-CG-CD2	-8.59	91.91	110.80
1	A	128	PHE	CE1-CZ-CE2	8.59	135.45	120.00
2	B	90	GLU	CG-CD-OE1	-8.58	98.66	118.40
1	A	113	LEU	CB-CA-C	-8.58	99.55	110.96
1	C	83	LEU	N-CA-CB	-8.58	97.00	110.46
1	A	61	LYS	CA-C-O	-8.57	108.84	119.38
1	A	7	LYS	N-CA-CB	-8.56	97.04	110.22
2	B	52	ASP	CB-CG-OD2	-8.56	98.72	118.40
2	D	76	ALA	N-CA-C	-8.56	92.58	110.80
2	B	84	THR	O-C-N	-8.55	111.85	122.20
1	C	91	LEU	N-CA-CB	-8.54	97.68	110.07
2	D	85	PHE	O-C-N	-8.54	109.75	122.39
2	B	145	TYR	O-C-N	8.54	132.68	123.11
2	B	103	PHE	N-CA-CB	8.53	122.38	110.01
2	B	101	GLU	O-C-N	-8.53	112.24	122.22
1	A	76	MET	CA-CB-CG	-8.53	97.05	114.10
2	D	21	ASP	OD1-CG-OD2	-8.51	102.49	122.90
2	D	56	GLY	CA-C-N	8.51	136.06	121.35
2	D	56	GLY	C-N-CA	8.51	136.06	121.35
2	D	118	PHE	CB-CG-CD1	8.51	135.16	120.70
2	B	116	HIS	CE1-NE2-CD2	-8.50	100.50	109.00
1	C	49	SER	N-CA-CB	8.50	122.41	110.17
2	B	14	LEU	CD1-CG-CD2	8.49	129.48	110.80
1	C	114	PRO	N-CD-CG	-8.49	90.46	103.20
2	D	122	PHE	N-CA-CB	-8.49	99.11	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	LYS	O-C-N	8.48	132.14	122.22
1	C	92	ARG	CA-C-O	8.48	131.37	121.28
1	C	58	HIS	CA-C-O	-8.47	111.92	120.82
2	B	132	LYS	CA-C-O	8.47	129.40	120.42
1	A	139	LYS	N-CA-C	-8.46	101.96	112.88
1	C	109	LEU	CD1-CG-CD2	8.46	129.40	110.80
2	B	66	LYS	CA-C-N	-8.45	108.88	120.46
2	B	66	LYS	C-N-CA	-8.45	108.88	120.46
1	C	28	ALA	O-C-N	8.45	131.07	122.12
2	B	36	PRO	N-CD-CG	8.44	115.86	103.20
1	A	68	ASN	O-C-N	-8.44	111.89	122.27
1	A	94	ASP	CA-CB-CG	-8.44	104.16	112.60
2	B	95	LYS	O-C-N	-8.43	112.27	122.48
2	B	113	VAL	CA-C-O	-8.43	111.36	120.47
2	D	144	LYS	O-C-N	-8.43	111.13	122.43
1	C	16	LYS	CD-CE-NZ	-8.42	84.96	111.90
2	B	28	LEU	O-C-N	-8.42	112.02	122.20
1	C	127	LYS	N-CA-C	-8.42	102.19	111.36
2	D	45	PHE	CG-CD2-CE2	8.40	134.99	120.70
1	A	87	HIS	CB-CG-CD2	8.40	142.12	131.20
1	C	1	VAL	N-CA-C	-8.40	87.48	111.00
2	B	30	ARG	NH1-CZ-NH2	-8.40	108.39	119.30
2	D	77	HIS	CB-CG-ND1	-8.40	110.11	122.70
2	B	71	PHE	CA-C-N	8.39	132.46	120.79
2	B	71	PHE	C-N-CA	8.39	132.46	120.79
1	C	76	MET	CA-C-N	-8.39	109.75	119.32
1	C	76	MET	C-N-CA	-8.39	109.75	119.32
1	A	132	VAL	CA-C-O	-8.38	112.23	120.95
1	C	87	HIS	CE1-NE2-CD2	8.38	117.38	109.00
2	B	33	VAL	O-C-N	8.37	132.15	121.94
1	C	60	LYS	CA-C-O	8.36	129.42	120.55
2	D	93	CYS	CA-C-N	-8.37	106.46	120.68
2	D	93	CYS	C-N-CA	-8.37	106.46	120.68
2	D	10	ALA	N-CA-CB	-8.34	97.36	110.28
2	B	89	SER	CA-C-O	8.34	129.57	120.82
2	B	35	TYR	CA-C-O	-8.33	110.35	121.02
1	A	24	TYR	CA-C-O	-8.33	111.59	120.42
2	B	9	SER	N-CA-CB	8.33	123.04	110.22
2	B	37	TRP	CZ3-CH2-CZ2	8.31	132.31	121.50
2	D	42	PHE	CA-C-N	-8.31	104.72	121.18
2	D	42	PHE	C-N-CA	-8.31	104.72	121.18
2	B	8	LYS	CG-CD-CE	8.30	130.40	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	10	ALA	CA-C-O	-8.29	110.43	119.97
2	D	28	LEU	O-C-N	-8.29	113.53	122.07
1	A	6	ASP	CA-C-O	-8.28	112.04	120.90
2	B	73	ASP	CA-C-O	8.28	129.33	120.55
2	D	125	PRO	N-CA-C	8.28	125.04	113.53
1	A	4	PRO	N-CD-CG	-8.27	90.80	103.20
1	A	55	VAL	N-CA-C	8.27	118.36	110.42
1	A	114	PRO	CA-CB-CG	8.27	120.21	104.50
2	D	17	LYS	CB-CG-CD	-8.27	92.29	111.30
1	A	39	THR	O-C-N	8.26	133.86	122.46
2	D	7	GLU	N-CA-C	-8.26	101.53	111.69
1	C	128	PHE	CB-CG-CD2	-8.26	106.66	120.70
2	D	92	HIS	N-CA-CB	-8.26	96.53	110.41
1	C	60	LYS	CA-CB-CG	-8.26	97.59	114.10
2	B	11	VAL	CB-CA-C	8.23	122.10	111.81
2	D	130	TYR	CD1-CE1-CZ	-8.22	104.80	119.60
1	A	64	ASP	CB-CG-OD2	-8.22	99.49	118.40
1	C	42	TYR	CA-CB-CG	-8.22	99.10	113.90
2	B	14	LEU	N-CA-CB	-8.22	98.09	110.01
2	B	132	LYS	CG-CD-CE	-8.22	92.40	111.30
1	A	23	GLU	N-CA-CB	-8.21	97.75	110.06
2	D	65	LYS	N-CA-CB	-8.21	97.56	110.28
1	C	85	ASP	N-CA-C	8.20	120.22	111.28
1	A	44	PRO	CB-CA-C	-8.19	99.33	110.88
2	B	57	ASN	CA-C-O	8.18	128.49	119.32
2	B	89	SER	N-CA-CB	-8.18	98.15	110.01
2	D	139	ASN	CB-CG-ND2	-8.18	104.13	116.40
2	D	55	MET	CB-CG-SD	8.18	137.22	112.70
2	B	71	PHE	CA-C-O	-8.16	111.90	120.55
2	D	141	LEU	CA-C-O	8.16	129.07	120.42
1	C	17	VAL	CA-C-N	-8.16	105.42	121.41
1	C	17	VAL	C-N-CA	-8.16	105.42	121.41
1	A	20	HIS	CA-CB-CG	8.15	121.95	113.80
1	C	41	THR	CA-C-N	8.15	135.99	122.54
1	C	41	THR	C-N-CA	8.15	135.99	122.54
2	B	7	GLU	N-CA-C	-8.14	93.45	110.80
1	C	135	VAL	N-CA-C	-8.14	102.40	110.30
2	B	44	SER	CA-C-N	8.13	137.08	121.54
2	B	44	SER	C-N-CA	8.13	137.08	121.54
2	D	146	HIS	CA-CB-CG	-8.13	105.67	113.80
2	B	59	LYS	CG-CD-CE	-8.13	92.60	111.30
1	A	4	PRO	CA-CB-CG	-8.13	89.06	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	THR	OG1-CB-CG2	8.13	125.56	109.30
1	C	4	PRO	CA-C-N	-8.13	109.92	120.65
1	C	4	PRO	C-N-CA	-8.13	109.92	120.65
1	A	87	HIS	ND1-CE1-NE2	8.11	116.51	108.40
1	C	95	PRO	O-C-N	-8.11	110.78	122.37
2	B	62	ALA	O-C-N	8.10	130.84	122.09
1	A	40	LYS	CA-C-O	8.09	129.46	119.11
2	B	15	TRP	CA-C-O	-8.09	110.96	120.10
2	B	112	CYS	O-C-N	8.07	130.68	122.12
1	A	109	LEU	CD1-CG-CD2	8.07	128.56	110.80
1	C	90	LYS	CD-CE-NZ	-8.07	86.07	111.90
2	D	2	HIS	CA-CB-CG	-8.07	105.73	113.80
2	D	71	PHE	CG-CD1-CE1	-8.07	106.98	120.70
2	D	66	LYS	CB-CA-C	8.06	123.37	110.96
2	B	17	LYS	CD-CE-NZ	-8.05	86.13	111.90
2	B	134	VAL	CA-CB-CG1	-8.05	96.72	110.40
1	A	96	VAL	CA-CB-CG2	-8.04	96.72	110.40
1	A	114	PRO	N-CA-C	-8.04	102.79	113.65
2	B	20	VAL	CA-C-O	8.05	129.18	120.57
2	D	92	HIS	ND1-CG-CD2	-8.04	98.06	106.10
1	C	99	LYS	CB-CG-CD	8.03	129.76	111.30
2	B	26	GLU	CA-C-N	-8.03	108.89	120.29
2	B	26	GLU	C-N-CA	-8.03	108.89	120.29
1	C	27	GLU	N-CA-C	-8.03	102.61	111.36
1	C	33	PHE	CG-CD2-CE2	-8.03	107.06	120.70
2	D	5	PRO	CA-C-O	8.03	128.07	118.92
2	D	77	HIS	CB-CG-CD2	-8.03	120.77	131.20
2	D	94	ASP	CA-CB-CG	8.02	120.62	112.60
2	D	15	TRP	N-CA-C	-8.01	102.96	112.89
1	A	84	SER	CA-C-N	-8.00	108.15	120.31
1	A	84	SER	C-N-CA	-8.00	108.15	120.31
2	D	121	GLU	CA-C-N	-8.00	110.17	122.16
2	D	121	GLU	C-N-CA	-8.00	110.17	122.16
1	A	84	SER	CA-CB-OG	-7.99	95.12	111.10
2	B	115	ALA	N-CA-CB	-7.98	98.39	110.12
2	B	84	THR	N-CA-CB	7.97	123.27	109.72
1	A	73	VAL	CB-CA-C	7.97	122.47	112.04
1	A	130	ALA	CA-C-O	7.97	128.87	120.42
2	B	75	LEU	CD1-CG-CD2	-7.96	93.28	110.80
2	D	95	LYS	CG-CD-CE	7.96	129.62	111.30
2	B	107	GLY	N-CA-C	-7.96	102.71	113.37
1	A	8	THR	O-C-N	-7.95	113.69	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	42	PHE	CD1-CE1-CZ	7.95	134.31	120.00
1	A	62	VAL	CA-C-O	-7.94	112.43	120.85
1	A	15	GLY	CA-C-N	7.94	136.70	121.54
1	A	15	GLY	C-N-CA	7.94	136.70	121.54
1	C	12	ALA	CB-CA-C	-7.93	98.31	110.92
2	D	90	GLU	N-CA-C	7.92	120.91	111.33
1	A	46	PHE	CA-C-N	-7.92	111.89	122.42
1	A	46	PHE	C-N-CA	-7.92	111.89	122.42
2	B	91	LEU	N-CA-CB	-7.92	98.53	110.01
2	D	92	HIS	CB-CA-C	-7.92	94.20	109.95
2	B	117	HIS	CA-C-N	7.91	135.59	121.66
2	B	117	HIS	C-N-CA	7.91	135.59	121.66
2	B	84	THR	CA-CB-OG1	-7.91	97.74	109.60
1	C	33	PHE	CA-CB-CG	7.91	121.71	113.80
1	C	140	TYR	CA-C-O	-7.90	111.17	120.10
1	A	12	ALA	N-CA-C	-7.90	101.80	112.94
1	C	98	PHE	CE1-CZ-CE2	-7.90	105.78	120.00
1	A	125	LEU	O-C-N	-7.90	112.55	122.27
2	D	31	LEU	CA-C-O	7.89	130.25	121.02
2	D	54	VAL	N-CA-CB	-7.88	99.82	110.54
1	C	83	LEU	CB-CA-C	-7.88	94.59	109.72
1	C	122	HIS	CB-CG-CD2	-7.88	120.95	131.20
1	C	103	HIS	CA-C-N	7.88	130.84	120.28
1	C	103	HIS	C-N-CA	7.88	130.84	120.28
1	A	134	THR	CA-CB-OG1	7.87	121.41	109.60
2	D	92	HIS	CG-ND1-CE1	-7.87	95.92	109.30
1	A	67	THR	CA-CB-OG1	7.86	121.39	109.60
2	D	23	VAL	CA-CB-CG2	-7.86	97.04	110.40
2	B	47	ASP	OD1-CG-OD2	-7.86	104.05	122.90
2	B	61	LYS	CG-CD-CE	-7.85	93.24	111.30
1	C	73	VAL	CA-C-O	-7.85	112.08	120.64
2	D	21	ASP	CA-C-N	7.85	136.53	121.54
2	D	21	ASP	C-N-CA	7.85	136.53	121.54
1	A	13	ALA	CA-C-N	-7.83	107.64	120.72
1	A	13	ALA	C-N-CA	-7.83	107.64	120.72
2	B	69	GLY	N-CA-C	7.83	122.13	112.73
2	D	92	HIS	CB-CG-ND1	-7.83	110.96	122.70
2	B	9	SER	CA-C-N	-7.83	107.38	120.68
2	B	9	SER	C-N-CA	-7.83	107.38	120.68
1	C	8	THR	CA-C-O	7.82	129.26	120.90
1	A	27	GLU	CA-C-O	-7.80	112.28	120.55
1	A	116	GLU	CB-CG-CD	-7.79	99.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	HIS	ND1-CE1-NE2	7.79	116.19	108.40
2	B	143	HIS	N-CA-C	-7.79	102.79	111.28
2	D	41	PHE	CZ-CE2-CD2	-7.79	105.99	120.00
1	C	12	ALA	CA-C-N	7.78	131.61	120.79
1	C	12	ALA	C-N-CA	7.78	131.61	120.79
1	C	28	ALA	CA-C-N	-7.78	109.85	120.28
1	C	28	ALA	C-N-CA	-7.78	109.85	120.28
1	C	64	ASP	OD1-CG-OD2	7.77	141.55	122.90
1	C	47	ASP	O-C-N	7.77	132.30	123.05
1	A	42	TYR	CA-CB-CG	-7.76	99.92	113.90
2	D	86	ALA	CB-CA-C	-7.75	97.93	110.79
1	A	109	LEU	CA-C-N	-7.75	109.12	120.28
1	A	109	LEU	C-N-CA	-7.75	109.12	120.28
1	C	3	SER	CA-C-O	7.75	130.77	120.16
1	C	38	THR	N-CA-CB	-7.75	98.73	110.12
2	B	85	PHE	CG-CD2-CE2	-7.74	107.55	120.70
2	D	141	LEU	O-C-N	-7.74	113.33	122.15
2	B	65	LYS	CB-CG-CD	-7.73	93.52	111.30
2	B	36	PRO	N-CA-CB	7.73	110.86	103.52
2	B	120	LYS	CG-CD-CE	-7.73	93.53	111.30
1	A	20	HIS	ND1-CG-CD2	-7.72	98.38	106.10
1	A	17	VAL	CA-C-N	-7.72	106.28	121.41
1	A	17	VAL	C-N-CA	-7.72	106.28	121.41
2	B	126	VAL	O-C-N	-7.72	111.24	121.82
1	C	17	VAL	CG1-CB-CG2	7.72	127.78	110.80
2	D	32	LEU	CB-CG-CD2	7.72	133.85	110.70
1	A	1	VAL	O-C-N	7.71	135.34	123.00
2	D	12	THR	N-CA-CB	-7.71	98.76	110.16
2	B	132	LYS	O-C-N	-7.69	113.38	122.15
2	B	145	TYR	CG-CD2-CE2	-7.68	109.69	121.20
1	A	87	HIS	CG-CD2-NE2	7.66	114.86	107.20
2	B	28	LEU	CB-CG-CD2	-7.66	87.71	110.70
1	C	48	LEU	N-CA-CB	-7.66	99.77	110.65
1	A	14	TRP	NE1-CE2-CZ2	7.66	141.59	130.10
2	B	90	GLU	CA-CB-CG	-7.66	98.79	114.10
2	B	54	VAL	O-C-N	-7.64	114.42	121.91
2	B	117	HIS	CE1-NE2-CD2	7.64	116.64	109.00
1	C	47	ASP	CB-CG-OD2	-7.64	100.82	118.40
1	A	15	GLY	O-C-N	-7.64	112.77	122.70
1	C	121	VAL	CB-CA-C	7.63	121.74	111.97
2	B	42	PHE	CG-CD2-CE2	7.63	133.67	120.70
1	A	4	PRO	CA-C-N	-7.63	108.24	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	PRO	C-N-CA	-7.63	108.24	121.66
1	C	21	ALA	CA-C-O	-7.63	109.61	120.51
2	D	58	PRO	CA-C-O	-7.62	106.73	120.60
2	B	6	GLU	CG-CD-OE1	-7.61	100.90	118.40
2	B	55	MET	CA-C-O	-7.61	111.22	119.97
1	A	27	GLU	O-C-N	7.60	130.18	122.12
2	B	112	CYS	CA-C-O	-7.59	112.50	120.55
2	B	37	TRP	CD1-NE1-CE2	7.59	122.56	108.90
1	C	9	ASN	CA-CB-CG	7.58	120.18	112.60
1	A	126	ASP	CA-CB-CG	7.57	120.17	112.60
2	B	94	ASP	CA-CB-CG	7.57	120.17	112.60
1	C	47	ASP	N-CA-CB	-7.57	97.88	110.37
2	B	77	HIS	CA-CB-CG	-7.57	106.23	113.80
1	A	132	VAL	CA-C-N	7.57	130.42	120.28
1	A	132	VAL	C-N-CA	7.57	130.42	120.28
2	D	99	ASP	OD1-CG-OD2	7.57	141.06	122.90
2	B	118	PHE	CA-C-O	-7.54	110.44	119.27
1	C	139	LYS	CA-CB-CG	-7.54	99.02	114.10
1	C	1	VAL	CA-C-O	7.54	133.61	120.80
2	D	19	ASN	CA-CB-CG	-7.54	105.06	112.60
2	D	63	HIS	CA-C-O	-7.54	111.87	120.24
1	A	77	PRO	N-CA-CB	7.53	111.15	103.25
2	B	9	SER	N-CA-C	7.52	120.36	111.71
2	D	71	PHE	O-C-N	7.51	130.08	122.12
1	A	89	HIS	ND1-CG-CD2	-7.51	98.59	106.10
2	B	108	ASN	CA-CB-CG	-7.50	105.09	112.60
2	B	36	PRO	CA-N-CD	-7.50	101.49	112.00
2	D	60	VAL	CG1-CB-CG2	7.50	127.31	110.80
2	B	64	GLY	N-CA-C	7.50	121.73	112.73
2	B	70	ALA	CA-C-O	7.50	128.69	120.82
1	C	98	PHE	CG-CD2-CE2	-7.49	107.97	120.70
1	C	131	SER	CA-CB-OG	-7.49	96.12	111.10
2	D	44	SER	CA-CB-OG	7.48	126.07	111.10
2	B	42	PHE	CA-CB-CG	-7.48	106.32	113.80
2	D	4	THR	N-CA-C	7.47	120.61	110.31
1	A	53	ALA	CB-CA-C	-7.46	95.09	109.95
2	B	18	VAL	O-C-N	-7.46	114.74	123.03
2	B	21	ASP	CB-CG-OD2	-7.46	101.24	118.40
2	B	66	LYS	CB-CA-C	-7.46	97.05	110.70
2	B	30	ARG	CA-C-O	-7.45	110.07	119.31
1	A	31	ARG	NE-CZ-NH1	7.45	128.95	121.50
1	A	8	THR	N-CA-CB	-7.44	99.18	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	74	GLY	CA-C-O	7.44	131.94	119.59
1	C	11	LYS	CB-CA-C	7.43	123.13	110.79
2	B	52	ASP	CA-C-O	7.43	128.43	120.55
1	A	72	HIS	CA-C-O	7.42	130.10	121.34
1	C	122	HIS	CB-CA-C	7.42	122.69	110.81
2	B	65	LYS	CA-CB-CG	-7.42	99.27	114.10
2	B	34	VAL	O-C-N	7.41	130.17	121.80
1	C	47	ASP	CB-CA-C	-7.41	98.92	110.78
2	D	79	ASP	CA-CB-CG	-7.41	105.19	112.60
2	B	45	PHE	CB-CG-CD2	7.41	133.29	120.70
2	D	104	ARG	O-C-N	7.40	130.08	122.09
1	A	98	PHE	N-CA-CB	7.40	121.11	110.16
1	A	70	VAL	CA-CB-CG1	7.39	122.96	110.40
2	D	126	VAL	CA-C-N	-7.38	109.75	120.82
2	D	126	VAL	C-N-CA	-7.38	109.75	120.82
2	D	94	ASP	CB-CG-OD2	-7.37	101.45	118.40
1	A	138	SER	CB-CA-C	-7.37	97.00	110.63
1	C	128	PHE	CA-CB-CG	7.36	121.16	113.80
1	C	10	VAL	N-CA-C	7.36	118.15	110.72
1	A	113	LEU	CA-C-N	7.35	127.37	119.28
1	A	113	LEU	C-N-CA	7.35	127.37	119.28
1	A	82	ALA	O-C-N	-7.35	114.39	122.03
2	B	123	THR	CA-C-O	-7.35	112.34	121.01
1	A	23	GLU	CB-CG-CD	-7.34	100.13	112.60
1	A	33	PHE	O-C-N	-7.33	113.64	122.22
2	D	122	PHE	CZ-CE2-CD2	-7.33	106.81	120.00
2	B	91	LEU	CA-C-O	7.32	128.51	120.82
1	C	3	SER	CB-CA-C	7.32	124.60	110.17
2	B	42	PHE	CG-CD1-CE1	-7.32	108.25	120.70
1	C	113	LEU	CD1-CG-CD2	7.32	126.90	110.80
2	D	139	ASN	O-C-N	-7.32	113.81	122.15
2	D	90	GLU	O-C-N	7.32	129.87	122.12
2	B	51	PRO	CA-C-O	7.31	130.09	119.34
1	A	48	LEU	CB-CG-CD2	7.31	132.62	110.70
1	C	44	PRO	N-CD-CG	-7.31	92.24	103.20
1	C	60	LYS	N-CA-C	7.29	119.23	111.28
1	C	125	LEU	O-C-N	-7.29	113.69	122.22
1	A	10	VAL	N-CA-C	-7.28	103.43	110.42
1	C	133	SER	CA-CB-OG	-7.28	96.53	111.10
2	D	124	PRO	CB-CA-C	7.28	119.81	110.92
2	D	75	LEU	CB-CA-C	7.28	122.88	110.79
2	D	133	VAL	CG1-CB-CG2	7.28	126.81	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	LYS	CB-CG-CD	7.26	128.01	111.30
2	D	121	GLU	OE1-CD-OE2	-7.26	105.47	122.90
1	C	99	LYS	CA-CB-CG	7.26	128.62	114.10
2	D	96	LEU	O-C-N	7.26	132.67	122.36
1	A	24	TYR	CA-CB-CG	-7.26	100.84	113.90
1	C	139	LYS	N-CA-C	-7.26	103.52	112.88
1	A	112	HIS	O-C-N	7.25	131.26	122.35
1	C	137	THR	O-C-N	7.25	131.01	122.24
1	A	117	PHE	O-C-N	7.24	132.22	122.59
1	C	52	SER	CA-C-N	7.24	131.67	120.82
1	C	52	SER	C-N-CA	7.24	131.67	120.82
2	D	145	TYR	CB-CG-CD2	-7.24	109.95	120.80
1	C	36	PHE	CA-C-N	-7.23	112.19	119.56
1	C	36	PHE	C-N-CA	-7.23	112.19	119.56
1	A	21	ALA	N-CA-C	-7.22	95.43	110.80
2	B	141	LEU	CB-CA-C	7.22	122.77	110.79
1	A	16	LYS	CA-C-O	7.21	130.83	120.51
2	D	86	ALA	CA-C-O	-7.21	112.91	120.55
2	B	20	VAL	CA-C-N	7.21	134.78	121.52
2	B	20	VAL	C-N-CA	7.21	134.78	121.52
2	D	85	PHE	N-CA-C	-7.21	104.48	113.20
2	D	36	PRO	N-CD-CG	7.21	114.01	103.20
2	D	144	LYS	N-CA-CB	7.21	122.35	110.39
1	C	122	HIS	CA-CB-CG	7.20	121.00	113.80
1	A	139	LYS	CA-C-N	7.19	130.64	120.28
1	A	139	LYS	C-N-CA	7.19	130.64	120.28
1	A	82	ALA	N-CA-C	-7.19	103.14	110.97
2	D	90	GLU	OE1-CD-OE2	-7.19	105.65	122.90
1	C	115	ALA	N-CA-CB	7.18	120.96	110.26
2	B	42	PHE	CA-C-O	7.18	128.64	119.95
2	B	118	PHE	CD1-CG-CD2	-7.18	107.83	118.60
1	A	126	ASP	CA-C-N	7.18	130.12	120.65
1	A	126	ASP	C-N-CA	7.18	130.12	120.65
2	D	24	GLY	CA-C-O	7.18	128.75	121.00
1	A	128	PHE	CG-CD2-CE2	7.17	132.89	120.70
2	B	131	GLN	N-CA-C	7.17	119.09	111.28
1	C	117	PHE	CE1-CZ-CE2	7.17	132.90	120.00
2	B	134	VAL	CB-CA-C	-7.16	102.64	112.02
2	D	131	GLN	CG-CD-OE1	-7.16	106.49	120.80
2	D	84	THR	CA-CB-OG1	-7.15	98.87	109.60
2	D	86	ALA	CA-C-N	-7.15	110.71	120.44
2	D	86	ALA	C-N-CA	-7.15	110.71	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	TRP	CD2-CE3-CZ3	7.15	127.90	118.60
1	C	56	LYS	CA-C-N	7.14	127.72	119.94
1	C	56	LYS	C-N-CA	7.14	127.72	119.94
1	C	14	TRP	N-CA-C	-7.14	103.83	112.54
1	C	47	ASP	CB-CG-OD1	-7.13	101.99	118.40
2	B	63	HIS	O-C-N	7.13	130.57	122.22
1	C	37	PRO	N-CD-CG	7.13	113.90	103.20
1	A	124	SER	O-C-N	7.13	130.28	122.15
1	C	26	ALA	O-C-N	-7.12	114.69	122.09
1	A	69	ALA	N-CA-CB	-7.11	99.34	110.30
1	C	87	HIS	CA-CB-CG	-7.11	106.69	113.80
1	A	61	LYS	CB-CA-C	-7.11	95.46	110.31
2	B	61	LYS	CD-CE-NZ	-7.10	89.17	111.90
2	D	61	LYS	CA-C-O	7.10	128.30	120.63
2	B	139	ASN	CB-CG-ND2	7.10	127.05	116.40
1	C	113	LEU	CB-CG-CD1	-7.09	89.44	110.70
2	B	124	PRO	CA-C-O	-7.08	110.29	120.56
2	D	75	LEU	N-CA-CB	-7.08	99.71	110.12
2	D	13	ALA	CA-C-N	-7.08	109.55	120.31
2	D	13	ALA	C-N-CA	-7.08	109.55	120.31
1	A	33	PHE	CB-CG-CD1	7.08	132.73	120.70
1	C	54	GLN	CA-C-N	-7.08	110.37	120.42
1	C	54	GLN	C-N-CA	-7.08	110.37	120.42
2	D	75	LEU	CB-CG-CD2	7.08	131.93	110.70
2	D	80	ASN	CB-CA-C	-7.08	96.34	110.42
2	D	19	ASN	O-C-N	-7.07	113.18	122.59
1	A	18	GLY	CA-C-O	-7.07	108.27	120.57
2	B	117	HIS	O-C-N	-7.07	114.73	122.09
1	C	83	LEU	CA-C-O	-7.07	110.77	119.18
1	C	79	ALA	N-CA-C	7.07	118.98	111.28
1	C	98	PHE	O-C-N	7.07	129.61	122.12
1	C	127	LYS	CA-C-O	-7.06	112.93	120.42
1	C	8	THR	CA-CB-OG1	-7.06	99.01	109.60
2	D	17	LYS	CA-C-N	7.05	131.40	121.66
2	D	17	LYS	C-N-CA	7.05	131.40	121.66
1	A	14	TRP	O-C-N	7.05	131.88	122.43
2	B	137	VAL	O-C-N	-7.05	115.03	121.87
1	A	24	TYR	N-CA-C	-7.05	103.67	111.36
2	B	145	TYR	CA-C-N	7.05	134.39	121.70
2	B	145	TYR	C-N-CA	7.05	134.39	121.70
1	C	20	HIS	CE1-NE2-CD2	7.05	116.05	109.00
2	D	17	LYS	N-CA-CB	7.05	121.44	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LEU	CB-CG-CD1	7.05	131.84	110.70
2	D	1	VAL	CB-CA-C	-7.04	98.02	111.40
1	A	106	LEU	CA-C-N	7.04	130.10	120.46
1	A	106	LEU	C-N-CA	7.04	130.10	120.46
2	D	60	VAL	CA-CB-CG1	-7.04	98.44	110.40
2	B	24	GLY	N-CA-C	7.03	120.66	112.50
1	A	54	GLN	N-CA-C	-7.03	103.04	111.69
1	A	57	GLY	CA-C-N	-7.03	110.31	120.29
1	A	57	GLY	C-N-CA	-7.03	110.31	120.29
1	C	65	ALA	O-C-N	-7.03	114.00	122.22
1	A	95	PRO	N-CA-C	-7.02	105.08	113.86
2	B	4	THR	CB-CA-C	7.02	124.00	110.17
1	C	17	VAL	N-CA-CB	7.01	122.80	111.23
1	C	100	LEU	CB-CA-C	7.01	121.89	110.88
1	A	116	GLU	OE1-CD-OE2	-7.01	106.08	122.90
2	D	7	GLU	CA-CB-CG	-7.01	100.08	114.10
2	B	85	PHE	CD1-CE1-CZ	7.01	132.61	120.00
1	A	50	HIS	N-CA-C	7.00	121.46	110.32
1	C	110	ALA	CA-C-N	7.00	129.67	120.28
1	C	110	ALA	C-N-CA	7.00	129.67	120.28
2	B	97	HIS	CB-CG-CD2	-7.00	122.10	131.20
1	A	31	ARG	CA-C-O	-7.00	113.47	120.82
1	C	60	LYS	CD-CE-NZ	-7.00	89.51	111.90
1	C	98	PHE	N-CA-CB	7.00	120.55	110.06
2	B	142	ALA	N-CA-C	-6.99	104.72	113.18
2	D	63	HIS	CA-C-N	-6.99	111.33	120.13
2	D	63	HIS	C-N-CA	-6.99	111.33	120.13
1	C	131	SER	CB-CA-C	-6.99	97.25	110.67
2	D	61	LYS	O-C-N	-6.99	114.71	122.12
1	A	100	LEU	CD1-CG-CD2	-6.99	95.43	110.80
1	C	113	LEU	CB-CG-CD2	6.99	131.66	110.70
1	A	85	ASP	CB-CG-OD1	6.98	134.46	118.40
2	B	3	LEU	CD1-CG-CD2	-6.98	95.44	110.80
2	D	45	PHE	CA-C-N	-6.98	107.73	121.41
2	D	45	PHE	C-N-CA	-6.98	107.73	121.41
2	B	73	ASP	CA-C-N	6.98	135.09	121.41
2	B	73	ASP	C-N-CA	6.98	135.09	121.41
2	D	93	CYS	CA-CB-SG	-6.97	98.36	114.40
1	C	118	THR	O-C-N	6.97	133.03	120.56
2	D	99	ASP	CA-C-N	6.97	127.55	119.47
2	D	99	ASP	C-N-CA	6.97	127.55	119.47
1	A	122	HIS	CG-CD2-NE2	6.96	114.16	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	LYS	CA-C-O	-6.96	110.19	119.11
2	D	48	LEU	O-C-N	6.96	130.62	122.19
1	A	27	GLU	N-CA-CB	-6.96	99.89	110.12
1	A	86	LEU	CA-C-O	6.96	127.79	120.42
1	A	63	ALA	N-CA-CB	-6.95	99.07	110.40
1	A	77	PRO	N-CA-C	6.95	126.78	112.47
2	B	21	ASP	N-CA-C	-6.95	103.80	112.90
1	A	117	PHE	CD1-CG-CD2	6.94	129.01	118.60
2	D	139	ASN	N-CA-C	-6.94	103.80	111.36
2	D	3	LEU	CA-CB-CG	-6.93	92.04	116.30
2	B	68	LEU	CB-CG-CD1	-6.93	89.92	110.70
1	C	75	ASP	N-CA-CB	-6.92	99.84	111.96
2	B	78	LEU	N-CA-C	-6.92	104.82	113.20
2	B	89	SER	CA-CB-OG	-6.92	97.26	111.10
1	C	58	HIS	CA-C-N	-6.92	111.50	120.14
1	C	58	HIS	C-N-CA	-6.92	111.50	120.14
1	A	97	ASN	CA-CB-CG	-6.92	105.69	112.60
1	C	94	ASP	O-C-N	6.91	128.42	121.30
1	C	95	PRO	CA-C-N	6.91	131.63	120.30
1	C	95	PRO	C-N-CA	6.91	131.63	120.30
2	B	10	ALA	CB-CA-C	-6.91	96.29	110.38
2	B	74	GLY	N-CA-C	6.90	129.54	113.18
2	D	40	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	C	117	PHE	CA-C-N	-6.89	112.09	122.29
1	C	117	PHE	C-N-CA	-6.89	112.09	122.29
2	D	125	PRO	CA-C-O	6.89	130.61	119.86
1	A	55	VAL	O-C-N	-6.89	115.16	121.91
1	C	48	LEU	CB-CG-CD1	6.89	131.36	110.70
1	A	76	MET	CG-SD-CE	6.88	116.04	100.90
2	D	144	LYS	CB-CA-C	6.88	124.69	110.31
2	B	34	VAL	CA-C-O	-6.88	113.04	120.47
1	C	81	SER	CA-C-N	-6.87	110.38	120.28
1	C	81	SER	C-N-CA	-6.87	110.38	120.28
2	D	144	LYS	CD-CE-NZ	6.87	133.89	111.90
2	D	81	LEU	CA-C-N	-6.86	110.98	120.38
2	D	81	LEU	C-N-CA	-6.86	110.98	120.38
1	C	105	LEU	CB-CG-CD2	-6.86	90.12	110.70
2	D	77	HIS	CG-ND1-CE1	-6.86	97.64	109.30
2	D	122	PHE	CD1-CG-CD2	-6.86	108.31	118.60
2	D	11	VAL	CA-C-N	-6.85	110.56	120.29
2	D	11	VAL	C-N-CA	-6.85	110.56	120.29
1	A	50	HIS	ND1-CE1-NE2	-6.85	101.55	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	ARG	CB-CG-CD	-6.85	95.55	111.30
2	D	37	TRP	CE3-CZ3-CH2	-6.85	112.20	121.10
1	C	43	PHE	CE1-CZ-CE2	-6.84	107.68	120.00
1	A	78	ASN	N-CA-C	-6.84	103.90	111.36
2	B	126	VAL	CG1-CB-CG2	-6.84	95.75	110.80
1	A	118	THR	N-CA-CB	-6.84	101.31	109.59
1	A	49	SER	O-C-N	-6.83	115.24	122.96
2	B	81	LEU	O-C-N	-6.82	114.89	122.12
1	A	87	HIS	CA-C-O	-6.82	110.86	119.31
1	C	58	HIS	ND1-CG-CD2	6.82	112.92	106.10
2	D	100	PRO	CA-N-CD	-6.81	102.47	112.00
1	A	43	PHE	CZ-CE2-CD2	-6.81	107.75	120.00
1	C	76	MET	N-CA-CB	-6.81	98.25	110.37
1	A	105	LEU	CA-C-O	-6.80	111.76	119.79
2	D	33	VAL	CB-CA-C	6.80	120.65	111.87
1	C	90	LYS	CA-CB-CG	-6.80	100.49	114.10
2	B	111	VAL	CB-CA-C	6.80	120.58	111.88
2	D	53	ALA	CA-C-N	-6.80	111.15	120.46
2	D	53	ALA	C-N-CA	-6.80	111.15	120.46
1	A	43	PHE	CG-CD2-CE2	6.80	132.25	120.70
1	A	84	SER	CB-CA-C	-6.80	97.62	110.67
2	B	45	PHE	CG-CD1-CE1	-6.79	109.15	120.70
2	B	61	LYS	CB-CA-C	-6.79	98.06	110.63
1	A	58	HIS	CG-ND1-CE1	-6.79	97.75	109.30
1	C	105	LEU	CA-C-N	-6.79	111.38	120.54
1	C	105	LEU	C-N-CA	-6.79	111.38	120.54
2	B	31	LEU	O-C-N	-6.78	114.82	122.08
1	A	71	ALA	CA-C-N	6.78	134.71	123.25
1	A	71	ALA	C-N-CA	6.78	134.71	123.25
1	C	133	SER	N-CA-CB	6.78	120.04	109.94
1	C	38	THR	N-CA-C	6.77	118.66	111.28
1	A	9	ASN	OD1-CG-ND2	-6.76	115.84	122.60
2	B	21	ASP	CB-CG-OD1	-6.76	102.85	118.40
2	D	128	ALA	O-C-N	6.76	129.29	122.12
2	D	85	PHE	CE1-CZ-CE2	-6.76	107.83	120.00
2	B	124	PRO	N-CA-CB	6.75	109.63	103.08
1	C	16	LYS	CA-C-O	6.75	127.76	119.79
1	C	126	ASP	N-CA-C	-6.75	104.00	111.36
1	A	20	HIS	CA-C-O	-6.75	111.67	119.56
2	B	17	LYS	CA-CB-CG	-6.74	100.62	114.10
1	C	130	ALA	CA-C-O	6.74	127.89	120.82
2	D	145	TYR	CG-CD1-CE1	6.73	131.30	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	HIS	CB-CA-C	-6.73	99.96	111.46
2	B	37	TRP	N-CA-CB	-6.72	99.53	110.42
1	A	10	VAL	CA-C-O	-6.72	114.05	121.17
2	D	57	ASN	CB-CG-ND2	-6.72	106.32	116.40
1	C	38	THR	CA-CB-CG2	-6.72	99.08	110.50
2	D	143	HIS	CA-C-N	6.72	131.94	120.72
2	D	143	HIS	C-N-CA	6.72	131.94	120.72
2	B	106	LEU	O-C-N	-6.72	114.49	122.15
2	D	19	ASN	CB-CA-C	6.71	123.78	110.42
2	B	41	PHE	N-CA-C	-6.71	105.13	113.38
1	C	118	THR	CB-CA-C	-6.71	96.12	111.89
1	C	29	LEU	N-CA-C	6.71	118.59	111.28
2	D	39	GLN	O-C-N	-6.70	111.69	122.41
2	D	79	ASP	O-C-N	6.70	130.50	122.26
2	D	88	LEU	CD1-CG-CD2	6.70	125.54	110.80
2	B	118	PHE	CB-CG-CD2	6.70	132.09	120.70
2	D	44	SER	CA-C-O	6.70	127.76	119.05
2	D	44	SER	CA-C-N	6.69	134.51	122.06
2	D	44	SER	C-N-CA	6.69	134.51	122.06
2	D	18	VAL	N-CA-C	-6.69	100.06	108.89
2	D	118	PHE	CA-CB-CG	-6.67	107.13	113.80
2	B	17	LYS	CB-CA-C	-6.67	98.95	110.09
1	A	91	LEU	O-C-N	6.67	130.24	122.17
1	C	113	LEU	O-C-N	6.67	128.99	121.32
1	C	115	ALA	N-CA-C	6.67	121.72	112.45
1	A	64	ASP	N-CA-CB	-6.66	100.05	110.30
2	D	143	HIS	ND1-CE1-NE2	6.65	115.05	108.40
2	B	78	LEU	CB-CG-CD2	6.65	130.65	110.70
1	A	74	ASP	CA-C-N	6.64	134.54	122.92
1	A	74	ASP	C-N-CA	6.64	134.54	122.92
1	A	83	LEU	O-C-N	-6.64	112.73	122.43
1	C	137	THR	N-CA-C	-6.64	104.40	113.30
2	D	5	PRO	CB-CG-CD	6.64	127.34	106.10
2	B	116	HIS	O-C-N	-6.63	114.93	122.09
2	B	27	ALA	O-C-N	-6.63	114.59	122.15
2	B	11	VAL	N-CA-CB	-6.63	103.40	110.62
1	A	30	GLU	CB-CG-CD	-6.62	101.34	112.60
2	B	23	VAL	CA-C-O	-6.62	114.06	120.95
1	A	85	ASP	O-C-N	-6.62	114.13	122.27
1	A	48	LEU	N-CA-C	6.62	121.25	112.25
1	A	84	SER	N-CA-C	6.60	119.48	111.82
1	A	22	GLY	N-CA-C	6.60	128.82	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	LEU	N-CA-C	-6.60	105.23	113.28
1	A	3	SER	CA-CB-OG	6.59	124.29	111.10
2	B	4	THR	N-CA-C	6.59	124.38	109.81
2	D	25	GLY	CA-C-O	-6.59	113.96	120.75
1	A	103	HIS	N-CA-CB	6.59	120.92	109.72
2	B	66	LYS	CA-CB-CG	6.58	127.27	114.10
1	C	104	CYS	O-C-N	6.58	129.10	122.12
2	B	126	VAL	CA-C-N	6.58	134.11	121.54
2	B	126	VAL	C-N-CA	6.58	134.11	121.54
2	B	66	LYS	CD-CE-NZ	-6.58	90.86	111.90
1	A	134	THR	CA-C-N	6.57	131.60	120.29
1	A	134	THR	C-N-CA	6.57	131.60	120.29
2	D	131	GLN	O-C-N	-6.57	115.15	122.12
1	A	90	LYS	CG-CD-CE	-6.57	96.18	111.30
2	D	53	ALA	O-C-N	-6.57	115.05	122.08
1	C	59	GLY	N-CA-C	6.57	121.85	113.24
1	A	103	HIS	CG-ND1-CE1	-6.57	98.14	109.30
2	B	106	LEU	CD1-CG-CD2	6.56	125.24	110.80
1	C	141	ARG	CG-CD-NE	-6.56	97.56	112.00
2	B	9	SER	O-C-N	6.56	129.90	122.22
2	D	72	SER	O-C-N	-6.56	113.86	122.59
2	B	36	PRO	O-C-N	-6.56	112.99	122.37
2	D	41	PHE	CA-CB-CG	-6.56	107.24	113.80
1	A	43	PHE	CA-C-N	-6.55	113.18	120.45
1	A	43	PHE	C-N-CA	-6.55	113.18	120.45
1	C	24	TYR	OH-CZ-CE2	-6.55	100.24	119.90
1	A	17	VAL	CA-CB-CG2	6.55	121.53	110.40
2	B	14	LEU	N-CA-C	6.55	118.07	111.07
1	A	48	LEU	CB-CA-C	-6.54	102.05	111.14
2	B	93	CYS	CA-C-N	-6.54	109.56	120.68
2	B	93	CYS	C-N-CA	-6.54	109.56	120.68
2	B	19	ASN	CB-CG-OD1	6.54	133.88	120.80
2	D	62	ALA	CA-C-O	6.53	127.47	120.55
1	A	18	GLY	CA-C-N	-6.51	112.44	122.60
1	A	18	GLY	C-N-CA	-6.51	112.44	122.60
1	A	39	THR	CA-C-N	-6.51	108.88	121.58
1	A	39	THR	C-N-CA	-6.51	108.88	121.58
1	C	23	GLU	O-C-N	6.51	128.78	122.07
1	C	74	ASP	N-CA-CB	-6.51	99.47	110.41
1	A	33	PHE	CZ-CE2-CD2	6.51	131.72	120.00
2	B	113	VAL	CA-C-N	6.51	129.33	120.54
2	B	113	VAL	C-N-CA	6.51	129.33	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	PHE	CA-CB-CG	-6.51	107.29	113.80
2	D	17	LYS	CD-CE-NZ	-6.51	91.08	111.90
1	A	43	PHE	CB-CG-CD2	6.50	131.75	120.70
1	C	64	ASP	CB-CG-OD2	-6.50	103.45	118.40
1	C	138	SER	CB-CA-C	-6.50	98.61	110.63
2	D	36	PRO	N-CA-CB	-6.50	97.30	103.41
2	B	101	GLU	CB-CG-CD	-6.50	101.56	112.60
2	B	106	LEU	CA-C-N	6.49	128.47	120.22
2	B	106	LEU	C-N-CA	6.49	128.47	120.22
1	C	48	LEU	CA-C-O	6.48	128.49	119.80
2	B	63	HIS	CA-C-N	-6.48	112.79	119.98
2	B	63	HIS	C-N-CA	-6.48	112.79	119.98
1	C	129	LEU	CA-C-N	6.48	128.86	120.44
1	C	129	LEU	C-N-CA	6.48	128.86	120.44
1	A	24	TYR	CB-CA-C	-6.48	99.84	110.85
1	A	62	VAL	CG1-CB-CG2	-6.47	96.57	110.80
1	C	130	ALA	N-CA-CB	6.47	119.39	110.01
1	A	35	SER	CA-C-O	6.46	127.15	119.60
2	B	22	GLU	O-C-N	6.46	129.98	122.17
2	B	100	PRO	CA-C-O	-6.45	110.47	118.99
1	A	98	PHE	CA-CB-CG	-6.44	107.36	113.80
2	B	6	GLU	CA-C-N	6.44	133.84	121.54
2	B	6	GLU	C-N-CA	6.44	133.84	121.54
1	A	67	THR	CA-C-O	6.44	127.79	120.90
2	D	142	ALA	CA-C-N	6.44	129.20	120.38
2	D	142	ALA	C-N-CA	6.44	129.20	120.38
2	B	82	LYS	CG-CD-CE	-6.43	96.50	111.30
2	B	58	PRO	N-CA-C	6.43	122.47	113.53
2	D	49	SER	CA-C-O	-6.43	111.82	119.15
2	B	91	LEU	CB-CA-C	6.42	120.97	110.88
2	B	139	ASN	N-CA-C	6.42	120.38	112.54
1	A	96	VAL	O-C-N	-6.42	115.39	121.87
1	A	84	SER	N-CA-CB	6.42	120.23	110.28
2	D	85	PHE	CZ-CE2-CD2	6.42	131.55	120.00
1	A	124	SER	CA-C-N	-6.41	110.57	120.31
