Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:31 PM EDT

PDB ID	:	1HBS / pdb_00001hbs
Title	:	REFINED CRYSTAL STRUCTURE OF DEOXYHEMOGLOBIN S. I. RESTRAINED LEAST-SQUARES REFINEMENT AT 3.0-ANGSTROMS RESOLUTION
Authors	:	Padlan, E.A.; Love, W.E.
Deposited on	:	1982-06-02
Resolution	:	3.00 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:

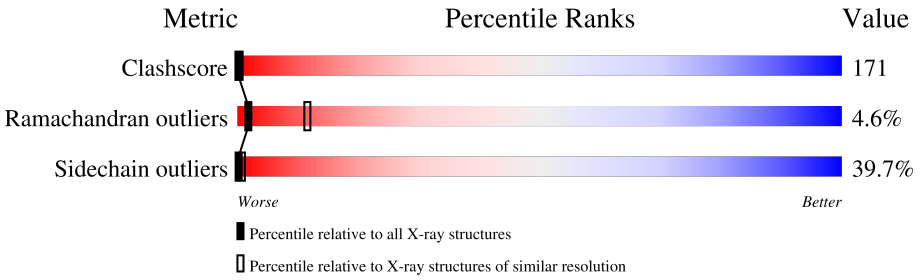
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	13% 62% 26%
1	C	141	9% 55% 36%
1	E	141	13% 53% 34%
1	G	141	12% 51% 37%
2	B	146	8% 63% 29%
2	D	146	10% 64% 26%
2	F	146	12% 58% 30%
2	H	146	• 11% 51% 38%

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	A	142	-	-	X	-
3	HEM	B	147	-	X	-	-
3	HEM	D	147	-	-	X	-
3	HEM	E	142	-	X	X	-
3	HEM	F	147	-	X	-	-
3	HEM	G	142	-	-	X	-
3	HEM	H	147	-	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9104 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 S (DEOXY) (ALPHA CHAIN).

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			
1	E	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	G	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

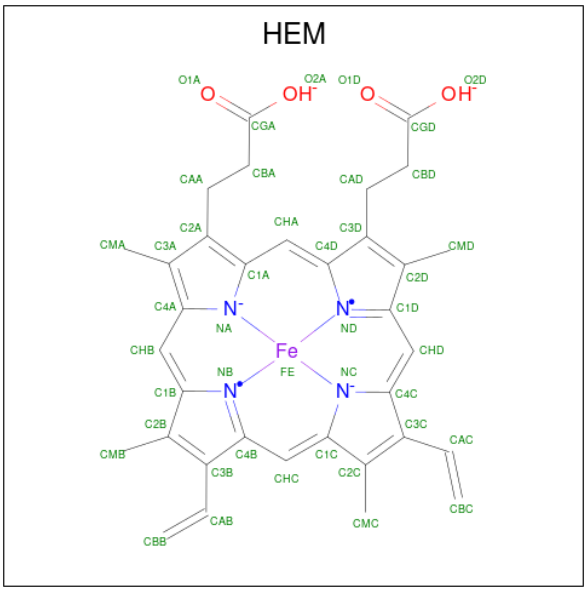
- Molecule 2 is a protein called HEMOGLOBIN S (DEOXY) (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			
2	D	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			
2	F	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			
2	H	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	VAL	GLU	conflict	UNP P68871
D	6	VAL	GLU	conflict	UNP P68871
F	6	VAL	GLU	conflict	UNP P68871
H	6	VAL	GLU	conflict	UNP P68871

- 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	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

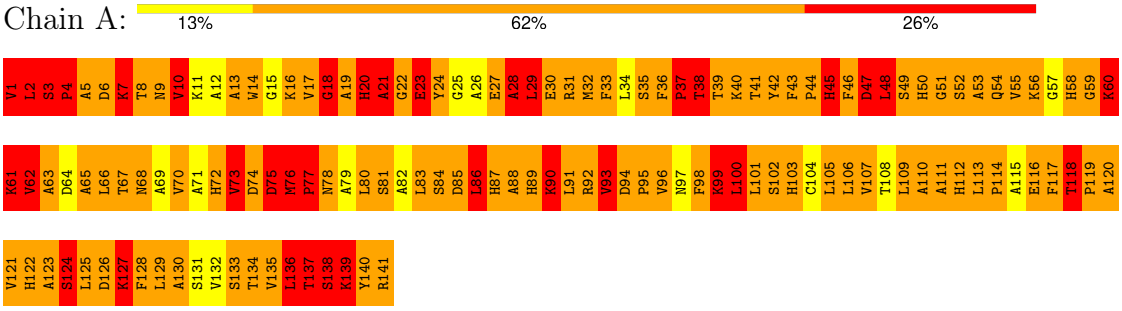
3 Residue-property plots (i)

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

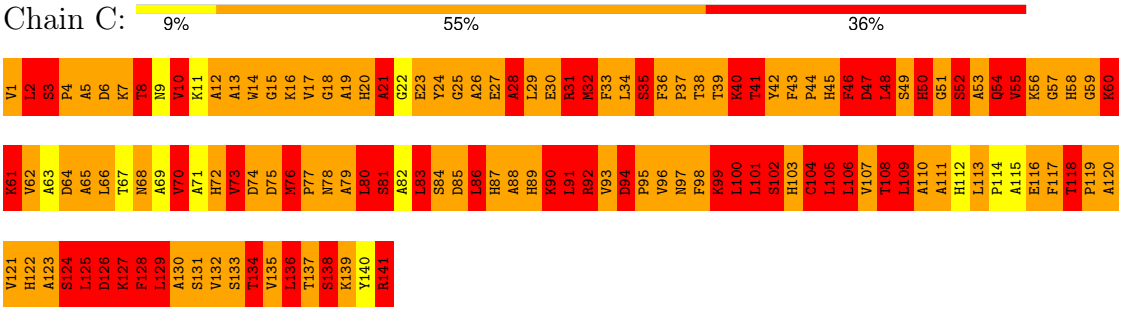
• Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)

Chain A:



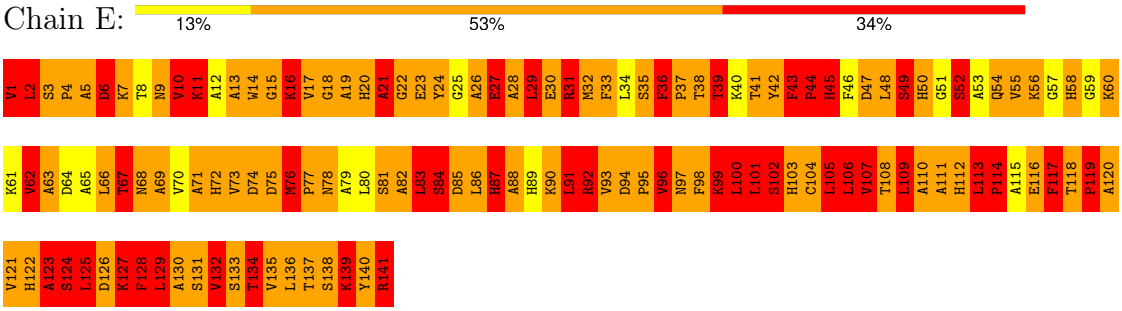
• Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)

Chain C:



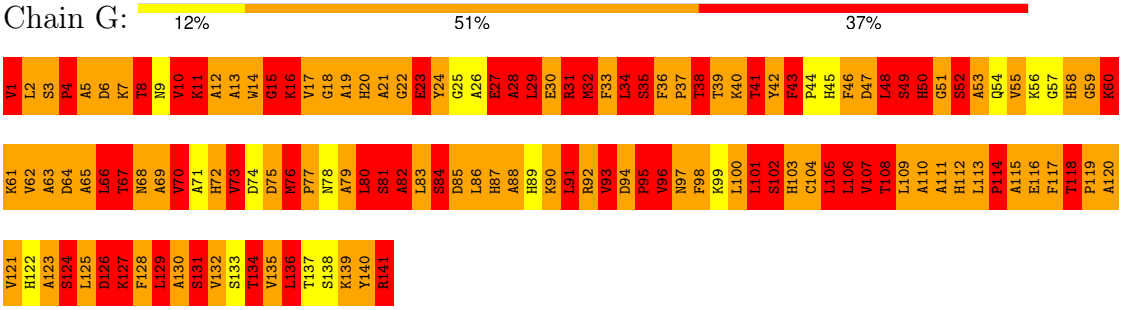
• Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)

Chain E:



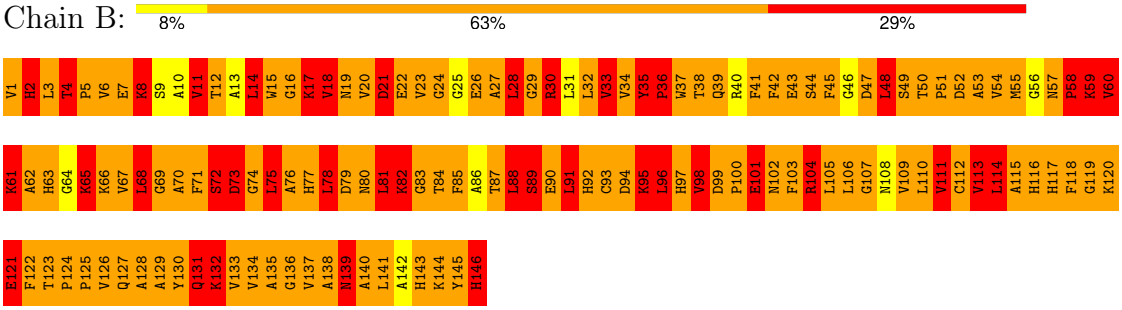
• Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)

Chain G:



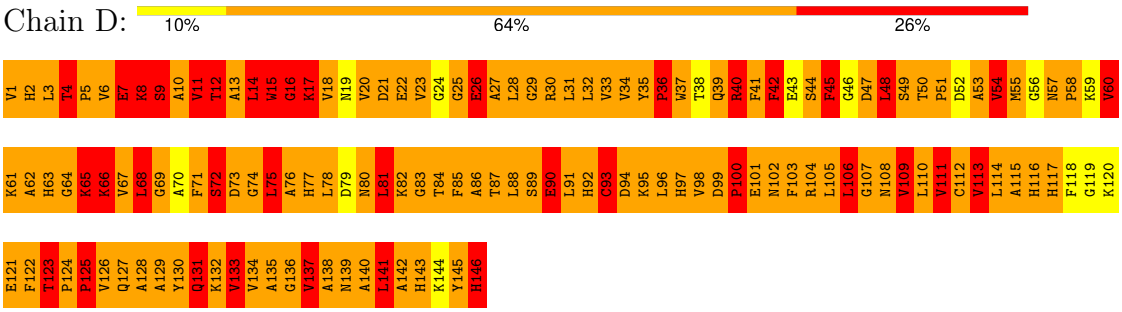
• Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain B:



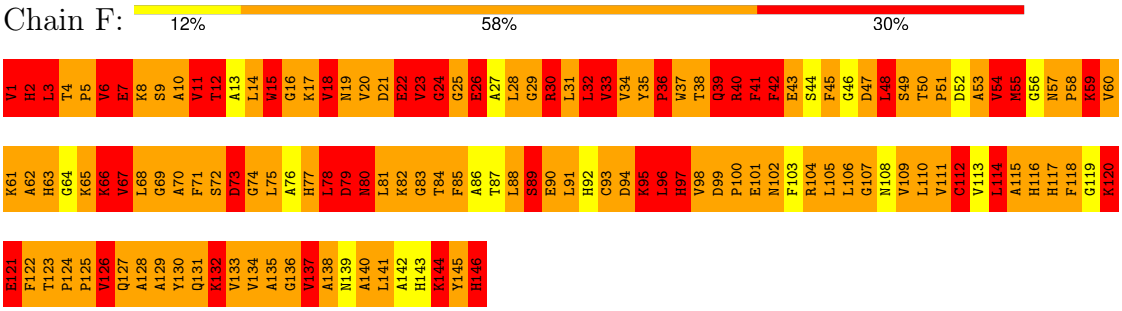
• Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain D:



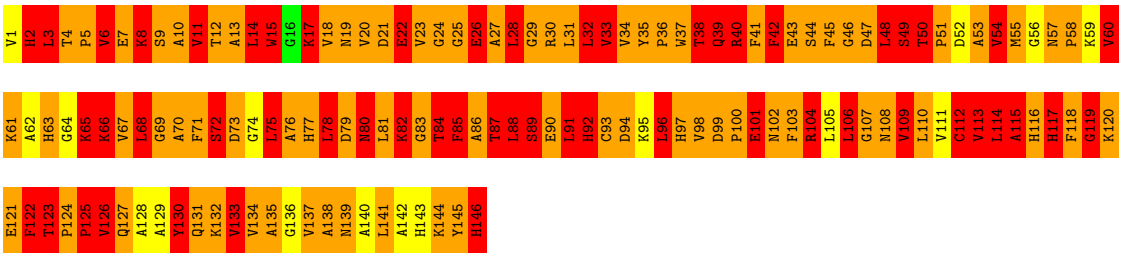
• Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain F:



• Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain H:


V1 H2 L3 T4 P5 V6 E7 K8 S9 A10 V11 T12 A13 L14 W15 G16 K17 V18 N19 V20 D21 E22 V23 G24 G25 E26 A27 L28 G29 R30 L31 L32 V33 V34 Y35 P36 W37 T38 Q39 R40 F41 F42 E43 S44 F45 G46 D47 L48 S49 T50 P51 D52 A53 V54 M55 G56 N57 P58 K59 V60
K61 A62 H63 G64 K65 K66 V67 L68 G69 A70 F71 S72 D73 G74 L75 A76 H77 L78 D79 N80 L81 K82 G83 T84 F85 A86 T87 L88 S89 E90 L91 H92 C93 D94 K95 L96 H97 V98 D99 P100 E101 N102 F103 R104 L105 L106 G107 N108 V109 L110 V111 C112 V113 L114 A115 H116 H117 F118 G119 K120
E121 F122 T123 P124 P125 V126 Q127 A128 A129 Y130 Q131 K132 V133 V134 A135 G136 V137 A138 N139 A140 L141 A142 H143 K144 Y145 H146

4 Data and refinement statistics (i)

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	63.33Å 185.66Å 52.97Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.254 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9104	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: 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	5.80	354/1097 (32.3%)	7.44	642/1491 (43.1%)
1	C	5.93	364/1097 (33.2%)	8.66	704/1491 (47.2%)
1	E	5.33	322/1097 (29.4%)	8.11	702/1491 (47.1%)
1	G	5.61	339/1097 (30.9%)	8.09	681/1491 (45.7%)
2	B	5.35	361/1151 (31.4%)	7.54	665/1564 (42.5%)
2	D	5.71	377/1151 (32.8%)	7.46	695/1564 (44.4%)
2	F	5.61	356/1151 (30.9%)	7.79	707/1564 (45.2%)
2	H	5.24	335/1151 (29.1%)	8.02	704/1564 (45.0%)
All	All	5.57	2808/8992 (31.2%)	7.89	5500/12220 (45.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	C	0	1
2	F	0	2
All	All	1	3