1	A	124	SER	C-N-CA	-6.41	110.57	120.31
1	A	140	TYR	N-CA-CB	6.41	120.08	110.22
2	B	19	ASN	O-C-N	6.40	130.61	122.93
1	A	106	LEU	CA-CB-CG	6.40	138.70	116.30
2	B	28	LEU	CB-CA-C	6.40	121.46	110.84
2	D	137	VAL	CA-C-O	6.40	127.38	120.47
2	B	81	LEU	N-CA-C	6.40	118.25	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	SER	CA-C-N	-6.40	112.62	122.60
1	C	138	SER	C-N-CA	-6.40	112.62	122.60
2	B	111	VAL	N-CA-C	-6.39	103.65	110.36
2	B	144	LYS	N-CA-C	-6.39	105.11	113.17
1	C	14	TRP	CE2-CD2-CE3	6.39	125.19	118.80
2	B	50	THR	CA-C-N	-6.39	112.42	119.19
2	B	50	THR	C-N-CA	-6.39	112.42	119.19
2	D	112	CYS	N-CA-CB	6.39	119.46	109.94
2	B	121	GLU	CB-CG-CD	-6.38	101.75	112.60
1	A	54	GLN	CA-C-N	-6.38	112.53	120.56
1	A	54	GLN	C-N-CA	-6.38	112.53	120.56
2	D	132	LYS	CG-CD-CE	-6.38	96.64	111.30
1	A	75	ASP	CA-C-N	-6.37	106.26	121.80
1	A	75	ASP	C-N-CA	-6.37	106.26	121.80
1	A	76	MET	N-CA-CB	-6.37	99.04	110.37
2	B	17	LYS	N-CA-CB	6.36	119.91	110.49
2	B	110	LEU	CB-CA-C	6.36	120.99	110.81
1	C	99	LYS	N-CA-C	6.36	118.22	111.28
1	A	130	ALA	O-C-N	-6.36	114.90	122.15
2	B	94	ASP	N-CA-C	-6.36	104.21	112.23
1	A	4	PRO	O-C-N	-6.36	112.82	122.74
2	D	105	LEU	CB-CG-CD1	6.36	129.77	110.70
2	D	113	VAL	O-C-N	-6.35	115.29	121.83
1	C	68	ASN	N-CA-C	6.35	118.20	111.28
2	B	8	LYS	CA-C-O	6.35	127.69	120.90
1	C	7	LYS	N-CA-C	6.35	121.85	111.37
1	C	117	PHE	N-CA-C	6.34	120.53	110.70
1	A	8	THR	CB-CA-C	6.34	121.31	110.79
1	C	141	ARG	NH1-CZ-NH2	6.33	127.53	119.30
1	A	73	VAL	CA-CB-CG1	6.33	121.16	110.40
2	B	5	PRO	N-CD-CG	-6.33	93.71	103.20
1	A	138	SER	N-CA-C	6.32	118.98	111.71
2	B	60	VAL	CG1-CB-CG2	6.32	124.71	110.80
1	C	110	ALA	CB-CA-C	6.32	121.33	110.84
1	C	101	LEU	CA-C-O	-6.32	112.70	119.97
2	D	45	PHE	CE1-CZ-CE2	-6.32	108.62	120.00
2	B	114	LEU	O-C-N	6.32	128.66	122.09
2	B	38	THR	CA-C-N	6.31	129.59	120.38
2	B	38	THR	C-N-CA	6.31	129.59	120.38
1	C	82	ALA	N-CA-C	6.31	118.96	111.71
2	D	78	LEU	O-C-N	-6.31	114.20	122.59
2	B	107	GLY	CA-C-O	-6.30	113.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	57	ASN	CB-CG-OD1	6.30	133.41	120.80
1	A	38	THR	CA-CB-CG2	-6.30	99.79	110.50
1	A	97	ASN	CA-C-O	-6.30	111.04	119.11
1	C	126	ASP	O-C-N	-6.30	114.97	122.15
2	B	96	LEU	CB-CG-CD2	-6.29	91.83	110.70
2	B	92	HIS	CG-ND1-CE1	-6.29	98.61	109.30
2	B	37	TRP	CD2-CE3-CZ3	-6.28	110.43	118.60
1	A	98	PHE	CB-CG-CD1	-6.28	110.02	120.70
1	C	104	CYS	CA-C-N	-6.28	111.90	120.44
1	C	104	CYS	C-N-CA	-6.28	111.90	120.44
2	D	47	ASP	CA-C-O	-6.28	114.05	120.71
2	D	71	PHE	CB-CG-CD2	-6.28	110.03	120.70
2	D	98	VAL	CA-C-O	-6.28	113.31	120.65
1	A	99	LYS	CA-CB-CG	6.27	126.64	114.10
2	D	98	VAL	CA-CB-CG2	-6.27	99.74	110.40
2	D	4	THR	CA-CB-OG1	-6.27	100.20	109.60
2	B	35	TYR	CD1-CG-CD2	-6.26	108.71	118.10
2	B	88	LEU	CD1-CG-CD2	-6.26	97.03	110.80
2	B	63	HIS	CE1-NE2-CD2	6.25	115.25	109.00
2	D	135	ALA	N-CA-CB	6.25	119.14	110.07
1	A	33	PHE	CB-CG-CD2	-6.24	110.09	120.70
1	C	37	PRO	CA-N-CD	-6.24	103.26	112.00
2	D	97	HIS	N-CA-CB	6.24	121.04	110.49
2	B	48	LEU	O-C-N	6.24	129.93	122.26
2	D	39	GLN	N-CA-CB	-6.24	99.44	110.42
2	B	71	PHE	N-CA-CB	-6.23	100.97	110.12
1	C	62	VAL	O-C-N	6.23	127.91	121.87
1	A	21	ALA	N-CA-CB	6.22	121.00	110.49
1	C	93	VAL	N-CA-CB	-6.22	103.75	110.53
1	C	14	TRP	CD1-CG-CD2	6.21	116.24	106.30
2	B	5	PRO	CB-CG-CD	6.21	125.97	106.10
2	B	133	VAL	CA-C-N	6.21	128.51	120.56
2	B	133	VAL	C-N-CA	6.21	128.51	120.56
2	B	99	ASP	OD1-CG-OD2	6.21	137.79	122.90
1	C	77	PRO	N-CA-CB	-6.20	96.19	103.26
1	C	1	VAL	CB-CA-C	-6.20	99.62	111.40
2	D	120	LYS	N-CA-CB	-6.20	102.00	110.56
2	B	27	ALA	N-CA-CB	-6.20	100.99	110.16
2	D	18	VAL	N-CA-CB	6.20	117.28	110.53
2	B	12	THR	CA-CB-CG2	-6.19	99.97	110.50
2	B	77	HIS	CA-C-O	-6.18	113.92	121.89
1	A	64	ASP	CB-CA-C	-6.18	97.78	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	ALA	CA-C-N	-6.17	112.64	120.60
1	C	69	ALA	C-N-CA	-6.17	112.64	120.60
2	B	82	LYS	CA-C-O	6.17	127.07	119.97
1	A	135	VAL	N-CA-C	-6.17	103.17	111.44
2	B	30	ARG	NE-CZ-NH1	-6.17	115.33	121.50
2	B	6	GLU	CB-CA-C	-6.16	97.81	110.38
2	B	97	HIS	CA-C-N	-6.16	115.02	122.90
2	B	97	HIS	C-N-CA	-6.16	115.02	122.90
1	C	119	PRO	N-CA-CB	6.16	109.71	103.25
1	A	24	TYR	CZ-CE2-CD2	-6.16	108.52	119.60
1	A	96	VAL	CA-CB-CG1	6.16	120.87	110.40
2	B	48	LEU	CB-CG-CD2	6.15	129.15	110.70
1	A	43	PHE	CD1-CE1-CZ	6.15	131.07	120.00
1	A	132	VAL	N-CA-C	-6.14	104.36	110.62
2	B	46	GLY	CA-C-O	-6.14	109.89	120.57
1	A	78	ASN	CB-CA-C	-6.13	100.42	110.85
2	D	122	PHE	CD1-CE1-CZ	-6.13	108.96	120.00
1	A	94	ASP	N-CA-C	-6.13	101.32	109.84
2	D	5	PRO	O-C-N	-6.13	111.05	122.33
1	A	83	LEU	CB-CA-C	-6.13	97.76	109.95
2	B	6	GLU	CG-CD-OE2	6.12	132.48	118.40
1	A	55	VAL	N-CA-CB	-6.12	103.39	110.55
2	D	144	LYS	CA-C-N	6.12	129.44	120.82
2	D	144	LYS	C-N-CA	6.12	129.44	120.82
1	A	42	TYR	CD1-CE1-CZ	6.11	130.60	119.60
1	A	122	HIS	N-CA-C	-6.11	97.79	110.80
1	C	137	THR	CA-C-O	-6.10	112.06	119.32
2	B	32	LEU	CA-C-O	6.10	126.87	119.31
2	D	7	GLU	CA-C-N	-6.10	111.04	120.31
2	D	7	GLU	C-N-CA	-6.10	111.04	120.31
2	D	68	LEU	N-CA-CB	6.10	120.34	110.40
2	B	102	ASN	CB-CG-ND2	-6.09	107.26	116.40
2	D	127	GLN	CB-CA-C	6.09	120.85	110.74
2	B	123	THR	CA-CB-OG1	6.09	118.73	109.60
1	A	45	HIS	CA-C-O	6.08	126.42	119.18
1	A	24	TYR	CD1-CE1-CZ	6.08	130.55	119.60
1	C	77	PRO	CA-CB-CG	6.08	116.05	104.50
2	D	66	LYS	CB-CG-CD	6.08	125.27	111.30
2	B	57	ASN	CB-CG-ND2	-6.07	107.30	116.40
1	C	80	LEU	CB-CA-C	-6.07	100.93	110.94
1	A	16	LYS	CB-CG-CD	-6.06	97.35	111.30
1	A	99	LYS	CA-C-O	-6.06	111.92	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	14	LEU	CA-C-N	-6.05	110.55	121.14
2	D	14	LEU	C-N-CA	-6.05	110.55	121.14
1	A	11	LYS	O-C-N	-6.04	114.33	122.43
1	C	33	PHE	O-C-N	-6.04	115.15	122.22
1	A	87	HIS	CB-CG-ND1	-6.04	113.64	122.70
2	D	77	HIS	O-C-N	-6.04	114.56	122.59
1	A	56	LYS	CB-CA-C	6.04	122.43	110.42
1	A	83	LEU	N-CA-CB	-6.04	100.27	110.41
2	D	15	TRP	CZ3-CH2-CZ2	6.03	129.34	121.50
1	C	10	VAL	CB-CA-C	-6.02	103.91	112.22
2	D	102	ASN	O-C-N	-6.02	114.86	122.27
1	A	59	GLY	N-CA-C	6.02	121.12	113.24
2	B	44	SER	N-CA-C	-6.02	103.68	111.02
2	D	117	HIS	CE1-NE2-CD2	6.01	115.01	109.00
2	D	122	PHE	CG-CD2-CE2	6.01	130.91	120.70
1	C	85	ASP	CB-CG-OD1	6.00	132.20	118.40
2	B	116	HIS	ND1-CE1-NE2	6.00	114.40	108.40
1	A	30	GLU	CA-CB-CG	-5.99	102.12	114.10
2	B	22	GLU	N-CA-CB	-5.99	101.27	110.13
2	B	70	ALA	N-CA-C	5.99	117.47	111.07
1	C	141	ARG	CA-C-O	-5.99	103.04	121.00
1	A	87	HIS	CE1-NE2-CD2	-5.98	103.02	109.00
2	B	23	VAL	CG1-CB-CG2	5.97	123.94	110.80
1	C	128	PHE	CB-CG-CD1	-5.97	110.55	120.70
2	B	13	ALA	CB-CA-C	-5.97	101.51	110.88
2	B	67	VAL	CG1-CB-CG2	5.97	123.93	110.80
1	A	50	HIS	CA-C-O	-5.96	114.21	121.36
2	D	22	GLU	CB-CG-CD	5.96	122.73	112.60
2	B	114	LEU	CA-C-O	-5.95	114.53	120.90
2	D	15	TRP	NE1-CE2-CZ2	5.95	139.03	130.10
1	A	60	LYS	CG-CD-CE	-5.94	97.63	111.30
2	D	29	GLY	O-C-N	5.94	130.43	122.70
2	B	120	LYS	CB-CA-C	-5.94	98.13	109.95
2	D	58	PRO	N-CA-CB	5.94	109.49	103.25
1	A	119	PRO	O-C-N	-5.94	114.63	122.64
2	D	116	HIS	CB-CG-CD2	-5.94	123.48	131.20
2	B	5	PRO	CB-CA-C	-5.93	103.65	112.55
2	B	30	ARG	N-CA-C	-5.93	105.54	112.89
1	C	112	HIS	CA-C-O	-5.92	112.72	119.41
2	B	103	PHE	N-CA-C	-5.92	104.73	111.07
1	C	128	PHE	CD1-CE1-CZ	5.92	130.66	120.00
1	A	87	HIS	CA-C-N	-5.92	112.39	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	HIS	C-N-CA	-5.92	112.39	120.44
2	B	45	PHE	CA-C-O	-5.92	112.05	120.51
2	D	143	HIS	CB-CA-C	5.92	120.74	110.68
2	B	119	GLY	O-C-N	-5.92	114.39	122.55
1	C	20	HIS	CA-CB-CG	5.91	119.71	113.80
2	D	60	VAL	CA-CB-CG2	5.91	120.45	110.40
2	B	28	LEU	N-CA-CB	5.91	119.77	109.72
1	A	114	PRO	CA-C-O	-5.91	110.57	119.55
2	B	102	ASN	O-C-N	-5.91	115.00	122.27
1	A	103	HIS	O-C-N	-5.90	115.06	122.20
1	C	109	LEU	N-CA-C	-5.90	103.83	111.02
2	B	79	ASP	OD1-CG-OD2	-5.89	108.75	122.90
1	C	76	MET	N-CA-C	5.89	122.82	109.81
1	C	118	THR	CA-C-O	-5.88	111.14	121.67
1	A	140	TYR	CD1-CE1-CZ	5.88	130.19	119.60
1	A	29	LEU	N-CA-C	5.88	117.36	111.07
2	B	89	SER	CB-CA-C	5.88	120.11	110.88
1	C	135	VAL	CA-C-O	-5.88	115.00	121.29
1	C	67	THR	N-CA-C	-5.88	104.78	111.07
1	A	70	VAL	CG1-CB-CG2	-5.87	97.88	110.80
2	B	43	GLU	CA-C-O	5.87	126.53	119.43
2	B	54	VAL	CG1-CB-CG2	5.87	123.72	110.80
1	A	30	GLU	O-C-N	5.87	128.34	122.12
2	B	136	GLY	N-CA-C	-5.87	105.69	112.50
1	C	133	SER	CA-C-N	5.87	128.14	120.28
1	C	133	SER	C-N-CA	5.87	128.14	120.28
1	C	51	GLY	O-C-N	-5.86	115.59	122.45
1	C	122	HIS	CG-CD2-NE2	-5.86	101.34	107.20
2	B	93	CYS	N-CA-CB	-5.86	101.46	110.07
1	A	122	HIS	CB-CG-ND1	-5.85	113.92	122.70
2	B	104	ARG	CG-CD-NE	-5.85	99.13	112.00
2	D	71	PHE	CB-CG-CD1	-5.85	110.75	120.70
2	B	90	GLU	CG-CD-OE2	-5.85	104.95	118.40
1	C	139	LYS	CB-CG-CD	-5.85	97.85	111.30
1	A	63	ALA	N-CA-C	5.84	120.14	112.89
1	A	58	HIS	CB-CG-CD2	-5.84	123.61	131.20
2	B	7	GLU	CA-C-O	-5.84	112.16	120.51
1	A	2	LEU	CA-C-N	-5.84	107.55	121.80
1	A	2	LEU	C-N-CA	-5.84	107.55	121.80
2	D	91	LEU	N-CA-CB	-5.84	101.54	110.12
1	C	14	TRP	CA-CB-CG	-5.84	102.51	113.60
2	D	90	GLU	N-CA-CB	-5.83	101.31	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	ARG	NE-CZ-NH2	-5.83	113.95	119.20
2	D	100	PRO	CA-C-O	-5.83	110.43	119.64
2	D	91	LEU	CA-C-N	-5.83	110.22	121.58
2	D	91	LEU	C-N-CA	-5.83	110.22	121.58
1	A	30	GLU	N-CA-C	5.82	118.38	111.33
1	A	90	LYS	CB-CG-CD	5.82	124.69	111.30
2	B	26	GLU	N-CA-C	-5.82	104.84	111.07
2	B	38	THR	N-CA-C	-5.82	105.02	111.71
2	B	117	HIS	CG-ND1-CE1	-5.82	99.41	109.30
2	D	9	SER	N-CA-C	5.81	119.55	112.23
1	A	60	LYS	CA-C-N	-5.80	111.03	120.72
1	A	60	LYS	C-N-CA	-5.80	111.03	120.72
1	A	5	ALA	N-CA-C	-5.80	106.03	113.23
1	A	40	LYS	CB-CA-C	-5.80	98.40	109.95
1	A	132	VAL	CA-CB-CG1	5.80	120.26	110.40
2	D	86	ALA	N-CA-C	-5.80	104.96	111.28
1	C	21	ALA	N-CA-CB	-5.80	100.69	110.49
1	A	39	THR	CA-CB-OG1	5.80	118.30	109.60
2	D	22	GLU	CB-CA-C	5.80	121.96	110.42
2	D	13	ALA	CB-CA-C	-5.79	101.54	110.81
1	A	87	HIS	N-CA-C	-5.79	105.71	112.89
2	B	81	LEU	CA-CB-CG	5.79	136.56	116.30
2	D	80	ASN	CB-CG-OD1	-5.79	109.22	120.80
2	B	126	VAL	CB-CA-C	-5.79	102.73	112.16
1	C	125	LEU	CA-C-O	5.78	126.63	120.10
2	D	131	GLN	N-CA-C	5.78	117.58	111.28
1	A	141	ARG	CB-CG-CD	-5.78	98.00	111.30
2	B	104	ARG	CA-C-O	5.78	126.61	119.97
2	D	35	TYR	O-C-N	5.77	126.61	121.36
1	C	7	LYS	O-C-N	-5.77	115.47	122.11
1	A	122	HIS	CE1-NE2-CD2	-5.77	103.23	109.00
2	B	41	PHE	CG-CD2-CE2	-5.76	110.90	120.70
2	B	52	ASP	CA-CB-CG	-5.76	106.84	112.60
2	D	98	VAL	CB-CA-C	-5.76	103.99	110.96
2	B	47	ASP	O-C-N	5.76	129.91	123.05
2	B	85	PHE	CB-CA-C	5.76	120.77	109.72
1	A	85	ASP	OD1-CG-OD2	-5.75	109.10	122.90
1	C	35	SER	O-C-N	-5.75	114.62	122.33
1	C	89	HIS	CB-CA-C	5.75	122.11	110.38
1	C	57	GLY	CA-C-O	5.75	127.34	120.90
2	D	139	ASN	CB-CA-C	-5.75	101.08	110.85
2	B	20	VAL	CA-CB-CG1	-5.75	100.63	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	VAL	CA-C-N	-5.74	110.38	121.58
1	C	73	VAL	C-N-CA	-5.74	110.38	121.58
2	D	106	LEU	O-C-N	-5.74	115.21	122.27
2	D	127	GLN	CG-CD-NE2	-5.74	107.79	116.40
2	D	40	ARG	NH1-CZ-NH2	5.74	126.76	119.30
1	C	31	ARG	NH1-CZ-NH2	5.74	126.76	119.30
2	B	101	GLU	CG-CD-OE1	-5.73	105.23	118.40
2	D	11	VAL	CA-C-O	-5.73	114.69	121.05
1	C	31	ARG	O-C-N	5.72	127.97	122.07
1	C	46	PHE	CD1-CE1-CZ	5.72	130.30	120.00
2	B	119	GLY	CA-C-O	5.72	129.06	121.51
1	C	78	ASN	CB-CA-C	5.72	121.80	110.42
2	D	122	PHE	CA-CB-CG	-5.72	108.08	113.80
2	B	71	PHE	CZ-CE2-CD2	5.71	130.29	120.00
1	A	72	HIS	CA-C-N	5.71	128.58	120.53
1	A	72	HIS	C-N-CA	5.71	128.58	120.53
2	D	62	ALA	CA-C-N	-5.70	110.83	120.58
2	D	62	ALA	C-N-CA	-5.70	110.83	120.58
2	D	113	VAL	CA-C-N	5.70	127.86	120.44
2	D	113	VAL	C-N-CA	5.70	127.86	120.44
1	A	23	GLU	CG-CD-OE2	-5.70	105.30	118.40
1	A	68	ASN	OD1-CG-ND2	-5.70	116.90	122.60
2	B	99	ASP	CA-C-N	5.70	126.44	120.12
2	B	99	ASP	C-N-CA	5.70	126.44	120.12
1	C	110	ALA	N-CA-C	-5.69	102.03	111.37
1	C	40	LYS	CB-CG-CD	-5.69	98.21	111.30
2	B	92	HIS	CA-CB-CG	-5.69	108.11	113.80
2	D	71	PHE	CZ-CE2-CD2	5.69	130.24	120.00
1	C	92	ARG	CG-CD-NE	-5.68	99.49	112.00
2	D	39	GLN	CA-CB-CG	-5.68	102.74	114.10
1	A	105	LEU	CB-CG-CD2	5.68	127.73	110.70
1	A	14	TRP	CD2-CE2-CZ2	-5.68	116.72	122.40
2	B	42	PHE	O-C-N	-5.68	114.84	122.22
2	B	91	LEU	N-CA-C	5.67	117.14	111.07
2	D	41	PHE	N-CA-CB	5.67	119.36	110.46
2	D	116	HIS	CB-CG-ND1	-5.66	114.21	122.70
2	B	9	SER	CA-C-O	5.66	126.49	120.10
2	D	126	VAL	CA-CB-CG1	-5.66	100.79	110.40
2	B	63	HIS	CG-ND1-CE1	-5.65	99.69	109.30
2	B	118	PHE	CB-CA-C	5.65	121.03	109.55
1	C	30	GLU	N-CA-CB	5.65	118.41	109.82
2	D	140	ALA	N-CA-C	-5.65	105.12	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	THR	N-CA-CB	5.65	118.20	110.01
1	C	58	HIS	N-CA-C	-5.65	105.03	111.07
1	C	139	LYS	N-CA-CB	-5.64	101.98	110.73
2	D	146	HIS	CB-CG-ND1	-5.64	114.23	122.70
2	B	132	LYS	N-CA-CB	5.64	118.50	110.16
2	D	135	ALA	CA-C-N	5.64	132.47	121.41
2	D	135	ALA	C-N-CA	5.64	132.47	121.41
2	D	145	TYR	CA-C-O	-5.64	114.49	120.92
1	A	98	PHE	CE1-CZ-CE2	5.63	130.14	120.00
1	A	85	ASP	CB-CG-OD2	-5.63	105.45	118.40
1	C	55	VAL	CA-CB-CG1	-5.61	100.86	110.40
1	A	90	LYS	CA-C-O	5.61	128.52	120.16
2	D	45	PHE	CA-CB-CG	-5.61	108.19	113.80
2	B	83	GLY	CA-C-O	-5.60	114.72	120.66
2	D	104	ARG	CA-CB-CG	-5.60	102.91	114.10
2	D	86	ALA	O-C-N	5.59	128.05	122.12
1	A	44	PRO	CA-N-CD	5.59	119.83	112.00
2	D	116	HIS	ND1-CE1-NE2	-5.59	102.81	108.40
2	D	51	PRO	N-CA-C	5.59	122.83	113.78
2	B	138	ALA	O-C-N	-5.58	116.22	122.03
1	A	56	LYS	CD-CE-NZ	-5.58	94.04	111.90
1	A	38	THR	CA-CB-OG1	5.58	117.97	109.60
2	D	81	LEU	N-CA-CB	-5.58	101.90	110.16
1	A	132	VAL	CG1-CB-CG2	-5.58	98.53	110.80
2	B	60	VAL	N-CA-CB	5.56	120.41	111.23
2	D	14	LEU	CB-CG-CD1	-5.56	94.01	110.70
2	B	63	HIS	ND1-CG-CD2	-5.56	100.54	106.10
2	D	21	ASP	CB-CA-C	-5.56	101.23	110.68
2	B	108	ASN	CB-CG-OD1	-5.55	109.70	120.80
1	A	137	THR	CA-C-O	-5.55	113.07	119.56
2	B	116	HIS	CG-ND1-CE1	-5.55	99.87	109.30
1	C	85	ASP	CA-C-O	5.54	126.43	120.55
2	B	134	VAL	N-CA-C	-5.54	105.32	110.53
1	C	43	PHE	CA-CB-CG	5.53	119.33	113.80
2	B	105	LEU	O-C-N	5.53	127.98	122.12
2	B	116	HIS	N-CA-C	-5.53	105.17	111.14
1	A	16	LYS	CD-CE-NZ	5.52	129.57	111.90
1	A	90	LYS	O-C-N	-5.52	114.74	121.92
2	D	100	PRO	N-CA-CB	5.52	109.48	103.30
1	A	30	GLU	CG-CD-OE2	-5.51	105.72	118.40
1	A	22	GLY	CA-C-N	5.51	127.93	120.38
1	A	22	GLY	C-N-CA	5.51	127.93	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	HIS	CA-CB-CG	-5.51	108.29	113.80
1	C	75	ASP	N-CA-C	-5.51	97.11	108.18
1	A	88	ALA	N-CA-CB	5.50	118.05	110.07
1	A	41	THR	OG1-CB-CG2	5.50	120.30	109.30
2	B	94	ASP	CB-CG-OD2	-5.50	105.76	118.40
1	C	33	PHE	CB-CG-CD1	-5.50	111.35	120.70
2	B	113	VAL	O-C-N	-5.49	115.59	121.80
2	B	23	VAL	N-CA-C	-5.49	105.02	110.62
1	A	58	HIS	N-CA-CB	-5.49	102.04	110.16
1	C	13	ALA	CB-CA-C	5.49	119.65	110.92
2	B	82	LYS	CA-C-N	-5.48	113.97	120.00
2	B	82	LYS	C-N-CA	-5.48	113.97	120.00
1	C	8	THR	CA-C-N	5.48	127.63	120.28
1	C	8	THR	C-N-CA	5.48	127.63	120.28
2	D	73	ASP	N-CA-CB	5.47	119.74	110.49
1	A	47	ASP	CB-CG-OD1	5.47	130.99	118.40
2	D	73	ASP	CB-CA-C	-5.47	99.53	110.42
1	C	61	LYS	CA-C-N	-5.47	112.97	120.46
1	C	61	LYS	C-N-CA	-5.47	112.97	120.46
1	C	69	ALA	CB-CA-C	5.47	119.47	110.88
1	C	108	THR	N-CA-C	-5.47	105.40	111.36
2	D	78	LEU	CD1-CG-CD2	5.47	122.83	110.80
1	C	119	PRO	CB-CA-C	5.46	120.58	111.56
1	C	12	ALA	N-CA-CB	5.46	118.12	109.82
2	B	33	VAL	CA-C-O	-5.46	113.94	121.15
1	C	36	PHE	CG-CD2-CE2	-5.46	111.42	120.70
2	B	14	LEU	CB-CA-C	5.46	119.45	110.88
1	C	84	SER	O-C-N	-5.46	116.34	122.12
2	D	84	THR	CA-C-N	-5.45	111.04	121.94
2	D	84	THR	C-N-CA	-5.45	111.04	121.94
2	B	45	PHE	CB-CG-CD1	-5.45	111.44	120.70
2	B	124	PRO	N-CD-CG	-5.44	95.03	103.20
2	B	78	LEU	CA-CB-CG	-5.44	97.25	116.30
1	A	127	LYS	CA-C-O	-5.44	115.29	121.00
2	D	145	TYR	N-CA-C	5.44	118.20	110.10
2	B	57	ASN	N-CA-CB	5.43	117.94	110.01
2	B	129	ALA	CA-C-N	-5.43	111.65	120.72
2	B	129	ALA	C-N-CA	-5.43	111.65	120.72
2	D	125	PRO	CA-C-N	-5.43	112.70	120.42
2	D	125	PRO	C-N-CA	-5.43	112.70	120.42
1	A	140	TYR	CB-CG-CD2	5.43	128.94	120.80
2	B	30	ARG	CD-NE-CZ	5.42	131.99	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	GLU	CB-CA-C	-5.42	101.63	110.85
2	D	48	LEU	CB-CG-CD2	5.42	126.95	110.70
1	C	11	LYS	N-CA-CB	-5.42	102.16	110.12
1	A	27	GLU	CA-CB-CG	-5.41	103.27	114.10
2	B	56	GLY	CA-C-N	5.41	130.28	121.83
2	B	56	GLY	C-N-CA	5.41	130.28	121.83
1	A	36	PHE	N-CA-CB	-5.41	103.57	111.20
2	D	123	THR	OG1-CB-CG2	-5.41	98.48	109.30
1	C	40	LYS	CD-CE-NZ	-5.41	94.60	111.90
1	A	81	SER	CB-CA-C	-5.41	99.01	110.31
1	C	100	LEU	N-CA-C	-5.41	105.28	111.07
2	D	40	ARG	CA-C-N	5.40	132.11	122.06
2	D	40	ARG	C-N-CA	5.40	132.11	122.06
1	A	44	PRO	N-CA-C	-5.40	107.60	114.35
1	A	3	SER	N-CA-CB	-5.40	100.76	110.37
1	A	76	MET	CA-C-N	-5.40	113.09	119.84
1	A	76	MET	C-N-CA	-5.40	113.09	119.84
1	C	112	HIS	ND1-CE1-NE2	5.40	113.80	108.40
1	C	51	GLY	N-CA-C	5.40	123.04	115.43
2	B	72	SER	CA-C-O	5.39	127.00	121.07
2	B	80	ASN	O-C-N	5.39	131.55	121.63
2	B	128	ALA	CA-C-N	5.39	127.95	120.29
2	B	128	ALA	C-N-CA	5.39	127.95	120.29
2	D	42	PHE	CA-C-O	5.39	127.28	120.65
2	B	30	ARG	O-C-N	5.39	129.90	122.46
2	D	78	LEU	CB-CG-CD1	-5.39	94.53	110.70
2	B	27	ALA	CA-C-N	5.39	129.76	121.19
2	B	27	ALA	C-N-CA	5.39	129.76	121.19
1	C	77	PRO	CA-C-N	5.38	131.82	121.54
1	C	77	PRO	C-N-CA	5.38	131.82	121.54
2	D	70	ALA	CA-C-O	5.38	126.12	120.42
1	C	54	GLN	N-CA-CB	5.38	118.03	110.12
1	A	47	ASP	N-CA-CB	-5.38	101.67	110.21
1	C	106	LEU	CB-CA-C	5.38	119.41	110.81
2	D	93	CYS	CA-C-O	-5.37	115.16	120.80
1	C	65	ALA	CB-CA-C	-5.37	100.70	110.63
1	C	96	VAL	CA-CB-CG1	-5.37	101.27	110.40
1	A	1	VAL	N-CA-CB	-5.36	102.39	111.50
2	B	7	GLU	CA-CB-CG	5.36	124.82	114.10
2	D	117	HIS	CA-C-N	5.36	131.10	121.66
2	D	117	HIS	C-N-CA	5.36	131.10	121.66
2	D	35	TYR	CA-C-N	-5.36	114.30	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	35	TYR	C-N-CA	-5.36	114.30	119.87
1	A	69	ALA	CA-C-N	-5.35	111.52	120.30
1	A	69	ALA	C-N-CA	-5.35	111.52	120.30
1	C	111	ALA	O-C-N	5.35	127.80	122.12
1	C	117	PHE	CG-CD2-CE2	5.35	129.80	120.70
2	B	15	TRP	NE1-CE2-CD2	-5.35	100.45	107.40
2	B	2	HIS	N-CA-C	5.35	117.12	108.41
1	C	43	PHE	CD1-CE1-CZ	5.34	129.62	120.00
2	B	104	ARG	CB-CG-CD	5.34	123.58	111.30
1	C	105	LEU	O-C-N	5.34	127.85	122.09
2	B	92	HIS	CB-CG-CD2	5.33	138.13	131.20
1	A	71	ALA	CB-CA-C	5.33	119.92	110.85
1	A	106	LEU	N-CA-C	5.33	117.84	111.71
2	D	71	PHE	CA-C-O	-5.33	114.90	120.55
2	B	23	VAL	O-C-N	5.32	127.03	121.87
2	D	60	VAL	N-CA-CB	-5.32	104.82	110.62
2	B	126	VAL	CA-C-O	-5.32	114.51	120.25
1	A	67	THR	OG1-CB-CG2	5.31	119.93	109.30
2	B	5	PRO	CA-C-N	-5.31	111.65	120.68
2	B	5	PRO	C-N-CA	-5.31	111.65	120.68
1	C	54	GLN	OE1-CD-NE2	5.31	127.91	122.60
2	B	144	LYS	N-CA-CB	-5.31	102.63	110.49
1	A	88	ALA	CA-C-N	-5.31	112.31	121.66
1	A	88	ALA	C-N-CA	-5.31	112.31	121.66
1	C	55	VAL	O-C-N	-5.31	116.36	121.83
1	C	117	PHE	CZ-CE2-CD2	-5.31	110.45	120.00
2	B	140	ALA	N-CA-C	-5.31	105.54	112.23
2	B	93	CYS	CA-C-O	-5.30	115.23	120.80
1	A	119	PRO	CA-C-O	5.30	130.25	120.60
2	B	131	GLN	CA-C-O	-5.30	114.93	120.55
1	C	88	ALA	O-C-N	5.30	127.54	122.03
2	D	102	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	A	64	ASP	O-C-N	5.30	129.43	122.33
1	C	140	TYR	CB-CG-CD1	5.30	128.75	120.80
2	D	108	ASN	CB-CG-OD1	-5.30	110.20	120.80
2	B	131	GLN	O-C-N	5.29	127.73	122.12
1	A	33	PHE	CG-CD1-CE1	5.29	129.69	120.70
1	C	121	VAL	N-CA-CB	5.29	116.73	110.55
1	C	76	MET	CB-CG-SD	-5.28	96.86	112.70
2	D	49	SER	N-CA-C	-5.28	106.89	113.38
2	D	54	VAL	CA-CB-CG2	5.28	119.37	110.40
2	D	133	VAL	N-CA-C	-5.28	105.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	LYS	CG-CD-CE	-5.27	99.17	111.30
2	B	34	VAL	N-CA-CB	-5.27	101.23	110.77
2	D	118	PHE	CG-CD2-CE2	-5.27	111.74	120.70
1	C	122	HIS	CB-CG-ND1	5.27	130.60	122.70
2	D	102	ASN	N-CA-C	-5.27	105.71	111.82
1	C	7	LYS	N-CA-CB	-5.27	101.20	109.78
2	B	42	PHE	CA-C-N	-5.26	113.51	122.56
2	B	42	PHE	C-N-CA	-5.26	113.51	122.56
2	B	77	HIS	CG-ND1-CE1	-5.26	100.35	109.30
1	C	24	TYR	O-C-N	-5.26	116.62	122.09
1	C	116	GLU	N-CA-C	-5.26	106.91	113.38
2	B	15	TRP	CG-CD1-NE1	5.26	117.04	110.20
2	B	39	GLN	CG-CD-OE1	-5.26	110.28	120.80
1	A	25	GLY	CA-C-O	5.26	129.72	120.57
1	A	42	TYR	N-CA-C	-5.26	106.86	113.28
1	C	19	ALA	N-CA-C	5.26	119.68	113.16
2	B	92	HIS	CE1-NE2-CD2	5.26	114.26	109.00
1	C	29	LEU	N-CA-CB	-5.25	102.40	110.12
2	D	124	PRO	CA-C-N	5.25	124.88	119.05
2	D	124	PRO	C-N-CA	5.25	124.88	119.05
2	D	142	ALA	N-CA-C	5.25	119.53	113.18
2	B	131	GLN	CG-CD-OE1	-5.25	110.31	120.80
1	C	74	ASP	N-CA-C	5.25	119.53	113.18
1	A	80	LEU	N-CA-C	-5.24	106.66	113.16
1	A	86	LEU	CB-CG-CD2	5.24	126.41	110.70
2	B	102	ASN	CA-CB-CG	-5.24	107.36	112.60
2	B	32	LEU	O-C-N	-5.23	115.24	122.46
2	D	11	VAL	N-CA-CB	-5.23	103.87	110.57
1	A	23	GLU	CA-CB-CG	-5.23	103.64	114.10
2	D	66	LYS	CA-C-N	-5.23	111.72	120.30
2	D	66	LYS	C-N-CA	-5.23	111.72	120.30
2	D	94	ASP	N-CA-C	-5.23	105.64	112.23
1	C	132	VAL	CA-C-O	5.23	126.71	121.17
2	B	53	ALA	N-CA-C	5.22	116.97	111.28
1	C	24	TYR	N-CA-C	5.22	117.38	111.11
2	D	48	LEU	CA-CB-CG	-5.22	98.02	116.30
1	C	35	SER	CA-C-N	5.22	128.27	122.74
1	C	35	SER	C-N-CA	5.22	128.27	122.74
2	B	52	ASP	OD1-CG-OD2	-5.21	110.38	122.90
1	A	74	ASP	O-C-N	-5.21	115.45	122.43
2	B	37	TRP	O-C-N	-5.21	114.69	122.39
2	D	12	THR	CA-C-O	5.20	125.93	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	LYS	CD-CE-NZ	5.20	128.54	111.90
2	D	102	ASN	CA-C-O	-5.19	114.00	119.97
1	A	117	PHE	CG-CD1-CE1	-5.19	111.88	120.70
2	D	58	PRO	CB-CA-C	-5.19	103.00	111.56
1	A	129	LEU	CA-C-N	5.19	127.66	120.29
1	A	129	LEU	C-N-CA	5.19	127.66	120.29
1	A	114	PRO	CB-CA-C	-5.18	104.13	112.21
1	A	56	LYS	CG-CD-CE	-5.18	99.39	111.30
1	A	8	THR	CA-CB-CG2	-5.17	101.71	110.50
2	D	17	LYS	CA-CB-CG	-5.17	103.76	114.10
1	A	108	THR	CA-CB-CG2	-5.17	101.71	110.50
2	B	60	VAL	CB-CA-C	5.17	119.77	111.29
2	D	46	GLY	N-CA-C	5.17	125.42	113.18
1	C	37	PRO	N-CA-CB	5.16	108.64	103.48
2	B	129	ALA	O-C-N	5.16	128.03	122.15
2	D	38	THR	OG1-CB-CG2	5.16	119.61	109.30
2	D	8	LYS	CB-CG-CD	-5.15	99.44	111.30
1	A	35	SER	CB-CA-C	-5.15	99.31	109.67
2	B	39	GLN	N-CA-CB	5.15	118.28	110.14
2	B	92	HIS	CB-CA-C	-5.15	99.23	109.99
1	A	34	LEU	N-CA-C	-5.14	105.30	112.45
1	A	39	THR	CA-CB-CG2	5.14	119.24	110.50
1	A	105	LEU	CA-C-N	-5.14	112.87	120.28
1	A	105	LEU	C-N-CA	-5.14	112.87	120.28
1	C	14	TRP	CB-CA-C	-5.14	99.56	110.31
2	D	118	PHE	O-C-N	-5.14	115.42	122.46
2	D	118	PHE	CB-CG-CD2	-5.14	111.97	120.70
2	D	138	ALA	CA-C-O	5.14	125.99	120.70
2	B	40	ARG	N-CA-C	-5.14	106.11	112.38
2	D	59	LYS	CA-C-O	-5.13	114.07	119.97
1	A	14	TRP	CE2-CD2-CE3	-5.13	113.67	118.80
2	B	117	HIS	ND1-CE1-NE2	-5.13	103.27	108.40
1	C	82	ALA	CA-C-N	-5.13	112.52	122.06
1	C	82	ALA	C-N-CA	-5.13	112.52	122.06
2	D	2	HIS	CG-CD2-NE2	-5.13	102.07	107.20
2	D	66	LYS	O-C-N	-5.13	116.69	122.03
2	B	143	HIS	CA-CB-CG	-5.13	108.67	113.80
2	D	68	LEU	CB-CA-C	-5.13	99.28	109.99
2	D	120	LYS	CA-C-N	5.13	130.68	121.66
2	D	120	LYS	C-N-CA	5.13	130.68	121.66
2	B	87	THR	CA-C-N	-5.12	112.90	120.28
2	B	87	THR	C-N-CA	-5.12	112.90	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	PHE	CD1-CG-CD2	5.12	126.29	118.60
2	B	142	ALA	N-CA-CB	5.12	119.02	110.41
1	A	140	TYR	CB-CA-C	-5.12	101.15	110.63
1	C	14	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	C	89	HIS	N-CA-C	5.12	118.69	112.23
1	C	96	VAL	O-C-N	-5.12	116.01	121.80
1	A	47	ASP	CA-C-N	-5.12	114.46	122.95
1	A	47	ASP	C-N-CA	-5.12	114.46	122.95
2	D	26	GLU	CA-CB-CG	-5.12	103.87	114.10
2	B	114	LEU	CA-C-N	-5.11	113.43	120.28
2	B	114	LEU	C-N-CA	-5.11	113.43	120.28
2	B	117	HIS	CB-CA-C	-5.11	102.63	110.81
2	D	109	VAL	O-C-N	5.11	126.83	121.87
1	A	32	MET	O-C-N	-5.11	116.70	122.12
2	B	3	LEU	CB-CA-C	-5.11	99.61	109.37
1	C	116	GLU	N-CA-CB	-5.11	102.92	110.53
2	D	108	ASN	N-CA-CB	5.11	117.72	110.16
1	A	5	ALA	N-CA-CB	-5.10	102.48	110.44
1	A	139	LYS	CA-C-O	-5.10	113.57	119.59
1	C	90	LYS	CA-C-O	5.10	127.80	120.51
1	A	10	VAL	CA-C-N	-5.09	112.21	120.72
1	A	10	VAL	C-N-CA	-5.09	112.21	120.72
1	A	98	PHE	CZ-CE2-CD2	-5.09	110.83	120.00
1	C	67	THR	CA-C-O	-5.09	115.47	120.82
2	D	15	TRP	N-CA-CB	-5.09	102.10	110.40
2	D	146	HIS	CA-C-O	5.09	136.28	121.00
2	D	59	LYS	N-CA-CB	5.09	118.17	110.28
2	D	61	LYS	N-CA-C	5.09	117.49	111.33
1	A	103	HIS	ND1-CG-CD2	5.09	111.19	106.10
1	A	80	LEU	CA-C-O	-5.09	113.12	119.28
2	B	127	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	45	HIS	O-C-N	-5.08	115.19	122.41
2	B	48	LEU	CA-C-O	-5.08	113.95	119.95
2	D	50	THR	CA-CB-CG2	-5.08	101.86	110.50
1	C	85	ASP	CB-CG-OD2	-5.08	106.71	118.40
2	B	141	LEU	CD1-CG-CD2	-5.08	99.63	110.80
1	C	45	HIS	CA-C-N	-5.08	111.86	122.07
1	C	45	HIS	C-N-CA	-5.08	111.86	122.07
2	D	42	PHE	CB-CG-CD2	5.08	129.33	120.70
1	A	95	PRO	CA-N-CD	-5.08	104.89	112.00
2	B	33	VAL	CA-C-N	-5.08	111.97	120.30
2	B	33	VAL	C-N-CA	-5.08	111.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	TYR	CA-CB-CG	5.07	123.03	113.90
2	D	97	HIS	CA-C-N	-5.07	116.03	122.37
2	D	97	HIS	C-N-CA	-5.07	116.03	122.37
2	D	99	ASP	CB-CG-OD1	-5.07	106.74	118.40
1	A	36	PHE	CB-CG-CD2	-5.07	112.08	120.70
2	B	21	ASP	OD1-CG-OD2	5.07	135.06	122.90
1	A	140	TYR	N-CA-C	5.07	117.54	111.71
2	B	63	HIS	CB-CG-ND1	-5.07	115.10	122.70
1	C	67	THR	CA-CB-CG2	-5.07	101.89	110.50
1	C	133	SER	CA-C-O	-5.06	115.48	120.90
1	A	14	TRP	CB-CG-CD1	-5.06	119.31	126.90
1	C	20	HIS	CA-C-O	-5.06	112.63	119.11
1	A	5	ALA	CB-CA-C	-5.06	99.28	109.55
1	A	95	PRO	CB-CA-C	-5.06	104.30	111.68
1	A	29	LEU	CB-CG-CD1	-5.05	95.54	110.70
2	B	90	GLU	CB-CG-CD	-5.05	104.01	112.60
1	A	31	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	C	67	THR	N-CA-CB	-5.04	102.69	110.01
1	C	43	PHE	CD1-CG-CD2	5.04	126.16	118.60
1	A	38	THR	O-C-N	-5.04	115.68	122.43
1	C	137	THR	CA-CB-CG2	-5.04	101.94	110.50
2	B	55	MET	CA-C-N	-5.04	111.54	121.41
2	B	55	MET	C-N-CA	-5.04	111.54	121.41
2	B	122	PHE	CD1-CE1-CZ	-5.04	110.93	120.00
1	A	71	ALA	N-CA-CB	-5.04	102.71	110.16
1	C	104	CYS	CA-C-O	-5.04	115.21	120.55
1	A	66	LEU	N-CA-CB	-5.03	102.55	110.30
1	C	127	LYS	CA-CB-CG	-5.03	104.03	114.10
1	A	7	LYS	CA-C-O	5.03	125.79	120.10
2	D	116	HIS	CA-CB-CG	-5.03	108.77	113.80
1	C	134	THR	CA-C-N	-5.03	114.42	120.70
1	C	134	THR	C-N-CA	-5.03	114.42	120.70
2	D	136	GLY	CA-C-O	5.03	129.31	120.57
1	A	106	LEU	CB-CG-CD1	5.02	125.77	110.70
2	B	78	LEU	O-C-N	-5.02	114.96	122.39
2	D	130	TYR	CB-CG-CD2	5.02	128.33	120.80
1	A	24	TYR	CG-CD2-CE2	5.02	128.73	121.20
2	B	21	ASP	CA-C-O	-5.02	113.73	119.60
1	C	114	PRO	CA-CB-CG	-5.02	94.97	104.50
2	B	50	THR	OG1-CB-CG2	-5.01	99.27	109.30
1	A	42	TYR	O-C-N	5.01	129.52	122.41
1	A	87	HIS	CG-ND1-CE1	-5.01	100.78	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	117	HIS	N-CA-C	-5.01	105.47	111.03
1	C	64	ASP	CB-CG-OD1	-5.00	106.89	118.40
2	B	37	TRP	CE3-CZ3-CH2	5.00	127.60	121.10