All (2808) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	THR	C-O	30.85	1.65	1.24
1	A	122	HIS	CE1-NE2	27.81	1.60	1.32
2	F	143	HIS	CE1-NE2	26.50	1.59	1.32
2	B	41	PHE	C-O	24.63	1.56	1.24
1	E	132	VAL	C-O	24.42	1.55	1.24
2	F	23	VAL	C-O	23.89	1.54	1.24
1	C	45	HIS	ND1-CE1	23.72	1.56	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	93	CYS	C-O	23.71	1.48	1.23
1	C	76	MET	C-O	23.69	1.54	1.24
1	A	125	LEU	C-N	23.50	1.62	1.33
1	G	56	LYS	C-O	23.20	1.53	1.24
2	H	116	HIS	CD2-NE2	23.11	1.63	1.37
1	A	27	GLU	C-O	22.82	1.52	1.24
2	F	83	GLY	C-O	22.65	1.51	1.23
2	B	129	ALA	C-O	22.51	1.53	1.24
1	C	77	PRO	C-O	22.43	1.50	1.24
1	A	70	VAL	C-O	22.43	1.50	1.24
2	F	134	VAL	C-O	22.37	1.49	1.24
1	A	78	ASN	C-O	22.12	1.49	1.24
2	D	14	LEU	C-O	22.02	1.52	1.24
1	C	90	LYS	C-O	21.99	1.51	1.24
2	D	43	GLU	C-O	21.33	1.56	1.23
2	F	34	VAL	C-O	21.10	1.47	1.24
2	D	127	GLN	C-O	21.04	1.48	1.24
1	C	70	VAL	C-O	-20.97	1.00	1.24
2	F	92	HIS	CG-ND1	-20.74	1.15	1.38
2	F	145	TYR	C-N	20.59	1.62	1.33
2	D	129	ALA	C-N	20.55	1.61	1.34
2	H	36	PRO	C-O	20.48	1.50	1.24
2	D	118	PHE	C-O	20.45	1.51	1.24
2	D	108	ASN	C-N	20.38	1.54	1.34
1	C	37	PRO	C-O	20.20	1.51	1.24
2	H	88	LEU	C-O	20.18	1.49	1.24
1	G	67	THR	N-CA	20.12	1.72	1.46
1	A	35	SER	C-O	19.89	1.50	1.24
1	G	23	GLU	C-N	-19.84	1.06	1.33
2	B	35	TYR	C-O	-19.62	1.01	1.24
1	C	15	GLY	C-O	19.56	1.50	1.23
1	G	64	ASP	C-O	-19.54	1.01	1.24
1	A	54	GLN	C-N	19.45	1.56	1.33
2	H	30	ARG	CD-NE	19.12	1.73	1.46
1	C	95	PRO	N-CA	-19.10	1.22	1.47
1	G	63	ALA	C-N	-19.06	1.10	1.33
1	A	23	GLU	CD-OE2	18.92	1.61	1.25
1	C	141	ARG	CD-NE	18.90	1.72	1.46
1	C	136	LEU	C-O	-18.85	1.02	1.24
1	A	95	PRO	C-N	-18.84	1.11	1.33
2	D	131	GLN	C-O	18.56	1.46	1.24
2	D	121	GLU	C-N	18.45	1.59	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	20	HIS	CE1-NE2	-18.44	1.14	1.32
1	C	39	THR	CB-OG1	18.42	1.73	1.43
1	G	19	ALA	C-O	18.41	1.48	1.24
1	A	103	HIS	CE1-NE2	-18.33	1.14	1.32
2	B	140	ALA	C-O	18.33	1.46	1.24
2	H	7	GLU	C-O	18.26	1.46	1.24
1	E	23	GLU	C-O	18.26	1.46	1.24
2	F	137	VAL	C-N	-18.08	1.10	1.33
2	F	110	LEU	CA-CB	18.07	1.81	1.53
2	B	35	TYR	CA-C	17.99	1.71	1.52
2	F	37	TRP	NE1-CE2	17.97	1.57	1.37
1	C	10	VAL	C-O	17.94	1.41	1.24
2	F	33	VAL	C-O	17.90	1.45	1.24
2	D	11	VAL	N-CA	-17.87	1.24	1.46
2	D	43	GLU	N-CA	17.86	1.67	1.46
1	G	14	TRP	C-O	-17.80	1.01	1.24
1	A	70	VAL	C-N	-17.80	1.09	1.33
1	G	62	VAL	C-O	17.74	1.43	1.23
2	D	100	PRO	C-O	17.70	1.48	1.24
1	G	30	GLU	C-N	-17.67	1.09	1.34
1	A	58	HIS	ND1-CE1	17.66	1.50	1.32
1	A	90	LYS	CA-C	17.62	1.69	1.53
1	C	13	ALA	C-O	17.57	1.47	1.24
2	F	112	CYS	C-N	-17.54	1.11	1.33
2	H	103	PHE	N-CA	17.41	1.67	1.46
1	E	134	THR	C-O	17.35	1.44	1.24
1	A	89	HIS	CE1-NE2	17.21	1.49	1.32
1	C	78	ASN	N-CA	17.19	1.69	1.46
1	E	50	HIS	CE1-NE2	-17.19	1.15	1.32
1	C	13	ALA	N-CA	17.15	1.68	1.46
2	F	64	GLY	N-CA	17.10	1.67	1.45
1	G	103	HIS	CG-CD2	17.04	1.54	1.35
1	G	47	ASP	CA-C	16.99	1.74	1.53
1	G	69	ALA	C-O	16.98	1.44	1.24
2	B	38	THR	N-CA	16.98	1.68	1.46
2	F	53	ALA	CA-C	16.96	1.74	1.52
2	H	99	ASP	N-CA	16.91	1.72	1.46
1	E	69	ALA	N-CA	16.89	1.68	1.46
1	A	41	THR	N-CA	16.87	1.67	1.46
2	D	124	PRO	C-N	16.85	1.50	1.34
1	G	103	HIS	CD2-NE2	16.82	1.56	1.37
1	A	37	PRO	CA-CB	16.61	1.77	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	96	LEU	C-N	-16.58	1.10	1.33
1	C	45	HIS	CG-CD2	-16.55	1.17	1.35
1	E	14	TRP	C-O	16.55	1.45	1.24
2	F	123	THR	CA-CB	16.52	1.73	1.53
2	H	15	TRP	C-O	16.51	1.44	1.24
1	C	118	THR	N-CA	16.49	1.69	1.45
2	H	46	GLY	N-CA	-16.48	1.29	1.45
1	E	20	HIS	N-CA	16.36	1.67	1.46
1	C	89	HIS	CD2-NE2	16.34	1.55	1.37
2	H	68	LEU	N-CA	16.33	1.68	1.46
2	D	124	PRO	N-CD	-16.32	1.25	1.47
1	E	20	HIS	CE1-NE2	-16.27	1.16	1.32
1	A	4	PRO	C-N	16.25	1.57	1.33
1	A	61	LYS	CA-C	16.19	1.73	1.52
1	G	112	HIS	ND1-CE1	16.18	1.48	1.32
1	C	103	HIS	CD2-NE2	16.16	1.55	1.37
1	G	51	GLY	N-CA	-16.14	1.22	1.45
2	D	92	HIS	CD2-NE2	-16.12	1.20	1.37
2	D	25	GLY	C-N	16.11	1.54	1.33
2	F	104	ARG	N-CA	16.00	1.65	1.46
2	F	97	HIS	CG-ND1	-15.96	1.20	1.38
1	G	63	ALA	N-CA	15.96	1.67	1.46
1	A	13	ALA	CA-C	15.95	1.73	1.52
1	A	75	ASP	C-O	15.94	1.41	1.24
1	A	58	HIS	N-CA	15.81	1.65	1.46
1	E	89	HIS	CG-ND1	15.80	1.55	1.38
1	C	13	ALA	CA-C	-15.80	1.31	1.52
1	G	37	PRO	C-N	-15.79	1.10	1.33
1	C	129	LEU	N-CA	15.79	1.67	1.46
2	H	82	LYS	N-CA	15.76	1.65	1.46
1	E	7	LYS	N-CA	15.74	1.65	1.46
1	C	139	LYS	C-O	15.70	1.45	1.24
1	E	24	TYR	C-N	15.64	1.56	1.33
2	B	12	THR	CB-OG1	15.63	1.68	1.43
1	G	23	GLU	C-O	15.61	1.42	1.24
2	F	62	ALA	C-O	15.60	1.42	1.24
1	A	140	TYR	C-O	15.60	1.42	1.24
2	F	36	PRO	N-CA	15.59	1.67	1.47
1	G	69	ALA	N-CA	15.59	1.66	1.46
1	C	112	HIS	ND1-CE1	15.48	1.48	1.32
1	C	45	HIS	CB-CG	15.41	1.71	1.50
1	C	89	HIS	CB-CG	15.41	1.71	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	36	PRO	C-O	15.38	1.44	1.24
1	E	109	LEU	C-N	-15.35	1.12	1.33
2	B	45	PHE	C-O	15.34	1.43	1.24
1	G	119	PRO	N-CA	-15.34	1.27	1.47
2	H	135	ALA	C-N	-15.32	1.11	1.33
1	C	83	LEU	C-N	15.32	1.53	1.33
2	F	138	ALA	C-O	15.25	1.41	1.24
2	D	87	THR	C-N	15.24	1.54	1.33
1	E	105	LEU	C-N	-15.23	1.12	1.33
1	G	30	GLU	C-O	15.17	1.41	1.24
2	F	40	ARG	CD-NE	15.16	1.67	1.46
2	B	133	VAL	N-CA	15.15	1.64	1.46
1	C	71	ALA	C-O	15.14	1.43	1.24
2	F	133	VAL	N-CA	15.14	1.66	1.46
1	G	112	HIS	CA-CB	15.12	1.79	1.53
1	A	121	VAL	N-CA	15.11	1.68	1.46
1	C	110	ALA	C-N	-15.09	1.13	1.33
1	A	34	LEU	N-CA	15.07	1.65	1.46
1	C	9	ASN	N-CA	-15.06	1.28	1.46
1	E	24	TYR	C-O	-15.05	1.06	1.24
1	A	87	HIS	N-CA	15.02	1.63	1.46
1	E	45	HIS	CD2-NE2	-14.99	1.21	1.37
1	C	75	ASP	CG-OD1	14.99	1.53	1.25
1	A	69	ALA	N-CA	14.97	1.65	1.46
2	B	109	VAL	CA-CB	14.97	1.72	1.54
1	E	31	ARG	NE-CZ	-14.97	1.16	1.33
1	A	76	MET	CA-CB	14.94	1.76	1.54
2	D	77	HIS	CG-CD2	14.93	1.52	1.35
1	C	103	HIS	CE1-NE2	-14.93	1.17	1.32
1	G	7	LYS	C-N	14.93	1.54	1.33
1	A	69	ALA	CA-CB	-14.91	1.29	1.53
2	F	134	VAL	C-N	-14.90	1.15	1.33
1	C	94	ASP	C-N	14.89	1.55	1.33
1	G	67	THR	C-O	14.87	1.43	1.24
2	D	26	GLU	CD-OE2	14.82	1.53	1.25
1	A	138	SER	C-N	-14.81	1.12	1.33
2	D	91	LEU	N-CA	-14.80	1.28	1.46
2	B	37	TRP	NE1-CE2	14.78	1.53	1.37
2	B	38	THR	CB-OG1	14.77	1.67	1.43
2	D	87	THR	C-O	-14.77	1.06	1.24
2	D	130	TYR	C-O	-14.76	1.05	1.24
2	B	97	HIS	ND1-CE1	14.76	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLY	C-N	14.76	1.52	1.33
1	E	15	GLY	C-N	14.69	1.54	1.33
1	C	30	GLU	N-CA	14.69	1.64	1.46
1	G	117	PHE	CA-CB	14.69	1.78	1.53
1	E	102	SER	CA-C	14.63	1.71	1.52
1	A	141	ARG	CD-NE	14.62	1.66	1.46
2	D	77	HIS	CA-CB	14.61	1.79	1.53
2	D	134	VAL	N-CA	14.61	1.63	1.46
1	G	59	GLY	N-CA	-14.61	1.26	1.45
2	H	55	MET	C-N	-14.60	1.12	1.33
2	B	53	ALA	C-O	14.59	1.41	1.24
2	B	129	ALA	N-CA	14.59	1.65	1.46
1	A	124	SER	C-O	14.58	1.40	1.24
2	B	16	GLY	C-N	14.56	1.54	1.33
2	B	130	TYR	C-O	14.55	1.43	1.24
2	F	12	THR	C-N	-14.55	1.14	1.33
1	A	27	GLU	N-CA	14.50	1.64	1.46
1	C	110	ALA	C-O	14.45	1.42	1.24
2	H	107	GLY	C-O	14.45	1.41	1.24
2	B	8	LYS	C-O	-14.41	1.07	1.24
2	H	143	HIS	C-N	-14.38	1.12	1.33
1	E	137	THR	CB-OG1	14.32	1.66	1.43
1	C	20	HIS	CD2-NE2	14.32	1.53	1.37
1	E	11	LYS	CA-CB	14.32	1.75	1.53
1	E	45	HIS	CE1-NE2	14.29	1.46	1.32
2	F	140	ALA	C-O	-14.29	1.07	1.24
1	A	128	PHE	N-CA	-14.29	1.29	1.46
1	A	128	PHE	C-N	14.28	1.52	1.33
2	D	35	TYR	CA-CB	-14.25	1.37	1.53
1	A	50	HIS	N-CA	14.24	1.64	1.46
1	G	125	LEU	N-CA	14.23	1.64	1.46
2	D	115	ALA	C-N	14.22	1.52	1.33
1	C	73	VAL	C-O	14.22	1.41	1.24
2	H	7	GLU	N-CA	14.21	1.64	1.46
2	H	83	GLY	N-CA	14.15	1.65	1.45
1	A	24	TYR	C-O	-14.12	1.05	1.24
2	B	63	HIS	CE1-NE2	14.12	1.46	1.32
2	D	145	TYR	N-CA	14.11	1.62	1.45
2	F	116	HIS	CG-CD2	14.08	1.51	1.35
2	D	2	HIS	C-O	14.05	1.41	1.23
1	G	10	VAL	C-O	14.04	1.39	1.24
2	B	11	VAL	N-CA	14.04	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	90	GLU	C-O	13.99	1.41	1.24
1	E	134	THR	C-N	-13.97	1.16	1.33
2	D	48	LEU	C-N	13.95	1.52	1.33
2	H	39	GLN	N-CA	13.95	1.64	1.46
1	A	35	SER	C-N	-13.95	1.16	1.33
2	B	2	HIS	CG-ND1	13.92	1.53	1.38
1	E	11	LYS	N-CA	-13.91	1.29	1.46
1	C	36	PHE	CA-C	13.90	1.69	1.52
1	C	95	PRO	CA-CB	13.88	1.73	1.53
1	E	15	GLY	N-CA	13.87	1.65	1.45
1	G	32	MET	CA-CB	13.84	1.75	1.53
2	H	29	GLY	C-N	13.83	1.52	1.34
1	A	20	HIS	C-O	13.82	1.44	1.24
2	D	55	MET	C-O	13.82	1.41	1.24
2	D	117	HIS	CG-CD2	-13.81	1.20	1.35
2	H	77	HIS	C-N	13.80	1.53	1.33
1	G	72	HIS	CG-CD2	13.79	1.51	1.35
2	D	34	VAL	N-CA	13.77	1.64	1.46
2	D	48	LEU	C-O	-13.77	1.03	1.24
1	C	94	ASP	N-CA	13.75	1.63	1.45
2	F	69	GLY	CA-C	13.72	1.71	1.51
1	A	122	HIS	CD2-NE2	-13.71	1.22	1.37
2	D	4	THR	CB-OG1	13.70	1.65	1.43
1	A	19	ALA	C-N	13.67	1.55	1.33
2	D	65	LYS	C-O	13.64	1.39	1.24
1	C	48	LEU	CA-CB	13.62	1.71	1.53
2	H	118	PHE	N-CA	-13.61	1.27	1.46
2	B	133	VAL	C-O	13.60	1.40	1.24
1	C	81	SER	C-N	-13.57	1.15	1.34
1	C	113	LEU	N-CA	13.57	1.61	1.46
1	C	20	HIS	CE1-NE2	-13.56	1.19	1.32
1	G	135	VAL	CA-CB	13.56	1.69	1.54
2	H	76	ALA	N-CA	-13.54	1.30	1.46
1	A	89	HIS	CG-CD2	13.52	1.50	1.35
1	C	39	THR	CA-C	-13.49	1.33	1.52
2	H	101	GLU	C-N	-13.49	1.16	1.33
1	C	38	THR	CA-CB	13.48	1.75	1.53
1	E	20	HIS	CG-CD2	-13.46	1.21	1.35
1	G	2	LEU	C-O	13.44	1.39	1.23
2	H	12	THR	C-O	13.44	1.41	1.24
2	D	8	LYS	C-O	13.43	1.41	1.24
2	D	120	LYS	N-CA	13.43	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	142	ALA	CA-CB	13.41	1.75	1.53
1	A	19	ALA	N-CA	13.38	1.63	1.45
2	H	70	ALA	C-O	-13.35	1.08	1.24
2	F	39	GLN	C-O	-13.34	1.07	1.24
1	G	40	LYS	C-N	-13.33	1.15	1.33
2	B	104	ARG	N-CA	13.32	1.63	1.46
1	E	95	PRO	C-O	13.31	1.43	1.24
2	H	132	LYS	C-N	13.30	1.50	1.33
1	E	36	PHE	N-CA	13.27	1.60	1.46
2	H	2	HIS	CA-CB	13.26	1.69	1.53
2	B	63	HIS	C-N	-13.23	1.17	1.33
2	H	98	VAL	C-O	13.21	1.38	1.24
2	D	61	LYS	N-CA	13.20	1.63	1.46
2	H	104	ARG	C-N	13.19	1.54	1.33
2	D	146	HIS	CG-ND1	-13.19	1.23	1.38
2	F	110	LEU	C-N	13.19	1.50	1.33
2	F	37	TRP	N-CA	13.19	1.63	1.46
2	B	135	ALA	CA-C	-13.18	1.36	1.52
2	F	78	LEU	C-N	-13.18	1.15	1.33
2	D	7	GLU	CA-CB	13.17	1.74	1.53
2	F	143	HIS	C-O	-13.16	1.07	1.24
1	C	58	HIS	C-N	-13.15	1.18	1.33
2	F	59	LYS	C-N	13.13	1.50	1.33
1	C	86	LEU	C-O	-13.12	1.07	1.24
1	E	31	ARG	CD-NE	-13.12	1.27	1.46
1	C	103	HIS	CG-ND1	13.09	1.52	1.38
1	E	90	LYS	C-O	13.09	1.40	1.23
2	F	23	VAL	N-CA	13.08	1.63	1.46
2	F	41	PHE	C-O	13.07	1.41	1.24
2	B	138	ALA	C-O	13.06	1.40	1.24
1	A	76	MET	C-O	13.06	1.37	1.24
1	G	47	ASP	CA-CB	-13.05	1.30	1.53
1	A	118	THR	C-N	13.02	1.50	1.34
1	G	42	TYR	CA-C	13.01	1.70	1.52
2	F	102	ASN	CG-OD1	13.00	1.48	1.23
1	A	129	LEU	C-N	-12.99	1.18	1.33
2	F	75	LEU	C-O	12.98	1.41	1.24
2	B	32	LEU	C-N	12.98	1.46	1.33
2	H	5	PRO	N-CD	12.97	1.66	1.47
2	B	125	PRO	C-O	12.96	1.40	1.24
1	A	93	VAL	N-CA	12.96	1.61	1.46
1	G	37	PRO	C-O	12.94	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	84	THR	CB-OG1	12.93	1.64	1.43
1	C	64	ASP	CA-CB	12.93	1.76	1.53
2	F	68	LEU	CA-CB	12.89	1.73	1.53
2	F	13	ALA	C-O	12.88	1.39	1.24
2	H	55	MET	C-O	12.88	1.40	1.24
2	H	58	PRO	C-O	12.88	1.40	1.24
2	B	103	PHE	C-O	-12.87	1.08	1.24
2	D	90	GLU	CD-OE2	12.86	1.49	1.25
2	B	7	GLU	C-N	-12.85	1.17	1.33
2	H	13	ALA	C-O	12.80	1.39	1.24
2	H	39	GLN	C-O	12.80	1.40	1.24
2	D	127	GLN	C-N	-12.77	1.16	1.33
2	F	37	TRP	CZ2-CH2	12.76	1.61	1.37
1	E	119	PRO	C-N	-12.75	1.14	1.33
1	E	112	HIS	CG-CD2	12.74	1.49	1.35
2	D	106	LEU	C-N	12.74	1.52	1.33
2	B	4	THR	CA-CB	12.72	1.72	1.53
1	C	58	HIS	N-CA	-12.71	1.31	1.46
1	G	6	ASP	N-CA	12.70	1.61	1.46
2	D	86	ALA	CA-CB	12.68	1.74	1.53
1	G	58	HIS	CG-CD2	12.68	1.49	1.35
2	D	49	SER	CA-CB	12.67	1.77	1.53
2	D	131	GLN	C-N	-12.67	1.14	1.33
1	E	137	THR	N-CA	12.65	1.60	1.46
2	D	146	HIS	CD2-NE2	12.64	1.51	1.37
1	E	14	TRP	N-CA	12.64	1.63	1.46
1	C	89	HIS	CG-ND1	-12.62	1.24	1.38
1	A	89	HIS	C-N	-12.62	1.14	1.33
2	B	126	VAL	N-CA	12.62	1.62	1.46
1	G	81	SER	CB-OG	12.61	1.67	1.42
1	E	141	ARG	CZ-NH2	-12.59	1.17	1.33
2	F	48	LEU	C-N	-12.57	1.16	1.33
1	A	101	LEU	C-O	-12.56	1.09	1.24
1	A	6	ASP	C-N	-12.56	1.18	1.33
1	C	43	PHE	CA-C	12.56	1.68	1.52
1	G	124	SER	N-CA	12.55	1.61	1.46
1	E	20	HIS	CD2-NE2	12.54	1.51	1.37
2	F	119	GLY	CA-C	-12.53	1.34	1.51
2	B	115	ALA	C-O	-12.52	1.09	1.24
1	A	96	VAL	C-O	-12.51	1.08	1.24
2	F	16	GLY	C-N	-12.50	1.16	1.33
2	H	79	ASP	CG-OD2	12.50	1.49	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	9	SER	C-N	12.48	1.48	1.33
2	F	35	TYR	C-O	12.45	1.40	1.24
1	G	127	LYS	C-O	12.43	1.39	1.24
1	G	109	LEU	N-CA	-12.43	1.30	1.46
2	H	134	VAL	N-CA	12.43	1.63	1.46
2	F	83	GLY	C-N	-12.42	1.16	1.33
2	D	109	VAL	CA-CB	12.41	1.68	1.54
1	G	81	SER	C-N	-12.40	1.16	1.33
2	F	109	VAL	C-N	12.38	1.50	1.33
1	C	88	ALA	C-O	12.38	1.38	1.24
2	D	129	ALA	CA-CB	12.38	1.73	1.53
2	D	120	LYS	C-O	12.37	1.39	1.24
1	A	45	HIS	CD2-NE2	-12.36	1.24	1.37
1	A	2	LEU	C-N	12.35	1.51	1.33
2	F	9	SER	CA-CB	12.33	1.73	1.53
2	H	6	VAL	C-O	12.32	1.38	1.23
2	H	97	HIS	CG-ND1	-12.31	1.24	1.38
2	H	91	LEU	N-CA	-12.30	1.30	1.46
1	E	56	LYS	N-CA	12.30	1.61	1.46
1	A	78	ASN	N-CA	12.30	1.61	1.46
1	A	84	SER	N-CA	12.29	1.61	1.46
1	E	41	THR	CA-C	12.29	1.69	1.52
2	F	125	PRO	N-CD	12.28	1.65	1.47
2	D	98	VAL	N-CA	12.27	1.61	1.46
1	E	75	ASP	CA-CB	12.26	1.71	1.53
1	C	71	ALA	C-N	12.25	1.50	1.33
1	E	35	SER	CB-OG	12.25	1.66	1.42
2	H	71	PHE	C-O	12.22	1.38	1.24
2	D	26	GLU	CD-OE1	-12.19	1.02	1.25
2	F	85	PHE	C-O	12.18	1.41	1.24
1	A	139	LYS	C-N	12.17	1.50	1.33
2	D	117	HIS	C-N	-12.17	1.14	1.33
1	A	136	LEU	C-N	12.16	1.50	1.34
1	C	45	HIS	CA-CB	12.14	1.70	1.53
1	G	120	ALA	CA-CB	12.14	1.72	1.53
2	D	92	HIS	CG-ND1	12.13	1.51	1.38
1	C	3	SER	CB-OG	12.12	1.66	1.42
2	D	70	ALA	CA-C	12.12	1.69	1.52
2	F	16	GLY	C-O	12.12	1.40	1.23
2	D	125	PRO	CA-CB	12.12	1.74	1.53
1	G	87	HIS	CD2-NE2	-12.12	1.24	1.37
2	B	74	GLY	CA-C	12.08	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	120	ALA	N-CA	-12.06	1.31	1.46
1	G	107	VAL	C-N	-12.04	1.18	1.33
2	H	104	ARG	C-O	-12.04	1.10	1.24
1	G	87	HIS	CG-ND1	12.04	1.51	1.38
1	A	58	HIS	CG-CD2	12.03	1.49	1.35
2	B	2	HIS	N-CA	12.02	1.63	1.47
1	E	102	SER	C-N	-12.00	1.17	1.33
1	G	49	SER	N-CA	12.00	1.60	1.46
1	E	87	HIS	ND1-CE1	11.99	1.44	1.32
2	H	57	ASN	C-N	-11.99	1.21	1.34
1	C	6	ASP	CA-CB	11.98	1.72	1.53
2	H	2	HIS	CE1-NE2	-11.98	1.20	1.32
1	C	56	LYS	N-CA	-11.96	1.32	1.46
2	D	57	ASN	C-O	11.95	1.39	1.24
2	D	14	LEU	N-CA	11.95	1.62	1.46
2	H	109	VAL	C-O	11.94	1.40	1.24
1	C	12	ALA	CA-C	11.93	1.68	1.52
1	C	117	PHE	N-CA	-11.91	1.30	1.46
1	E	45	HIS	N-CA	-11.90	1.32	1.46
1	E	3	SER	N-CA	11.90	1.62	1.46
2	F	53	ALA	N-CA	-11.89	1.32	1.46
1	A	43	PHE	CA-C	-11.89	1.40	1.53
2	F	2	HIS	ND1-CE1	11.89	1.44	1.32
2	F	129	ALA	N-CA	11.89	1.60	1.46
2	D	15	TRP	N-CA	11.88	1.60	1.46
2	D	117	HIS	CA-CB	11.88	1.72	1.53
2	B	8	LYS	N-CA	11.85	1.60	1.46
1	A	35	SER	N-CA	11.84	1.61	1.46
2	F	29	GLY	N-CA	11.84	1.60	1.45
2	B	87	THR	C-O	11.83	1.37	1.24
2	F	121	GLU	CA-CB	11.83	1.71	1.53
1	G	76	MET	C-O	11.80	1.39	1.24
1	E	39	THR	C-O	11.80	1.41	1.24
1	C	59	GLY	N-CA	-11.79	1.31	1.45
1	C	118	THR	C-O	11.79	1.38	1.23
1	E	123	ALA	CA-C	11.79	1.68	1.52
2	B	135	ALA	C-O	11.78	1.37	1.24
1	G	129	LEU	N-CA	-11.77	1.30	1.46
2	F	97	HIS	CD2-NE2	11.77	1.50	1.37
1	G	50	HIS	CA-CB	11.76	1.73	1.53
2	H	115	ALA	C-N	-11.76	1.18	1.34
1	C	92	ARG	NE-CZ	11.71	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	132	VAL	CA-CB	-11.68	1.41	1.54
1	G	81	SER	CA-C	11.67	1.68	1.52
1	A	100	LEU	C-N	-11.67	1.18	1.33
2	H	117	HIS	N-CA	-11.66	1.31	1.46
2	D	85	PHE	N-CA	11.66	1.60	1.46
2	D	146	HIS	CE1-NE2	-11.65	1.20	1.32
1	A	3	SER	CA-CB	-11.65	1.38	1.53
2	D	52	ASP	C-O	11.63	1.37	1.24
1	A	124	SER	CA-C	-11.63	1.37	1.52
1	A	79	ALA	C-N	-11.63	1.18	1.33
1	A	45	HIS	CG-ND1	11.62	1.51	1.38
2	D	4	THR	N-CA	11.62	1.63	1.45
2	H	94	ASP	N-CA	11.62	1.60	1.46
1	C	114	PRO	N-CD	11.58	1.64	1.47
1	A	117	PHE	CA-CB	11.57	1.68	1.52
2	D	89	SER	C-O	11.50	1.39	1.24
1	G	44	PRO	CA-CB	11.50	1.70	1.53
1	C	72	HIS	N-CA	11.47	1.59	1.46
2	D	81	LEU	N-CA	11.47	1.60	1.46
1	G	108	THR	C-O	-11.46	1.10	1.24
2	H	66	LYS	CA-C	11.46	1.68	1.52
1	C	71	ALA	N-CA	11.45	1.61	1.46
2	D	101	GLU	CA-CB	-11.44	1.33	1.53
2	B	145	TYR	C-O	11.44	1.38	1.23
1	C	50	HIS	CG-ND1	-11.44	1.25	1.38
1	C	35	SER	C-N	-11.43	1.18	1.33
2	D	72	SER	C-N	-11.43	1.20	1.33
2	H	67	VAL	C-O	11.43	1.36	1.24
1	G	8	THR	C-O	-11.42	1.10	1.24
2	D	31	LEU	C-N	-11.41	1.18	1.34
1	E	6	ASP	CG-OD1	11.41	1.47	1.25
2	D	12	THR	CB-OG1	11.40	1.61	1.43
1	E	45	HIS	CA-CB	11.40	1.68	1.53
1	E	81	SER	C-O	11.40	1.37	1.24
2	F	97	HIS	CG-CD2	11.40	1.48	1.35
2	F	90	GLU	C-O	-11.39	1.10	1.24
1	G	63	ALA	C-O	11.38	1.39	1.24
2	F	38	THR	CA-C	11.38	1.67	1.52
2	B	102	ASN	CG-OD1	11.37	1.45	1.23
1	G	90	LYS	C-N	-11.37	1.17	1.33
1	E	54	GLN	C-N	-11.36	1.19	1.33
2	F	83	GLY	N-CA	11.36	1.63	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	134	THR	CA-C	11.36	1.67	1.52
1	E	121	VAL	C-N	-11.34	1.18	1.33
1	A	66	LEU	CA-C	11.32	1.67	1.52
1	A	67	THR	CB-OG1	11.32	1.61	1.43
2	D	31	LEU	CA-C	11.32	1.66	1.52
2	F	63	HIS	CE1-NE2	-11.32	1.21	1.32
1	E	28	ALA	C-N	11.32	1.48	1.33
1	C	77	PRO	N-CD	11.31	1.63	1.47
2	B	63	HIS	C-O	11.31	1.37	1.24
1	C	110	ALA	CA-CB	11.30	1.72	1.53
1	E	54	GLN	C-O	11.31	1.37	1.24
2	F	40	ARG	CZ-NH1	11.30	1.48	1.32
1	A	52	SER	N-CA	-11.30	1.32	1.46
1	G	61	LYS	C-O	11.30	1.37	1.24
1	A	55	VAL	C-N	-11.29	1.18	1.33
1	G	114	PRO	N-CD	11.28	1.63	1.47
2	H	56	GLY	C-O	11.27	1.39	1.23
1	E	92	ARG	NE-CZ	11.24	1.45	1.33
2	F	40	ARG	C-O	11.24	1.38	1.24
1	A	100	LEU	C-O	11.23	1.37	1.24
1	C	45	HIS	CD2-NE2	11.23	1.50	1.37
1	C	67	THR	C-O	11.22	1.38	1.24
2	H	59	LYS	C-O	11.21	1.38	1.24