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	137	THR	CB
2	B	12	THR	CB
2	B	50	THR	CB
1	C	78	ASN	CA
1	C	118	THR	CB
2	D	2	HIS	CA
2	D	72	SER	CA
2	D	73	ASP	CA
2	D	78	LEU	CA
2	D	144	LYS	CA

All (206) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Mainchain
1	A	101	LEU	Mainchain
1	A	11	LYS	Mainchain
1	A	111	ALA	Mainchain
1	A	114	PRO	Mainchain
1	A	118	THR	Mainchain
1	A	12	ALA	Mainchain
1	A	122	HIS	Mainchain
1	A	126	ASP	Sidechain
1	A	141	ARG	Sidechain
1	A	15	GLY	Mainchain
1	A	18	GLY	Peptide
1	A	19	ALA	Mainchain
1	A	20	HIS	Sidechain
1	A	21	ALA	Mainchain
1	A	22	GLY	Mainchain
1	A	23	GLU	Sidechain
1	A	24	TYR	Sidechain
1	A	3	SER	Mainchain
1	A	36	PHE	Sidechain
1	A	4	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	A	41	THR	Mainchain
1	A	45	HIS	Sidechain
1	A	46	PHE	Mainchain
1	A	48	LEU	Mainchain
1	A	50	HIS	Sidechain
1	A	52	SER	Mainchain
1	A	54	GLN	Sidechain
1	A	56	LYS	Mainchain
1	A	59	GLY	Mainchain
1	A	61	LYS	Mainchain
1	A	63	ALA	Mainchain
1	A	64	ASP	Sidechain
1	A	72	HIS	Sidechain
1	A	74	ASP	Mainchain
1	A	75	ASP	Mainchain
1	A	76	MET	Mainchain
1	A	78	ASN	Mainchain,Sidechain
1	A	81	SER	Mainchain
1	A	82	ALA	Mainchain
1	A	83	LEU	Mainchain
1	A	85	ASP	Mainchain,Sidechain
1	A	88	ALA	Mainchain
1	A	9	ASN	Mainchain
1	A	90	LYS	Mainchain
1	A	92	ARG	Sidechain
1	A	97	ASN	Mainchain
1	A	99	LYS	Mainchain
2	B	1	VAL	Mainchain
2	B	100	PRO	Mainchain
2	B	101	GLU	Mainchain
2	B	104	ARG	Sidechain
2	B	114	LEU	Mainchain
2	B	117	HIS	Sidechain
2	B	118	PHE	Sidechain
2	B	121	GLU	Sidechain
2	B	123	THR	Mainchain
2	B	126	VAL	Mainchain
2	B	131	GLN	Mainchain
2	B	139	ASN	Mainchain
2	B	14	LEU	Mainchain
2	B	141	LEU	Mainchain
2	B	143	HIS	Sidechain