1	E	38	THR	CA-C	11.21	1.67	1.52
1	E	7	LYS	CA-CB	-11.20	1.35	1.53
1	E	4	PRO	C-N	-11.19	1.17	1.33
1	E	125	LEU	C-N	11.19	1.48	1.33
1	A	7	LYS	C-O	11.19	1.36	1.24
2	D	43	GLU	C-N	-11.18	1.19	1.33
1	E	31	ARG	CZ-NH2	11.18	1.48	1.33
1	A	14	TRP	C-O	-11.16	1.10	1.24
2	F	18	VAL	C-O	11.15	1.36	1.24
2	B	63	HIS	CD2-NE2	-11.14	1.25	1.37
1	E	132	VAL	C-N	-11.14	1.19	1.34
2	B	122	PHE	C-O	11.14	1.35	1.23
2	H	60	VAL	C-O	11.14	1.36	1.24
2	F	116	HIS	C-N	-11.12	1.19	1.33
1	G	50	HIS	C-N	-11.11	1.17	1.33
2	B	12	THR	C-O	11.11	1.36	1.24
1	A	86	LEU	CA-C	11.11	1.67	1.53
1	A	103	HIS	ND1-CE1	11.10	1.43	1.32
1	C	36	PHE	C-N	-11.10	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	VAL	C-O	11.09	1.36	1.24
1	C	105	LEU	C-O	-11.09	1.11	1.24
1	E	72	HIS	CG-ND1	11.09	1.50	1.38
1	E	58	HIS	CA-CB	11.09	1.71	1.53
2	F	13	ALA	N-CA	11.09	1.59	1.46
2	H	127	GLN	C-O	11.09	1.38	1.24
2	H	95	LYS	C-N	-11.08	1.18	1.33
1	E	92	ARG	C-N	11.08	1.47	1.33
2	F	84	THR	CA-CB	11.07	1.71	1.53
1	A	57	GLY	C-N	-11.06	1.19	1.33
1	E	102	SER	CA-CB	-11.06	1.35	1.53
2	F	136	GLY	CA-C	11.06	1.67	1.51
2	B	19	ASN	CA-C	11.04	1.67	1.52
1	A	113	LEU	CA-CB	11.03	1.67	1.53
2	B	127	GLN	CA-CB	11.02	1.70	1.53
2	D	97	HIS	CA-CB	11.02	1.69	1.53
2	H	11	VAL	C-N	11.01	1.49	1.33
1	C	69	ALA	N-CA	-11.01	1.33	1.46
2	F	28	LEU	N-CA	-11.01	1.33	1.46
2	H	73	ASP	C-O	11.01	1.40	1.24
1	C	72	HIS	CG-ND1	-11.00	1.26	1.38
1	A	64	ASP	C-O	10.99	1.37	1.24
2	D	19	ASN	N-CA	10.99	1.60	1.46
1	C	72	HIS	CG-CD2	10.97	1.48	1.35
1	G	31	ARG	CZ-NH1	-10.97	1.17	1.32
1	G	52	SER	C-N	10.95	1.48	1.33
1	G	125	LEU	CA-CB	-10.95	1.35	1.53
2	D	63	HIS	ND1-CE1	10.94	1.43	1.32
1	E	41	THR	C-N	-10.94	1.17	1.33
2	H	38	THR	CA-C	10.94	1.67	1.52
2	H	124	PRO	C-N	-10.94	1.22	1.34
1	G	4	PRO	C-O	10.92	1.38	1.24
2	H	61	LYS	C-O	10.92	1.38	1.24
1	C	120	ALA	N-CA	-10.91	1.33	1.46
1	A	21	ALA	CA-CB	10.91	1.72	1.53
1	C	36	PHE	N-CA	-10.90	1.35	1.46
1	A	86	LEU	C-N	-10.90	1.20	1.33
1	G	133	SER	C-N	10.90	1.48	1.33
2	B	111	VAL	CA-C	10.90	1.68	1.52
1	C	81	SER	CA-CB	10.89	1.71	1.53
1	A	106	LEU	N-CA	10.89	1.60	1.46
2	B	123	THR	CA-CB	10.88	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	32	MET	C-O	10.88	1.36	1.24
1	G	136	LEU	N-CA	-10.86	1.31	1.46
1	E	40	LYS	N-CA	10.86	1.60	1.46
2	D	66	LYS	C-N	10.85	1.47	1.33
2	D	74	GLY	CA-C	10.84	1.67	1.51
1	G	132	VAL	C-O	-10.84	1.11	1.24
2	D	97	HIS	C-N	10.84	1.47	1.33
1	E	139	LYS	C-O	10.83	1.38	1.23
2	D	118	PHE	CA-C	-10.83	1.37	1.52
1	G	129	LEU	CA-CB	10.82	1.72	1.53
1	A	47	ASP	CG-OD1	10.82	1.46	1.25
1	G	44	PRO	C-O	10.82	1.37	1.24
1	A	106	LEU	C-O	-10.80	1.10	1.24
2	D	134	VAL	C-N	-10.80	1.19	1.33
2	H	78	LEU	CA-CB	-10.80	1.38	1.53
2	D	137	VAL	N-CA	10.80	1.59	1.46
1	G	36	PHE	N-CA	-10.79	1.35	1.46
1	C	62	VAL	CA-C	-10.78	1.37	1.52
1	C	100	LEU	N-CA	10.78	1.59	1.46
2	D	23	VAL	CA-CB	10.78	1.68	1.54
1	E	130	ALA	CA-CB	10.78	1.70	1.53
1	G	67	THR	C-N	-10.77	1.19	1.34
2	H	140	ALA	C-O	-10.77	1.11	1.24
2	H	41	PHE	C-O	10.77	1.38	1.24
1	C	9	ASN	C-N	-10.76	1.20	1.33
2	D	118	PHE	CA-CB	10.76	1.71	1.53
1	G	121	VAL	CA-CB	10.75	1.69	1.54
2	F	4	THR	C-N	-10.75	1.22	1.34
1	A	130	ALA	N-CA	-10.74	1.33	1.46
2	H	54	VAL	N-CA	10.74	1.59	1.46
1	G	103	HIS	CE1-NE2	10.74	1.43	1.32
2	F	50	THR	C-O	10.73	1.38	1.24
1	A	49	SER	C-O	10.73	1.36	1.24
2	B	91	LEU	C-O	10.73	1.38	1.24
2	D	137	VAL	C-O	-10.72	1.11	1.24
1	E	30	GLU	CA-C	10.72	1.67	1.52
2	D	118	PHE	N-CA	10.71	1.60	1.46
2	D	116	HIS	CD2-NE2	10.71	1.49	1.37
2	B	101	GLU	CD-OE2	10.68	1.45	1.25
2	H	90	GLU	C-N	-10.68	1.18	1.33
2	F	48	LEU	CB-CG	10.67	1.74	1.53
1	E	107	VAL	N-CA	-10.66	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	41	THR	N-CA	-10.65	1.32	1.46
1	G	130	ALA	N-CA	10.65	1.60	1.46
1	G	83	LEU	C-N	-10.64	1.20	1.33
2	H	97	HIS	ND1-CE1	10.61	1.43	1.32
2	H	131	GLN	C-O	-10.61	1.10	1.24
2	D	15	TRP	C-N	-10.60	1.18	1.33
1	C	47	ASP	C-O	10.60	1.37	1.24
1	C	119	PRO	N-CA	10.59	1.61	1.47
1	E	121	VAL	C-O	10.59	1.36	1.23
1	A	45	HIS	C-N	10.59	1.48	1.33
2	F	146	HIS	ND1-CE1	-10.59	1.22	1.32
2	H	22	GLU	C-N	10.59	1.46	1.34
1	E	66	LEU	C-O	10.58	1.36	1.24
1	C	128	PHE	C-N	-10.57	1.19	1.33
2	F	49	SER	N-CA	-10.57	1.32	1.46
2	H	135	ALA	CA-CB	-10.57	1.35	1.53
2	F	119	GLY	N-CA	10.56	1.60	1.45
2	H	96	LEU	CA-CB	10.56	1.71	1.53
2	H	72	SER	C-O	10.56	1.36	1.24
2	D	1	VAL	C-N	-10.54	1.20	1.33
2	D	63	HIS	CA-CB	10.54	1.70	1.53
1	C	63	ALA	C-N	-10.53	1.19	1.33
2	B	20	VAL	C-O	10.53	1.35	1.24
1	E	72	HIS	CD2-NE2	10.53	1.49	1.37
1	C	135	VAL	C-N	-10.52	1.20	1.33
2	D	2	HIS	CA-CB	10.50	1.71	1.53
2	F	108	ASN	C-O	10.49	1.37	1.24
1	C	124	SER	C-N	-10.49	1.19	1.33
1	E	22	GLY	C-N	10.46	1.48	1.33
1	C	61	LYS	C-O	-10.45	1.11	1.24
2	D	98	VAL	C-O	-10.43	1.12	1.24
1	G	45	HIS	CE1-NE2	-10.42	1.22	1.32
1	C	72	HIS	CA-C	-10.41	1.39	1.52
2	D	3	LEU	C-O	-10.40	1.08	1.23
2	H	54	VAL	CA-C	-10.40	1.39	1.52
2	F	92	HIS	CD2-NE2	-10.39	1.26	1.37
2	D	63	HIS	CD2-NE2	10.39	1.49	1.37
1	G	21	ALA	N-CA	-10.39	1.34	1.46
2	B	21	ASP	N-CA	10.37	1.60	1.46
1	A	92	ARG	C-O	10.37	1.37	1.23
1	E	98	PHE	CA-C	10.36	1.66	1.52
1	G	84	SER	CB-OG	10.36	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	45	HIS	C-O	10.35	1.39	1.24
1	E	104	CYS	N-CA	-10.35	1.34	1.46
2	B	5	PRO	C-O	-10.34	1.10	1.24
2	F	25	GLY	CA-C	10.34	1.68	1.51
2	F	17	LYS	N-CA	-10.33	1.32	1.46
2	D	104	ARG	NE-CZ	10.30	1.44	1.33
1	E	130	ALA	C-N	10.29	1.46	1.33
1	A	125	LEU	N-CA	10.28	1.59	1.46
2	D	133	VAL	N-CA	10.27	1.58	1.46
2	B	52	ASP	C-N	-10.27	1.20	1.33
2	D	35	TYR	N-CA	10.27	1.58	1.46
2	F	77	HIS	CA-CB	10.27	1.67	1.53
1	G	128	PHE	C-O	10.27	1.35	1.24
2	B	144	LYS	N-CA	10.26	1.59	1.46
2	H	3	LEU	CA-C	10.26	1.65	1.52
2	H	44	SER	N-CA	10.25	1.59	1.45
2	H	65	LYS	N-CA	10.25	1.59	1.46
1	G	140	TYR	CA-CB	-10.25	1.36	1.53
2	B	103	PHE	CA-CB	-10.24	1.37	1.53
1	C	85	ASP	C-O	-10.24	1.11	1.24
2	H	15	TRP	C-N	-10.23	1.18	1.33
1	A	45	HIS	CG-CD2	-10.23	1.24	1.35
1	G	98	PHE	N-CA	10.22	1.58	1.46
2	D	77	HIS	C-O	10.22	1.35	1.23
2	H	32	LEU	CA-CB	10.20	1.70	1.53
2	B	95	LYS	CE-NZ	10.20	1.79	1.49
2	D	146	HIS	ND1-CE1	10.20	1.42	1.32
2	D	100	PRO	N-CA	10.20	1.59	1.47
1	G	141	ARG	N-CA	10.20	1.65	1.46
2	B	143	HIS	ND1-CE1	-10.19	1.22	1.32
2	F	15	TRP	CZ2-CH2	-10.18	1.18	1.37
1	G	78	ASN	C-N	10.18	1.46	1.33
2	F	83	GLY	CA-C	-10.17	1.34	1.51
1	C	50	HIS	CA-C	-10.17	1.39	1.52
1	G	19	ALA	C-N	10.17	1.48	1.33
2	D	77	HIS	CG-ND1	-10.16	1.27	1.38
1	A	37	PRO	C-O	10.16	1.37	1.24
2	D	87	THR	CB-OG1	10.16	1.60	1.43
1	G	140	TYR	C-N	10.16	1.47	1.33
2	F	115	ALA	C-O	10.15	1.36	1.24
1	C	124	SER	CB-OG	10.15	1.62	1.42
1	E	42	TYR	C-O	10.14	1.37	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	THR	N-CA	10.14	1.58	1.46
2	H	92	HIS	N-CA	10.13	1.58	1.46
1	E	116	GLU	C-O	-10.13	1.11	1.24
1	G	105	LEU	N-CA	-10.12	1.34	1.46
2	H	43	GLU	C-O	-10.12	1.10	1.23
1	C	10	VAL	CA-C	-10.10	1.40	1.52
2	F	97	HIS	ND1-CE1	10.10	1.42	1.32
2	H	66	LYS	C-O	-10.10	1.11	1.24
2	D	119	GLY	C-N	-10.09	1.20	1.34
1	A	87	HIS	CG-ND1	-10.08	1.27	1.38
2	D	80	ASN	CA-C	-10.08	1.39	1.53
1	A	82	ALA	CA-C	-10.07	1.40	1.52
1	E	117	PHE	C-O	10.07	1.37	1.23
1	A	12	ALA	N-CA	10.07	1.59	1.46
1	A	30	GLU	N-CA	10.07	1.58	1.46
2	D	30	ARG	NE-CZ	10.07	1.44	1.33
2	D	44	SER	N-CA	-10.06	1.33	1.46
2	H	20	VAL	CA-C	10.06	1.64	1.52
2	H	17	LYS	CA-CB	10.06	1.71	1.53
1	A	16	LYS	CA-CB	10.05	1.71	1.53
2	B	78	LEU	CA-C	-10.05	1.39	1.52
1	E	2	LEU	C-O	-10.05	1.12	1.23
2	B	44	SER	N-CA	10.05	1.59	1.46
1	E	3	SER	C-N	-10.05	1.23	1.34
1	C	90	LYS	C-N	-10.04	1.18	1.33
1	C	30	GLU	C-O	10.04	1.35	1.24
1	A	60	LYS	CE-NZ	10.02	1.79	1.49
1	C	126	ASP	CG-OD2	10.02	1.44	1.25
2	D	110	LEU	C-N	-10.02	1.20	1.33
2	F	63	HIS	CA-C	10.01	1.66	1.52
1	E	117	PHE	N-CA	10.01	1.60	1.46
2	B	37	TRP	CD1-NE1	-10.00	1.16	1.37
1	A	101	LEU	CB-CG	10.00	1.73	1.53
2	B	15	TRP	N-CA	9.99	1.59	1.46
1	C	54	GLN	CD-OE1	9.99	1.42	1.23
1	C	9	ASN	CG-OD1	9.98	1.42	1.23
2	D	60	VAL	C-O	9.98	1.35	1.24
1	A	50	HIS	C-O	-9.97	1.11	1.23
1	C	133	SER	N-CA	9.97	1.59	1.46
1	C	62	VAL	C-O	9.97	1.36	1.24
1	A	59	GLY	N-CA	9.96	1.58	1.45
1	E	40	LYS	C-O	9.96	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	56	GLY	C-O	9.95	1.37	1.23
2	H	9	SER	CA-CB	9.95	1.70	1.53
1	A	122	HIS	C-O	9.95	1.35	1.24
1	C	16	LYS	CG-CD	9.94	1.82	1.52
1	A	77	PRO	CA-C	9.94	1.66	1.52
2	B	24	GLY	C-N	-9.94	1.22	1.33
2	B	73	ASP	CA-CB	9.93	1.70	1.53
1	C	65	ALA	CA-C	9.93	1.66	1.52
1	C	134	THR	N-CA	-9.93	1.33	1.46
1	E	41	THR	CB-OG1	9.93	1.59	1.43
1	E	119	PRO	N-CA	-9.92	1.34	1.47
2	D	123	THR	CA-C	9.91	1.65	1.53
2	D	121	GLU	CD-OE2	9.90	1.44	1.25
1	E	88	ALA	C-N	9.89	1.47	1.33
2	H	139	ASN	CA-CB	9.87	1.69	1.53
1	C	37	PRO	C-N	-9.86	1.20	1.34
1	G	134	THR	CA-CB	9.86	1.68	1.53
1	E	100	LEU	C-N	9.85	1.48	1.33
1	E	42	TYR	CE1-CZ	9.84	1.61	1.38
1	A	111	ALA	C-O	9.84	1.37	1.24
2	F	1	VAL	N-CA	9.84	1.65	1.46
2	D	116	HIS	N-CA	-9.83	1.34	1.46
1	G	128	PHE	N-CA	-9.83	1.34	1.46
1	G	110	ALA	C-N	9.82	1.44	1.33
1	C	35	SER	C-O	9.80	1.36	1.24
1	E	74	ASP	CG-OD1	9.79	1.44	1.25
2	F	82	LYS	CD-CE	9.79	1.81	1.52
2	H	145	TYR	C-O	9.79	1.35	1.24
1	G	56	LYS	N-CA	9.78	1.58	1.46
1	A	105	LEU	C-O	9.78	1.35	1.24
2	F	39	GLN	CG-CD	9.78	1.76	1.52
2	D	107	GLY	N-CA	-9.77	1.32	1.45
2	F	123	THR	C-O	9.77	1.39	1.23
2	F	117	HIS	CD2-NE2	9.76	1.48	1.37
1	C	116	GLU	C-O	9.76	1.35	1.24
2	D	97	HIS	C-O	-9.76	1.10	1.23
2	D	2	HIS	CG-ND1	9.75	1.49	1.38
1	A	131	SER	C-O	9.75	1.35	1.24
1	C	119	PRO	CA-C	9.74	1.67	1.52
2	D	117	HIS	CB-CG	9.73	1.63	1.50
2	F	114	LEU	CB-CG	9.73	1.73	1.53
2	D	115	ALA	C-O	-9.73	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	112	HIS	CG-CD2	-9.73	1.25	1.35
2	H	126	VAL	C-O	-9.71	1.14	1.24
2	D	123	THR	C-O	9.71	1.36	1.23
1	G	45	HIS	CG-ND1	-9.71	1.27	1.38
2	F	5	PRO	N-CD	-9.71	1.34	1.47
2	F	52	ASP	CA-C	9.69	1.64	1.52
1	C	59	GLY	CA-C	9.69	1.62	1.52
1	C	92	ARG	CD-NE	9.69	1.59	1.46
2	H	77	HIS	CE1-NE2	9.69	1.42	1.32
2	D	37	TRP	NE1-CE2	-9.68	1.26	1.37
1	A	92	ARG	NE-CZ	9.68	1.43	1.33
2	D	116	HIS	CA-CB	9.67	1.68	1.53
1	C	55	VAL	C-N	-9.66	1.22	1.33
2	D	139	ASN	C-O	-9.66	1.11	1.24
1	G	135	VAL	C-N	9.65	1.47	1.33
1	A	72	HIS	ND1-CE1	9.65	1.42	1.32
2	B	25	GLY	N-CA	9.64	1.59	1.45
1	E	108	THR	CB-OG1	9.64	1.59	1.43
2	F	30	ARG	CZ-NH2	-9.64	1.21	1.33
2	D	116	HIS	CE1-NE2	-9.64	1.23	1.32
1	C	112	HIS	CG-ND1	-9.63	1.27	1.38
2	D	126	VAL	N-CA	9.63	1.56	1.46
2	F	136	GLY	N-CA	-9.63	1.31	1.45
2	B	107	GLY	CA-C	9.62	1.64	1.51
1	C	89	HIS	CE1-NE2	-9.62	1.23	1.32
1	G	45	HIS	C-N	-9.62	1.20	1.33
1	E	8	THR	C-O	-9.62	1.13	1.24
1	E	48	LEU	C-N	9.62	1.46	1.33
1	G	116	GLU	C-O	9.61	1.38	1.23
2	H	17	LYS	C-N	9.61	1.44	1.33
2	F	145	TYR	CA-CB	-9.60	1.38	1.53
1	G	14	TRP	NE1-CE2	-9.59	1.26	1.37
1	A	14	TRP	N-CA	9.58	1.58	1.46
1	E	72	HIS	C-O	-9.57	1.13	1.24
2	H	11	VAL	N-CA	9.57	1.57	1.46
1	E	103	HIS	CG-CD2	-9.56	1.25	1.35
2	F	90	GLU	CG-CD	9.56	1.75	1.52
1	C	34	LEU	CB-CG	9.55	1.72	1.53
2	D	138	ALA	C-O	-9.55	1.13	1.24
1	A	34	LEU	CA-CB	-9.55	1.38	1.53
1	E	103	HIS	CA-CB	9.55	1.68	1.53
2	B	109	VAL	N-CA	-9.54	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	THR	CA-CB	9.53	1.69	1.52
2	F	79	ASP	CA-CB	-9.53	1.38	1.53
1	G	118	THR	N-CA	9.53	1.56	1.45
2	B	21	ASP	C-N	-9.52	1.21	1.33
2	D	122	PHE	CA-CB	-9.52	1.37	1.53
1	G	35	SER	C-O	9.52	1.36	1.24
1	G	72	HIS	ND1-CE1	-9.52	1.23	1.32
1	G	134	THR	N-CA	-9.52	1.34	1.46
1	C	40	LYS	CG-CD	9.52	1.81	1.52
1	A	124	SER	N-CA	9.51	1.57	1.46
2	H	87	THR	CA-C	9.50	1.65	1.52
2	F	33	VAL	N-CA	9.50	1.58	1.46
2	B	117	HIS	CG-CD2	9.49	1.46	1.35
1	A	79	ALA	C-O	9.48	1.34	1.24
1	G	141	ARG	C-O	9.48	1.42	1.23
1	G	115	ALA	CA-C	-9.48	1.39	1.53
1	C	23	GLU	CD-OE2	9.47	1.43	1.25
2	F	5	PRO	C-O	9.47	1.37	1.24
1	E	58	HIS	ND1-CE1	-9.46	1.23	1.32
2	D	142	ALA	N-CA	-9.46	1.33	1.46
2	F	8	LYS	CB-CG	9.46	1.80	1.52
1	C	16	LYS	C-O	-9.45	1.11	1.24
2	H	129	ALA	N-CA	-9.45	1.34	1.46
2	H	27	ALA	CA-C	9.44	1.65	1.52
1	E	122	HIS	CG-ND1	9.43	1.48	1.38
1	C	95	PRO	N-CD	9.43	1.60	1.47
1	C	103	HIS	C-N	-9.43	1.19	1.33
2	B	134	VAL	C-O	9.43	1.35	1.24
2	H	135	ALA	C-O	9.42	1.35	1.24
2	D	97	HIS	CG-CD2	9.42	1.46	1.35
1	G	121	VAL	N-CA	-9.42	1.34	1.46
1	A	89	HIS	CG-ND1	-9.41	1.27	1.38
1	A	105	LEU	N-CA	-9.41	1.34	1.46
2	B	37	TRP	CZ2-CH2	9.41	1.55	1.37
1	A	47	ASP	N-CA	9.41	1.58	1.46
1	C	9	ASN	CA-C	9.41	1.65	1.52
1	E	32	MET	C-N	-9.41	1.21	1.33
2	H	97	HIS	CE1-NE2	9.40	1.42	1.32
1	E	83	LEU	N-CA	9.40	1.58	1.46
1	A	27	GLU	CD-OE2	9.39	1.43	1.25
2	B	104	ARG	CZ-NH1	9.39	1.46	1.32
2	B	14	LEU	C-N	-9.39	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	17	LYS	CA-CB	9.38	1.69	1.53
2	F	41	PHE	N-CA	9.38	1.57	1.46
2	H	86	ALA	CA-CB	-9.38	1.38	1.54
2	D	39	GLN	CD-OE1	9.37	1.41	1.23
2	H	40	ARG	N-CA	9.37	1.58	1.46
1	C	128	PHE	CA-CB	9.36	1.68	1.53
2	D	80	ASN	CA-CB	9.36	1.70	1.53
1	E	82	ALA	N-CA	-9.36	1.34	1.46
1	E	132	VAL	N-CA	9.36	1.58	1.46
2	F	40	ARG	CA-CB	9.36	1.69	1.53
2	H	90	GLU	CA-CB	-9.36	1.38	1.53
2	B	145	TYR	CA-CB	9.35	1.68	1.53
1	C	99	LYS	CA-C	9.35	1.66	1.52
1	G	114	PRO	N-CA	-9.34	1.35	1.47
2	F	67	VAL	C-O	9.34	1.35	1.24
2	F	68	LEU	CB-CG	9.34	1.72	1.53
2	B	92	HIS	CD2-NE2	-9.32	1.27	1.37
1	E	79	ALA	C-N	9.31	1.47	1.33
1	E	134	THR	CB-OG1	9.31	1.58	1.43
2	H	2	HIS	CG-ND1	9.31	1.48	1.38
2	F	16	GLY	CA-C	9.31	1.65	1.51
1	E	87	HIS	CG-ND1	9.30	1.48	1.38
1	G	114	PRO	CA-C	9.30	1.65	1.52
1	G	71	ALA	N-CA	9.30	1.58	1.46
1	C	103	HIS	C-O	9.30	1.35	1.24
2	B	53	ALA	C-N	-9.29	1.22	1.33
2	D	116	HIS	CG-CD2	9.29	1.46	1.35
2	D	71	PHE	N-CA	-9.28	1.35	1.46
2	H	31	LEU	CA-CB	-9.28	1.38	1.53
1	G	54	GLN	C-O	9.27	1.36	1.24
2	D	42	PHE	C-N	-9.27	1.23	1.33
2	F	36	PRO	N-CD	-9.26	1.34	1.47
2	H	27	ALA	C-N	9.26	1.46	1.33
2	H	139	ASN	N-CA	-9.25	1.34	1.46
1	G	93	VAL	C-O	-9.25	1.14	1.24
1	A	34	LEU	C-O	9.25	1.36	1.24
2	D	34	VAL	C-O	9.24	1.34	1.24
1	C	33	PHE	N-CA	-9.24	1.34	1.46
2	D	111	VAL	C-O	-9.24	1.12	1.24
2	H	127	GLN	CB-CG	9.24	1.80	1.52
2	F	27	ALA	C-N	-9.23	1.22	1.33
2	B	113	VAL	C-N	-9.23	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	VAL	C-O	9.22	1.35	1.24
2	D	127	GLN	N-CA	-9.22	1.35	1.46
2	B	38	THR	C-N	-9.22	1.22	1.33
2	B	137	VAL	N-CA	9.22	1.57	1.46
2	H	26	GLU	CD-OE2	9.22	1.42	1.25
1	G	122	HIS	CG-ND1	9.21	1.48	1.38
1	C	56	LYS	CA-C	9.21	1.64	1.52
1	C	95	PRO	C-O	-9.21	1.11	1.24
1	A	111	ALA	CA-C	9.20	1.66	1.52
2	B	118	PHE	CA-CB	9.19	1.68	1.53
1	C	87	HIS	C-N	9.20	1.46	1.33
1	G	15	GLY	CA-C	9.19	1.64	1.51
2	B	136	GLY	N-CA	-9.18	1.32	1.45
1	A	13	ALA	C-O	9.18	1.35	1.24
1	E	4	PRO	N-CA	9.17	1.58	1.47
1	G	123	ALA	C-O	-9.17	1.13	1.24
2	H	145	TYR	C-N	-9.17	1.20	1.33
1	C	133	SER	C-O	9.17	1.35	1.24
2	F	49	SER	C-O	-9.16	1.12	1.24
1	C	141	ARG	CZ-NH2	9.16	1.45	1.33
1	A	88	ALA	CA-C	-9.15	1.40	1.52
2	F	40	ARG	CG-CD	9.15	1.79	1.52
2	B	19	ASN	CG-OD1	9.15	1.41	1.23
1	E	86	LEU	CA-C	9.15	1.65	1.52
2	H	23	VAL	C-O	-9.14	1.14	1.24
2	F	50	THR	CB-OG1	9.14	1.58	1.43
1	A	61	LYS	CD-CE	9.14	1.79	1.52
2	D	68	LEU	C-O	9.13	1.36	1.24
2	F	143	HIS	CD2-NE2	-9.13	1.27	1.37
2	H	127	GLN	C-N	-9.13	1.22	1.33
1	E	100	LEU	N-CA	9.12	1.57	1.46
2	B	117	HIS	CA-C	-9.12	1.40	1.52
2	D	100	PRO	CA-C	-9.12	1.38	1.52
1	G	70	VAL	N-CA	9.12	1.57	1.46
1	G	94	ASP	CG-OD2	9.12	1.42	1.25
1	A	126	ASP	CA-CB	-9.11	1.39	1.53
1	E	58	HIS	CE1-NE2	9.11	1.41	1.32
1	C	81	SER	CA-C	9.11	1.65	1.52
2	B	78	LEU	C-N	-9.10	1.21	1.34
1	G	8	THR	C-N	-9.10	1.22	1.33
2	H	84	THR	N-CA	9.10	1.56	1.46
2	D	97	HIS	CD2-NE2	9.09	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	THR	C-O	9.08	1.35	1.24
1	G	39	THR	CA-C	9.08	1.65	1.52
2	H	9	SER	C-O	9.08	1.36	1.24
2	F	77	HIS	CE1-NE2	-9.06	1.23	1.32
2	B	68	LEU	C-N	9.05	1.48	1.33
1	G	53	ALA	CA-CB	9.05	1.70	1.53
2	B	50	THR	C-O	-9.04	1.13	1.24
1	E	128	PHE	C-O	9.04	1.34	1.24
2	H	23	VAL	CA-CB	9.04	1.66	1.54
2	B	56	GLY	C-N	9.04	1.48	1.33
1	G	133	SER	C-O	9.04	1.35	1.24
2	D	2	HIS	ND1-CE1	-9.03	1.23	1.32
2	F	15	TRP	CZ3-CH2	9.03	1.63	1.40
2	D	138	ALA	CA-CB	9.02	1.67	1.53
1	C	25	GLY	CA-C	9.01	1.62	1.52
2	D	3	LEU	C-N	-9.01	1.19	1.33
1	G	108	THR	C-N	9.01	1.46	1.33
2	B	86	ALA	CA-CB	9.01	1.67	1.53
2	D	105	LEU	CA-CB	-9.01	1.38	1.53
2	D	124	PRO	C-O	-9.00	1.14	1.24
2	B	37	TRP	CA-CB	8.99	1.69	1.53
1	C	68	ASN	CA-C	8.98	1.64	1.52
1	E	45	HIS	CG-CD2	-8.98	1.25	1.35
1	C	29	LEU	N-CA	-8.97	1.35	1.46
1	G	32	MET	N-CA	-8.97	1.35	1.46
2	F	19	ASN	C-N	8.96	1.43	1.34
2	D	93	CYS	N-CA	8.94	1.57	1.46
1	C	74	ASP	C-N	8.94	1.46	1.33
2	D	113	VAL	N-CA	-8.94	1.35	1.46
1	C	98	PHE	CB-CG	8.93	1.71	1.50
2	D	2	HIS	CE1-NE2	8.93	1.41	1.32
2	D	25	GLY	N-CA	8.93	1.60	1.45
2	B	123	THR	CA-C	-8.92	1.42	1.52
1	G	42	TYR	C-N	8.92	1.44	1.33
2	H	61	LYS	C-N	-8.92	1.21	1.33
2	B	112	CYS	C-O	8.92	1.34	1.24
2	H	44	SER	CA-CB	-8.92	1.40	1.54
1	C	80	LEU	N-CA	8.91	1.57	1.46
2	D	106	LEU	CA-CB	8.91	1.67	1.53
2	H	24	GLY	CA-C	8.91	1.63	1.51
2	H	28	LEU	CA-C	8.90	1.64	1.52
1	E	92	ARG	N-CA	8.90	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	ALA	CA-C	8.90	1.63	1.52
2	H	19	ASN	CA-C	8.89	1.65	1.53
2	H	127	GLN	CD-NE2	8.89	1.51	1.33
1	C	34	LEU	C-N	-8.86	1.21	1.33
1	G	92	ARG	NE-CZ	-8.86	1.23	1.33
2	B	69	GLY	N-CA	8.85	1.57	1.45
1	C	41	THR	CB-OG1	8.85	1.57	1.43
2	H	25	GLY	C-N	-8.85	1.22	1.33
1	A	52	SER	CA-C	8.84	1.64	1.52
1	G	93	VAL	CA-C	8.84	1.63	1.52
2	H	36	PRO	CA-C	-8.84	1.39	1.52
1	A	81	SER	N-CA	8.83	1.57	1.46
2	D	53	ALA	CA-CB	8.82	1.67	1.53
1	A	21	ALA	C-N	8.82	1.46	1.33
1	E	10	VAL	C-O	8.82	1.34	1.24
2	F	22	GLU	CA-C	8.82	1.64	1.52
2	B	5	PRO	CA-CB	8.81	1.67	1.53
1	C	21	ALA	N-CA	-8.80	1.34	1.46