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Mol	Chain	Res	Type	Group
2	B	146	HIS	Sidechain
2	B	19	ASN	Sidechain
2	B	2	HIS	Sidechain
2	B	21	ASP	Mainchain,Sidechain
2	B	22	GLU	Sidechain
2	B	26	GLU	Sidechain
2	B	3	LEU	Mainchain
2	B	38	THR	Mainchain
2	B	4	THR	Mainchain
2	B	43	GLU	Mainchain
2	B	44	SER	Mainchain
2	B	47	ASP	Mainchain,Sidechain
2	B	49	SER	Peptide,Mainchain
2	B	52	ASP	Sidechain
2	B	56	GLY	Mainchain
2	B	59	LYS	Mainchain
2	B	6	GLU	Sidechain
2	B	60	VAL	Mainchain
2	B	61	LYS	Mainchain
2	B	62	ALA	Mainchain
2	B	63	HIS	Mainchain,Sidechain
2	B	7	GLU	Mainchain
2	B	78	LEU	Mainchain
2	B	79	ASP	Mainchain,Sidechain
2	B	80	ASN	Mainchain,Sidechain
2	B	84	THR	Mainchain
2	B	90	GLU	Mainchain,Sidechain
1	C	109	LEU	Mainchain
1	C	110	ALA	Mainchain
1	C	111	ALA	Mainchain
1	C	112	HIS	Mainchain
1	C	113	LEU	Mainchain
1	C	114	PRO	Mainchain
1	C	116	GLU	Mainchain,Sidechain
1	C	119	PRO	Mainchain
1	C	125	LEU	Mainchain
1	C	126	ASP	Sidechain
1	C	135	VAL	Mainchain
1	C	138	SER	Mainchain
1	C	14	TRP	Mainchain
1	C	141	ARG	Sidechain
1	C	17	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	C	18	GLY	Mainchain
1	C	20	HIS	Sidechain
1	C	21	ALA	Mainchain
1	C	23	GLU	Sidechain
1	C	25	GLY	Mainchain
1	C	3	SER	Mainchain
1	C	44	PRO	Mainchain
1	C	45	HIS	Mainchain,Sidechain
1	C	46	PHE	Mainchain,Sidechain
1	C	47	ASP	Mainchain,Sidechain
1	C	48	LEU	Mainchain
1	C	5	ALA	Mainchain
1	C	64	ASP	Sidechain
1	C	69	ALA	Mainchain
1	C	71	ALA	Mainchain
1	C	72	HIS	Mainchain
1	C	74	ASP	Mainchain
1	C	75	ASP	Mainchain,Sidechain
1	C	78	ASN	Sidechain
1	C	80	LEU	Mainchain
1	C	83	LEU	Mainchain
1	C	88	ALA	Mainchain
1	C	9	ASN	Sidechain
1	C	92	ARG	Sidechain
1	C	95	PRO	Mainchain
2	D	1	VAL	Mainchain
2	D	101	GLU	Sidechain
2	D	104	ARG	Sidechain
2	D	108	ASN	Sidechain
2	D	117	HIS	Mainchain,Sidechain
2	D	118	PHE	Sidechain
2	D	120	LYS	Mainchain
2	D	121	GLU	Sidechain
2	D	127	GLN	Sidechain
2	D	137	VAL	Mainchain
2	D	139	ASN	Sidechain
2	D	143	HIS	Sidechain
2	D	144	LYS	Mainchain
2	D	146	HIS	Sidechain
2	D	17	LYS	Mainchain
2	D	18	VAL	Peptide
2	D	19	ASN	Sidechain

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Mol	Chain	Res	Type	Group
2	D	2	HIS	Mainchain,Sidechain
2	D	21	ASP	Mainchain,Sidechain
2	D	22	GLU	Mainchain,Sidechain
2	D	26	GLU	Sidechain
2	D	3	LEU	Peptide,Mainchain
2	D	33	VAL	Mainchain
2	D	34	VAL	Mainchain
2	D	40	ARG	Sidechain
2	D	42	PHE	Mainchain
2	D	43	GLU	Sidechain
2	D	46	GLY	Mainchain
2	D	48	LEU	Peptide,Mainchain
2	D	49	SER	Peptide,Mainchain
2	D	5	PRO	Mainchain
2	D	52	ASP	Mainchain,Sidechain
2	D	56	GLY	Mainchain
2	D	6	GLU	Sidechain
2	D	60	VAL	Mainchain
2	D	63	HIS	Sidechain
2	D	64	GLY	Mainchain
2	D	66	LYS	Mainchain
2	D	7	GLU	Sidechain
2	D	73	ASP	Mainchain
2	D	75	LEU	Mainchain
2	D	76	ALA	Mainchain
2	D	77	HIS	Sidechain
2	D	79	ASP	Mainchain,Sidechain
2	D	8	LYS	Mainchain
2	D	80	ASN	Mainchain
2	D	83	GLY	Mainchain
2	D	84	THR	Mainchain
2	D	90	GLU	Sidechain
2	D	92	HIS	Mainchain,Sidechain
2	D	94	ASP	Sidechain
2	D	96	LEU	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	1069	0	1069	242	0
1	C	1069	0	1066	255	1
2	B	1123	0	1107	327	0
2	D	1123	0	1116	427	0
3	A	43	0	30	6	0
3	B	43	0	30	10	0
3	C	43	0	30	15	0
3	D	43	0	30	12	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	56	0	0	1	0
5	B	57	0	0	1	2
5	C	59	0	0	0	1
5	D	49	0	0	1	0
All	All	4779	0	4478	1286	2

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 142.

All (1286) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:CA	1:C:118:THR:CB	1.75	1.63
1:C:113:LEU:CD1	1:C:113:LEU:CG	1.75	1.63
2:D:2:HIS:CD2	2:D:2:HIS:CG	1.85	1.63
2:B:50:THR:CG2	2:B:50:THR:CB	1.75	1.63
1:A:40:LYS:CA	1:A:40:LYS:CB	1.75	1.61
2:D:48:LEU:CG	2:D:48:LEU:CD1	1.75	1.61
2:D:67:VAL:CA	2:D:67:VAL:CB	1.76	1.61
1:C:70:VAL:C	1:C:70:VAL:CA	1.74	1.61
1:C:54:GLN:CA	1:C:54:GLN:C	1.75	1.60
1:A:29:LEU:CB	1:A:29:LEU:CA	1.79	1.60
2:D:113:VAL:CG2	2:D:113:VAL:CB	1.74	1.60
2:B:8:LYS:CD	2:B:8:LYS:CG	1.78	1.59
2:B:8:LYS:CB	2:B:8:LYS:CA	1.74	1.59
2:D:52:ASP:CG	2:D:52:ASP:CB	1.75	1.59
2:B:9:SER:CB	2:B:9:SER:CA	1.79	1.59
1:C:105:LEU:CD1	1:C:105:LEU:CG	1.79	1.59
2:D:59:LYS:C	2:D:59:LYS:CA	1.76	1.59
2:B:145:TYR:C	2:B:145:TYR:CA	1.75	1.58
1:C:16:LYS:CD	1:C:16:LYS:CG	1.81	1.58
2:D:47:ASP:CG	2:D:47:ASP:CB	1.76	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:HIS:CB	2:D:77:HIS:CA	1.75	1.58
1:C:48:LEU:CD2	1:C:48:LEU:CG	1.74	1.58
2:D:126:VAL:CB	2:D:126:VAL:CA	1.81	1.58
2:B:7:GLU:CG	2:B:7:GLU:CB	1.77	1.57
2:B:52:ASP:CG	2:B:52:ASP:CB	1.77	1.57
2:B:143:HIS:ND1	2:B:143:HIS:CG	1.70	1.57
2:B:47:ASP:CA	2:B:47:ASP:C	1.75	1.57
2:B:104:ARG:CD	2:B:104:ARG:CG	1.76	1.57
2:B:41:PHE:C	2:B:41:PHE:CA	1.77	1.57
1:C:38:THR:CB	1:C:38:THR:CA	1.81	1.57
1:A:5:ALA:CB	1:A:5:ALA:CA	1.77	1.57
2:D:92:HIS:C	2:D:92:HIS:CA	1.76	1.57
1:A:87:HIS:C	1:A:87:HIS:CA	1.75	1.56
1:C:73:VAL:CB	1:C:73:VAL:CA	1.80	1.56
2:B:65:LYS:CB	2:B:65:LYS:CA	1.80	1.56
2:D:78:LEU:CA	2:D:78:LEU:CB	1.79	1.56
2:D:121:GLU:CB	2:D:121:GLU:CA	1.79	1.56
1:A:14:TRP:CA	1:A:14:TRP:CB	1.83	1.56
1:A:62:VAL:C	1:A:62:VAL:CA	1.75	1.56
2:B:5:PRO:C	2:B:5:PRO:CA	1.78	1.55
2:D:18:VAL:CB	2:D:18:VAL:CG2	1.80	1.55
1:A:141:ARG:CB	1:A:141:ARG:CG	1.79	1.55
1:C:84:SER:CB	1:C:84:SER:CA	1.79	1.55
1:A:58:HIS:C	1:A:58:HIS:CA	1.76	1.55
2:D:123:THR:CG2	2:D:123:THR:CB	1.80	1.55
2:D:8:LYS:CA	2:D:8:LYS:CB	1.85	1.55
1:C:70:VAL:CA	1:C:70:VAL:N	1.68	1.55
2:D:141:LEU:CG	2:D:141:LEU:CD2	1.78	1.55
1:A:72:HIS:CA	1:A:72:HIS:CB	1.78	1.54
2:B:10:ALA:C	2:B:10:ALA:CA	1.78	1.54
1:C:61:LYS:C	1:C:61:LYS:CA	1.76	1.54
1:C:61:LYS:CE	1:C:61:LYS:CD	1.81	1.54
1:C:137:THR:C	1:C:137:THR:CA	1.74	1.54
2:B:49:SER:CA	2:B:49:SER:CB	1.83	1.54
2:B:90:GLU:CB	2:B:90:GLU:CA	1.84	1.54
2:D:10:ALA:C	2:D:10:ALA:CA	1.75	1.54
2:B:6:GLU:C	2:B:6:GLU:CA	1.77	1.54
1:C:40:LYS:CE	1:C:40:LYS:NZ	1.69	1.54
2:D:4:THR:CB	2:D:4:THR:CA	1.82	1.54
2:D:8:LYS:CB	2:D:8:LYS:CG	1.79	1.54
2:D:53:ALA:C	2:D:53:ALA:CA	1.76	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:VAL:N	2:B:1:VAL:CA	1.68	1.53
1:C:8:THR:CB	1:C:8:THR:CA	1.84	1.53
1:C:99:LYS:CD	1:C:99:LYS:CG	1.82	1.53
1:A:84:SER:CB	1:A:84:SER:CA	1.82	1.53
2:B:3:LEU:CA	2:B:3:LEU:CB	1.77	1.53
2:D:21:ASP:CG	2:D:21:ASP:CB	1.78	1.53
2:D:131:GLN:CD	2:D:131:GLN:CG	1.77	1.53
1:A:2:LEU:C	1:A:2:LEU:CA	1.77	1.53
2:B:117:HIS:CE1	2:B:117:HIS:ND1	1.75	1.53
1:C:10:VAL:C	1:C:10:VAL:CA	1.81	1.53
2:D:7:GLU:C	2:D:7:GLU:CA	1.75	1.53
2:D:22:GLU:CG	2:D:22:GLU:CA	1.85	1.53
2:D:50:THR:N	2:D:50:THR:CA	1.71	1.53
2:D:73:ASP:CA	2:D:73:ASP:CB	1.86	1.53
2:B:47:ASP:CA	2:B:47:ASP:N	1.67	1.52
2:B:80:ASN:CG	2:B:80:ASN:CB	1.75	1.52
1:C:16:LYS:C	1:C:16:LYS:CA	1.82	1.52
1:C:87:HIS:C	1:C:87:HIS:CA	1.82	1.52
2:D:46:GLY:CA	2:D:46:GLY:C	1.82	1.52
1:A:90:LYS:CE	1:A:90:LYS:CD	1.84	1.52
1:C:2:LEU:C	1:C:2:LEU:CA	1.79	1.52
1:C:78:ASN:CB	1:C:78:ASN:CG	1.77	1.52
2:D:94:ASP:N	2:D:94:ASP:CA	1.68	1.52
2:B:81:LEU:N	2:B:81:LEU:CA	1.68	1.52
2:B:143:HIS:C	2:B:143:HIS:CA	1.76	1.52
1:C:72:HIS:CB	1:C:72:HIS:CA	1.86	1.52
2:D:108:ASN:CG	2:D:108:ASN:CB	1.83	1.52
1:A:56:LYS:CE	1:A:56:LYS:CD	1.84	1.51
2:B:49:SER:CA	2:B:49:SER:N	1.67	1.51
2:B:80:ASN:C	2:B:80:ASN:CA	1.80	1.51
2:D:22:GLU:CA	2:D:22:GLU:C	1.83	1.51
1:A:31:ARG:NE	1:A:31:ARG:CD	1.68	1.51
2:B:1:VAL:CA	2:B:1:VAL:CB	1.86	1.51
1:A:1:VAL:CB	1:A:1:VAL:CA	1.84	1.51
1:C:131:SER:C	1:C:131:SER:CA	1.76	1.51
2:D:8:LYS:CA	2:D:8:LYS:N	1.68	1.51
2:D:48:LEU:CA	2:D:48:LEU:N	1.72	1.51
2:B:142:ALA:C	2:B:142:ALA:CA	1.82	1.50
1:C:82:ALA:C	1:C:83:LEU:N	1.69	1.50
2:D:12:THR:N	2:D:12:THR:CA	1.68	1.50
2:D:18:VAL:N	2:D:18:VAL:CA	1.70	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ASN:CA	2:B:80:ASN:N	1.73	1.50
2:B:12:THR:CG2	2:B:12:THR:CA	1.89	1.50
1:C:56:LYS:NZ	1:C:56:LYS:CE	1.72	1.50
2:D:7:GLU:CG	2:D:7:GLU:CB	1.88	1.50
2:D:79:ASP:C	2:D:79:ASP:CA	1.83	1.50
1:A:74:ASP:CG	1:A:74:ASP:CB	1.80	1.49
2:B:108:ASN:CB	2:B:108:ASN:CG	1.84	1.49
2:B:74:GLY:C	2:B:75:LEU:N	1.70	1.49
3:B:148:HEM:CBD	3:B:148:HEM:CGD	1.85	1.49
2:D:45:PHE:C	2:D:46:GLY:CA	1.78	1.49
2:D:80:ASN:N	2:D:80:ASN:CA	1.75	1.49
1:A:52:SER:N	1:A:52:SER:CA	1.75	1.49
2:B:2:HIS:C	2:B:2:HIS:CA	1.84	1.49
2:B:22:GLU:CD	2:B:22:GLU:CG	1.85	1.49
1:C:16:LYS:CE	1:C:16:LYS:NZ	1.71	1.49
2:D:82:LYS:CD	2:D:82:LYS:CG	1.89	1.49
2:D:49:SER:C	2:D:49:SER:CA	1.86	1.48
2:B:77:HIS:CG	2:B:77:HIS:CD2	1.83	1.48
1:C:90:LYS:CE	1:C:90:LYS:CD	1.91	1.48
1:A:76:MET:CG	1:A:76:MET:SD	2.02	1.48
1:C:1:VAL:C	1:C:1:VAL:CA	1.83	1.48
2:D:59:LYS:CE	2:D:59:LYS:CD	1.88	1.48
1:A:16:LYS:CD	1:A:16:LYS:CE	1.92	1.48
1:A:61:LYS:CE	1:A:61:LYS:NZ	1.74	1.48
1:C:7:LYS:N	1:C:7:LYS:CA	1.75	1.47
1:A:18:GLY:C	1:A:18:GLY:CA	1.86	1.47
1:A:44:PRO:C	1:A:44:PRO:CA	1.83	1.47
2:B:21:ASP:CG	2:B:21:ASP:CB	1.84	1.47
2:B:61:LYS:NZ	2:B:61:LYS:CE	1.75	1.47
1:C:20:HIS:CE1	1:C:20:HIS:ND1	1.79	1.47
2:D:117:HIS:CG	2:D:117:HIS:ND1	1.74	1.47
1:C:75:ASP:N	1:C:75:ASP:CA	1.71	1.47
2:D:12:THR:CA	2:D:12:THR:CB	1.93	1.47
2:B:9:SER:CA	2:B:9:SER:C	1.87	1.46
2:D:52:ASP:N	2:D:52:ASP:CA	1.76	1.46
1:A:75:ASP:CG	1:A:75:ASP:CA	1.88	1.46
3:B:148:HEM:CBA	3:B:148:HEM:CGA	1.91	1.46
1:C:90:LYS:CD	1:C:90:LYS:CG	1.90	1.46
3:C:142:HEM:CGD	3:C:142:HEM:CBD	1.93	1.46
1:A:137:THR:CB	1:A:137:THR:CA	1.91	1.45
2:D:1:VAL:N	2:D:1:VAL:CA	1.77	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:LYS:CD	2:B:61:LYS:CG	1.93	1.45
1:C:7:LYS:CD	1:C:7:LYS:CG	1.95	1.45
1:C:139:LYS:CE	1:C:139:LYS:CD	1.95	1.45
1:C:76:MET:CG	1:C:76:MET:SD	2.05	1.44
1:A:60:LYS:CE	1:A:60:LYS:CD	1.93	1.44
2:B:82:LYS:CE	2:B:82:LYS:CG	1.93	1.44
2:B:139:ASN:CG	2:B:139:ASN:CA	1.87	1.44
2:D:19:ASN:ND2	2:D:19:ASN:CG	1.71	1.44
1:C:114:PRO:C	1:C:114:PRO:CA	1.90	1.44
2:D:43:GLU:CG	2:D:43:GLU:CA	1.95	1.44
2:D:47:ASP:CB	2:D:47:ASP:CA	1.94	1.43
1:A:11:LYS:CE	1:A:11:LYS:CD	1.96	1.43
1:A:99:LYS:CE	1:A:99:LYS:CD	1.95	1.43
2:B:87:THR:CB	2:B:87:THR:CA	1.95	1.43
1:C:16:LYS:CG	1:C:16:LYS:CB	1.93	1.43
2:D:146:HIS:CG	2:D:146:HIS:ND1	1.85	1.43
1:A:137:THR:CB	1:A:137:THR:OG1	1.66	1.42
2:B:2:HIS:CG	2:B:2:HIS:CD2	2.05	1.42
2:D:43:GLU:CG	2:D:43:GLU:CD	1.92	1.42
2:D:58:PRO:CD	2:D:58:PRO:N	1.71	1.42
1:A:127:LYS:CD	1:A:127:LYS:CG	1.97	1.42
1:C:72:HIS:CG	1:C:72:HIS:ND1	1.80	1.42
2:D:55:MET:C	2:D:55:MET:CA	1.90	1.42
2:B:65:LYS:CA	2:B:65:LYS:CG	1.98	1.42
2:D:26:GLU:CD	2:D:26:GLU:CG	1.90	1.42
2:D:77:HIS:CD2	2:D:77:HIS:NE2	1.88	1.41
2:B:66:LYS:CE	2:B:66:LYS:NZ	1.81	1.41
2:D:104:ARG:CD	2:D:104:ARG:NE	1.84	1.41
1:A:138:SER:CA	1:A:138:SER:OG	1.69	1.41
2:D:43:GLU:CA	2:D:43:GLU:C	1.94	1.41
2:B:2:HIS:CG	2:B:2:HIS:ND1	1.88	1.40
1:C:139:LYS:CE	1:C:139:LYS:NZ	1.84	1.40
1:A:20:HIS:ND1	1:A:20:HIS:CG	1.70	1.40
1:A:64:ASP:CG	1:A:64:ASP:CB	1.95	1.39
2:D:5:PRO:N	2:D:5:PRO:CA	1.84	1.39
2:D:2:HIS:ND1	2:D:2:HIS:CE1	1.90	1.39
1:A:75:ASP:CA	1:A:75:ASP:CB	1.97	1.39
1:A:81:SER:CB	1:A:81:SER:CA	2.00	1.39
2:D:90:GLU:OE1	2:D:90:GLU:CD	1.64	1.39
1:A:17:VAL:C	1:A:17:VAL:CA	1.96	1.38
2:B:49:SER:CB	2:B:49:SER:OG	1.71	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:PRO:N	2:B:125:PRO:CD	1.67	1.38
1:A:16:LYS:CD	1:A:16:LYS:CG	2.01	1.38
2:B:146:HIS:CB	2:B:146:HIS:CG	2.05	1.38
3:D:148:HEM:CGD	3:D:148:HEM:CBD	2.01	1.38
2:B:2:HIS:CA	2:B:2:HIS:CB	2.01	1.38
2:B:124:PRO:CD	2:B:124:PRO:N	1.70	1.38
2:B:144:LYS:CE	2:B:144:LYS:CD	2.01	1.38
2:D:80:ASN:CG	2:D:80:ASN:OD1	1.66	1.38
1:A:92:ARG:CD	1:A:92:ARG:CZ	2.01	1.38
1:C:30:GLU:CD	1:C:30:GLU:CG	1.96	1.37
2:D:2:HIS:CE1	2:D:2:HIS:NE2	1.90	1.37
2:D:143:HIS:CD2	2:D:143:HIS:CG	1.85	1.37
1:A:15:GLY:O	1:A:15:GLY:C	1.67	1.37
2:B:87:THR:CB	2:B:87:THR:CG2	2.02	1.37
2:D:77:HIS:CE1	2:D:77:HIS:ND1	1.91	1.37
1:C:92:ARG:NH1	1:C:92:ARG:CZ	1.87	1.37
2:D:146:HIS:ND1	2:D:146:HIS:CD2	1.91	1.36
1:C:138:SER:CA	1:C:138:SER:OG	1.73	1.36
2:B:79:ASP:CG	2:B:79:ASP:OD2	1.67	1.36
1:A:50:HIS:CB	1:A:50:HIS:CA	2.02	1.36
2:B:1:VAL:CB	2:B:1:VAL:CG1	2.03	1.36
2:B:6:GLU:OE1	2:B:6:GLU:CD	1.67	1.35
2:B:117:HIS:ND1	2:B:117:HIS:CG	1.94	1.35
1:A:127:LYS:CG	1:A:127:LYS:CA	2.02	1.35
2:D:6:GLU:CD	2:D:6:GLU:CG	1.97	1.35
1:A:30:GLU:CD	1:A:30:GLU:CG	2.00	1.35
2:D:8:LYS:CD	2:D:8:LYS:CE	2.03	1.35
2:B:104:ARG:CZ	2:B:104:ARG:NH1	1.87	1.34
2:D:139:ASN:CG	2:D:139:ASN:OD1	1.68	1.34
2:D:121:GLU:CD	2:D:121:GLU:CG	2.01	1.34
2:B:132:LYS:NZ	2:B:132:LYS:CE	1.88	1.34
2:D:20:VAL:CA	2:D:20:VAL:CG2	2.05	1.34
2:D:26:GLU:CD	2:D:26:GLU:OE2	1.71	1.33
1:A:16:LYS:CE	1:A:16:LYS:CG	2.06	1.33
2:B:59:LYS:CE	2:B:59:LYS:NZ	1.92	1.33
2:B:146:HIS:CE1	2:B:146:HIS:ND1	1.84	1.33
2:B:1:VAL:O	2:B:1:VAL:C	1.70	1.33
1:A:56:LYS:CD	1:A:56:LYS:CG	2.06	1.32
2:D:43:GLU:C	2:D:43:GLU:HB2	1.53	1.32
1:A:61:LYS:CE	1:A:61:LYS:CG	2.06	1.32
1:A:72:HIS:CA	1:A:72:HIS:CG	2.12	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:GLU:CG	2:B:101:GLU:CD	2.02	1.32
2:D:66:LYS:CD	2:D:66:LYS:CG	2.06	1.32
1:C:11:LYS:CE	1:C:11:LYS:NZ	1.91	1.32
2:D:1:VAL:CA	2:D:1:VAL:C	2.02	1.32
1:A:78:ASN:CB	1:A:78:ASN:ND2	1.87	1.31
1:A:85:ASP:CG	1:A:85:ASP:OD2	1.73	1.31
1:A:23:GLU:OE1	1:A:23:GLU:CD	1.72	1.31
2:B:143:HIS:ND1	2:B:143:HIS:CE1	1.99	1.31
2:D:82:LYS:NZ	2:D:82:LYS:CE	1.94	1.31
2:D:20:VAL:CA	2:D:20:VAL:CB	2.10	1.30
1:C:40:LYS:CE	1:C:40:LYS:CG	2.07	1.30
2:D:66:LYS:NZ	2:D:66:LYS:CE	1.95	1.29
3:A:142:HEM:CGD	3:A:142:HEM:CBD	2.09	1.29
3:D:148:HEM:CGA	3:D:148:HEM:O2A	1.77	1.29
2:D:50:THR:CA	2:D:50:THR:CB	2.11	1.29
2:D:8:LYS:CE	2:D:8:LYS:NZ	1.94	1.29
2:D:76:ALA:N	2:D:76:ALA:CA	1.94	1.29
1:C:40:LYS:NZ	1:C:40:LYS:CD	1.95	1.28
1:A:139:LYS:CE	1:A:139:LYS:NZ	1.96	1.28
1:A:138:SER:CA	1:A:138:SER:CB	2.12	1.28
1:C:105:LEU:CG	1:C:105:LEU:CD2	2.12	1.27
2:B:90:GLU:CD	2:B:90:GLU:CG	2.07	1.27
2:D:101:GLU:CD	2:D:101:GLU:CG	2.07	1.27
1:A:1:VAL:CA	1:A:1:VAL:CG2	2.13	1.27
2:B:22:GLU:CD	2:B:22:GLU:OE1	1.77	1.27
1:C:61:LYS:CE	1:C:61:LYS:NZ	1.98	1.26
2:D:3:LEU:O	2:D:3:LEU:C	1.77	1.26
1:C:114:PRO:CA	1:C:114:PRO:N	1.72	1.26
1:A:21:ALA:C	1:A:21:ALA:CA	2.09	1.26
1:C:1:VAL:CG1	1:C:1:VAL:CG2	2.13	1.26
2:B:6:GLU:CD	2:B:6:GLU:CG	2.07	1.26
2:B:121:GLU:CD	2:B:121:GLU:CG	2.07	1.26
2:B:1:VAL:CA	2:B:1:VAL:C	2.09	1.26
2:D:17:LYS:CE	2:D:17:LYS:NZ	1.98	1.26
2:B:104:ARG:CZ	2:B:104:ARG:NH2	1.97	1.25
2:D:125:PRO:CD	2:D:125:PRO:N	1.67	1.25
2:B:8:LYS:CG	2:B:8:LYS:CA	2.13	1.25
1:A:23:GLU:CD	1:A:23:GLU:CG	2.10	1.25
1:C:138:SER:CA	1:C:138:SER:CB	2.14	1.24
2:D:4:THR:HB	2:D:6:GLU:OE2	1.29	1.24
2:B:47:ASP:CG	2:B:47:ASP:OD2	1.78	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LYS:CE	2:B:144:LYS:NZ	1.99	1.24
1:C:1:VAL:CG2	1:C:1:VAL:HG13	1.64	1.24
2:D:95:LYS:NZ	2:D:95:LYS:CE	1.99	1.24
2:B:49:SER:C	2:B:49:SER:O	1.79	1.24
2:D:26:GLU:CD	2:D:26:GLU:OE1	1.79	1.23
2:B:5:PRO:N	2:B:5:PRO:CD	1.81	1.23
2:B:12:THR:CG2	2:B:12:THR:OG1	1.78	1.23
1:A:14:TRP:CA	1:A:14:TRP:CG	2.22	1.22
1:A:75:ASP:CG	1:A:75:ASP:OD1	1.82	1.22
2:D:95:LYS:CD	2:D:95:LYS:CG	2.16	1.22
1:A:78:ASN:CG	1:A:78:ASN:CA	2.11	1.22
1:C:46:PHE:CE2	1:C:46:PHE:CG	2.02	1.22
2:D:43:GLU:CD	2:D:43:GLU:CB	2.13	1.22
1:C:60:LYS:NZ	1:C:60:LYS:CE	2.02	1.21
1:C:112:HIS:CG	1:C:112:HIS:ND1	1.78	1.21
2:B:2:HIS:CD2	2:B:2:HIS:NE2	2.09	1.21
1:C:1:VAL:CA	1:C:1:VAL:CG1	2.18	1.21
2:D:26:GLU:CG	2:D:26:GLU:CB	2.18	1.21
1:C:99:LYS:CG	1:C:99:LYS:CA	2.17	1.20
2:D:73:ASP:CA	2:D:73:ASP:CG	2.14	1.20
1:C:23:GLU:CG	1:C:23:GLU:CD	2.15	1.19
2:D:58:PRO:CD	2:D:58:PRO:CB	2.20	1.19
1:A:92:ARG:CD	1:A:92:ARG:NH1	2.03	1.19
2:B:49:SER:CB	2:B:49:SER:C	2.15	1.18
1:C:90:LYS:CE	1:C:90:LYS:NZ	2.06	1.18
2:B:121:GLU:CD	2:B:121:GLU:OE1	1.87	1.18
1:C:113:LEU:CD1	1:C:113:LEU:CB	2.22	1.18
2:D:65:LYS:CE	2:D:65:LYS:CD	2.20	1.18
1:C:92:ARG:HH21	1:C:92:ARG:NE	1.42	1.17
1:C:16:LYS:CD	1:C:16:LYS:CE	2.23	1.17
2:D:2:HIS:CB	2:D:2:HIS:CA	2.21	1.17
2:D:49:SER:C	2:D:50:THR:CA	2.17	1.17
2:B:139:ASN:CG	2:B:139:ASN:ND2	2.01	1.17
1:A:127:LYS:CD	1:A:127:LYS:CB	2.23	1.16
1:C:1:VAL:CG1	1:C:1:VAL:CB	2.22	1.16
2:B:104:ARG:CD	2:B:104:ARG:CZ	2.24	1.15
2:B:108:ASN:CB	2:B:108:ASN:ND2	2.10	1.15
2:D:46:GLY:C	2:D:47:ASP:CA	2.20	1.15
1:A:1:VAL:HG23	1:A:1:VAL:N	1.61	1.15
2:B:26:GLU:HG2	2:B:26:GLU:OE2	1.46	1.15
2:D:77:HIS:NE2	2:D:77:HIS:CG	2.15	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:PRO:CD	2:B:58:PRO:N	1.78	1.14
1:A:1:VAL:CG2	1:A:1:VAL:N	2.09	1.14
2:B:26:GLU:OE2	2:B:26:GLU:CG	1.95	1.14
1:C:73:VAL:CA	1:C:73:VAL:CG1	2.26	1.14
1:A:72:HIS:CG	1:A:72:HIS:ND1	1.85	1.14
2:D:43:GLU:CD	2:D:43:GLU:HB3	1.71	1.14
2:D:47:ASP:CA	2:D:47:ASP:N	2.09	1.13
1:C:56:LYS:CD	1:C:56:LYS:CG	2.27	1.13
1:C:99:LYS:CD	1:C:99:LYS:CE	2.26	1.13
2:D:82:LYS:CD	2:D:82:LYS:NZ	2.12	1.13
2:D:66:LYS:CD	2:D:66:LYS:CE	2.27	1.12
1:A:92:ARG:NH1	1:A:92:ARG:HD3	1.60	1.12
2:B:104:ARG:CZ	2:B:104:ARG:NE	2.13	1.12
2:D:65:LYS:CD	2:D:65:LYS:CG	2.27	1.11
3:C:142:HEM:CGA	3:C:142:HEM:O2A	0.82	1.11
2:B:2:HIS:ND1	2:B:2:HIS:CE1	2.18	1.11
2:D:8:LYS:CA	2:D:8:LYS:CG	2.29	1.11
2:D:6:GLU:CG	2:D:6:GLU:CA	2.28	1.10
3:C:142:HEM:CGA	3:C:142:HEM:CBA	2.29	1.10
2:D:22:GLU:CA	2:D:22:GLU:HG3	1.61	1.10
2:D:43:GLU:C	2:D:43:GLU:CB	2.23	1.10
2:D:4:THR:CB	2:D:6:GLU:OE2	2.00	1.10
2:D:10:ALA:C	2:D:10:ALA:CB	2.23	1.10
2:D:78:LEU:CD2	2:D:78:LEU:CD1	2.30	1.09
1:A:90:LYS:CE	1:A:90:LYS:CG	2.29	1.08
2:D:144:LYS:CE	2:D:144:LYS:NZ	2.16	1.08
2:B:117:HIS:NE2	2:B:117:HIS:CD2	2.21	1.08
1:A:75:ASP:HB3	1:A:75:ASP:OD2	1.54	1.08
1:A:92:ARG:CD	1:A:92:ARG:HH11	1.65	1.07
2:B:48:LEU:C	2:B:49:SER:CA	2.27	1.07
1:C:1:VAL:CG1	1:C:1:VAL:HG22	1.77	1.07
2:D:5:PRO:CA	2:D:5:PRO:CB	2.31	1.07
1:A:16:LYS:CG	1:A:16:LYS:HE2	1.82	1.07
3:A:142:HEM:CGA	3:A:142:HEM:CBA	2.32	1.07
1:C:16:LYS:CD	1:C:16:LYS:CB	2.33	1.07
2:D:76:ALA:N	2:D:76:ALA:CB	2.17	1.07
2:D:6:GLU:CG	2:D:6:GLU:HB3	1.55	1.07
2:D:8:LYS:CB	2:D:8:LYS:CD	2.33	1.06
1:A:75:ASP:CB	1:A:75:ASP:OD2	2.02	1.06
1:C:116:GLU:CG	1:C:116:GLU:CB	2.33	1.06
2:D:6:GLU:CG	2:D:6:GLU:HB2	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:ASP:CG	2:D:79:ASP:OD2	1.98	1.06
2:D:4:THR:C	2:D:5:PRO:CA	2.27	1.05
2:D:26:GLU:CG	2:D:26:GLU:OE1	2.05	1.05
1:C:84:SER:CA	1:C:84:SER:OG	2.04	1.05
2:D:78:LEU:CB	2:D:78:LEU:CD2	2.33	1.05
1:A:99:LYS:CE	1:A:99:LYS:NZ	2.20	1.05
2:B:46:GLY:C	2:B:47:ASP:CA	2.29	1.05
2:D:79:ASP:CG	2:D:79:ASP:OD1	1.99	1.05
2:D:53:ALA:C	2:D:53:ALA:CB	2.30	1.05
1:A:78:ASN:CG	1:A:78:ASN:HB2	1.50	1.04
2:B:65:LYS:CD	2:B:65:LYS:CE	2.35	1.04
1:C:30:GLU:CD	1:C:30:GLU:OE2	0.80	1.04
1:C:40:LYS:CD	1:C:40:LYS:HE3	1.53	1.04
2:D:6:GLU:CA	2:D:6:GLU:C	2.31	1.04
1:A:16:LYS:HE2	1:A:16:LYS:HG3	1.38	1.04
2:D:77:HIS:CB	2:D:77:HIS:C	2.29	1.04
2:D:141:LEU:CD2	2:D:141:LEU:CD1	2.34	1.04
2:D:47:ASP:C	2:D:48:LEU:CA	2.30	1.04
1:A:74:ASP:CG	1:A:74:ASP:OD1	0.80	1.03
2:D:6:GLU:CB	2:D:6:GLU:HG2	1.51	1.03
2:B:59:LYS:CE	2:B:59:LYS:CD	2.36	1.03
2:B:66:LYS:CE	2:B:66:LYS:CD	2.37	1.02
2:B:81:LEU:N	2:B:81:LEU:CB	2.22	1.02
1:C:1:VAL:CB	1:C:1:VAL:N	2.22	1.02
2:B:139:ASN:ND2	2:B:139:ASN:OD1	1.91	1.02
1:C:99:LYS:CD	1:C:99:LYS:CB	2.36	1.02
1:A:78:ASN:CG	1:A:78:ASN:HB3	1.50	1.02
2:B:8:LYS:CG	2:B:8:LYS:HB2	1.52	1.02
1:C:40:LYS:CD	1:C:40:LYS:HE2	1.53	1.02
2:B:49:SER:N	2:B:49:SER:C	2.18	1.01
1:C:38:THR:H	1:C:38:THR:HG22	1.23	1.01
1:C:92:ARG:HH21	1:C:92:ARG:CD	1.72	1.01
2:D:79:ASP:C	2:D:79:ASP:CB	2.31	1.01
1:C:40:LYS:CE	1:C:40:LYS:HD2	1.50	1.01
2:D:58:PRO:CD	2:D:58:PRO:CA	2.37	1.01
2:B:1:VAL:CA	2:B:2:HIS:N	2.23	1.01
2:D:6:GLU:CB	2:D:6:GLU:HG3	1.51	1.01
3:D:148:HEM:CGA	3:D:148:HEM:CBA	2.39	1.01
2:B:101:GLU:CG	2:B:101:GLU:OE2	2.09	1.00
1:C:90:LYS:CD	1:C:90:LYS:CB	2.39	1.00
1:A:75:ASP:CG	1:A:75:ASP:OD2	2.04	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:CZ	1:A:92:ARG:NH2	0.85	1.00
2:D:78:LEU:CG	2:D:78:LEU:HD21	1.51	1.00
2:B:8:LYS:CG	2:B:8:LYS:HB3	1.52	1.00
1:A:85:ASP:CG	1:A:85:ASP:OD1	0.75	1.00
1:C:56:LYS:CE	1:C:56:LYS:CD	2.39	1.00
2:D:18:VAL:CG2	2:D:18:VAL:CG1	2.40	1.00
2:D:45:PHE:C	2:D:46:GLY:HA3	1.85	0.99
2:D:79:ASP:C	2:D:80:ASN:CA	2.35	0.99
1:C:40:LYS:CE	1:C:40:LYS:HD3	1.50	0.99
2:D:1:VAL:CA	2:D:2:HIS:N	2.23	0.99
2:D:47:ASP:CB	2:D:47:ASP:N	2.25	0.99
1:A:17:VAL:C	1:A:17:VAL:O	0.75	0.99
2:D:12:THR:CA	2:D:12:THR:CG2	2.39	0.99
2:D:104:ARG:CD	2:D:104:ARG:HH11	1.76	0.99
2:B:90:GLU:CA	2:B:90:GLU:CG	2.41	0.98
2:D:20:VAL:CA	2:D:20:VAL:HG22	1.92	0.98
2:D:82:LYS:CD	2:D:82:LYS:CE	2.41	0.98
2:D:146:HIS:ND1	2:D:146:HIS:NE2	2.10	0.98
1:A:78:ASN:CG	1:A:78:ASN:OD1	2.07	0.98
1:A:2:LEU:CA	1:A:3:SER:N	2.27	0.98
2:D:43:GLU:CB	2:D:43:GLU:HG3	1.47	0.97
2:D:92:HIS:C	2:D:92:HIS:CB	2.37	0.97
2:B:8:LYS:NZ	2:B:8:LYS:CE	2.27	0.97
2:B:132:LYS:NZ	2:B:132:LYS:CD	2.26	0.97
2:D:45:PHE:CA	2:D:46:GLY:N	2.27	0.97
2:D:52:ASP:CB	2:D:52:ASP:N	2.28	0.97
1:C:139:LYS:CD	1:C:139:LYS:NZ	2.27	0.97
2:D:43:GLU:CB	2:D:43:GLU:HG2	1.47	0.97
1:A:92:ARG:NH1	1:A:92:ARG:HD2	1.75	0.97
1:A:75:ASP:CG	1:A:75:ASP:HB2	1.42	0.97
2:D:73:ASP:CB	2:D:73:ASP:C	2.38	0.97
1:A:92:ARG:CZ	1:A:92:ARG:HD2	1.94	0.96
2:D:45:PHE:C	2:D:46:GLY:N	0.87	0.96
1:A:75:ASP:CG	1:A:75:ASP:HB3	1.43	0.96
3:C:142:HEM:O2A	3:C:142:HEM:CBA	2.14	0.96
3:B:148:HEM:CGA	3:B:148:HEM:O2A	0.66	0.96
2:B:2:HIS:C	2:B:2:HIS:CB	2.39	0.95
1:C:1:VAL:C	1:C:1:VAL:CB	2.38	0.95
2:D:7:GLU:C	2:D:8:LYS:CA	2.37	0.95
2:D:22:GLU:CG	2:D:22:GLU:CD	2.39	0.95
2:B:2:HIS:CA	2:B:3:LEU:N	2.28	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:CG	1:A:127:LYS:CE	2.44	0.95
2:D:78:LEU:HG	2:D:78:LEU:HD22	0.96	0.95
1:A:61:LYS:CE	1:A:61:LYS:HD2	1.44	0.95
1:C:38:THR:CA	1:C:38:THR:CG2	2.44	0.95
2:D:20:VAL:CA	2:D:20:VAL:HG23	1.91	0.95
2:D:20:VAL:CA	2:D:20:VAL:CG1	2.45	0.95
1:C:61:LYS:CD	1:C:61:LYS:NZ	2.29	0.95
1:A:1:VAL:HG23	1:A:1:VAL:H3	1.12	0.95
1:C:7:LYS:CG	1:C:7:LYS:CE	2.45	0.95
2:B:9:SER:CA	2:B:9:SER:OG	2.13	0.95
1:C:1:VAL:N	1:C:1:VAL:HB	1.81	0.94
1:A:61:LYS:CE	1:A:61:LYS:HD3	1.44	0.94
2:D:120:LYS:NZ	2:D:120:LYS:CE	2.29	0.94
2:B:80:ASN:C	2:B:81:LEU:CA	2.40	0.94
1:C:84:SER:CB	1:C:84:SER:C	2.39	0.94
2:B:139:ASN:CG	2:B:139:ASN:HB3	1.37	0.94
3:B:148:HEM:CBA	3:B:148:HEM:O2A	2.15	0.94
2:B:8:LYS:CB	2:B:8:LYS:HG2	1.44	0.94
2:D:76:ALA:N	2:D:76:ALA:C	2.26	0.94
2:D:22:GLU:CG	2:D:22:GLU:HB2	1.43	0.94
2:B:8:LYS:CB	2:B:8:LYS:HG3	1.44	0.93
2:D:121:GLU:CA	2:D:121:GLU:CG	2.45	0.93
1:A:85:ASP:OD1	1:A:85:ASP:CB	2.15	0.93
1:C:1:VAL:HG13	1:C:1:VAL:HG22	0.95	0.93
2:D:6:GLU:CG	2:D:6:GLU:CB	0.94	0.93
2:B:12:THR:C	2:B:12:THR:HG23	1.93	0.93
2:D:141:LEU:CD2	2:D:141:LEU:CB	2.45	0.93
2:D:22:GLU:CG	2:D:22:GLU:HB3	1.43	0.93
2:D:78:LEU:CG	2:D:78:LEU:HD22	1.51	0.93
1:A:90:LYS:CE	1:A:90:LYS:HG3	1.98	0.93
1:A:78:ASN:CB	1:A:78:ASN:CG	0.88	0.92
2:D:126:VAL:CA	2:D:126:VAL:CG2	2.46	0.92
3:D:148:HEM:CBA	3:D:148:HEM:O1A	2.18	0.92
2:B:22:GLU:CD	2:B:22:GLU:OE2	2.12	0.92
1:A:61:LYS:CD	1:A:61:LYS:HE2	1.42	0.92
2:B:47:ASP:C	2:B:47:ASP:CB	2.41	0.92
2:B:43:GLU:CD	2:B:43:GLU:CG	2.43	0.92
2:B:82:LYS:CE	2:B:82:LYS:HD3	1.40	0.92
2:B:104:ARG:CZ	2:B:104:ARG:HD3	1.98	0.92
1:C:72:HIS:CB	1:C:72:HIS:C	2.41	0.92
2:D:79:ASP:CA	2:D:80:ASN:N	2.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:CA	1:A:137:THR:CG2	2.45	0.92
2:D:90:GLU:CD	2:D:90:GLU:CG	2.43	0.92
1:A:62:VAL:CA	1:A:63:ALA:N	2.33	0.92
1:C:1:VAL:CG2	1:C:1:VAL:CB	2.48	0.92
2:D:52:ASP:CB	2:D:52:ASP:OD1	2.17	0.92
2:D:126:VAL:CA	2:D:126:VAL:CG1	2.48	0.91
1:A:51:GLY:C	1:A:52:SER:CA	2.43	0.91
1:A:72:HIS:CB	1:A:72:HIS:C	2.42	0.91
2:D:47:ASP:CA	2:D:47:ASP:C	2.43	0.91
2:B:10:ALA:C	2:B:10:ALA:CB	2.41	0.91
1:C:46:PHE:CE2	1:C:46:PHE:CD2	0.92	0.91
1:A:61:LYS:CD	1:A:61:LYS:HE3	1.42	0.91
2:B:80:ASN:CB	2:B:80:ASN:ND2	2.33	0.91
2:D:108:ASN:CB	2:D:108:ASN:ND2	2.33	0.91
2:B:65:LYS:CA	2:B:65:LYS:HG2	2.01	0.91
2:B:87:THR:CG2	2:B:87:THR:OG1	2.16	0.91
2:D:67:VAL:CA	2:D:67:VAL:CG1	2.47	0.91
2:D:22:GLU:HG3	2:D:22:GLU:CB	1.39	0.91
2:D:65:LYS:CD	2:D:65:LYS:CB	2.48	0.91
2:B:2:HIS:CD2	2:B:2:HIS:CB	2.53	0.91
2:B:65:LYS:CA	2:B:65:LYS:HG3	2.01	0.91
2:B:82:LYS:CD	2:B:82:LYS:HE3	1.39	0.91
2:B:139:ASN:CG	2:B:139:ASN:HB2	1.37	0.91
2:D:77:HIS:CE1	2:D:77:HIS:CG	2.52	0.91
1:A:127:LYS:CB	1:A:127:LYS:HG3	1.40	0.90
2:B:82:LYS:CD	2:B:82:LYS:HE2	1.39	0.90
2:B:82:LYS:CG	2:B:82:LYS:HE2	1.74	0.90
2:B:82:LYS:CE	2:B:82:LYS:NZ	2.35	0.90
1:C:1:VAL:CA	1:C:1:VAL:N	2.33	0.90
2:B:12:THR:CG2	2:B:12:THR:C	2.45	0.90
2:B:82:LYS:CE	2:B:82:LYS:HD2	1.40	0.90
1:A:137:THR:OG1	1:A:137:THR:CG2	2.14	0.90
2:B:139:ASN:OD1	2:B:139:ASN:CB	2.20	0.90
2:D:139:ASN:OD1	2:D:139:ASN:CB	2.19	0.90
2:B:8:LYS:CD	2:B:8:LYS:CB	2.49	0.90
2:B:65:LYS:CG	2:B:65:LYS:CD	2.49	0.90
2:D:49:SER:C	2:D:49:SER:CB	2.44	0.90
2:D:3:LEU:O	2:D:4:THR:N	2.03	0.90
1:A:61:LYS:NZ	1:A:61:LYS:CD	2.34	0.89
1:C:30:GLU:CG	1:C:30:GLU:OE2	2.20	0.89
2:D:26:GLU:CG	2:D:26:GLU:OE2	2.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:CB	1:A:127:LYS:HG2	1.40	0.89
1:A:56:LYS:CD	1:A:56:LYS:CB	2.50	0.89
2:D:104:ARG:HH11	2:D:104:ARG:HD2	1.37	0.89
1:A:44:PRO:C	1:A:44:PRO:CB	2.46	0.89
1:A:127:LYS:CG	1:A:127:LYS:HB2	1.37	0.89
2:D:22:GLU:CB	2:D:22:GLU:HG2	1.39	0.89
2:D:66:LYS:NZ	3:D:148:HEM:O1A	2.06	0.89
1:A:1:VAL:CA	1:A:1:VAL:CG1	2.51	0.89
2:D:7:GLU:CB	2:D:7:GLU:CD	2.45	0.89
2:D:20:VAL:CG2	2:D:20:VAL:C	2.45	0.89
1:C:72:HIS:CA	1:C:72:HIS:CG	2.54	0.88
2:D:93:CYS:C	2:D:94:ASP:CA	2.45	0.88
1:A:75:ASP:CB	1:A:75:ASP:C	2.45	0.88
2:D:78:LEU:CD2	2:D:78:LEU:CG	0.88	0.88
2:D:80:ASN:N	2:D:80:ASN:HB3	1.89	0.88
2:B:2:HIS:CG	2:B:2:HIS:CB	0.83	0.88
1:C:1:VAL:CA	1:C:1:VAL:CG2	2.51	0.88
2:B:8:LYS:CA	2:B:8:LYS:HG3	2.02	0.88
1:C:16:LYS:CD	1:C:16:LYS:HB3	2.03	0.88
1:A:127:LYS:CG	1:A:127:LYS:HB3	1.37	0.88
2:B:2:HIS:CG	2:B:2:HIS:HB3	1.42	0.88
2:B:2:HIS:CG	2:B:2:HIS:HB2	1.42	0.88
1:C:99:LYS:CB	1:C:99:LYS:HG3	1.36	0.87
2:D:67:VAL:CB	2:D:67:VAL:N	2.36	0.87
2:B:5:PRO:C	2:B:5:PRO:N	2.31	0.87
1:C:38:THR:H	1:C:38:THR:CG2	1.88	0.87
1:C:99:LYS:CG	1:C:99:LYS:HB3	1.36	0.87
2:B:8:LYS:CG	2:B:8:LYS:CB	0.87	0.87
2:D:94:ASP:N	2:D:94:ASP:CB	2.38	0.87
2:D:146:HIS:ND1	2:D:146:HIS:CE1	0.67	0.86
1:A:141:ARG:CG	1:A:141:ARG:CA	2.53	0.86
2:B:117:HIS:ND1	2:B:117:HIS:CB	2.37	0.86
3:C:142:HEM:O2A	3:C:142:HEM:O1A	1.92	0.86
1:C:99:LYS:CB	1:C:99:LYS:HG2	1.36	0.86
1:C:99:LYS:CG	1:C:99:LYS:HB2	1.36	0.86
1:A:17:VAL:CA	1:A:18:GLY:N	2.38	0.85
1:A:50:HIS:CB	1:A:50:HIS:N	2.37	0.85
1:C:38:THR:HG22	1:C:38:THR:N	1.91	0.85
1:C:40:LYS:CE	1:C:40:LYS:CD	0.85	0.85
1:A:58:HIS:CA	1:A:59:GLY:N	2.39	0.85
2:B:108:ASN:CB	2:B:108:ASN:HD22	1.88	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:THR:CG2	1:C:38:THR:N	2.39	0.85
1:C:46:PHE:CE2	1:C:46:PHE:HD2	1.59	0.85
2:B:5:PRO:CA	2:B:6:GLU:N	2.40	0.85
2:D:20:VAL:HG23	2:D:20:VAL:C	2.01	0.85
2:B:47:ASP:N	2:B:47:ASP:CB	2.39	0.84
1:C:56:LYS:CE	1:C:56:LYS:CG	2.55	0.84
1:A:31:ARG:CD	1:A:31:ARG:CZ	2.54	0.84
2:D:59:LYS:CA	2:D:60:VAL:N	2.40	0.84
1:C:118:THR:CB	1:C:118:THR:N	2.40	0.84
2:B:65:LYS:HG3	2:B:65:LYS:C	2.03	0.84
1:C:8:THR:CA	1:C:8:THR:CG2	2.55	0.84
1:A:50:HIS:CB	1:A:50:HIS:C	2.50	0.84
1:C:40:LYS:NZ	1:C:40:LYS:HD3	1.92	0.84
1:A:127:LYS:CD	1:A:127:LYS:HB2	2.06	0.84
1:A:141:ARG:CB	1:A:141:ARG:CD	2.55	0.84
2:B:49:SER:CA	2:B:49:SER:O	2.26	0.84
3:B:148:HEM:CBA	3:B:148:HEM:O1A	2.24	0.84
1:C:74:ASP:C	1:C:75:ASP:CA	2.51	0.84
1:C:60:LYS:NZ	1:C:60:LYS:CD	2.41	0.84
1:A:99:LYS:CE	1:A:99:LYS:CG	2.52	0.83
1:C:69:ALA:C	1:C:70:VAL:CA	2.50	0.83
2:D:50:THR:CB	2:D:50:THR:C	2.51	0.83
1:C:139:LYS:CE	1:C:139:LYS:CG	2.56	0.83
2:D:19:ASN:ND2	2:D:19:ASN:OD1	2.10	0.83
2:D:77:HIS:CA	2:D:77:HIS:CG	2.61	0.83
1:A:137:THR:CA	1:A:137:THR:OG1	2.25	0.83
2:D:11:VAL:C	2:D:12:THR:CA	2.52	0.83
2:B:61:LYS:NZ	2:B:61:LYS:CD	2.42	0.83
2:D:78:LEU:HG	2:D:78:LEU:HD23	0.83	0.83
1:A:92:ARG:CZ	1:A:92:ARG:HD3	1.96	0.82
2:B:8:LYS:CA	2:B:8:LYS:HG2	2.08	0.82
2:D:78:LEU:CD2	2:D:78:LEU:HG	0.56	0.82
1:A:92:ARG:HD3	1:A:92:ARG:HH11	1.20	0.82
2:B:143:HIS:ND1	2:B:143:HIS:CB	2.43	0.82
2:D:48:LEU:N	2:D:48:LEU:CB	2.42	0.82
2:B:65:LYS:CB	2:B:65:LYS:HG2	1.32	0.82
2:B:65:LYS:CB	2:B:65:LYS:HG3	1.32	0.82
1:C:105:LEU:CD2	1:C:105:LEU:CB	2.56	0.82
2:B:47:ASP:CA	2:B:48:LEU:N	2.41	0.82
2:B:121:GLU:CD	2:B:121:GLU:CB	2.52	0.82
2:D:146:HIS:ND1	2:D:146:HIS:HE1	1.35	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:ASN:N	2:D:80:ASN:CB	2.40	0.82
1:C:48:LEU:CD2	1:C:48:LEU:CD1	2.57	0.81
2:D:2:HIS:CG	2:D:2:HIS:ND1	2.48	0.81
1:A:61:LYS:CE	1:A:61:LYS:CD	0.81	0.81
1:A:92:ARG:CZ	1:A:92:ARG:HH22	1.48	0.81
2:B:65:LYS:CG	2:B:65:LYS:HB2	1.31	0.81
2:D:113:VAL:CG2	2:D:113:VAL:CG1	2.58	0.81
1:A:21:ALA:CA	1:A:22:GLY:N	2.43	0.81
1:A:40:LYS:CB	1:A:40:LYS:C	2.53	0.81
2:B:3:LEU:CB	2:B:3:LEU:N	2.42	0.81
2:B:65:LYS:CG	2:B:65:LYS:CE	2.58	0.81
1:C:105:LEU:CD1	1:C:105:LEU:CB	2.58	0.81
1:A:5:ALA:CB	1:A:5:ALA:N	2.43	0.81
1:A:92:ARG:CZ	1:A:92:ARG:HH21	1.48	0.81
2:B:87:THR:CB	2:B:87:THR:C	2.52	0.81
1:C:76:MET:SD	1:C:76:MET:CB	2.68	0.81
1:C:118:THR:CB	1:C:118:THR:C	2.52	0.81
2:D:4:THR:CA	2:D:4:THR:CG2	2.54	0.81
2:B:121:GLU:CG	2:B:121:GLU:OE2	2.27	0.81
1:A:60:LYS:CE	1:A:60:LYS:CG	2.57	0.81
2:D:18:VAL:CG2	2:D:18:VAL:CA	2.58	0.81
1:A:72:HIS:CG	1:A:72:HIS:N	2.48	0.81
2:B:2:HIS:ND1	2:B:2:HIS:CB	2.44	0.81
1:C:23:GLU:OE2	1:C:23:GLU:CB	2.29	0.81
2:D:48:LEU:CD1	2:D:48:LEU:CB	2.58	0.81
1:C:23:GLU:CG	1:C:23:GLU:OE2	2.28	0.80
2:D:8:LYS:CG	2:D:8:LYS:CE	2.59	0.80
2:D:49:SER:O	2:D:50:THR:HA	1.81	0.80
2:D:55:MET:CA	2:D:56:GLY:N	2.43	0.80
1:A:84:SER:CA	1:A:84:SER:OG	2.28	0.80
2:B:65:LYS:CG	2:B:65:LYS:HB3	1.31	0.80
1:C:105:LEU:CD1	1:C:105:LEU:CD2	2.58	0.80
2:D:43:GLU:CG	2:D:43:GLU:HB2	1.29	0.80
2:B:7:GLU:CG	2:B:7:GLU:CA	2.47	0.80
1:C:92:ARG:NE	1:C:92:ARG:NH2	2.27	0.80
2:B:65:LYS:CB	2:B:65:LYS:CD	2.59	0.80
1:A:76:MET:SD	1:A:76:MET:CB	2.66	0.80
2:B:12:THR:HG23	2:B:12:THR:CB	1.28	0.80
2:B:43:GLU:O	2:B:44:SER:C	2.23	0.79
2:D:12:THR:C	2:D:12:THR:HG22	2.07	0.79
1:A:1:VAL:CA	1:A:1:VAL:HG22	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:THR:CB	2:B:12:THR:HG22	1.28	0.79
2:B:59:LYS:CE	2:B:59:LYS:CG	2.61	0.79
1:C:73:VAL:CA	1:C:73:VAL:CG2	2.59	0.79
2:D:73:ASP:CG	2:D:73:ASP:OD2	2.26	0.79
3:A:142:HEM:CBA	3:A:142:HEM:O1A	2.31	0.79
1:A:81:SER:CB	1:A:81:SER:N	2.45	0.79
2:D:17:LYS:NZ	2:D:17:LYS:CD	2.46	0.79