1	G	9	ASN	C-O	-8.80	1.14	1.24
1	G	35	SER	CA-C	8.80	1.64	1.52
1	G	137	THR	C-O	8.79	1.35	1.24
1	A	27	GLU	CA-CB	-8.79	1.38	1.53
1	A	35	SER	CA-C	-8.79	1.40	1.52
2	F	39	GLN	CA-CB	-8.79	1.38	1.53
2	F	135	ALA	C-O	-8.79	1.14	1.24
1	A	61	LYS	CB-CG	8.78	1.78	1.52
2	F	140	ALA	CA-CB	-8.78	1.39	1.53
1	A	83	LEU	N-CA	8.78	1.57	1.46
1	E	72	HIS	ND1-CE1	-8.78	1.23	1.32
2	D	80	ASN	C-O	8.76	1.33	1.23
2	D	91	LEU	C-O	8.76	1.34	1.24
1	G	111	ALA	N-CA	-8.75	1.36	1.46
2	F	49	SER	CA-C	8.75	1.65	1.52
2	B	87	THR	CA-CB	8.73	1.67	1.53
1	A	96	VAL	C-N	8.73	1.47	1.33
2	F	52	ASP	N-CA	-8.72	1.36	1.46
1	G	126	ASP	CG-OD1	-8.72	1.08	1.25
2	D	106	LEU	C-O	8.71	1.35	1.24
1	G	116	GLU	C-N	-8.71	1.21	1.33
2	B	59	LYS	N-CA	-8.71	1.35	1.46
2	H	103	PHE	CA-CB	-8.70	1.39	1.53
1	A	39	THR	C-N	-8.70	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129	LEU	CA-C	-8.69	1.40	1.52
1	C	43	PHE	N-CA	-8.69	1.37	1.46
2	B	30	ARG	CA-CB	8.69	1.68	1.53
2	D	101	GLU	CG-CD	8.69	1.73	1.52
1	G	52	SER	N-CA	-8.68	1.34	1.46
2	B	114	LEU	CA-CB	8.68	1.67	1.53
2	F	82	LYS	CA-C	8.68	1.64	1.52
2	H	21	ASP	C-O	8.68	1.34	1.24
2	B	102	ASN	C-N	8.67	1.45	1.33
2	F	53	ALA	C-N	8.67	1.44	1.33
1	A	75	ASP	C-N	-8.67	1.24	1.33
1	C	5	ALA	N-CA	8.67	1.56	1.46
2	B	66	LYS	C-N	-8.66	1.23	1.33
1	A	24	TYR	C-N	8.66	1.44	1.33
1	G	8	THR	CA-CB	8.64	1.67	1.53
1	A	103	HIS	C-O	8.63	1.34	1.24
2	B	43	GLU	CD-OE1	8.62	1.41	1.25
1	C	116	GLU	N-CA	-8.61	1.36	1.46
1	E	129	LEU	C-O	-8.61	1.14	1.24
1	C	141	ARG	CB-CG	-8.61	1.26	1.52
2	D	80	ASN	CG-ND2	8.60	1.51	1.33
1	E	72	HIS	N-CA	8.60	1.59	1.46
2	H	91	LEU	CA-CB	8.60	1.67	1.53
1	C	29	LEU	CA-CB	-8.60	1.40	1.53
1	C	6	ASP	C-O	-8.59	1.14	1.24
1	A	103	HIS	CD2-NE2	8.59	1.47	1.37
2	B	113	VAL	N-CA	8.59	1.57	1.46
1	G	26	ALA	N-CA	-8.59	1.35	1.46
2	D	97	HIS	CA-C	-8.59	1.42	1.53
1	E	16	LYS	CA-CB	8.59	1.68	1.53
1	A	68	ASN	C-O	8.59	1.34	1.24
2	D	46	GLY	CA-C	-8.59	1.42	1.52
1	A	128	PHE	CA-C	8.58	1.63	1.52
1	A	85	ASP	C-O	-8.57	1.12	1.24
2	F	103	PHE	CA-CB	8.57	1.67	1.53
2	D	85	PHE	C-N	-8.57	1.21	1.33
2	F	71	PHE	CA-CB	8.57	1.68	1.53
1	A	56	LYS	C-O	-8.56	1.13	1.24
1	E	45	HIS	C-N	-8.56	1.21	1.33
1	G	64	ASP	N-CA	-8.56	1.36	1.46
2	H	22	GLU	CB-CG	8.56	1.78	1.52
1	E	87	HIS	C-N	-8.55	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	130	TYR	CE2-CZ	8.55	1.58	1.38
1	C	84	SER	N-CA	-8.55	1.36	1.46
2	F	72	SER	C-N	-8.55	1.21	1.33
1	G	112	HIS	N-CA	-8.54	1.35	1.46
2	B	124	PRO	C-O	8.54	1.34	1.24
2	F	98	VAL	CA-CB	8.54	1.63	1.53
2	D	117	HIS	CG-ND1	8.53	1.47	1.38
2	D	92	HIS	CE1-NE2	8.53	1.41	1.32
1	C	132	VAL	CB-CG1	8.53	1.80	1.52
2	F	17	LYS	C-O	8.52	1.35	1.24
1	C	76	MET	CA-CB	8.52	1.66	1.53
1	E	121	VAL	CA-C	8.52	1.64	1.52
2	D	134	VAL	C-O	-8.52	1.14	1.24
2	B	122	PHE	CA-CB	-8.51	1.41	1.52
2	B	128	ALA	CA-C	8.51	1.65	1.52
2	H	77	HIS	CD2-NE2	-8.51	1.28	1.37
1	E	124	SER	N-CA	8.49	1.56	1.46
1	G	61	LYS	N-CA	8.49	1.56	1.46
2	B	45	PHE	CG-CD1	8.49	1.56	1.38
2	F	8	LYS	CA-CB	-8.49	1.39	1.53
2	B	97	HIS	CE1-NE2	-8.49	1.24	1.32
2	F	38	THR	CB-OG1	8.49	1.57	1.43
1	G	28	ALA	N-CA	-8.49	1.35	1.46
1	A	46	PHE	CA-C	-8.48	1.41	1.52
1	A	65	ALA	C-O	8.48	1.35	1.24
2	H	34	VAL	N-CA	8.48	1.56	1.46
2	B	12	THR	N-CA	-8.47	1.36	1.46
1	C	82	ALA	N-CA	8.46	1.56	1.46
2	F	75	LEU	CA-CB	8.46	1.66	1.53
2	H	130	TYR	CG-CD1	8.46	1.57	1.39
2	F	10	ALA	N-CA	-8.46	1.36	1.46
2	D	40	ARG	CZ-NH1	8.46	1.44	1.32
2	F	85	PHE	CG-CD1	8.45	1.56	1.38
1	G	119	PRO	CA-CB	8.45	1.65	1.53
1	A	38	THR	C-N	8.45	1.45	1.33
1	A	141	ARG	CA-CB	8.45	1.70	1.53
1	A	112	HIS	C-N	-8.44	1.22	1.33
2	B	19	ASN	CA-CB	-8.45	1.42	1.53
2	B	91	LEU	C-N	-8.44	1.22	1.33
1	A	109	LEU	CA-CB	8.44	1.67	1.53
2	H	130	TYR	C-N	8.43	1.46	1.33
1	E	122	HIS	C-N	-8.43	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	103	PHE	C-O	8.43	1.33	1.24
1	E	139	LYS	C-N	-8.43	1.21	1.33
1	C	80	LEU	CB-CG	-8.42	1.36	1.53
2	B	84	THR	C-N	8.42	1.44	1.33
1	G	64	ASP	CA-C	8.42	1.63	1.52
2	B	35	TYR	CE2-CZ	8.41	1.58	1.38
2	F	93	CYS	C-O	8.41	1.34	1.24
1	A	62	VAL	C-O	8.41	1.33	1.24
2	B	117	HIS	CD2-NE2	-8.41	1.28	1.37
2	B	113	VAL	C-O	-8.40	1.14	1.24
1	C	18	GLY	CA-C	8.39	1.63	1.51
2	F	35	TYR	CA-CB	8.39	1.66	1.53
1	A	25	GLY	N-CA	8.39	1.56	1.45
2	H	24	GLY	C-N	-8.39	1.24	1.33
2	H	57	ASN	C-O	8.38	1.35	1.24
1	C	132	VAL	C-O	8.38	1.33	1.24
1	E	104	CYS	C-N	8.38	1.44	1.33
2	B	115	ALA	N-CA	8.38	1.56	1.46
2	B	146	HIS	CE1-NE2	8.37	1.41	1.32
1	G	26	ALA	C-O	8.36	1.34	1.24
1	G	54	GLN	CG-CD	8.36	1.73	1.52
1	G	82	ALA	CA-CB	8.35	1.67	1.53
1	E	45	HIS	CG-ND1	8.35	1.47	1.38
1	C	129	LEU	CA-CB	8.35	1.67	1.53
2	D	134	VAL	CA-CB	-8.34	1.44	1.54
1	G	23	GLU	CD-OE1	8.34	1.41	1.25
2	B	139	ASN	CA-C	8.33	1.64	1.52
1	C	47	ASP	N-CA	8.33	1.56	1.46
1	E	118	THR	N-CA	8.33	1.58	1.45
2	H	65	LYS	C-N	8.33	1.43	1.33
2	B	85	PHE	N-CA	-8.33	1.36	1.46
1	G	109	LEU	CG-CD1	8.32	1.80	1.52
2	B	37	TRP	CE2-CZ2	-8.32	1.22	1.39
2	D	128	ALA	C-N	-8.32	1.22	1.33
2	F	77	HIS	ND1-CE1	-8.32	1.24	1.32
1	E	129	LEU	C-N	8.31	1.44	1.33
1	G	57	GLY	CA-C	8.31	1.62	1.51
1	E	32	MET	N-CA	-8.30	1.36	1.46
1	A	76	MET	N-CA	-8.30	1.36	1.46
2	B	84	THR	C-O	-8.30	1.13	1.24
1	A	74	ASP	CA-C	8.29	1.64	1.52
2	B	114	LEU	C-N	8.29	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	143	HIS	CE1-NE2	-8.29	1.24	1.32
1	G	97	ASN	C-N	-8.29	1.23	1.33
2	D	36	PRO	C-O	8.29	1.34	1.24
2	F	90	GLU	CA-CB	8.29	1.66	1.53
1	E	138	SER	C-O	8.29	1.33	1.24
1	E	50	HIS	CG-ND1	-8.28	1.29	1.38
2	H	52	ASP	CG-OD2	8.28	1.41	1.25
2	D	97	HIS	CG-ND1	-8.28	1.29	1.38
2	B	87	THR	CB-OG1	8.28	1.56	1.43
1	E	6	ASP	N-CA	8.28	1.56	1.46
1	E	138	SER	N-CA	-8.28	1.36	1.46
1	A	50	HIS	CG-CD2	8.27	1.45	1.35
1	E	110	ALA	CA-CB	8.26	1.67	1.53
1	A	91	LEU	C-O	8.26	1.33	1.24
2	D	62	ALA	C-O	8.26	1.33	1.24
2	H	38	THR	C-N	-8.26	1.22	1.33
2	B	19	ASN	N-CA	8.25	1.56	1.46
2	F	15	TRP	CD1-NE1	-8.25	1.20	1.37
2	H	107	GLY	N-CA	8.24	1.57	1.45
2	H	20	VAL	N-CA	-8.24	1.37	1.46
1	A	33	PHE	CA-C	8.24	1.64	1.52
2	F	122	PHE	C-O	8.23	1.33	1.23
1	G	89	HIS	CA-CB	-8.23	1.42	1.54
2	H	131	GLN	CD-OE1	8.23	1.39	1.23
2	B	97	HIS	CD2-NE2	8.22	1.46	1.37
2	H	41	PHE	C-N	8.22	1.43	1.33
1	C	106	LEU	CB-CG	8.21	1.69	1.53
2	D	78	LEU	C-O	8.21	1.33	1.24
2	D	8	LYS	CA-CB	-8.21	1.39	1.53
2	F	146	HIS	CE1-NE2	8.20	1.40	1.32
2	D	130	TYR	CG-CD1	8.20	1.56	1.39
1	E	4	PRO	C-O	8.20	1.34	1.24
2	H	34	VAL	CA-CB	-8.19	1.43	1.54
1	A	96	VAL	N-CA	8.19	1.57	1.46
1	C	87	HIS	CG-ND1	8.19	1.47	1.38
2	F	82	LYS	C-N	-8.18	1.20	1.33
2	H	40	ARG	CZ-NH2	8.18	1.44	1.33
1	A	62	VAL	C-N	-8.18	1.21	1.33
1	A	137	THR	CB-OG1	8.18	1.56	1.43
1	C	84	SER	C-N	8.18	1.45	1.34
2	D	64	GLY	N-CA	8.18	1.56	1.45
2	B	64	GLY	N-CA	8.17	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	12	ALA	N-CA	-8.17	1.36	1.46
1	C	102	SER	CB-OG	-8.17	1.25	1.42
2	H	102	ASN	C-N	-8.16	1.23	1.33
1	A	118	THR	CA-CB	8.16	1.65	1.53
1	C	124	SER	N-CA	-8.16	1.36	1.46
1	E	6	ASP	CB-CG	-8.16	1.31	1.52
2	B	112	CYS	C-N	-8.16	1.24	1.34
2	D	42	PHE	CA-CB	8.16	1.64	1.53
2	F	89	SER	C-N	8.16	1.43	1.33
1	A	19	ALA	C-O	8.15	1.34	1.23
1	C	54	GLN	CA-C	8.15	1.63	1.52
1	A	113	LEU	C-O	-8.15	1.14	1.24
1	A	41	THR	CA-C	-8.14	1.41	1.52
2	D	95	LYS	CA-C	-8.14	1.44	1.52
1	G	55	VAL	C-N	8.14	1.45	1.34
1	G	14	TRP	CA-CB	8.14	1.66	1.53
1	G	87	HIS	CE1-NE2	8.14	1.40	1.32
2	D	20	VAL	C-N	-8.13	1.23	1.33
1	G	118	THR	CA-CB	8.13	1.65	1.53
1	A	110	ALA	C-O	8.13	1.33	1.24
1	A	104	CYS	CA-CB	8.12	1.67	1.53
2	B	110	LEU	C-N	8.12	1.43	1.33
1	G	105	LEU	C-O	8.11	1.33	1.24
1	C	85	ASP	N-CA	8.10	1.56	1.46
1	E	104	CYS	CA-CB	8.10	1.66	1.53
1	C	60	LYS	N-CA	8.10	1.56	1.46
1	C	22	GLY	CA-C	8.09	1.62	1.51
2	D	138	ALA	C-N	8.09	1.46	1.33
1	E	75	ASP	C-O	8.09	1.31	1.23
1	A	84	SER	CA-CB	-8.09	1.40	1.53
2	B	14	LEU	CA-C	8.09	1.63	1.52
1	C	136	LEU	C-N	8.09	1.46	1.33
2	H	13	ALA	N-CA	-8.09	1.36	1.46
2	D	6	VAL	C-N	-8.08	1.24	1.33
2	B	102	ASN	N-CA	8.07	1.56	1.46
1	C	112	HIS	CB-CG	8.07	1.61	1.50
2	B	136	GLY	C-N	8.07	1.43	1.33
2	H	15	TRP	CZ3-CH2	-8.07	1.20	1.40
1	C	2	LEU	N-CA	8.07	1.55	1.46
2	D	135	ALA	C-O	8.06	1.33	1.24
2	F	95	LYS	C-O	8.06	1.33	1.24
1	A	12	ALA	C-N	8.05	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	99	ASP	CG-OD1	-8.05	1.10	1.25
1	G	78	ASN	CA-C	8.05	1.63	1.52
1	G	86	LEU	C-O	-8.05	1.13	1.24
1	A	127	LYS	C-N	8.05	1.44	1.33
2	F	55	MET	N-CA	8.05	1.56	1.46
1	E	123	ALA	C-N	-8.04	1.23	1.33
2	H	98	VAL	CA-C	-8.04	1.44	1.52
1	G	126	ASP	C-N	-8.04	1.23	1.34
1	A	137	THR	CA-CB	8.03	1.66	1.53
1	C	118	THR	CA-C	-8.03	1.43	1.53
2	F	103	PHE	C-O	-8.02	1.14	1.24
1	C	97	ASN	C-N	-8.01	1.24	1.33
1	G	45	HIS	CD2-NE2	8.00	1.46	1.37
2	H	20	VAL	CA-CB	8.00	1.62	1.54
2	D	45	PHE	CA-CB	8.00	1.67	1.53
2	F	84	THR	C-N	7.99	1.44	1.33
2	F	45	PHE	CG-CD2	7.99	1.55	1.38
1	G	91	LEU	N-CA	-7.98	1.35	1.46