1:A:74:ASP:OD1	1:A:74:ASP:OD2	2.00	0.79
2:B:5:PRO:C	2:B:5:PRO:CB	2.54	0.79
2:D:43:GLU:CG	2:D:43:GLU:HB3	1.29	0.79
1:C:61:LYS:CE	1:C:61:LYS:CG	2.59	0.79
1:C:138:SER:CA	1:C:138:SER:HG	1.94	0.78
2:D:82:LYS:CD	2:D:82:LYS:HZ2	1.97	0.78
2:B:146:HIS:CB	2:B:146:HIS:CD2	2.66	0.78
2:D:22:GLU:C	2:D:22:GLU:HG3	2.09	0.78
2:D:49:SER:O	2:D:50:THR:CA	2.31	0.78
1:C:1:VAL:CG2	1:C:1:VAL:HA	2.12	0.78
2:B:2:HIS:CA	2:B:2:HIS:CG	2.65	0.78
2:B:7:GLU:CB	2:B:7:GLU:CD	2.56	0.78
2:B:82:LYS:HE2	2:B:82:LYS:CB	2.14	0.78
1:A:84:SER:CB	1:A:84:SER:C	2.57	0.78
2:B:80:ASN:CA	2:B:80:ASN:O	2.31	0.78
2:D:7:GLU:C	2:D:7:GLU:CB	2.57	0.78
2:B:2:HIS:CD2	2:B:2:HIS:CE1	2.72	0.77
2:D:43:GLU:CG	2:D:43:GLU:CB	0.78	0.77
2:D:78:LEU:CB	2:D:78:LEU:C	2.58	0.77
2:B:139:ASN:ND2	2:B:139:ASN:CB	2.47	0.77
2:D:10:ALA:C	2:D:10:ALA:HB3	2.08	0.77
1:C:46:PHE:CD2	1:C:46:PHE:HE2	1.48	0.77
2:D:82:LYS:NZ	2:D:82:LYS:HD2	1.98	0.77
2:B:117:HIS:CG	2:B:117:HIS:NE2	2.52	0.77
1:C:75:ASP:N	1:C:75:ASP:C	2.43	0.77
1:C:90:LYS:CE	1:C:90:LYS:CG	2.63	0.77
1:C:82:ALA:C	1:C:83:LEU:CA	2.58	0.77
1:A:138:SER:CA	1:A:138:SER:HG	1.95	0.77
2:B:6:GLU:C	2:B:6:GLU:CB	2.58	0.77
1:C:116:GLU:CB	1:C:116:GLU:CD	2.57	0.77
2:D:7:GLU:CA	2:D:7:GLU:CG	2.63	0.76
2:B:6:GLU:C	2:B:6:GLU:N	2.43	0.76
2:B:41:PHE:CA	2:B:41:PHE:O	2.31	0.76
2:B:87:THR:CA	2:B:87:THR:OG1	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:CA	1:C:70:VAL:O	2.32	0.76
2:D:6:GLU:OE2	2:D:6:GLU:OE1	2.02	0.76
2:D:12:THR:CG2	2:D:12:THR:C	2.58	0.76
1:A:50:HIS:C	1:A:50:HIS:CG	2.64	0.76
2:B:41:PHE:CA	2:B:42:PHE:N	2.46	0.76
1:C:131:SER:CA	1:C:131:SER:O	2.34	0.76
1:A:40:LYS:CA	1:A:40:LYS:CG	2.61	0.76
1:C:70:VAL:CA	1:C:71:ALA:N	2.36	0.76
3:A:142:HEM:CBA	3:A:142:HEM:O2A	2.33	0.76
2:D:46:GLY:CA	2:D:46:GLY:O	2.33	0.76
2:D:47:ASP:CB	2:D:47:ASP:OD1	2.34	0.76
2:B:146:HIS:CB	2:B:146:HIS:ND1	2.42	0.76
1:A:50:HIS:CA	1:A:50:HIS:CG	2.68	0.76
2:B:61:LYS:CE	2:B:61:LYS:CG	2.64	0.76
2:D:22:GLU:CG	2:D:22:GLU:CB	0.76	0.75
1:C:16:LYS:C	1:C:16:LYS:N	2.43	0.75
1:A:138:SER:OG	1:A:138:SER:HA	1.81	0.75
2:D:59:LYS:C	2:D:59:LYS:CB	2.57	0.75
2:D:78:LEU:CB	2:D:78:LEU:N	2.49	0.75
2:D:132:LYS:NZ	2:D:132:LYS:CE	2.49	0.75
1:C:1:VAL:C	1:C:1:VAL:CG1	2.59	0.75
1:C:30:GLU:CD	1:C:50:HIS:HD2	1.94	0.75
1:C:54:GLN:C	1:C:54:GLN:CB	2.59	0.75
2:D:101:GLU:CG	2:D:101:GLU:OE2	2.33	0.75
3:D:148:HEM:CBD	3:D:148:HEM:O1D	2.34	0.75
1:A:2:LEU:CA	1:A:2:LEU:O	2.33	0.75
2:B:49:SER:OG	2:B:49:SER:C	2.29	0.75
2:B:61:LYS:CD	2:B:61:LYS:CB	2.62	0.75
1:A:17:VAL:CA	1:A:17:VAL:O	2.34	0.75
2:B:49:SER:O	2:B:50:THR:N	2.19	0.75
1:A:11:LYS:CE	1:A:11:LYS:CG	2.64	0.75
1:C:2:LEU:C	1:C:2:LEU:CB	2.57	0.75
1:A:18:GLY:CA	1:A:19:ALA:N	2.49	0.74
1:A:74:ASP:CG	1:A:74:ASP:CA	2.60	0.74
2:B:65:LYS:CG	2:B:65:LYS:C	2.60	0.74
1:A:133:SER:O	1:A:137:THR:HG22	1.85	0.74
2:B:3:LEU:CB	2:B:3:LEU:C	2.61	0.74
2:B:8:LYS:HG2	2:B:8:LYS:C	2.12	0.74
2:D:104:ARG:NE	2:D:104:ARG:CG	2.49	0.74
1:C:30:GLU:CG	1:C:30:GLU:OE1	2.35	0.74
1:C:1:VAL:C	1:C:1:VAL:HG12	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:C	1:A:87:HIS:CB	2.60	0.74
1:C:2:LEU:CA	1:C:2:LEU:O	2.36	0.74
1:C:61:LYS:C	1:C:61:LYS:CB	2.60	0.74
1:C:99:LYS:CG	1:C:99:LYS:CB	0.74	0.74
2:D:59:LYS:CE	2:D:59:LYS:CG	2.52	0.74
1:A:81:SER:CA	1:A:81:SER:OG	2.35	0.74
1:C:7:LYS:N	1:C:7:LYS:CB	2.49	0.74
2:B:43:GLU:CG	2:B:43:GLU:OE2	2.36	0.73
2:D:45:PHE:O	2:D:46:GLY:N	2.14	0.73
3:A:142:HEM:CBD	3:A:142:HEM:O1D	2.35	0.73
2:D:82:LYS:CD	2:D:82:LYS:HZ3	2.02	0.73
2:B:143:HIS:C	2:B:143:HIS:CB	2.60	0.73
1:C:54:GLN:CA	1:C:55:VAL:N	2.51	0.73
2:D:104:ARG:CD	2:D:104:ARG:NH1	2.52	0.73
1:A:74:ASP:CB	1:A:74:ASP:OD1	2.37	0.73
1:A:1:VAL:CG2	1:A:1:VAL:H1	1.99	0.73
2:D:95:LYS:CD	2:D:95:LYS:CB	2.67	0.73
1:A:75:ASP:CG	1:A:75:ASP:CB	0.68	0.73
3:B:148:HEM:CBD	3:B:148:HEM:O1D	2.35	0.73
2:D:79:ASP:OD2	2:D:79:ASP:CB	2.37	0.73
2:B:2:HIS:C	2:B:2:HIS:CG	2.66	0.73
1:C:131:SER:C	1:C:131:SER:CB	2.61	0.72
1:C:70:VAL:N	1:C:70:VAL:CB	2.49	0.72
2:D:49:SER:CA	2:D:50:THR:N	2.52	0.72
2:B:145:TYR:C	2:B:145:TYR:CB	2.55	0.72
2:B:12:THR:HG21	2:B:12:THR:HB	0.75	0.72
2:D:143:HIS:CD2	2:D:143:HIS:CB	2.68	0.72
1:A:56:LYS:CD	1:A:56:LYS:NZ	2.52	0.72
1:C:16:LYS:HB3	1:C:16:LYS:HD3	1.70	0.72
2:D:2:HIS:CG	2:D:2:HIS:CA	2.70	0.72
2:D:113:VAL:CG2	2:D:113:VAL:CA	2.65	0.72
2:D:132:LYS:NZ	2:D:132:LYS:CD	2.53	0.72
2:B:59:LYS:NZ	2:B:59:LYS:CD	2.53	0.72
1:C:40:LYS:NZ	1:C:40:LYS:HD2	2.01	0.72
1:A:5:ALA:CB	1:A:5:ALA:C	2.62	0.72
2:B:8:LYS:CB	2:B:8:LYS:N	2.49	0.72
2:D:8:LYS:CB	2:D:8:LYS:C	2.60	0.72
2:D:47:ASP:N	2:D:47:ASP:HB3	2.04	0.72
2:D:50:THR:N	2:D:50:THR:CB	2.53	0.72
1:C:92:ARG:CD	1:C:92:ARG:NH2	2.52	0.71
2:D:78:LEU:CG	2:D:78:LEU:HD23	1.51	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:HIS:CG	2:B:2:HIS:CE1	2.77	0.71
2:D:43:GLU:CA	2:D:44:SER:N	2.53	0.71
1:A:87:HIS:CA	1:A:88:ALA:N	2.50	0.71
2:B:146:HIS:CG	2:B:146:HIS:CA	2.73	0.71
1:A:52:SER:N	1:A:52:SER:CB	2.54	0.71
1:A:127:LYS:CG	1:A:127:LYS:CB	0.71	0.71
2:B:7:GLU:CG	2:B:7:GLU:HA	2.19	0.71
2:B:145:TYR:CA	2:B:145:TYR:O	2.38	0.71
2:D:139:ASN:OD1	2:D:139:ASN:HB3	1.91	0.71
2:B:12:THR:CB	2:B:12:THR:HG21	1.28	0.71
2:B:139:ASN:CG	2:B:139:ASN:CB	0.66	0.71
1:C:75:ASP:N	1:C:75:ASP:CB	2.54	0.71
2:B:1:VAL:CA	2:B:1:VAL:CG2	2.64	0.70
1:A:52:SER:N	1:A:52:SER:C	2.46	0.70
2:D:22:GLU:CA	2:D:23:VAL:N	2.53	0.70
2:D:92:HIS:C	2:D:92:HIS:N	2.49	0.70
2:D:141:LEU:CD2	2:D:141:LEU:HD13	2.21	0.70
1:C:113:LEU:CD1	1:C:113:LEU:HB3	2.21	0.70
1:A:30:GLU:CD	1:A:30:GLU:CB	2.63	0.70
3:C:142:HEM:CBD	3:C:142:HEM:O1D	2.32	0.70
2:D:4:THR:O	2:D:5:PRO:CA	2.40	0.70
1:C:6:ASP:C	1:C:7:LYS:CA	2.62	0.70
1:C:10:VAL:C	1:C:10:VAL:CB	2.65	0.70
2:D:1:VAL:HB	2:D:2:HIS:N	2.06	0.70
2:D:45:PHE:O	2:D:46:GLY:HA3	1.90	0.70
2:B:82:LYS:CE	2:B:82:LYS:CD	0.70	0.70
1:C:10:VAL:CA	1:C:11:LYS:N	2.52	0.69
1:A:62:VAL:C	1:A:62:VAL:CB	2.63	0.69
2:B:12:THR:CA	2:B:12:THR:HG23	1.88	0.69
2:B:5:PRO:N	2:B:6:GLU:N	2.40	0.69
2:D:73:ASP:OD2	5:D:174:HOH:O	2.10	0.69
2:B:90:GLU:CG	2:B:90:GLU:OE1	2.38	0.69
1:C:56:LYS:NZ	1:C:56:LYS:CD	2.56	0.69
2:B:57:ASN:C	2:B:58:PRO:CD	2.64	0.69
2:D:8:LYS:CG	2:D:8:LYS:C	2.65	0.69
2:D:131:GLN:CG	2:D:131:GLN:NE2	2.49	0.69
1:A:137:THR:CB	1:A:137:THR:C	2.64	0.69
2:B:74:GLY:CA	2:B:75:LEU:N	2.51	0.69
1:A:127:LYS:CG	1:A:127:LYS:HA	2.15	0.69
1:C:46:PHE:CD2	1:C:46:PHE:CZ	2.39	0.69
2:D:17:LYS:NZ	2:D:17:LYS:HD3	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LYS:CD	1:C:56:LYS:CB	2.70	0.69
1:A:11:LYS:CD	1:A:11:LYS:NZ	2.56	0.68
1:A:92:ARG:CD	1:A:92:ARG:NH2	2.56	0.68
3:B:148:HEM:CBD	3:B:148:HEM:O2D	2.38	0.68
2:B:12:THR:CA	2:B:12:THR:HG22	1.88	0.68
3:C:142:HEM:CBD	3:C:142:HEM:O2D	2.35	0.68
2:D:67:VAL:CG1	2:D:67:VAL:C	2.66	0.68
2:B:90:GLU:CB	2:B:90:GLU:C	2.67	0.68
1:C:38:THR:CB	1:C:38:THR:N	2.56	0.68
2:D:6:GLU:CD	2:D:6:GLU:CB	2.67	0.68
2:D:8:LYS:CB	2:D:8:LYS:N	2.55	0.68
2:D:82:LYS:CD	2:D:82:LYS:CB	2.68	0.68
1:A:78:ASN:ND2	1:A:78:ASN:OD1	2.26	0.68
2:B:52:ASP:CB	2:B:52:ASP:OD2	2.41	0.68
2:D:12:THR:CA	2:D:12:THR:OG1	2.40	0.68
2:D:47:ASP:CA	2:D:48:LEU:N	2.55	0.68
1:A:85:ASP:OD2	1:A:85:ASP:OD1	2.10	0.68
2:D:7:GLU:CA	2:D:8:LYS:N	2.49	0.68
1:C:16:LYS:CG	1:C:16:LYS:HA	2.22	0.68
1:A:92:ARG:CZ	1:A:92:ARG:NE	2.57	0.68
2:D:8:LYS:CB	2:D:8:LYS:HD3	2.21	0.68
1:A:81:SER:CB	1:A:81:SER:C	2.66	0.68
1:A:137:THR:OG1	1:A:137:THR:HG22	1.93	0.68
2:B:9:SER:CA	2:B:10:ALA:N	2.56	0.67
2:D:7:GLU:CA	2:D:7:GLU:O	2.38	0.67
2:D:24:GLY:HA2	2:D:68:LEU:HD22	1.76	0.67
1:C:1:VAL:CG1	1:C:1:VAL:HA	2.23	0.67
2:B:52:ASP:CG	2:B:52:ASP:CA	2.64	0.67
2:B:117:HIS:CE1	2:B:117:HIS:CG	2.82	0.67
1:C:38:THR:CA	1:C:38:THR:OG1	2.42	0.67
2:D:12:THR:N	2:D:12:THR:C	2.49	0.67
2:D:121:GLU:CB	2:D:121:GLU:C	2.68	0.67
1:C:23:GLU:CD	1:C:23:GLU:OE1	2.37	0.67
2:D:123:THR:CG2	2:D:123:THR:OG1	2.42	0.67
2:B:80:ASN:CG	2:B:80:ASN:CA	2.62	0.67
2:D:121:GLU:CG	2:D:121:GLU:OE2	2.42	0.67
2:D:104:ARG:NE	2:D:104:ARG:CZ	2.58	0.67
2:D:123:THR:CG2	2:D:123:THR:CA	2.70	0.67
2:B:41:PHE:C	2:B:41:PHE:CB	2.67	0.67
2:B:49:SER:CB	2:B:49:SER:N	2.57	0.67
2:D:92:HIS:CA	2:D:92:HIS:O	2.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:HIS:C	1:C:87:HIS:CB	2.66	0.67
1:C:113:LEU:HD22	1:C:116:GLU:HG3	1.77	0.67
2:D:1:VAL:CB	2:D:2:HIS:N	2.57	0.67
3:C:142:HEM:HBB2	3:C:142:HEM:CMB	2.25	0.66
2:D:22:GLU:C	2:D:22:GLU:N	2.52	0.66
2:D:5:PRO:CB	2:D:5:PRO:C	2.68	0.66
2:D:82:LYS:CG	2:D:82:LYS:CE	2.73	0.66
2:B:108:ASN:CG	2:B:108:ASN:CA	2.64	0.66
2:D:43:GLU:HB3	2:D:43:GLU:OE1	1.95	0.66
2:D:79:ASP:N	2:D:80:ASN:N	2.43	0.66
2:B:65:LYS:CE	2:B:65:LYS:NZ	2.59	0.66
2:D:24:GLY:CA	2:D:68:LEU:HD22	2.24	0.66
1:A:75:ASP:CB	1:A:75:ASP:OD1	2.44	0.66
2:B:65:LYS:CE	2:B:65:LYS:HG3	2.24	0.66
2:D:26:GLU:OE2	2:D:26:GLU:CB	2.43	0.66
1:C:135:VAL:O	1:C:138:SER:HB2	1.95	0.65
2:B:82:LYS:CD	2:B:82:LYS:NZ	2.59	0.65
1:A:21:ALA:CA	1:A:21:ALA:O	2.44	0.65
1:A:44:PRO:CA	1:A:45:HIS:N	2.55	0.65
1:A:75:ASP:CG	1:A:75:ASP:C	2.65	0.65
1:A:139:LYS:NZ	1:A:139:LYS:CD	2.57	0.65
2:B:65:LYS:CB	2:B:65:LYS:C	2.66	0.65
2:B:6:GLU:CA	2:B:7:GLU:N	2.54	0.65
2:D:104:ARG:HD2	2:D:104:ARG:NH1	2.10	0.65
2:D:48:LEU:CD1	2:D:48:LEU:CD2	2.72	0.65
1:C:139:LYS:CD	1:C:139:LYS:HZ3	2.10	0.65
1:C:1:VAL:CA	1:C:2:LEU:N	2.55	0.64
1:C:27:GLU:OE2	1:C:112:HIS:HE1	1.80	0.64
2:D:7:GLU:C	2:D:7:GLU:N	2.55	0.64
2:D:65:LYS:CD	2:D:65:LYS:NZ	2.59	0.64
2:D:67:VAL:CB	2:D:67:VAL:C	2.64	0.64
2:D:82:LYS:HZ2	2:D:82:LYS:HD2	1.59	0.64
2:B:50:THR:CG2	2:B:50:THR:OG1	2.43	0.64
2:B:74:GLY:O	2:B:75:LEU:N	2.28	0.64
1:C:92:ARG:NH1	1:C:92:ARG:HD2	2.12	0.64
2:D:1:VAL:CA	2:D:2:HIS:H	2.07	0.64
2:D:101:GLU:CG	2:D:101:GLU:OE1	2.43	0.64
2:B:80:ASN:C	2:B:80:ASN:N	2.55	0.64
1:C:16:LYS:CB	1:C:16:LYS:HD3	2.22	0.64
2:D:8:LYS:CA	2:D:8:LYS:HG3	2.26	0.64
3:C:142:HEM:CGD	3:C:142:HEM:CAD	2.73	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:ASP:N	2:D:94:ASP:C	2.50	0.64
2:D:51:PRO:C	2:D:52:ASP:CA	2.71	0.64
2:D:131:GLN:CG	2:D:131:GLN:OE1	2.39	0.64
2:B:90:GLU:CB	2:B:90:GLU:CD	2.69	0.64
2:B:104:ARG:CG	2:B:104:ARG:NE	2.60	0.64
1:C:105:LEU:CD2	1:C:105:LEU:HD13	2.28	0.64
2:D:12:THR:CB	2:D:12:THR:C	2.66	0.64
2:B:21:ASP:CB	2:B:21:ASP:OD1	2.42	0.63
1:C:48:LEU:CD2	1:C:48:LEU:CB	2.66	0.63
2:D:21:ASP:CB	2:D:21:ASP:OD2	2.42	0.63
1:A:127:LYS:HG3	1:A:127:LYS:HA	1.77	0.63
2:B:124:PRO:C	2:B:125:PRO:CD	2.60	0.63
2:B:6:GLU:OE1	2:B:6:GLU:OE2	2.09	0.63
1:C:23:GLU:CD	1:C:23:GLU:CB	2.67	0.63
1:C:23:GLU:OE2	1:C:23:GLU:HB2	1.96	0.63
3:C:142:HEM:HBB2	3:C:142:HEM:HMB1	1.80	0.63
2:D:52:ASP:N	2:D:52:ASP:C	2.56	0.63
1:C:8:THR:CA	1:C:8:THR:OG1	2.46	0.63
2:D:52:ASP:N	2:D:52:ASP:HB2	2.12	0.63
1:C:60:LYS:NZ	1:C:60:LYS:HD3	2.13	0.63
2:D:80:ASN:OD1	2:D:80:ASN:CB	2.39	0.63
1:C:7:LYS:CG	1:C:7:LYS:HE3	2.27	0.63
1:C:73:VAL:H	1:C:73:VAL:HG12	1.64	0.63
2:D:65:LYS:CE	2:D:65:LYS:CG	2.77	0.63
1:A:29:LEU:CA	1:A:29:LEU:CG	2.70	0.62
1:C:2:LEU:C	1:C:2:LEU:N	2.55	0.62
2:B:82:LYS:CE	2:B:82:LYS:HG2	2.20	0.62
1:C:87:HIS:CA	1:C:88:ALA:N	2.61	0.62
2:D:77:HIS:CD2	2:D:77:HIS:CE1	2.70	0.62
2:B:48:LEU:O	2:B:49:SER:CA	2.47	0.62
2:B:80:ASN:OD1	2:B:80:ASN:HA	2.00	0.62
2:D:59:LYS:CD	2:D:59:LYS:NZ	2.63	0.62
1:A:78:ASN:CG	1:A:78:ASN:HA	2.20	0.62
2:D:58:PRO:CG	2:D:58:PRO:HD3	1.11	0.62
1:A:99:LYS:CE	1:A:99:LYS:HG3	2.29	0.62
1:C:82:ALA:CA	1:C:83:LEU:N	2.58	0.62
3:C:142:HEM:CBA	3:C:142:HEM:O1A	2.48	0.62
2:D:10:ALA:C	2:D:10:ALA:N	2.57	0.62
2:D:4:THR:CA	2:D:4:THR:OG1	2.46	0.61
1:A:15:GLY:O	1:A:16:LYS:N	2.19	0.61
1:A:90:LYS:CD	1:A:90:LYS:NZ	2.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:SER:CA	2:B:9:SER:HG	2.14	0.61
2:B:9:SER:C	2:B:9:SER:OG	2.43	0.61
1:C:105:LEU:CD2	1:C:105:LEU:HB2	2.30	0.61
2:D:76:ALA:N	2:D:76:ALA:HB3	2.13	0.61
2:B:26:GLU:OE2	2:B:26:GLU:CD	2.43	0.61
2:D:46:GLY:CA	2:D:47:ASP:N	2.60	0.61
2:D:55:MET:CA	2:D:55:MET:O	2.42	0.61
2:D:58:PRO:CG	2:D:58:PRO:HD2	1.11	0.61
2:B:146:HIS:CG	2:B:146:HIS:C	2.79	0.61
2:B:65:LYS:HG3	2:B:65:LYS:HE2	1.82	0.61
2:B:142:ALA:CA	2:B:143:HIS:N	2.54	0.61
1:C:92:ARG:HD2	1:C:92:ARG:HH11	1.65	0.61
1:A:17:VAL:N	1:A:18:GLY:N	2.48	0.61
2:D:45:PHE:O	2:D:46:GLY:CA	2.44	0.61
2:B:142:ALA:C	2:B:142:ALA:CB	2.72	0.61
1:A:127:LYS:CG	1:A:127:LYS:HE2	2.27	0.61
2:D:4:THR:OG1	2:D:6:GLU:OE2	2.19	0.61
2:D:20:VAL:HG22	2:D:20:VAL:C	2.18	0.61
1:A:16:LYS:CD	1:A:16:LYS:CB	2.78	0.60
2:B:142:ALA:C	2:B:142:ALA:N	2.54	0.60
2:D:19:ASN:ND2	2:D:19:ASN:CB	2.63	0.60
2:D:52:ASP:CG	2:D:52:ASP:OD2	2.44	0.60
1:C:73:VAL:CA	1:C:73:VAL:HG12	2.30	0.60
2:D:18:VAL:CB	2:D:18:VAL:N	2.53	0.60
2:D:47:ASP:CG	2:D:47:ASP:CA	2.74	0.60
1:A:75:ASP:CB	1:A:75:ASP:N	2.64	0.60
2:D:47:ASP:N	2:D:47:ASP:C	2.60	0.60
2:D:53:ALA:CA	2:D:54:VAL:N	2.63	0.60
1:A:16:LYS:CE	1:A:16:LYS:HG2	2.22	0.60
2:D:141:LEU:HD13	2:D:141:LEU:HD22	1.82	0.60
2:B:4:THR:C	2:B:5:PRO:CD	2.73	0.60
1:C:118:THR:CA	1:C:118:THR:CG2	2.59	0.60
2:B:8:LYS:CG	2:B:8:LYS:C	2.70	0.59
1:A:92:ARG:HH11	1:A:92:ARG:HD2	1.47	0.59
1:C:61:LYS:CA	1:C:62:VAL:N	2.62	0.59
2:B:63:HIS:HE1	3:B:148:HEM:C4D	2.20	0.59
2:D:78:LEU:CD1	2:D:78:LEU:HD21	2.19	0.59
2:D:124:PRO:C	2:D:125:PRO:CD	2.67	0.59
2:B:66:LYS:CE	2:B:66:LYS:HG3	2.32	0.59
2:D:76:ALA:N	2:D:76:ALA:HB2	2.13	0.59
2:B:41:PHE:C	2:B:41:PHE:N	2.57	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:CE	2:B:66:LYS:CG	2.80	0.59
2:D:2:HIS:CG	2:D:2:HIS:NE2	2.67	0.59
1:A:51:GLY:C	1:A:52:SER:C	2.71	0.59
2:B:82:LYS:HE2	2:B:82:LYS:HB3	1.82	0.59
1:C:114:PRO:C	1:C:114:PRO:N	2.60	0.59
1:C:56:LYS:CD	1:C:56:LYS:HB3	2.32	0.58
2:D:1:VAL:HB	2:D:2:HIS:H	1.67	0.58
2:B:2:HIS:CB	2:B:2:HIS:N	2.66	0.58
1:C:73:VAL:CA	1:C:73:VAL:HG13	2.30	0.58
2:B:101:GLU:CD	2:B:101:GLU:CB	2.75	0.58
2:D:132:LYS:NZ	2:D:132:LYS:HD3	2.18	0.58
2:B:80:ASN:CB	2:B:80:ASN:OD1	2.50	0.58
2:D:67:VAL:C	2:D:67:VAL:HG12	2.29	0.58
1:A:40:LYS:CB	1:A:40:LYS:N	2.59	0.58
1:A:90:LYS:CE	1:A:90:LYS:NZ	2.67	0.58
1:C:92:ARG:HH21	1:C:92:ARG:HD2	1.68	0.58
2:D:79:ASP:O	2:D:80:ASN:CA	2.51	0.58
2:D:50:THR:CA	2:D:50:THR:CG2	2.81	0.58
2:B:12:THR:CG2	2:B:12:THR:CB	0.58	0.58
1:A:14:TRP:CB	1:A:14:TRP:N	2.63	0.57
2:B:65:LYS:CB	2:B:65:LYS:CG	0.58	0.57
1:C:137:THR:C	1:C:137:THR:N	2.59	0.57
1:A:20:HIS:O	1:A:21:ALA:C	2.46	0.57
2:B:47:ASP:C	2:B:47:ASP:HB3	2.29	0.57
1:A:14:TRP:CG	1:A:14:TRP:HA	2.34	0.57
1:C:113:LEU:CD1	1:C:113:LEU:HB2	2.28	0.57
1:C:73:VAL:HG12	1:C:73:VAL:N	2.19	0.57
1:C:76:MET:CG	1:C:76:MET:CE	2.81	0.57
2:B:26:GLU:OE2	2:B:26:GLU:CB	2.52	0.57
2:B:77:HIS:CD2	2:B:77:HIS:CB	2.84	0.57
1:A:127:LYS:CD	1:A:127:LYS:HB3	2.28	0.57
1:C:73:VAL:CG1	1:C:73:VAL:N	2.68	0.57
2:B:143:HIS:C	2:B:143:HIS:N	2.60	0.57
2:D:18:VAL:N	2:D:18:VAL:C	2.63	0.57
1:A:58:HIS:CA	1:A:58:HIS:O	2.45	0.57
2:B:80:ASN:CB	2:B:80:ASN:N	2.57	0.57
1:C:137:THR:CA	1:C:138:SER:N	2.58	0.57
1:C:16:LYS:CD	1:C:16:LYS:NZ	2.68	0.56
1:A:60:LYS:CE	1:A:60:LYS:NZ	2.69	0.56
1:C:47:ASP:C	1:C:47:ASP:OD1	2.43	0.56
2:D:126:VAL:CB	2:D:126:VAL:N	2.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:GLU:HB2	2:D:44:SER:N	2.16	0.56
2:B:90:GLU:CG	2:B:90:GLU:N	2.68	0.56
1:C:118:THR:CA	1:C:118:THR:HB	2.16	0.56
1:A:1:VAL:HG22	1:A:1:VAL:H1	1.70	0.56
1:A:64:ASP:CB	1:A:64:ASP:OD2	2.51	0.56
1:C:7:LYS:CG	1:C:7:LYS:HE2	2.34	0.56
1:C:118:THR:HG23	1:C:121:VAL:H	1.71	0.56
2:D:21:ASP:OD1	2:D:65:LYS:HG3	2.06	0.56
2:D:108:ASN:CG	2:D:108:ASN:CA	2.74	0.56
2:D:90:GLU:OE1	2:D:90:GLU:CG	2.53	0.56
2:B:8:LYS:CB	2:B:8:LYS:C	2.69	0.56
1:A:2:LEU:C	1:A:2:LEU:CB	2.75	0.56
2:B:10:ALA:C	2:B:10:ALA:N	2.54	0.55
2:B:12:THR:CG2	2:B:12:THR:HB	1.04	0.55
1:C:70:VAL:C	1:C:70:VAL:CB	2.70	0.55
1:A:75:ASP:HB3	1:A:75:ASP:O	2.07	0.55
2:D:79:ASP:C	2:D:79:ASP:HB2	2.25	0.55
1:A:75:ASP:CB	1:A:75:ASP:O	2.53	0.55
2:B:143:HIS:ND1	2:B:143:HIS:HB3	2.21	0.55
1:C:8:THR:CB	1:C:8:THR:C	2.67	0.55
1:A:29:LEU:CB	1:A:29:LEU:C	2.74	0.55
2:D:65:LYS:CD	2:D:65:LYS:HB3	2.36	0.55
1:A:1:VAL:CG2	1:A:1:VAL:H3	1.89	0.55
2:B:90:GLU:HG3	2:B:90:GLU:H	1.72	0.55
1:C:61:LYS:NZ	1:C:61:LYS:HD2	2.19	0.55
1:A:62:VAL:CA	1:A:62:VAL:O	2.44	0.54
1:A:17:VAL:C	1:A:18:GLY:C	2.75	0.54
1:A:137:THR:CB	1:A:137:THR:HG1	2.10	0.54
2:D:58:PRO:CD	2:D:58:PRO:HG2	1.03	0.54
1:C:40:LYS:HD3	1:C:40:LYS:HZ3	1.69	0.54
1:C:16:LYS:C	1:C:16:LYS:CB	2.71	0.54
1:C:137:THR:C	1:C:137:THR:CB	2.76	0.54
3:A:142:HEM:CGA	3:A:142:HEM:CAA	2.82	0.54
2:D:8:LYS:C	2:D:8:LYS:HG2	2.33	0.54
1:C:138:SER:OG	1:C:138:SER:HA	1.96	0.54
2:D:59:LYS:CE	2:D:59:LYS:HG2	2.38	0.54
2:D:79:ASP:N	2:D:80:ASN:H	2.04	0.54
1:A:17:VAL:C	1:A:17:VAL:CG1	2.81	0.54
2:B:108:ASN:HD22	2:B:108:ASN:HB2	1.70	0.54
1:C:84:SER:HB2	1:C:139:LYS:HD2	1.90	0.54
2:D:1:VAL:C	2:D:1:VAL:CB	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:GLY:C	2:B:75:LEU:CA	2.73	0.53
1:C:90:LYS:CD	1:C:90:LYS:NZ	2.71	0.53
2:D:4:THR:CB	2:D:4:THR:C	2.76	0.53
2:B:79:ASP:C	2:B:80:ASN:CA	2.77	0.53
2:B:123:THR:C	2:B:124:PRO:CD	2.63	0.53
2:D:18:VAL:CG2	2:D:18:VAL:HG11	2.37	0.53
2:D:121:GLU:CB	2:D:121:GLU:CD	2.68	0.53
1:A:138:SER:CB	1:A:138:SER:C	2.81	0.53
1:C:8:THR:CB	1:C:8:THR:N	2.67	0.53
1:C:61:LYS:CD	1:C:61:LYS:HZ3	2.19	0.53
2:D:58:PRO:CD	2:D:58:PRO:HG3	1.03	0.53
1:A:23:GLU:CD	1:A:23:GLU:CB	2.80	0.53
1:C:7:LYS:CD	1:C:7:LYS:CB	2.80	0.53
2:D:76:ALA:CB	2:D:76:ALA:H	2.12	0.53
1:A:133:SER:O	1:A:137:THR:CG2	2.57	0.53
1:C:138:SER:CB	1:C:138:SER:N	2.72	0.53
2:D:3:LEU:O	2:D:4:THR:CA	2.55	0.53
2:D:6:GLU:C	2:D:6:GLU:CB	2.81	0.53
2:D:73:ASP:O	2:D:76:ALA:HB3	2.08	0.53
3:D:148:HEM:O1A	3:D:148:HEM:CAA	2.56	0.53
2:D:10:ALA:HB3	2:D:11:VAL:N	2.24	0.53
2:B:80:ASN:CA	2:B:80:ASN:OD1	2.57	0.52
2:D:95:LYS:HA	2:D:95:LYS:HD3	1.92	0.52
2:D:73:ASP:CG	2:D:73:ASP:N	2.65	0.52
1:A:23:GLU:OE1	1:A:23:GLU:CG	2.57	0.52
2:B:79:ASP:OD2	2:B:79:ASP:CA	2.56	0.52
2:D:67:VAL:CA	2:D:67:VAL:CG2	2.77	0.52
2:D:104:ARG:NE	2:D:104:ARG:HH21	2.06	0.52
2:B:81:LEU:N	2:B:81:LEU:HB2	2.18	0.52
2:B:22:GLU:OE1	2:B:22:GLU:OE2	2.28	0.52
2:B:41:PHE:N	2:B:42:PHE:N	2.57	0.52
2:D:2:HIS:ND1	2:D:2:HIS:NE2	2.57	0.52
2:D:79:ASP:O	2:D:80:ASN:HA	2.10	0.52
2:B:1:VAL:CA	2:B:1:VAL:CG1	2.88	0.52
1:C:92:ARG:CZ	1:C:92:ARG:HD2	2.40	0.52
2:D:90:GLU:CB	2:D:90:GLU:OE2	2.58	0.52
1:A:18:GLY:C	1:A:18:GLY:N	2.61	0.52
1:C:99:LYS:CG	1:C:99:LYS:CE	2.89	0.52
2:D:3:LEU:O	2:D:3:LEU:CA	2.58	0.51
2:B:1:VAL:O	2:B:2:HIS:HA	2.11	0.51
1:C:137:THR:CA	1:C:137:THR:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:THR:O	2:B:54:VAL:HG23	2.11	0.51
1:C:92:ARG:CZ	1:C:92:ARG:CD	2.89	0.51
2:B:2:HIS:ND1	2:B:2:HIS:HB3	2.20	0.51
1:C:139:LYS:NZ	1:C:139:LYS:HD2	2.20	0.51
2:D:20:VAL:HG13	2:D:20:VAL:N	2.26	0.51
2:B:22:GLU:CG	2:B:22:GLU:OE1	2.59	0.51
1:A:44:PRO:C	1:A:44:PRO:N	2.63	0.51
2:D:73:ASP:CB	2:D:73:ASP:OD2	2.59	0.51
2:D:131:GLN:CD	2:D:131:GLN:CB	2.70	0.51
1:A:2:LEU:HA	1:A:3:SER:N	2.21	0.50
1:A:87:HIS:CA	1:A:87:HIS:O	2.44	0.50
2:B:65:LYS:CG	2:B:65:LYS:HE2	2.39	0.50
1:C:90:LYS:CD	1:C:90:LYS:HB3	2.38	0.50
2:D:104:ARG:NE	2:D:104:ARG:NH2	2.59	0.50
2:D:121:GLU:CA	2:D:121:GLU:HG3	2.37	0.50
1:A:15:GLY:O	1:A:15:GLY:CA	2.56	0.50
1:A:87:HIS:C	1:A:87:HIS:N	2.62	0.50
2:D:92:HIS:C	2:D:92:HIS:HB3	2.29	0.50
1:A:81:SER:CB	1:A:81:SER:H	2.22	0.50
2:D:47:ASP:CB	2:D:47:ASP:C	2.84	0.50
2:D:58:PRO:HD3	2:D:58:PRO:HG2	1.04	0.50
2:B:6:GLU:C	2:B:6:GLU:HB2	2.36	0.50
1:C:1:VAL:HB	1:C:1:VAL:H1	1.74	0.50
2:D:5:PRO:CA	2:D:5:PRO:CG	2.81	0.50
2:D:55:MET:N	2:D:56:GLY:N	2.59	0.50
2:D:121:GLU:CB	2:D:121:GLU:N	2.60	0.50
1:C:40:LYS:HG2	1:C:48:LEU:HD13	1.94	0.50
1:C:103:HIS:HE1	2:D:131:GLN:OE1	1.94	0.50
2:D:1:VAL:CB	2:D:2:HIS:H	2.23	0.50
2:D:73:ASP:OD2	2:D:73:ASP:OD1	2.30	0.50
2:B:3:LEU:CA	2:B:3:LEU:CG	2.81	0.50
1:A:76:MET:O	1:A:77:PRO:C	2.49	0.49
2:D:121:GLU:CG	2:D:121:GLU:OE1	2.60	0.49
2:D:12:THR:N	2:D:12:THR:CB	2.75	0.49
2:D:90:GLU:CD	2:D:90:GLU:CB	2.85	0.49
2:D:26:GLU:OE2	2:D:26:GLU:OE1	2.29	0.49
1:C:105:LEU:HD13	1:C:105:LEU:HD22	1.93	0.49
1:C:82:ALA:O	1:C:83:LEU:CA	2.59	0.49
2:D:43:GLU:HB2	2:D:43:GLU:HG3	1.34	0.49
2:D:123:THR:HB	2:D:124:PRO:CD	2.42	0.49
1:C:16:LYS:N	1:C:17:VAL:N	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:LYS:CE	2:D:82:LYS:HG3	2.41	0.49
2:B:21:ASP:CB	2:B:21:ASP:OD2	2.56	0.48
2:B:65:LYS:CB	2:B:65:LYS:CE	2.91	0.48
2:B:142:ALA:CA	2:B:142:ALA:O	2.55	0.48
1:A:44:PRO:C	1:A:44:PRO:HB2	2.33	0.48
2:B:96:LEU:HD13	3:B:148:HEM:C3D	2.49	0.48
1:A:16:LYS:CG	1:A:16:LYS:NZ	2.71	0.48
1:C:7:LYS:N	1:C:7:LYS:CG	2.76	0.48
1:C:56:LYS:CG	1:C:56:LYS:HE3	2.42	0.48
1:C:118:THR:CA	1:C:118:THR:OG1	2.54	0.48
2:D:8:LYS:N	2:D:8:LYS:C	2.54	0.48
3:D:148:HEM:CGD	3:D:148:HEM:CAD	2.85	0.48
1:A:50:HIS:HA	5:A:173:HOH:O	2.13	0.48
2:B:65:LYS:CB	2:B:65:LYS:N	2.65	0.48
2:D:6:GLU:HB2	2:D:6:GLU:C	2.38	0.48
2:D:9:SER:C	2:D:10:ALA:C	2.82	0.48
3:C:142:HEM:HMB1	3:C:142:HEM:CBB	2.44	0.48
2:D:12:THR:CA	2:D:12:THR:HG23	2.41	0.48
2:D:47:ASP:CA	2:D:47:ASP:OD2	2.62	0.48
1:A:55:VAL:O	1:A:56:LYS:C	2.53	0.48
2:B:22:GLU:CG	2:B:22:GLU:OE2	2.61	0.48
1:C:10:VAL:CA	1:C:10:VAL:O	2.47	0.48
1:A:29:LEU:CB	1:A:29:LEU:N	2.74	0.48
1:A:75:ASP:OD1	1:A:75:ASP:OD2	2.33	0.47
1:C:131:SER:CA	1:C:132:VAL:N	2.60	0.47
2:D:20:VAL:CA	2:D:20:VAL:HG12	2.41	0.47
2:B:87:THR:CA	2:B:87:THR:CG2	2.92	0.47
1:A:21:ALA:C	1:A:21:ALA:N	2.72	0.47
1:A:50:HIS:CB	1:A:50:HIS:H	2.23	0.47
2:D:22:GLU:CG	2:D:22:GLU:C	2.80	0.47
2:B:4:THR:HA	2:B:5:PRO:CD	2.44	0.47
1:C:87:HIS:C	1:C:87:HIS:N	2.65	0.47
2:D:22:GLU:CD	2:D:22:GLU:CB	2.87	0.47
2:D:53:ALA:C	2:D:53:ALA:HB1	2.33	0.47
1:A:58:HIS:C	1:A:58:HIS:CB	2.78	0.47
1:A:137:THR:CG2	1:A:137:THR:N	2.78	0.47
2:B:5:PRO:N	2:B:6:GLU:H	2.10	0.47
2:D:49:SER:N	2:D:50:THR:N	2.63	0.47
2:D:5:PRO:HA	2:D:8:LYS:HB3	1.96	0.47
2:B:2:HIS:ND1	2:B:2:HIS:O	2.48	0.47
2:B:145:TYR:C	2:B:145:TYR:N	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:LYS:HD3	2:D:143:HIS:NE2	2.31	0.46
1:A:72:HIS:CB	1:A:72:HIS:O	2.62	0.46
2:B:90:GLU:CB	2:B:90:GLU:N	2.64	0.46
2:B:10:ALA:CA	2:B:11:VAL:N	2.66	0.46
1:C:116:GLU:CB	1:C:116:GLU:OE1	2.63	0.46
2:D:10:ALA:CA	2:D:10:ALA:O	2.52	0.46
1:C:138:SER:CB	1:C:138:SER:C	2.89	0.46
2:D:8:LYS:HG3	2:D:8:LYS:HA	1.95	0.46
2:B:2:HIS:CG	2:B:2:HIS:O	2.69	0.46
1:C:3:SER:O	1:C:7:LYS:HG3	2.16	0.46
2:D:48:LEU:N	2:D:49:SER:N	2.63	0.46
1:A:84:SER:CA	1:A:84:SER:HG	2.28	0.46
2:B:6:GLU:CD	2:B:6:GLU:CB	2.69	0.46
2:D:20:VAL:HG22	2:D:21:ASP:N	2.30	0.46
2:B:143:HIS:CA	2:B:144:LYS:N	2.62	0.46
2:D:55:MET:C	2:D:55:MET:CB	2.85	0.46
1:C:56:LYS:HE3	1:C:56:LYS:HG3	1.98	0.45
1:A:84:SER:HB2	1:A:139:LYS:HD2	1.97	0.45
2:D:15:TRP:HE1	2:D:72:SER:HB3	1.80	0.45
2:D:141:LEU:CD2	2:D:141:LEU:HB3	2.44	0.45
2:D:6:GLU:CA	2:D:7:GLU:N	2.77	0.45
2:D:2:HIS:ND1	2:D:2:HIS:CB	2.76	0.45
1:C:113:LEU:HB3	1:C:113:LEU:HD13	1.96	0.45
1:C:56:LYS:CE	1:C:56:LYS:HG3	2.46	0.45
3:D:148:HEM:CBD	3:D:148:HEM:O2D	2.42	0.45
2:B:1:VAL:N	5:B:197:HOH:O	2.50	0.45
2:B:57:ASN:CA	2:B:58:PRO:CD	2.95	0.45
2:D:6:GLU:C	2:D:7:GLU:C	2.85	0.45
2:B:1:VAL:O	2:B:2:HIS:CA	2.63	0.45
2:B:79:ASP:O	2:B:80:ASN:CA	2.65	0.45
2:B:90:GLU:CB	2:B:90:GLU:OE1	2.63	0.45
1:C:30:GLU:CD	1:C:50:HIS:CD2	2.85	0.45
2:B:80:ASN:ND2	2:B:80:ASN:HB3	2.27	0.44
2:B:89:SER:OG	2:B:144:LYS:HB2	2.17	0.44
1:A:16:LYS:HG2	1:A:16:LYS:NZ	2.31	0.44
1:A:17:VAL:C	1:A:17:VAL:CB	2.80	0.44
1:A:43:PHE:N	1:A:44:PRO:CD	2.80	0.44
3:D:148:HEM:HBC2	3:D:148:HEM:HMC2	1.98	0.44
2:B:80:ASN:CG	2:B:80:ASN:HA	2.42	0.44
2:D:17:LYS:HE3	2:D:121:GLU:OE1	2.17	0.44
2:D:121:GLU:CB	2:D:121:GLU:OE2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:HIS:HE1	2:B:131:GLN:OE1	2.00	0.44
3:C:142:HEM:CGA	3:C:142:HEM:CAA	2.95	0.44
2:D:6:GLU:C	2:D:6:GLU:N	2.74	0.44
1:A:61:LYS:CG	1:A:61:LYS:HE2	2.11	0.44
2:B:90:GLU:N	2:B:90:GLU:HG3	2.32	0.44
1:A:56:LYS:CD	1:A:56:LYS:HB3	2.44	0.44
3:D:148:HEM:O1D	3:D:148:HEM:HBD1	2.17	0.44
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.82	0.44
2:B:41:PHE:N	2:B:42:PHE:H	2.16	0.44
2:B:79:ASP:OD2	2:B:79:ASP:HA	2.17	0.44
2:B:2:HIS:CB	2:B:2:HIS:O	2.66	0.44
1:C:30:GLU:OE2	1:C:50:HIS:HD2	1.99	0.44
1:C:72:HIS:CG	1:C:72:HIS:N	2.86	0.44
1:C:105:LEU:HD23	1:C:129:LEU:HD22	2.00	0.44
2:B:144:LYS:CE	2:B:144:LYS:HD2	2.29	0.43
1:A:78:ASN:ND2	1:A:78:ASN:HA	2.31	0.43
2:B:145:TYR:C	2:B:145:TYR:HB3	2.40	0.43
1:C:30:GLU:OE1	1:C:30:GLU:CB	2.66	0.43
2:D:8:LYS:CE	2:D:8:LYS:HG2	2.46	0.43
2:D:20:VAL:CA	2:D:20:VAL:HG13	2.41	0.43
2:D:63:HIS:CE1	3:D:148:HEM:C4D	3.06	0.43
2:D:67:VAL:CB	2:D:67:VAL:H	2.24	0.43
2:B:59:LYS:CD	2:B:59:LYS:HZ2	2.30	0.43
2:B:144:LYS:CE	2:B:144:LYS:HD3	2.29	0.43
1:A:7:LYS:O	1:A:11:LYS:HG3	2.19	0.43
1:A:28:ALA:CB	1:A:105:LEU:HD23	2.48	0.43
1:C:113:LEU:HD13	1:C:116:GLU:HB2	1.99	0.43
1:C:78:ASN:CB	1:C:78:ASN:ND2	2.66	0.43
2:B:82:LYS:CE	2:B:82:LYS:CB	2.78	0.43
1:C:40:LYS:CG	1:C:40:LYS:HE2	2.20	0.43
1:C:94:ASP:OD2	1:C:96:VAL:HG13	2.18	0.43
2:D:47:ASP:CA	2:D:48:LEU:H	2.29	0.43
1:C:72:HIS:CB	1:C:72:HIS:N	2.63	0.43
2:D:79:ASP:C	2:D:80:ASN:HB3	2.39	0.42
2:B:123:THR:CA	2:B:124:PRO:CD	2.97	0.42
2:D:6:GLU:N	2:D:7:GLU:N	2.67	0.42
2:D:43:GLU:CG	2:D:43:GLU:N	2.78	0.42
2:D:47:ASP:HB3	2:D:47:ASP:O	2.19	0.42
2:B:12:THR:CG2	2:B:12:THR:HG1	2.20	0.42
2:B:139:ASN:CA	2:B:139:ASN:OD1	2.61	0.42
1:A:64:ASP:CB	1:A:64:ASP:OD1	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ASP:HB3	2:D:47:ASP:H	1.80	0.42
1:C:76:MET:SD	1:C:76:MET:HB3	2.55	0.42
2:D:78:LEU:HD21	2:D:78:LEU:HD11	2.00	0.42
2:D:52:ASP:CB	2:D:52:ASP:H	2.28	0.42
2:D:59:LYS:N	2:D:60:VAL:N	2.67	0.42
2:B:65:LYS:CD	2:B:65:LYS:HB3	2.45	0.42
2:D:1:VAL:CA	2:D:1:VAL:O	2.61	0.42
1:A:56:LYS:CE	1:A:56:LYS:CG	2.98	0.42
2:B:63:HIS:CE1	3:B:148:HEM:C4D	3.05	0.42
2:D:123:THR:HB	2:D:124:PRO:HD2	2.02	0.42
1:C:86:LEU:CD2	3:C:142:HEM:HBA2	2.49	0.41
2:B:49:SER:CB	2:B:49:SER:HG	2.14	0.41
1:C:131:SER:C	1:C:131:SER:N	2.72	0.41
3:C:142:HEM:CMB	3:C:142:HEM:CBB	2.98	0.41
1:A:16:LYS:HG3	1:A:16:LYS:O	2.20	0.41
2:B:8:LYS:CD	2:B:8:LYS:HG3	2.21	0.41
2:D:20:VAL:HG23	2:D:20:VAL:HA	1.93	0.41
2:D:79:ASP:C	2:D:80:ASN:CB	2.89	0.41
2:B:121:GLU:CD	2:B:121:GLU:HB3	2.40	0.41
1:C:43:PHE:N	1:C:44:PRO:CD	2.84	0.41
2:D:80:ASN:OD1	2:D:80:ASN:HB2	2.19	0.41
1:A:85:ASP:OD2	1:A:85:ASP:CB	2.62	0.41
1:A:87:HIS:N	1:A:88:ALA:N	2.67	0.41
2:D:28:LEU:HD12	2:D:28:LEU:HA	1.88	0.41
1:A:60:LYS:CD	1:A:60:LYS:NZ	2.84	0.41
2:B:12:THR:C	2:B:12:THR:HG22	2.31	0.41
2:D:79:ASP:CA	2:D:79:ASP:OD2	2.68	0.41
2:D:92:HIS:HA	2:D:96:LEU:HB2	2.02	0.41
2:D:94:ASP:N	2:D:94:ASP:HB2	2.29	0.41
2:B:77:HIS:CD2	2:B:77:HIS:HA	2.56	0.41
2:D:3:LEU:HD23	2:D:3:LEU:HA	1.72	0.41
2:D:17:LYS:O	2:D:18:VAL:CA	2.68	0.41
2:B:74:GLY:O	2:B:75:LEU:CA	2.67	0.41
2:D:141:LEU:HD23	2:D:141:LEU:HA	2.03	0.40
2:B:6:GLU:N	2:B:7:GLU:N	2.65	0.40
2:B:57:ASN:HA	2:B:58:PRO:CD	2.52	0.40

All (2) 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)
1:C:85:ASP:OD2	5:B:204:HOH:O[2_657]	1.41	0.79
5:B:204:HOH:O	5:C:161:HOH:O[2_647]	2.02	0.18

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	139/141 (99%)	122 (88%)	14 (10%)	3 (2%)	5	0
1	C	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
2	B	144/146 (99%)	129 (90%)	14 (10%)	1 (1%)	18	6
2	D	144/146 (99%)	128 (89%)	13 (9%)	3 (2%)	5	0
All	All	566/574 (99%)	505 (89%)	54 (10%)	7 (1%)	10	2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
2	D	73	ASP
1	A	21	ALA
2	D	77	HIS
2	B	4	THR
2	D	78	LEU
1	A	3	SER

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	113/113 (100%)	104 (92%)	9 (8%)	11	1
1	C	113/113 (100%)	109 (96%)	4 (4%)	32	9
2	B	118/118 (100%)	107 (91%)	11 (9%)	8	1
2	D	118/118 (100%)	98 (83%)	20 (17%)	2	0
All	All	462/462 (100%)	418 (90%)	44 (10%)	8	0

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	4	PRO
1	A	17	VAL
1	A	75	ASP
1	A	83	LEU
1	A	84	SER
1	A	95	PRO
1	A	137	THR
1	A	138	SER
2	B	1	VAL
2	B	6	GLU
2	B	9	SER
2	B	32	LEU
2	B	50	THR
2	B	51	PRO
2	B	59	LYS
2	B	65	LYS
2	B	68	LEU
2	B	117	HIS
2	B	146	HIS
1	C	16	LYS
1	C	84	SER
1	C	114	PRO
1	C	138	SER
2	D	1	VAL
2	D	6	GLU
2	D	9	SER
2	D	12	THR
2	D	21	ASP
2	D	22	GLU
2	D	26	GLU
2	D	43	GLU
2	D	47	ASP

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Mol	Chain	Res	Type
2	D	59	LYS
2	D	66	LYS
2	D	67	VAL
2	D	68	LEU
2	D	72	SER
2	D	75	LEU
2	D	80	ASN
2	D	92	HIS
2	D	120	LYS
2	D	139	ASN
2	D	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	72	HIS
1	A	78	ASN
1	A	103	HIS
2	B	63	HIS
2	B	77	HIS
1	C	50	HIS
1	C	68	ASN
1	C	72	HIS
1	C	103	HIS
1	C	112	HIS
2	D	63	HIS
2	D	77	HIS
2	D	80	ASN
2	D	139	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are modelled with single atom - leaving 4 for Mogul analysis.

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	148	2	50,50,50	5.47	26 (52%)	67,82,82	5.59	43 (64%)
3	HEM	C	142	1	50,50,50	6.85	35 (70%)	67,82,82	4.54	42 (62%)
3	HEM	D	148	2	50,50,50	8.46	37 (74%)	67,82,82	4.73	42 (62%)
3	HEM	A	142	1	50,50,50	7.85	32 (64%)	67,82,82	6.01	40 (59%)

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	148	2	-	3/14/54/54	-
3	HEM	C	142	1	-	3/14/54/54	-
3	HEM	D	148	2	-	5/14/54/54	-
3	HEM	A	142	1	-	5/14/54/54	-

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	148	HEM	CBA-CGA	38.36	2.39	1.50
3	A	142	HEM	CBA-CGA	35.57	2.32	1.50
3	C	142	HEM	CBA-CGA	34.03	2.29	1.50
3	A	142	HEM	CBD-CGD	25.29	2.09	1.50
3	D	148	HEM	CBD-CGD	22.13	2.01	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	148	HEM	O2A-CGA	-19.44	0.66	1.30
3	C	142	HEM	CBD-CGD	18.43	1.93	1.50
3	B	148	HEM	CBA-CGA	17.83	1.91	1.50
3	B	148	HEM	CBD-CGD	15.17	1.85	1.50
3	C	142	HEM	O2A-CGA	-14.68	0.82	1.30
3	D	148	HEM	O2A-CGA	14.19	1.77	1.30
3	A	142	HEM	O2D-CGD	-13.07	0.87	1.30
3	D	148	HEM	O2D-CGD	-12.10	0.90	1.30
3	D	148	HEM	O1D-CGD	12.02	1.61	1.22
3	D	148	HEM	C1C-C2C	9.70	1.64	1.45
3	D	148	HEM	C4A-NA	-9.54	1.21	1.39
3	D	148	HEM	CHD-C1D	9.43	1.60	1.39
3	A	142	HEM	FE-NB	8.95	2.22	1.94
3	A	142	HEM	C4D-C3D	-8.87	1.30	1.45
3	D	148	HEM	CHA-C4D	-8.58	1.21	1.38
3	A	142	HEM	FE-NC	8.47	2.23	1.95
3	D	148	HEM	C4A-C3A	8.42	1.62	1.43
3	B	148	HEM	CHD-C4C	8.41	1.54	1.38
3	D	148	HEM	CBA-CAA	-8.13	1.23	1.51
3	A	142	HEM	C1A-C2A	8.07	1.60	1.44
3	D	148	HEM	C3D-C2D	7.99	1.54	1.36
3	B	148	HEM	C3C-C2C	7.95	1.53	1.37
3	A	142	HEM	C3C-C4C	7.80	1.59	1.46
3	C	142	HEM	O1D-CGD	-7.64	0.97	1.22
3	B	148	HEM	O1A-CGA	7.52	1.46	1.22
3	A	142	HEM	CBD-CAD	-7.39	1.26	1.51
3	A	142	HEM	O2A-CGA	7.36	1.55	1.30
3	C	142	HEM	C1D-C2D	7.04	1.58	1.44
3	B	148	HEM	CMB-C2B	-7.04	1.36	1.50
3	A	142	HEM	FE-ND	6.80	2.15	1.94
3	B	148	HEM	C3B-C4B	6.78	1.58	1.44
3	A	142	HEM	O1A-CGA	6.77	1.44	1.22
3	D	148	HEM	CAA-C2A	6.74	1.68	1.51
3	D	148	HEM	CBB-CAB	-6.66	0.98	1.30
3	A	142	HEM	CBA-CAA	-6.54	1.29	1.51
3	D	148	HEM	C1A-C2A	6.53	1.57	1.44
3	A	142	HEM	FE-NA	6.33	2.16	1.95
3	A	142	HEM	CHB-C1B	-6.00	1.26	1.38
3	B	148	HEM	CHC-C1C	5.96	1.50	1.38
3	C	142	HEM	CMB-C2B	-5.92	1.38	1.50
3	C	142	HEM	CAB-C3B	5.85	1.63	1.47
3	B	148	HEM	C4A-C3A	5.83	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	FE-NB	5.76	2.12	1.94
3	A	142	HEM	CHA-C1A	-5.72	1.26	1.39
3	D	148	HEM	FE-NC	5.68	2.13	1.95
3	B	148	HEM	C1B-C2B	5.67	1.56	1.44
3	A	142	HEM	C1D-C2D	5.60	1.55	1.44
3	D	148	HEM	CHC-C1C	-5.59	1.27	1.38
3	A	142	HEM	C4D-ND	5.57	1.49	1.40
3	C	142	HEM	CHC-C1C	-5.45	1.27	1.38
3	D	148	HEM	C1B-C2B	-5.41	1.33	1.44
3	C	142	HEM	FE-ND	5.38	2.11	1.94
3	A	142	HEM	C4C-NC	-5.38	1.29	1.39
3	C	142	HEM	C1B-C2B	5.32	1.55	1.44
3	D	148	HEM	CHD-C4C	5.31	1.48	1.38
3	B	148	HEM	CAB-C3B	5.23	1.61	1.47
3	C	142	HEM	O1A-CGA	5.15	1.38	1.22
3	A	142	HEM	C1D-ND	-5.12	1.28	1.38
3	C	142	HEM	CHD-C4C	-5.08	1.28	1.38
3	C	142	HEM	O2D-CGD	-5.07	1.14	1.30
3	D	148	HEM	O1A-CGA	5.05	1.38	1.22
3	D	148	HEM	C4D-ND	5.01	1.48	1.40
3	D	148	HEM	CAB-C3B	4.99	1.60	1.47
3	D	148	HEM	CMC-C2C	4.98	1.61	1.50
3	D	148	HEM	FE-NA	4.72	2.10	1.95
3	D	148	HEM	CMB-C2B	-4.70	1.41	1.50
3	A	142	HEM	C3B-C2B	4.58	1.46	1.37
3	C	142	HEM	C4D-C3D	-4.47	1.37	1.45
3	A	142	HEM	CMD-C2D	4.38	1.59	1.50
3	B	148	HEM	CAD-C3D	4.36	1.62	1.51
3	C	142	HEM	C1C-C2C	4.33	1.53	1.45
3	D	148	HEM	C3B-C2B	-4.29	1.28	1.37
3	D	148	HEM	FE-ND	4.29	2.08	1.94
3	C	142	HEM	FE-NC	4.24	2.09	1.95
3	D	148	HEM	CAC-C3C	-4.23	1.36	1.47
3	C	142	HEM	C4B-NB	-4.22	1.30	1.38
3	A	142	HEM	CHD-C4C	-4.21	1.30	1.38
3	A	142	HEM	C4A-C3A	4.18	1.52	1.43
3	B	148	HEM	CMA-C3A	-4.15	1.42	1.50
3	A	142	HEM	C4B-NB	4.14	1.47	1.38
3	D	148	HEM	C1B-NB	4.09	1.47	1.40
3	C	142	HEM	FE-NA	4.09	2.08	1.95
3	B	148	HEM	C3B-C2B	-4.06	1.28	1.37
3	D	148	HEM	C2A-C3A	-4.03	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	C4A-C3A	4.02	1.52	1.43
3	D	148	HEM	C4D-C3D	-3.89	1.38	1.45
3	A	142	HEM	C1A-NA	-3.86	1.32	1.39
3	D	148	HEM	CMA-C3A	-3.74	1.43	1.50
3	A	142	HEM	C1B-C2B	-3.70	1.37	1.44
3	C	142	HEM	CHD-C1D	3.69	1.47	1.39
3	C	142	HEM	CBC-CAC	3.58	1.47	1.30
3	D	148	HEM	C1A-NA	-3.52	1.33	1.39
3	B	148	HEM	C3C-C4C	3.51	1.52	1.46
3	C	142	HEM	CAD-C3D	3.50	1.60	1.51
3	D	148	HEM	CBD-CAD	-3.29	1.40	1.51
3	C	142	HEM	CAC-C3C	-3.26	1.38	1.47
3	C	142	HEM	C1A-NA	-3.23	1.33	1.39
3	C	142	HEM	CBD-CAD	-3.22	1.40	1.51
3	A	142	HEM	C1C-NC	3.20	1.45	1.39
3	D	148	HEM	FE-NB	3.14	2.04	1.94
3	B	148	HEM	FE-NA	3.13	2.05	1.95
3	C	142	HEM	C3C-C2C	3.12	1.43	1.37
3	D	148	HEM	C1D-C2D	-3.08	1.38	1.44
3	C	142	HEM	C3B-C4B	3.07	1.50	1.44
3	B	148	HEM	C4D-ND	3.05	1.45	1.40
3	B	148	HEM	C4B-NB	-2.86	1.33	1.38
3	B	148	HEM	C1D-ND	-2.83	1.33	1.38
3	C	142	HEM	C1A-C2A	2.81	1.50	1.44
3	C	142	HEM	C2A-C3A	-2.80	1.31	1.38
3	C	142	HEM	C4D-ND	-2.59	1.35	1.40
3	C	142	HEM	C1B-NB	2.59	1.44	1.40
3	C	142	HEM	C3B-C2B	-2.51	1.32	1.37
3	B	148	HEM	FE-ND	2.43	2.02	1.94
3	A	142	HEM	C1C-C2C	-2.37	1.40	1.45
3	C	142	HEM	CHA-C4D	-2.31	1.33	1.38
3	C	142	HEM	CMA-C3A	-2.27	1.46	1.50
3	A	142	HEM	CMC-C2C	-2.27	1.46	1.50
3	A	142	HEM	C3D-C2D	-2.22	1.32	1.36
3	D	148	HEM	C4B-NB	-2.17	1.34	1.38
3	B	148	HEM	CAA-C2A	2.17	1.56	1.51
3	B	148	HEM	FE-NB	2.10	2.01	1.94
3	B	148	HEM	CAC-C3C	-2.09	1.41	1.47
3	B	148	HEM	O2D-CGD	-2.04	1.24	1.30
3	A	142	HEM	CHC-C1C	2.04	1.42	1.38
3	B	148	HEM	CHA-C1A	-2.02	1.34	1.39