1	A	82	ALA	CA-CB	7.97	1.65	1.53
1	C	20	HIS	CB-CG	7.97	1.61	1.50
2	B	13	ALA	C-O	7.97	1.33	1.24
2	B	73	ASP	CG-OD2	7.97	1.40	1.25
1	C	47	ASP	CG-OD1	7.96	1.40	1.25
2	B	80	ASN	CB-CG	7.96	1.72	1.52
1	C	62	VAL	C-N	-7.96	1.23	1.33
2	B	34	VAL	CA-C	-7.95	1.43	1.52
2	D	75	LEU	N-CA	7.95	1.57	1.46
1	G	50	HIS	CG-CD2	7.95	1.44	1.35
2	B	29	GLY	C-N	-7.95	1.23	1.33
1	A	116	GLU	CA-CB	7.94	1.67	1.54
1	A	21	ALA	N-CA	-7.94	1.35	1.46
2	D	64	GLY	C-O	7.94	1.33	1.23
1	A	127	LYS	N-CA	7.94	1.55	1.46
1	E	11	LYS	CA-C	7.94	1.62	1.52
1	G	55	VAL	CA-C	7.94	1.65	1.52
1	A	81	SER	C-N	-7.94	1.23	1.33
1	A	103	HIS	CG-ND1	-7.93	1.29	1.38
1	E	12	ALA	C-O	-7.93	1.14	1.24
1	G	61	LYS	CG-CD	7.93	1.76	1.52
1	E	134	THR	N-CA	-7.93	1.36	1.46
2	F	18	VAL	CA-CB	7.93	1.64	1.54
1	G	31	ARG	NE-CZ	-7.92	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	89	HIS	CE1-NE2	-7.92	1.24	1.32
1	E	2	LEU	CA-CB	-7.92	1.41	1.53
1	E	4	PRO	N-CD	-7.92	1.36	1.47
2	B	107	GLY	C-O	7.91	1.33	1.23
1	E	42	TYR	CG-CD1	7.91	1.55	1.39
1	G	101	LEU	CG-CD1	7.91	1.78	1.52
2	B	5	PRO	N-CA	-7.91	1.37	1.47
2	D	56	GLY	C-O	7.90	1.34	1.23
2	D	128	ALA	CA-CB	7.90	1.65	1.53
1	A	121	VAL	C-O	7.90	1.32	1.23
1	C	127	LYS	C-O	7.90	1.33	1.24
1	A	49	SER	C-N	7.89	1.44	1.33
1	G	122	HIS	C-N	-7.89	1.23	1.33
1	C	3	SER	C-O	-7.89	1.14	1.24
2	D	82	LYS	N-CA	7.88	1.55	1.46
1	C	60	LYS	C-O	-7.88	1.14	1.24
2	F	34	VAL	C-N	-7.88	1.17	1.33
2	F	127	GLN	C-N	7.88	1.44	1.34
1	E	103	HIS	CB-CG	7.87	1.61	1.50
1	E	16	LYS	C-N	7.87	1.43	1.33
2	H	58	PRO	N-CD	7.87	1.58	1.47
2	D	86	ALA	CA-C	-7.87	1.42	1.52
2	D	17	LYS	CG-CD	-7.87	1.28	1.52
1	A	107	VAL	C-O	7.87	1.33	1.24
1	C	67	THR	N-CA	7.87	1.56	1.46
2	F	146	HIS	CA-CB	7.85	1.69	1.53
1	A	98	PHE	N-CA	7.85	1.55	1.46
2	B	37	TRP	CG-CD2	7.85	1.57	1.43
2	F	131	GLN	CA-C	7.85	1.63	1.52
2	B	122	PHE	C-N	7.84	1.44	1.33
1	C	11	LYS	C-O	-7.84	1.15	1.24
2	B	90	GLU	C-N	-7.84	1.21	1.33
2	B	116	HIS	C-N	7.83	1.45	1.33
2	H	100	PRO	C-O	-7.83	1.13	1.24
2	D	44	SER	CA-CB	7.83	1.67	1.54
2	B	140	ALA	N-CA	-7.83	1.36	1.46
1	E	50	HIS	CG-CD2	-7.82	1.27	1.35
1	E	3	SER	CA-C	-7.82	1.43	1.52
2	H	6	VAL	C-N	7.82	1.44	1.34
1	C	32	MET	CG-SD	7.82	2.00	1.80
2	F	11	VAL	N-CA	7.81	1.56	1.46
1	E	62	VAL	C-N	-7.81	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	136	GLY	CA-C	7.81	1.62	1.51
2	H	106	LEU	N-CA	7.81	1.56	1.46
1	C	133	SER	C-N	-7.81	1.23	1.33
2	H	126	VAL	N-CA	7.81	1.55	1.46
2	F	142	ALA	CA-CB	7.80	1.66	1.54
2	B	118	PHE	CA-C	-7.80	1.42	1.52
1	C	8	THR	C-N	-7.80	1.24	1.33
2	H	61	LYS	CE-NZ	7.80	1.72	1.49
1	G	37	PRO	CA-CB	-7.79	1.42	1.53
1	A	104	CYS	N-CA	-7.79	1.36	1.46
2	F	74	GLY	CA-C	7.79	1.65	1.51
2	D	92	HIS	C-O	-7.79	1.14	1.24
2	B	92	HIS	N-CA	7.79	1.55	1.46
2	D	15	TRP	C-O	7.79	1.33	1.24
2	H	63	HIS	CA-C	7.78	1.62	1.52
2	B	8	LYS	CB-CG	7.78	1.75	1.52
2	B	114	LEU	N-CA	-7.78	1.36	1.46
1	C	61	LYS	CA-C	7.78	1.62	1.52
1	E	47	ASP	CG-OD1	-7.78	1.10	1.25
2	F	30	ARG	CZ-NH1	7.78	1.43	1.32
1	C	114	PRO	C-O	-7.77	1.14	1.24
2	F	85	PHE	N-CA	7.77	1.55	1.46
2	D	65	LYS	CE-NZ	7.77	1.72	1.49
1	A	38	THR	CA-CB	7.76	1.65	1.53
2	B	18	VAL	CB-CG1	7.76	1.78	1.52
2	B	103	PHE	CA-C	7.76	1.63	1.52
2	D	126	VAL	CA-C	7.76	1.64	1.52
1	G	92	ARG	CZ-NH2	7.76	1.43	1.33
2	B	36	PRO	CA-CB	7.76	1.64	1.53
2	B	98	VAL	CB-CG2	7.76	1.78	1.52
1	G	82	ALA	N-CA	-7.76	1.36	1.46
2	F	117	HIS	CG-ND1	7.76	1.46	1.38
2	B	44	SER	CA-C	-7.76	1.41	1.52
1	C	103	HIS	ND1-CE1	7.75	1.40	1.32
2	D	117	HIS	CD2-NE2	7.75	1.46	1.37
2	F	121	GLU	N-CA	-7.75	1.37	1.46
1	G	83	LEU	CA-CB	-7.75	1.40	1.53
2	H	101	GLU	CA-CB	-7.74	1.40	1.53
1	G	30	GLU	CA-CB	-7.74	1.41	1.53
1	G	68	ASN	CA-C	7.74	1.63	1.52
1	A	24	TYR	CG-CD1	-7.74	1.23	1.39
2	F	22	GLU	CA-CB	7.74	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	86	LEU	CB-CG	7.73	1.69	1.53
1	E	112	HIS	CA-C	-7.73	1.42	1.52
2	F	28	LEU	C-O	7.73	1.33	1.24
2	D	50	THR	C-O	-7.73	1.14	1.24
2	D	52	ASP	CG-OD1	7.73	1.40	1.25
2	B	89	SER	CB-OG	7.72	1.57	1.42
2	D	13	ALA	C-N	-7.72	1.23	1.33
1	E	63	ALA	CA-CB	7.72	1.65	1.53
1	G	7	LYS	CA-CB	7.72	1.65	1.53
2	F	111	VAL	N-CA	-7.71	1.36	1.46
1	A	94	ASP	CA-C	7.71	1.61	1.52
2	F	14	LEU	N-CA	7.71	1.56	1.46
1	G	42	TYR	CB-CG	7.71	1.68	1.51
2	D	63	HIS	CE1-NE2	7.71	1.40	1.32
1	E	86	LEU	N-CA	7.70	1.56	1.46
1	C	49	SER	N-CA	7.70	1.56	1.45
1	E	87	HIS	CG-CD2	-7.70	1.27	1.35
2	B	100	PRO	C-N	7.70	1.44	1.34
2	F	80	ASN	N-CA	7.69	1.56	1.46
2	B	56	GLY	CA-C	-7.69	1.41	1.51
1	A	91	LEU	CB-CG	7.69	1.68	1.53
1	G	46	PHE	N-CA	7.68	1.55	1.45
1	E	73	VAL	C-N	7.68	1.44	1.33
2	F	146	HIS	CG-ND1	7.68	1.46	1.38
2	H	14	LEU	CB-CG	-7.68	1.38	1.53
1	C	64	ASP	CG-OD2	-7.68	1.10	1.25
2	B	146	HIS	ND1-CE1	-7.68	1.24	1.32
1	G	78	ASN	N-CA	7.67	1.55	1.46
1	C	65	ALA	N-CA	-7.67	1.36	1.46
1	C	125	LEU	C-O	7.67	1.33	1.24
2	D	48	LEU	N-CA	7.67	1.54	1.46
2	F	117	HIS	C-O	7.67	1.33	1.24
2	D	29	GLY	N-CA	7.66	1.56	1.45
1	C	31	ARG	CA-C	7.66	1.63	1.52
1	C	48	LEU	C-O	-7.66	1.13	1.23
1	C	87	HIS	CA-CB	7.66	1.66	1.53
1	E	130	ALA	CA-C	-7.66	1.43	1.52
2	H	141	LEU	N-CA	-7.65	1.37	1.46
1	E	41	THR	C-O	-7.65	1.14	1.24
1	E	89	HIS	C-O	7.65	1.34	1.24
2	H	12	THR	C-N	-7.65	1.24	1.33
1	G	79	ALA	CA-C	7.65	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	30	ARG	CB-CG	7.64	1.75	1.52
2	F	66	LYS	C-N	7.64	1.44	1.33
1	C	63	ALA	CA-CB	7.64	1.65	1.53
2	F	115	ALA	C-N	-7.63	1.24	1.33
1	E	139	LYS	CA-CB	7.63	1.63	1.53
2	B	97	HIS	CG-ND1	-7.63	1.29	1.38
1	G	43	PHE	C-O	7.63	1.32	1.24
2	H	103	PHE	C-O	7.63	1.33	1.24
1	G	125	LEU	C-O	-7.63	1.14	1.24
1	A	40	LYS	CA-CB	-7.62	1.39	1.53
1	G	18	GLY	N-CA	7.62	1.56	1.45
2	D	92	HIS	C-N	7.62	1.44	1.33
2	D	90	GLU	C-O	-7.62	1.15	1.24
1	G	80	LEU	CA-CB	-7.62	1.40	1.53
1	E	132	VAL	CA-CB	-7.62	1.43	1.54
2	D	6	VAL	C-O	-7.61	1.15	1.24
2	H	10	ALA	C-N	-7.61	1.25	1.34
2	D	141	LEU	CG-CD1	7.61	1.77	1.52
2	B	26	GLU	CD-OE1	-7.60	1.10	1.25
2	D	131	GLN	CA-C	7.60	1.62	1.52
1	G	111	ALA	C-O	7.59	1.35	1.23
2	D	9	SER	N-CA	-7.59	1.36	1.46
1	E	8	THR	CB-OG1	-7.59	1.31	1.43
2	D	108	ASN	CG-OD1	7.59	1.38	1.23
1	C	91	LEU	CG-CD2	7.59	1.77	1.52
2	F	77	HIS	CG-CD2	7.59	1.44	1.35
1	C	86	LEU	CB-CG	7.58	1.68	1.53
1	E	106	LEU	CG-CD1	7.58	1.77	1.52
2	D	125	PRO	N-CA	-7.58	1.38	1.47
2	B	130	TYR	C-N	-7.57	1.23	1.33
2	B	3	LEU	CA-CB	-7.57	1.41	1.53
1	G	84	SER	CA-C	7.57	1.62	1.52
2	F	80	ASN	C-O	-7.57	1.14	1.24
1	A	95	PRO	C-O	7.57	1.33	1.24
2	D	46	GLY	N-CA	7.57	1.56	1.45
2	B	22	GLU	C-O	7.57	1.32	1.24
2	B	40	ARG	CD-NE	7.57	1.56	1.46
1	A	116	GLU	CA-C	-7.56	1.41	1.52
1	C	103	HIS	CG-CD2	-7.55	1.27	1.35
2	D	133	VAL	C-O	7.55	1.32	1.24
2	D	145	TYR	CE2-CZ	7.55	1.56	1.38
2	H	100	PRO	CG-CD	7.55	1.76	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	PHE	N-CA	7.55	1.55	1.46
2	D	66	LYS	N-CA	7.55	1.55	1.46
1	E	117	PHE	CE1-CZ	7.55	1.61	1.38
1	E	97	ASN	C-O	7.54	1.33	1.24
1	C	51	GLY	C-O	7.54	1.34	1.24
1	C	36	PHE	C-O	7.54	1.32	1.23
2	B	129	ALA	CA-C	-7.53	1.42	1.52
1	G	48	LEU	N-CA	-7.53	1.36	1.46
2	B	17	LYS	CG-CD	7.53	1.75	1.52
2	H	131	GLN	N-CA	7.53	1.56	1.46
1	A	22	GLY	N-CA	7.53	1.56	1.45
2	F	7	GLU	CD-OE1	-7.53	1.11	1.25
2	H	2	HIS	ND1-CE1	-7.52	1.25	1.32
2	B	3	LEU	CG-CD2	7.52	1.77	1.52
1	A	132	VAL	N-CA	-7.52	1.37	1.46
2	D	90	GLU	CA-C	7.52	1.62	1.52
1	C	64	ASP	CG-OD1	7.52	1.39	1.25
2	F	56	GLY	C-O	7.52	1.34	1.23
2	F	57	ASN	N-CA	7.51	1.59	1.46
1	C	117	PHE	CA-C	7.50	1.62	1.52
1	C	112	HIS	CA-C	7.49	1.61	1.52
2	B	63	HIS	CG-ND1	7.48	1.46	1.38
1	C	17	VAL	CA-C	7.48	1.62	1.52
2	D	22	GLU	N-CA	7.48	1.55	1.46
2	D	132	LYS	C-N	7.48	1.43	1.33
2	F	8	LYS	C-N	7.48	1.42	1.33
2	B	47	ASP	N-CA	7.47	1.55	1.46
2	F	143	HIS	CA-CB	7.47	1.66	1.53
1	C	9	ASN	C-O	-7.47	1.15	1.24
2	H	9	SER	C-N	7.47	1.43	1.33
1	A	120	ALA	C-O	-7.46	1.14	1.24
2	D	99	ASP	CG-OD2	7.46	1.39	1.25
2	D	125	PRO	CA-C	-7.46	1.40	1.52
1	E	99	LYS	CE-NZ	7.46	1.71	1.49
1	E	129	LEU	CA-CB	7.46	1.65	1.53
2	H	8	LYS	N-CA	7.46	1.55	1.46
2	B	37	TRP	N-CA	7.46	1.55	1.46
1	E	38	THR	N-CA	7.46	1.55	1.46
1	E	108	THR	C-O	-7.46	1.15	1.24
2	F	63	HIS	C-N	-7.45	1.24	1.33
1	A	140	TYR	CA-C	7.45	1.62	1.52
1	G	11	LYS	C-O	7.45	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	VAL	N-CA	7.45	1.55	1.46
2	B	67	VAL	CA-C	7.45	1.61	1.52
1	G	22	GLY	C-O	7.44	1.33	1.23
2	B	30	ARG	CA-C	-7.44	1.42	1.52
2	F	99	ASP	N-CA	-7.44	1.33	1.46
1	G	64	ASP	CG-OD2	7.44	1.39	1.25
2	F	100	PRO	CA-C	-7.44	1.41	1.52
2	F	125	PRO	C-O	7.44	1.33	1.24
1	E	12	ALA	CA-C	7.43	1.62	1.52
1	G	5	ALA	C-N	7.43	1.43	1.33
1	C	62	VAL	N-CA	7.43	1.55	1.46
1	E	135	VAL	C-O	-7.43	1.15	1.24
2	H	137	VAL	CB-CG2	7.43	1.77	1.52
1	C	72	HIS	CA-CB	7.42	1.63	1.53
2	F	57	ASN	C-O	7.42	1.33	1.24
1	A	30	GLU	CA-CB	-7.42	1.41	1.53
2	B	77	HIS	CD2-NE2	7.42	1.46	1.37
1	G	27	GLU	C-O	7.41	1.33	1.24
1	G	22	GLY	N-CA	7.41	1.56	1.45