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	O2A-CGA-O1A	-23.84	62.01	123.33
3	D	148	HEM	O1A-CGA-CBA	-18.59	64.13	123.09
3	B	148	HEM	C4C-C3C-C2C	-16.82	92.23	106.81
3	A	142	HEM	O1A-CGA-CBA	-16.32	71.34	123.09
3	C	142	HEM	O2A-CGA-CBA	-14.12	69.38	114.00
3	D	148	HEM	O1D-CGD-CBD	-13.76	79.45	123.09
3	A	142	HEM	O2A-CGA-CBA	-13.65	70.86	114.00
3	C	142	HEM	O1A-CGA-CBA	-13.38	80.66	123.09
3	B	148	HEM	O1A-CGA-CBA	-12.94	82.05	123.09
3	A	142	HEM	O1D-CGD-CBD	-11.25	87.41	123.09
3	A	142	HEM	CHD-C1D-ND	11.16	136.43	124.42
3	B	148	HEM	O2A-CGA-O1A	10.90	151.37	123.33
3	A	142	HEM	C2A-C1A-NA	-10.85	98.11	110.15
3	C	142	HEM	CHD-C1D-ND	10.60	135.83	124.42
3	B	148	HEM	CHA-C4D-ND	10.22	137.00	124.37
3	B	148	HEM	C4C-NC-C1C	-10.13	89.31	105.82
3	D	148	HEM	O2A-CGA-O1A	-10.09	97.39	123.33
3	B	148	HEM	C4A-C3A-C2A	-9.31	96.16	106.82
3	B	148	HEM	CAD-C3D-C2D	-9.30	110.45	127.87
3	B	148	HEM	CHD-C4C-NC	-9.23	114.40	124.45
3	A	142	HEM	CHD-C4C-NC	9.21	134.48	124.45
3	B	148	HEM	C1D-C2D-C3D	-9.12	97.39	106.98
3	A	142	HEM	C4A-NA-C1A	9.12	120.68	105.82
3	D	148	HEM	CHB-C1B-NB	-8.78	113.51	124.37
3	C	142	HEM	CHC-C1C-NC	8.75	133.98	124.45
3	B	148	HEM	O1D-CGD-CBD	-8.26	96.88	123.09
3	A	142	HEM	C3D-C4D-ND	-8.01	101.38	110.17
3	A	142	HEM	CHA-C4D-ND	-8.00	114.47	124.37
3	D	148	HEM	CHA-C4D-ND	-7.93	114.56	124.37
3	A	142	HEM	O2D-CGD-O1D	7.63	142.95	123.33
3	B	148	HEM	C3B-C2B-C1B	-7.56	100.74	106.41
3	B	148	HEM	C3D-C4D-ND	-7.49	101.96	110.17
3	B	148	HEM	C1A-C2A-C3A	7.46	118.41	106.87
3	B	148	HEM	C2C-C1C-NC	7.44	123.39	109.64
3	B	148	HEM	CHC-C4B-NB	7.32	132.30	124.42
3	A	142	HEM	CHB-C1B-NB	-7.21	115.44	124.37
3	D	148	HEM	CHD-C4C-NC	7.19	132.28	124.45
3	A	142	HEM	C2D-C1D-ND	-7.17	101.61	109.90
3	A	142	HEM	CHC-C4B-NB	7.00	131.95	124.42
3	C	142	HEM	CMB-C2B-C1B	-6.92	114.22	125.03
3	C	142	HEM	O1D-CGD-CBD	-6.77	101.63	123.09
3	B	148	HEM	CHC-C1C-C2C	-6.49	111.99	125.49
3	D	148	HEM	C1D-C2D-C3D	-6.49	100.16	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	148	HEM	CHD-C4C-C3C	-6.45	114.34	125.21
3	B	148	HEM	CMB-C2B-C3B	6.42	143.95	128.43
3	B	148	HEM	CMB-C2B-C1B	-6.39	115.05	125.03
3	B	148	HEM	CHD-C4C-C3C	-6.39	114.44	125.21
3	C	142	HEM	O2D-CGD-O1D	6.36	139.69	123.33
3	C	142	HEM	CMA-C3A-C2A	6.35	139.09	125.62
3	A	142	HEM	CHA-C4D-C3D	6.29	136.82	125.23
3	D	148	HEM	C4C-C3C-C2C	-6.28	101.36	106.81
3	D	148	HEM	O2D-CGD-O1D	-6.26	107.23	123.33
3	B	148	HEM	C2D-C1D-ND	6.16	117.03	109.90
3	A	142	HEM	C4C-NC-C1C	6.14	115.83	105.82
3	D	148	HEM	C3D-C4D-ND	-6.08	103.50	110.17
3	C	142	HEM	CHA-C1A-NA	6.08	134.89	123.86
3	A	142	HEM	C3B-C4B-NB	-5.95	105.19	109.47
3	A	142	HEM	C4D-ND-C1D	5.92	112.22	105.21
3	C	142	HEM	C1D-C2D-C3D	-5.91	100.77	106.98
3	D	148	HEM	CHD-C1D-C2D	-5.77	115.92	125.03
3	D	148	HEM	C2C-C1C-NC	-5.70	99.09	109.64
3	C	142	HEM	CAA-C2A-C3A	-5.70	114.29	127.07
3	A	142	HEM	CAA-CBA-CGA	-5.69	98.57	113.67
3	D	148	HEM	C3C-C2C-C1C	5.67	112.41	107.05
3	C	142	HEM	C1B-NB-C4B	5.64	111.89	105.21
3	A	142	HEM	CHC-C1C-NC	5.62	130.57	124.45
3	D	148	HEM	CAD-C3D-C2D	-5.62	117.34	127.87
3	C	142	HEM	C2B-C1B-NB	-5.57	103.44	109.84
3	C	142	HEM	CAA-CBA-CGA	-5.53	99.00	113.67
3	B	148	HEM	C4B-C3B-C2B	5.45	112.29	107.28
3	B	148	HEM	C4D-C3D-C2D	5.44	114.81	106.89
3	C	142	HEM	O2D-CGD-CBD	-5.38	97.01	114.00
3	D	148	HEM	C3B-C2B-C1B	5.36	110.44	106.41
3	C	142	HEM	C4C-NC-C1C	5.30	114.47	105.82
3	B	148	HEM	C2A-C1A-NA	-5.27	104.30	110.15
3	A	142	HEM	C4D-C3D-C2D	5.27	114.57	106.89
3	A	142	HEM	C3C-C2C-C1C	5.25	112.01	107.05
3	B	148	HEM	CMC-C2C-C1C	5.11	133.73	124.73
3	D	148	HEM	O2A-CGA-CBA	-5.02	98.14	114.00
3	B	148	HEM	CAA-CBA-CGA	5.01	126.95	113.67
3	C	142	HEM	CHC-C4B-NB	5.00	129.81	124.42
3	A	142	HEM	C4A-CHB-C1B	4.97	137.93	126.25
3	B	148	HEM	O2D-CGD-CBD	-4.86	98.65	114.00
3	D	148	HEM	C4C-NC-C1C	4.80	113.65	105.82
3	B	148	HEM	CHD-C1D-ND	-4.78	119.28	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	HEM	CAD-C3D-C2D	-4.68	119.11	127.87
3	B	148	HEM	C1C-CHC-C4B	-4.65	116.13	126.02
3	C	142	HEM	CHD-C1D-C2D	-4.64	117.71	125.03
3	B	148	HEM	CMD-C2D-C3D	4.60	138.60	126.15
3	D	148	HEM	C1A-CHA-C4D	4.57	137.00	126.25
3	B	148	HEM	O2D-CGD-O1D	4.57	135.09	123.33
3	A	142	HEM	CHA-C1A-NA	4.56	132.13	123.86
3	C	142	HEM	C4D-C3D-C2D	4.55	113.52	106.89
3	C	142	HEM	CMA-C3A-C4A	-4.54	118.51	125.42
3	B	148	HEM	CMA-C3A-C2A	4.46	135.08	125.62
3	A	142	HEM	C3A-C4A-NA	-4.43	103.04	110.14
3	C	142	HEM	CHD-C4C-NC	4.32	129.16	124.45
3	D	148	HEM	C4C-CHD-C1D	-4.29	116.90	126.02
3	D	148	HEM	C1B-NB-C4B	-4.22	100.20	105.21
3	C	142	HEM	CAA-C2A-C1A	4.16	133.07	124.94
3	C	142	HEM	C4A-C3A-C2A	-4.16	102.05	106.82
3	D	148	HEM	CHA-C4D-C3D	4.13	132.84	125.23
3	D	148	HEM	CHC-C1C-NC	4.11	128.93	124.45
3	B	148	HEM	C1A-CHA-C4D	-4.06	116.69	126.25
3	A	142	HEM	C3B-C2B-C1B	4.04	109.44	106.41
3	C	142	HEM	C4C-CHD-C1D	-4.04	117.44	126.02
3	A	142	HEM	C4C-CHD-C1D	-3.99	117.54	126.02
3	D	148	HEM	C4A-CHB-C1B	3.92	135.48	126.25
3	A	142	HEM	CMB-C2B-C1B	-3.92	118.90	125.03
3	C	142	HEM	C2D-C1D-ND	-3.91	105.38	109.90
3	C	142	HEM	CHA-C4D-ND	-3.88	119.57	124.37
3	B	148	HEM	CHA-C4D-C3D	-3.80	118.21	125.23
3	B	148	HEM	CAA-C2A-C3A	-3.77	118.61	127.07
3	C	142	HEM	C2A-C1A-NA	-3.73	106.01	110.15
3	B	148	HEM	CAC-C3C-C4C	3.68	133.61	124.82
3	C	142	HEM	C1A-C2A-C3A	3.67	112.56	106.87
3	B	148	HEM	O2A-CGA-CBA	-3.67	102.40	114.00
3	A	142	HEM	CMC-C2C-C3C	-3.55	119.83	128.43
3	D	148	HEM	CMB-C2B-C1B	-3.53	119.51	125.03
3	A	142	HEM	CAD-C3D-C2D	-3.52	121.28	127.87
3	C	142	HEM	CMB-C2B-C3B	3.48	136.85	128.43
3	C	142	HEM	C4D-ND-C1D	3.41	109.25	105.21
3	A	142	HEM	C1A-CHA-C4D	3.35	134.12	126.25
3	C	142	HEM	C3B-C4B-NB	-3.32	107.08	109.47
3	D	148	HEM	C4D-C3D-C2D	3.32	111.72	106.89
3	C	142	HEM	CMD-C2D-C3D	3.31	135.11	126.15
3	A	142	HEM	C1B-NB-C4B	3.30	109.11	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	148	HEM	C3C-C2C-C1C	-3.28	103.94	107.05
3	C	142	HEM	C4B-C3B-C2B	3.27	110.28	107.28
3	C	142	HEM	CBB-CAB-C3B	-3.23	111.40	127.53
3	D	148	HEM	CHC-C1C-C2C	3.11	131.96	125.49
3	A	142	HEM	O2D-CGD-CBD	-3.09	104.23	114.00
3	C	142	HEM	C4C-C3C-C2C	3.07	109.48	106.81
3	A	142	HEM	C2C-C1C-NC	-3.07	103.95	109.64
3	B	148	HEM	C2B-C1B-NB	3.07	113.36	109.84
3	D	148	HEM	C3B-C4B-NB	3.00	111.62	109.47
3	C	142	HEM	CHA-C1A-C2A	-2.99	118.76	125.30
3	A	142	HEM	C4C-C3C-C2C	-2.99	104.22	106.81
3	D	148	HEM	CBA-CAA-C2A	-2.89	104.54	112.53
3	D	148	HEM	CMA-C3A-C2A	2.87	131.71	125.62
3	D	148	HEM	CMC-C2C-C1C	-2.86	119.70	124.73
3	D	148	HEM	C4A-C3A-C2A	-2.85	103.55	106.82
3	C	142	HEM	CHA-C4D-C3D	2.85	130.47	125.23
3	D	148	HEM	C4A-NA-C1A	2.81	110.40	105.82
3	D	148	HEM	CAA-CBA-CGA	2.79	121.07	113.67
3	B	148	HEM	CHA-C1A-NA	2.78	128.90	123.86
3	D	148	HEM	CMD-C2D-C1D	2.73	129.31	125.03
3	D	148	HEM	O2D-CGD-CBD	-2.72	105.41	114.00
3	C	142	HEM	C2C-C1C-NC	-2.72	104.61	109.64
3	A	142	HEM	C1A-C2A-C3A	2.71	111.06	106.87
3	B	148	HEM	CBD-CAD-C3D	2.66	119.88	112.53
3	D	148	HEM	CHB-C1B-C2B	2.63	134.41	126.95
3	B	148	HEM	C3B-C4B-NB	-2.57	107.62	109.47
3	B	148	HEM	CHC-C4B-C3B	-2.55	119.99	125.07
3	B	148	HEM	CMC-C2C-C3C	-2.53	122.31	128.43
3	C	142	HEM	CHB-C1B-NB	-2.49	121.28	124.37
3	D	148	HEM	CBB-CAB-C3B	-2.44	115.34	127.53
3	D	148	HEM	C2D-C1D-ND	2.39	112.66	109.90
3	D	148	HEM	CHC-C4B-NB	-2.36	121.89	124.42
3	A	142	HEM	C2B-C1B-NB	-2.34	107.14	109.84
3	D	148	HEM	CAA-C2A-C3A	2.25	132.13	127.07
3	C	142	HEM	C4A-NA-C1A	2.25	109.48	105.82
3	A	142	HEM	CHD-C4C-C3C	-2.16	121.56	125.21
3	D	148	HEM	C4D-ND-C1D	2.14	107.75	105.21
3	C	142	HEM	CHC-C1C-C2C	-2.13	121.05	125.49
3	A	142	HEM	CHB-C1B-C2B	2.10	132.93	126.95
3	A	142	HEM	CAD-CBD-CGD	2.03	119.06	113.67

There are no chirality outliers.

All (16) torsion outliers are listed below:

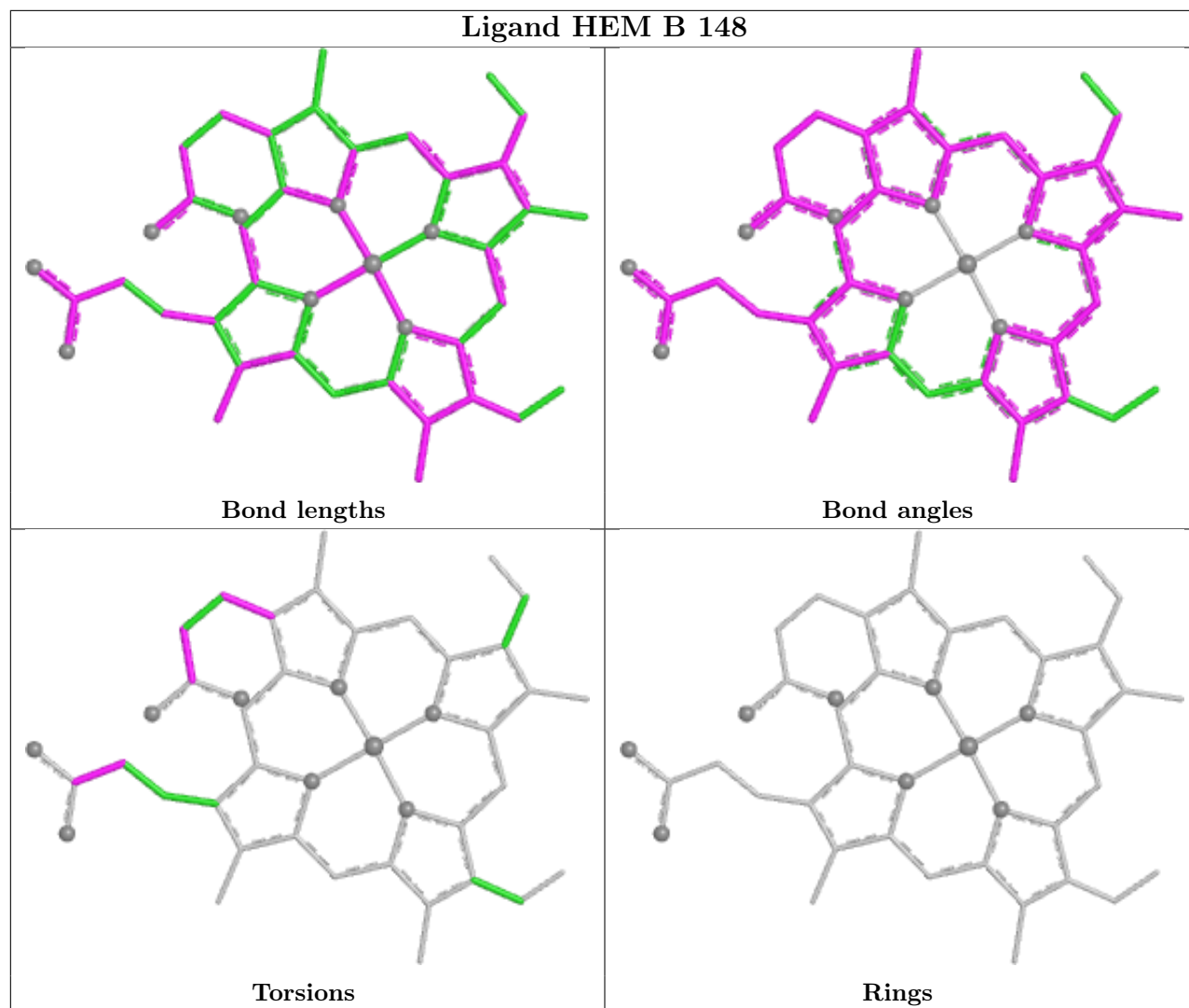
Mol	Chain	Res	Type	Atoms
3	B	148	HEM	C4D-C3D-CAD-CBD
3	A	142	HEM	C2B-C3B-CAB-CBB
3	D	148	HEM	C2B-C3B-CAB-CBB
3	C	142	HEM	CAA-CBA-CGA-O1A
3	C	142	HEM	CAD-CBD-CGD-O2D
3	D	148	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAA-CBA-CGA-O1A
3	B	148	HEM	CAA-CBA-CGA-O1A
3	D	148	HEM	C4B-C3B-CAB-CBB
3	D	148	HEM	CAD-CBD-CGD-O2D
3	D	148	HEM	CAA-CBA-CGA-O2A
3	C	142	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAD-CBD-CGD-O2D
3	B	148	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	C2C-C3C-CAC-CBC

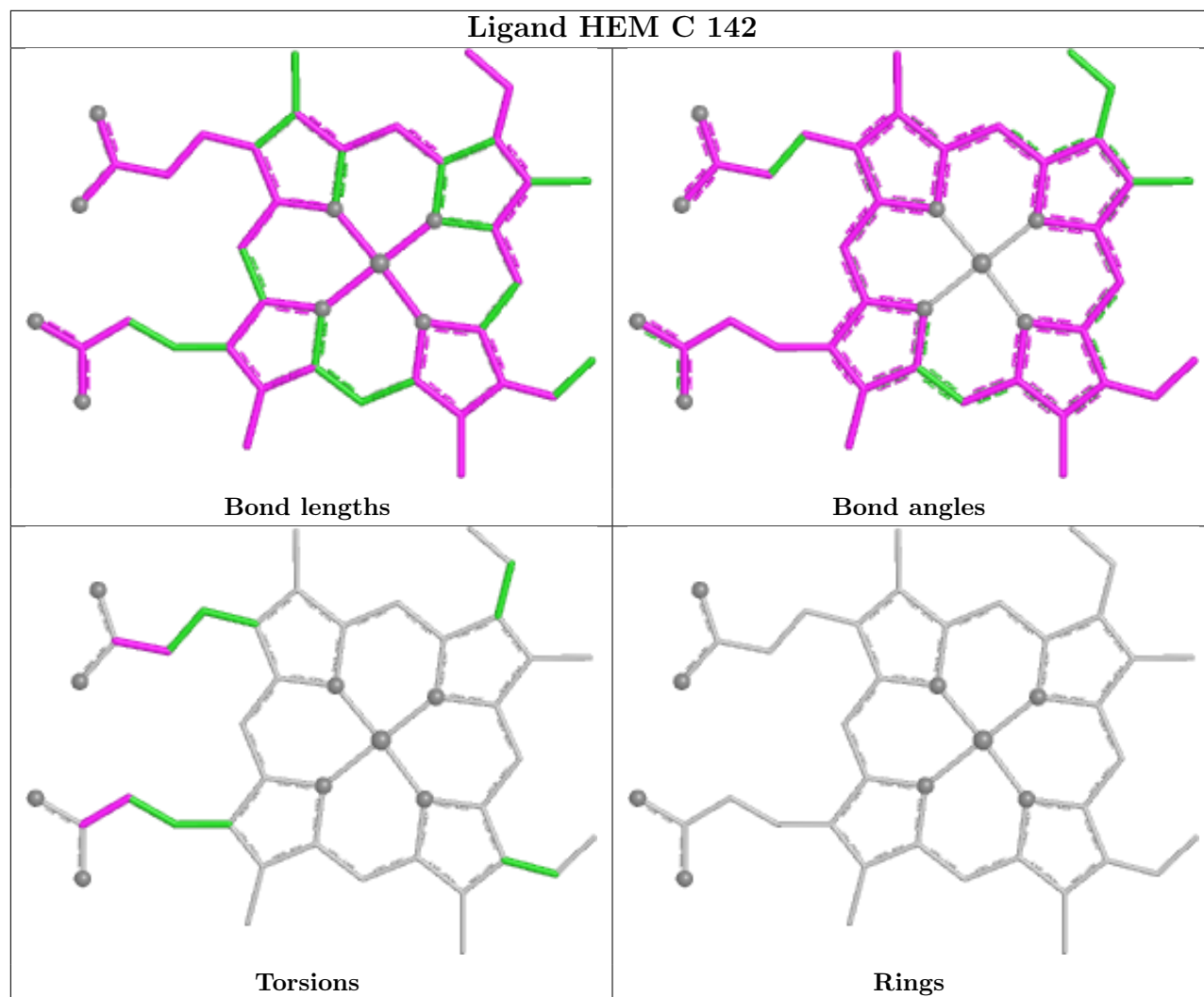
There are no ring outliers.

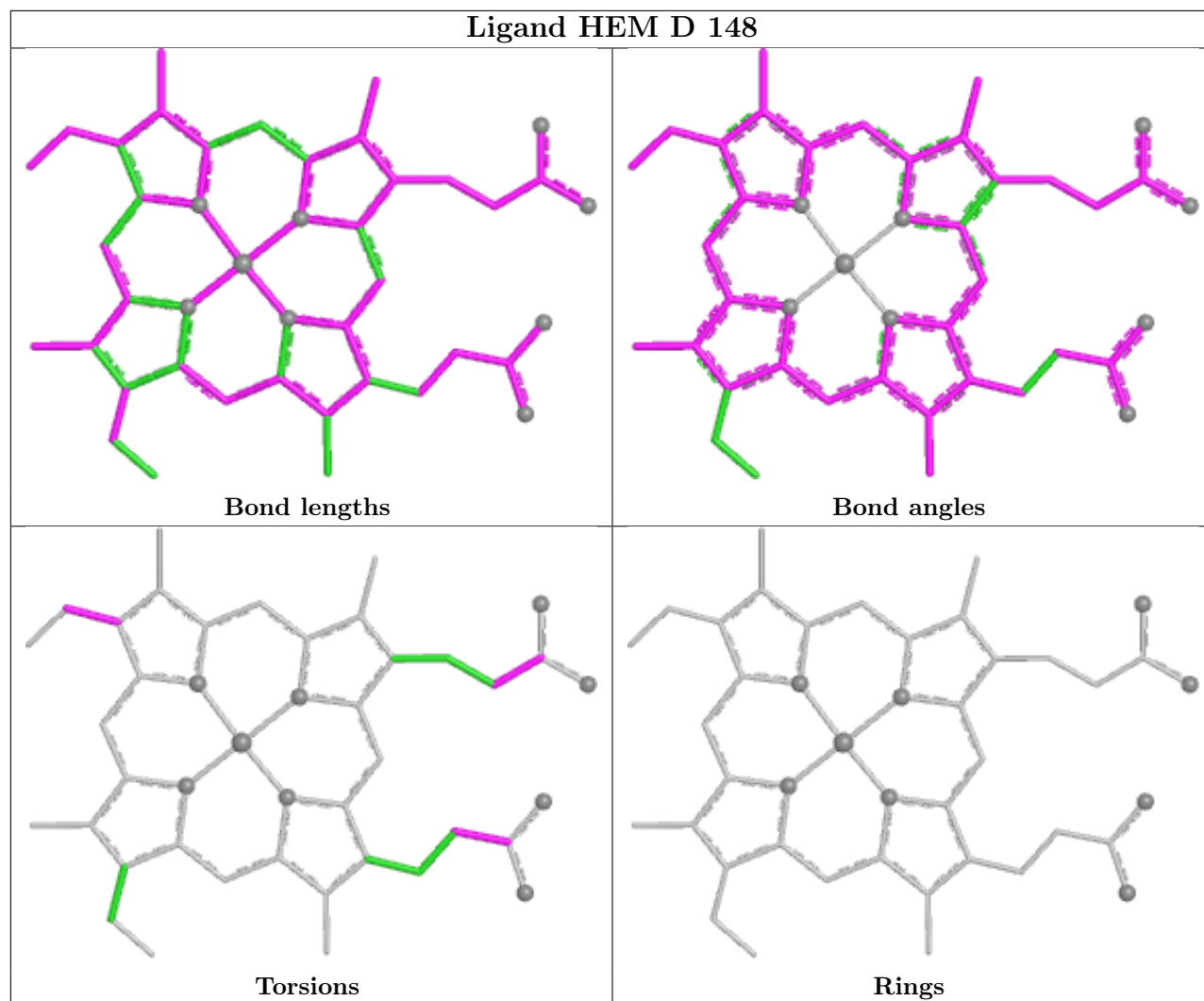
4 monomers are involved in 43 short contacts:

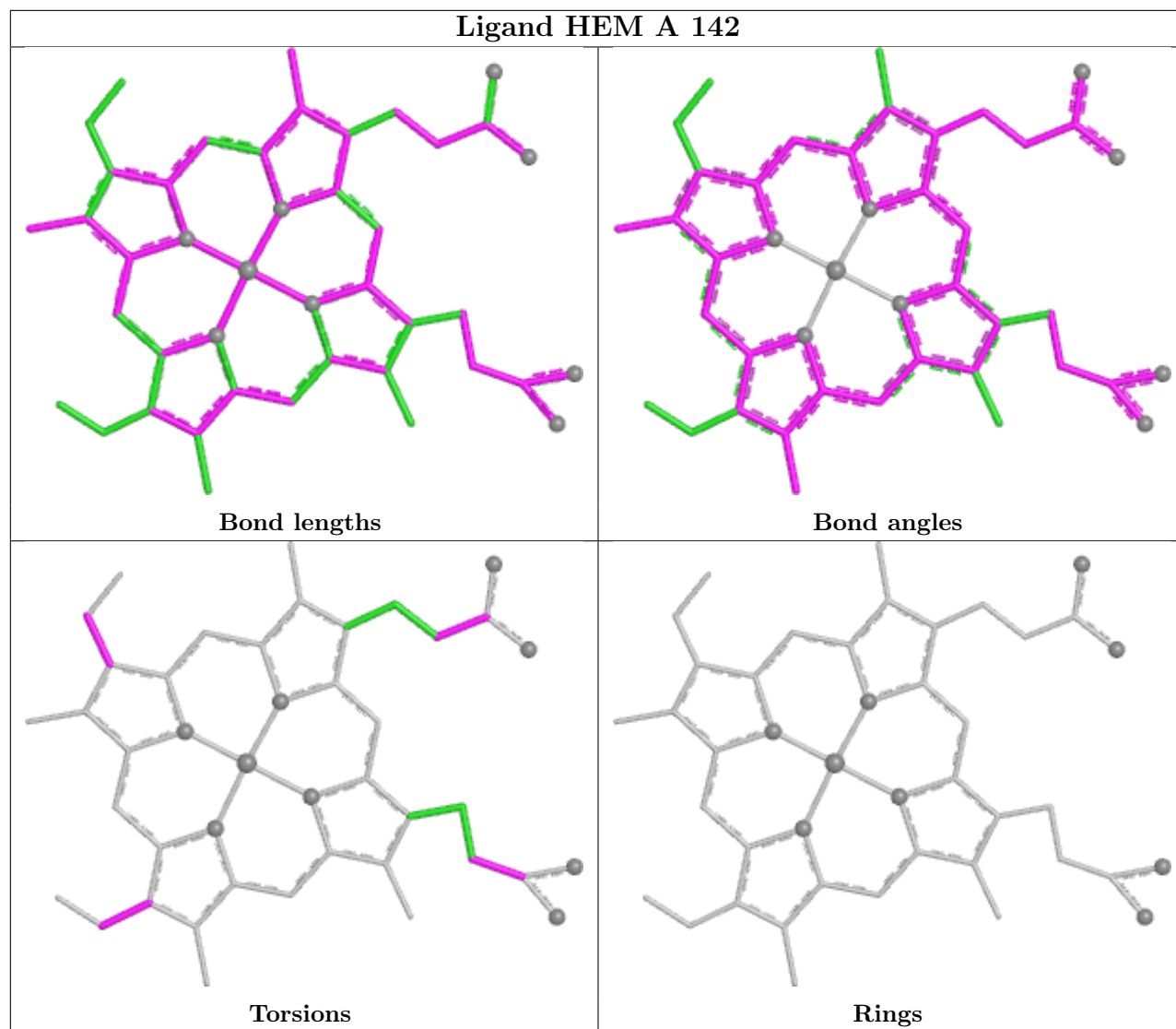
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	148	HEM	10	0
3	C	142	HEM	15	0
3	D	148	HEM	12	0
3	A	142	HEM	6	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	13
2	D	13
1	A	10
1	C	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	74:GLY	C	75:LEU	N	1.70
1	C	82:ALA	C	83:LEU	N	1.69
1	B	81:LEU	C	82:LYS	N	1.66
1	B	76:ALA	C	77:HIS	N	1.64
1	D	95:LYS	C	96:LEU	N	1.64
1	A	3:SER	C	4:PRO	N	1.62
1	A	45:HIS	C	46:PHE	N	1.62
1	D	17:LYS	C	18:VAL	N	1.61
1	D	73:ASP	C	74:GLY	N	1.61
1	B	6:GLU	C	7:GLU	N	1.20
1	B	124:PRO	C	125:PRO	N	1.20
1	C	2:LEU	C	3:SER	N	1.20
1	D	140:ALA	C	141:LEU	N	1.20
1	A	44:PRO	C	45:HIS	N	1.19
1	B	123:THR	C	124:PRO	N	1.19
1	D	30:ARG	C	31:LEU	N	1.19
1	D	47:ASP	C	48:LEU	N	1.19
1	C	133:SER	C	134:THR	N	1.18
1	D	1:VAL	C	2:HIS	N	1.18
1	D	7:GLU	C	8:LYS	N	1.18
1	D	18:VAL	C	19:ASN	N	1.18
1	A	120:ALA	C	121:VAL	N	1.17
1	C	21:ALA	C	22:GLY	N	1.17
1	C	112:HIS	C	113:LEU	N	1.17
1	A	127:LYS	C	128:PHE	N	1.16
1	D	58:PRO	C	59:LYS	N	1.16
1	B	142:ALA	C	143:HIS	N	1.15
1	D	19:ASN	C	20:VAL	N	1.15
1	A	47:ASP	C	48:LEU	N	1.13
1	B	40:ARG	C	41:PHE	N	1.13
1	B	2:HIS	C	3:LEU	N	1.12
1	C	44:PRO	C	45:HIS	N	1.11
1	C	15:GLY	C	16:LYS	N	1.09
1	B	46:GLY	C	47:ASP	N	1.07
1	C	118:THR	C	119:PRO	N	1.07
1	B	71:PHE	C	72:SER	N	1.05
1	A	2:LEU	C	3:SER	N	1.02
1	C	70:VAL	C	71:ALA	N	0.99
1	B	145:TYR	C	146:HIS	N	0.97
1	D	4:THR	C	5:PRO	N	0.97
1	A	50:HIS	C	51:GLY	N	0.96
1	A	15:GLY	C	16:LYS	N	0.92
1	A	74:ASP	C	75:ASP	N	0.92

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	45:PHE	C	46:GLY	N	0.87
1	B	1:VAL	C	2:HIS	N	0.79

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.