2	H	145	TYR	N-CA	7.41	1.55	1.46
1	G	62	VAL	N-CA	7.40	1.57	1.46
1	C	72	HIS	C-N	-7.40	1.23	1.33
1	E	112	HIS	CE1-NE2	-7.40	1.25	1.32
2	B	141	LEU	CA-C	-7.40	1.42	1.52
1	C	96	VAL	C-O	7.39	1.33	1.24
2	D	14	LEU	CG-CD1	7.38	1.76	1.52
2	F	96	LEU	N-CA	7.38	1.55	1.46
1	G	131	SER	C-O	7.38	1.32	1.24
2	H	115	ALA	N-CA	-7.38	1.36	1.46
2	F	47	ASP	CG-OD1	7.37	1.39	1.25
1	A	70	VAL	CA-CB	-7.37	1.45	1.54
2	B	34	VAL	N-CA	7.36	1.55	1.46
1	C	76	MET	SD-CE	7.36	1.98	1.79
1	C	114	PRO	C-N	-7.36	1.24	1.33
2	F	53	ALA	CA-CB	7.36	1.64	1.53
2	B	71	PHE	CD1-CE1	7.36	1.60	1.38
1	G	54	GLN	CA-C	7.35	1.62	1.52
2	F	120	LYS	N-CA	7.35	1.55	1.46
2	F	70	ALA	C-N	7.35	1.44	1.33
2	D	88	LEU	CA-CB	7.34	1.66	1.53
2	D	104	ARG	CB-CG	7.34	1.74	1.52
1	G	131	SER	CA-CB	7.34	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	THR	CA-CB	7.34	1.65	1.53
1	A	50	HIS	CA-CB	-7.34	1.42	1.53
1	C	131	SER	CB-OG	7.34	1.56	1.42
1	E	123	ALA	C-O	-7.34	1.14	1.24
2	H	59	LYS	CA-CB	7.34	1.65	1.53
1	G	137	THR	CB-OG1	7.34	1.55	1.43
2	F	8	LYS	N-CA	7.33	1.55	1.46
1	A	79	ALA	N-CA	-7.33	1.37	1.46
2	F	95	LYS	C-N	-7.33	1.23	1.33
2	H	129	ALA	C-O	-7.33	1.15	1.24
1	A	116	GLU	C-N	-7.33	1.24	1.33
1	A	135	VAL	C-O	-7.32	1.15	1.24
1	E	12	ALA	CA-CB	7.32	1.65	1.53
2	F	106	LEU	CA-C	7.32	1.62	1.52
1	C	87	HIS	CE1-NE2	-7.32	1.25	1.32
2	F	47	ASP	CG-OD2	7.32	1.39	1.25
2	H	138	ALA	CA-C	7.32	1.62	1.52
2	B	9	SER	CB-OG	7.32	1.56	1.42
2	H	71	PHE	CA-C	-7.31	1.43	1.52
2	H	58	PRO	CA-C	7.31	1.63	1.52
2	D	73	ASP	C-O	7.31	1.32	1.24
2	F	119	GLY	C-N	-7.31	1.23	1.34
1	G	72	HIS	CA-C	-7.30	1.43	1.52
1	A	140	TYR	CZ-OH	7.30	1.53	1.38
2	F	48	LEU	CA-C	7.30	1.61	1.52
1	C	46	PHE	CG-CD1	7.30	1.54	1.38
2	B	105	LEU	CA-C	7.30	1.62	1.52
2	D	76	ALA	C-N	-7.30	1.23	1.33
1	E	68	ASN	C-O	7.30	1.32	1.24
2	D	52	ASP	C-N	-7.29	1.24	1.33
1	C	24	TYR	N-CA	7.29	1.55	1.46
1	G	44	PRO	C-N	-7.29	1.23	1.33
2	B	42	PHE	C-O	7.29	1.34	1.23
2	H	28	LEU	C-O	7.29	1.32	1.24
1	E	118	THR	C-N	7.28	1.44	1.33
1	C	37	PRO	N-CA	7.28	1.57	1.47
1	C	140	TYR	C-O	7.28	1.32	1.24
2	F	77	HIS	CD2-NE2	-7.27	1.29	1.37
2	F	91	LEU	C-O	7.27	1.32	1.24
2	H	50	THR	C-O	7.27	1.35	1.23
2	B	7	GLU	CB-CG	7.27	1.74	1.52
2	D	72	SER	N-CA	-7.27	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	62	ALA	CA-CB	7.27	1.65	1.53
1	G	24	TYR	CA-CB	-7.26	1.41	1.53
1	C	33	PHE	CA-CB	7.26	1.65	1.53
2	B	29	GLY	CA-C	7.26	1.59	1.52
2	B	73	ASP	C-O	7.26	1.33	1.24
1	E	72	HIS	CA-CB	-7.26	1.42	1.53
2	H	124	PRO	CA-CB	-7.26	1.44	1.54
1	E	126	ASP	CA-CB	7.25	1.64	1.53
2	F	70	ALA	C-O	7.25	1.32	1.24
1	E	26	ALA	N-CA	7.24	1.55	1.46
1	E	88	ALA	N-CA	-7.24	1.36	1.46
2	B	11	VAL	CA-C	-7.24	1.43	1.52
2	B	21	ASP	CA-CB	-7.23	1.41	1.53
1	A	122	HIS	CB-CG	-7.23	1.40	1.50
2	B	109	VAL	C-O	7.23	1.31	1.24
2	B	142	ALA	CA-CB	-7.23	1.44	1.54
2	F	97	HIS	C-O	-7.23	1.15	1.23
2	F	71	PHE	N-CA	-7.23	1.36	1.46
2	F	135	ALA	N-CA	-7.23	1.37	1.46
2	F	12	THR	C-O	7.22	1.33	1.24
2	F	144	LYS	CA-CB	7.22	1.63	1.53
1	G	65	ALA	C-N	7.22	1.44	1.34
1	A	61	LYS	CE-NZ	7.22	1.71	1.49
2	D	61	LYS	C-N	7.22	1.42	1.33
1	E	26	ALA	C-O	7.22	1.33	1.24
1	E	55	VAL	CA-CB	-7.22	1.44	1.54
1	C	29	LEU	CA-C	7.21	1.61	1.52
1	G	130	ALA	CA-CB	-7.21	1.41	1.53
1	A	105	LEU	CB-CG	-7.21	1.39	1.53
2	F	95	LYS	CA-CB	7.20	1.65	1.53
2	F	26	GLU	C-N	-7.20	1.25	1.33
2	F	110	LEU	C-O	-7.20	1.15	1.24
1	G	6	ASP	C-N	7.20	1.42	1.33
1	C	58	HIS	CA-C	7.20	1.61	1.52
2	D	143	HIS	CA-CB	7.20	1.65	1.53
1	A	45	HIS	CE1-NE2	7.20	1.39	1.32
1	C	84	SER	CA-CB	7.20	1.64	1.53
2	B	77	HIS	N-CA	7.20	1.57	1.46
2	B	67	VAL	C-N	-7.19	1.23	1.33
2	F	1	VAL	C-O	7.19	1.38	1.23
2	F	130	TYR	N-CA	-7.19	1.36	1.46
2	F	114	LEU	CA-CB	7.19	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	36	PRO	C-N	-7.18	1.22	1.33
2	F	40	ARG	C-N	7.18	1.43	1.33
2	F	101	GLU	C-O	-7.17	1.15	1.24
1	C	48	LEU	CA-C	-7.17	1.44	1.53
1	G	36	PHE	CA-C	7.17	1.61	1.52
1	A	31	ARG	C-O	7.17	1.32	1.24
1	A	23	GLU	CB-CG	7.17	1.74	1.52
1	C	80	LEU	CA-C	-7.17	1.41	1.52
1	E	23	GLU	CD-OE2	-7.17	1.11	1.25
2	H	52	ASP	CA-CB	7.17	1.65	1.53
2	H	91	LEU	CG-CD1	7.16	1.76	1.52
2	D	14	LEU	C-N	7.16	1.43	1.33
1	E	49	SER	C-O	7.16	1.32	1.23
1	G	60	LYS	CA-C	7.15	1.62	1.52
2	F	125	PRO	C-N	7.15	1.42	1.33
1	G	112	HIS	CE1-NE2	-7.15	1.25	1.32
1	C	57	GLY	N-CA	7.15	1.56	1.45
2	H	130	TYR	CA-C	7.15	1.62	1.52
1	A	80	LEU	C-O	7.14	1.33	1.24
2	H	14	LEU	CG-CD2	7.14	1.76	1.52
1	G	50	HIS	CG-ND1	-7.14	1.30	1.38
1	G	58	HIS	ND1-CE1	7.14	1.39	1.32
1	A	98	PHE	C-O	7.13	1.32	1.24
1	E	37	PRO	CA-CB	-7.13	1.43	1.53
1	C	91	LEU	C-N	7.12	1.43	1.33
2	D	14	LEU	CA-C	-7.12	1.42	1.52
2	H	43	GLU	C-N	7.12	1.44	1.33
2	D	104	ARG	CA-CB	7.12	1.65	1.53
2	B	57	ASN	N-CA	7.12	1.57	1.46
2	F	113	VAL	N-CA	7.12	1.54	1.46
2	B	82	LYS	CG-CD	7.12	1.73	1.52
1	C	6	ASP	CG-OD1	7.12	1.38	1.25
2	D	31	LEU	N-CA	-7.12	1.38	1.46
2	F	116	HIS	CG-ND1	-7.12	1.30	1.38
1	A	30	GLU	CA-C	7.11	1.62	1.52
1	C	50	HIS	CA-CB	7.11	1.63	1.53
1	C	51	GLY	C-N	-7.11	1.23	1.33
1	A	85	ASP	CG-OD1	7.11	1.38	1.25
1	E	109	LEU	C-O	-7.11	1.15	1.24
1	A	83	LEU	CA-C	-7.11	1.43	1.52
1	C	112	HIS	CG-CD2	-7.11	1.28	1.35
2	D	84	THR	CA-CB	7.11	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	SER	N-CA	7.10	1.55	1.46
2	B	117	HIS	ND1-CE1	7.10	1.39	1.32
2	B	34	VAL	CA-CB	7.10	1.62	1.54
2	B	97	HIS	CB-CG	7.09	1.60	1.50
2	B	98	VAL	N-CA	7.09	1.55	1.46
1	G	34	LEU	CB-CG	-7.09	1.39	1.53
2	D	122	PHE	C-O	7.08	1.32	1.24
2	D	22	GLU	C-O	7.08	1.33	1.24
2	D	99	ASP	C-N	-7.08	1.27	1.34
1	A	75	ASP	CG-OD2	7.08	1.38	1.25
1	G	31	ARG	CG-CD	-7.07	1.31	1.52
1	G	105	LEU	CA-CB	7.07	1.64	1.53
2	H	20	VAL	C-O	-7.07	1.16	1.24
2	D	29	GLY	C-O	-7.07	1.14	1.23
2	D	136	GLY	CA-C	7.07	1.60	1.51
2	F	138	ALA	CA-C	7.06	1.61	1.52
1	C	101	LEU	CA-C	7.05	1.61	1.52
2	D	95	LYS	C-O	7.05	1.34	1.23
2	H	92	HIS	C-O	-7.05	1.15	1.24
2	H	144	LYS	CA-C	-7.05	1.41	1.52
2	F	40	ARG	CA-C	-7.04	1.43	1.52
2	F	140	ALA	N-CA	7.04	1.54	1.46
2	D	8	LYS	C-N	-7.04	1.23	1.33
2	B	22	GLU	N-CA	7.04	1.55	1.46
2	D	49	SER	N-CA	-7.04	1.36	1.46
2	H	45	PHE	CA-C	7.04	1.62	1.52
1	C	4	PRO	C-O	7.03	1.32	1.24
2	D	126	VAL	CA-CB	-7.03	1.46	1.54
1	G	83	LEU	CB-CG	-7.03	1.39	1.53
1	C	88	ALA	CA-CB	-7.03	1.42	1.53
2	D	142	ALA	C-N	-7.02	1.24	1.34
2	H	101	GLU	N-CA	-7.02	1.37	1.46
1	A	139	LYS	CD-CE	7.02	1.73	1.52
2	H	64	GLY	C-O	7.02	1.32	1.23
2	B	52	ASP	CA-C	7.01	1.62	1.53
1	E	100	LEU	CA-CB	7.01	1.64	1.53
2	D	140	ALA	CA-C	7.01	1.62	1.52
1	E	26	ALA	CA-C	-7.01	1.43	1.52
2	B	88	LEU	C-N	7.01	1.43	1.33
2	F	38	THR	C-O	-7.00	1.15	1.24
1	C	88	ALA	N-CA	7.00	1.54	1.46
1	C	105	LEU	CA-C	-7.00	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	SER	CA-CB	-7.00	1.41	1.53
1	C	76	MET	C-N	-6.99	1.25	1.34
1	G	52	SER	C-O	6.99	1.32	1.24
2	B	92	HIS	CE1-NE2	-6.99	1.25	1.32
1	E	31	ARG	CA-C	-6.98	1.44	1.52
2	B	134	VAL	CA-CB	-6.98	1.46	1.54
2	F	72	SER	N-CA	6.98	1.55	1.46
1	A	90	LYS	C-O	6.98	1.29	1.23
2	B	139	ASN	CA-CB	-6.97	1.42	1.53
2	D	99	ASP	CA-CB	-6.97	1.42	1.53
2	H	76	ALA	CA-CB	6.97	1.64	1.53
1	E	5	ALA	N-CA	6.97	1.55	1.46
1	A	140	TYR	N-CA	6.97	1.55	1.46
1	C	37	PRO	CA-C	-6.97	1.40	1.52
1	E	52	SER	CA-C	6.97	1.62	1.53
1	G	106	LEU	CB-CG	-6.97	1.39	1.53
2	H	63	HIS	C-N	-6.97	1.24	1.33
1	A	137	THR	C-N	-6.97	1.25	1.33
1	C	114	PRO	CA-C	6.97	1.64	1.52
1	E	13	ALA	CA-C	6.97	1.61	1.52
1	G	103	HIS	ND1-CE1	-6.96	1.25	1.32
2	B	72	SER	N-CA	-6.96	1.37	1.46
1	E	27	GLU	CA-C	6.96	1.62	1.52
1	A	24	TYR	CA-CB	6.96	1.64	1.53
2	H	3	LEU	C-O	-6.96	1.15	1.23
2	D	116	HIS	C-O	6.96	1.32	1.24
1	E	60	LYS	CA-C	-6.95	1.43	1.52
2	D	40	ARG	C-O	6.95	1.32	1.24
2	F	25	GLY	C-O	6.95	1.31	1.24
1	C	32	MET	SD-CE	6.95	1.97	1.79
2	B	94	ASP	CG-OD2	6.95	1.38	1.25
2	F	50	THR	C-N	-6.94	1.25	1.33
2	B	106	LEU	CB-CG	-6.94	1.39	1.53
2	H	38	THR	N-CA	-6.93	1.37	1.46
1	C	82	ALA	CA-C	-6.93	1.43	1.52
1	C	39	THR	N-CA	6.92	1.55	1.46
2	H	84	THR	C-N	-6.92	1.25	1.33
2	F	17	LYS	CE-NZ	6.91	1.70	1.49
1	A	134	THR	C-N	6.91	1.43	1.33
2	H	84	THR	CA-CB	6.91	1.64	1.53
1	E	53	ALA	N-CA	6.91	1.55	1.46
2	B	70	ALA	C-O	6.90	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	PHE	CA-CB	6.90	1.65	1.53
2	F	3	LEU	CA-C	6.89	1.61	1.52
1	A	55	VAL	CA-CB	6.89	1.63	1.54
2	B	9	SER	C-N	-6.89	1.25	1.33
2	H	133	VAL	CA-CB	-6.89	1.46	1.54
2	D	74	GLY	N-CA	6.89	1.55	1.45
1	E	122	HIS	CA-CB	6.89	1.64	1.53
1	A	6	ASP	N-CA	6.88	1.54	1.46
2	B	8	LYS	CA-C	-6.88	1.43	1.52
2	D	40	ARG	CD-NE	-6.88	1.36	1.46
1	A	56	LYS	N-CA	-6.88	1.37	1.46
2	H	117	HIS	CD2-NE2	-6.87	1.30	1.37
2	F	44	SER	N-CA	-6.87	1.37	1.46
1	A	5	ALA	N-CA	-6.87	1.37	1.46
2	H	14	LEU	CA-C	6.87	1.61	1.52
2	B	38	THR	CA-C	-6.86	1.43	1.52
1	E	65	ALA	CA-C	-6.86	1.43	1.52
2	F	105	LEU	N-CA	6.86	1.54	1.46
1	A	87	HIS	ND1-CE1	6.86	1.39	1.32
2	H	123	THR	CB-CG2	6.86	1.75	1.52
1	C	125	LEU	C-N	-6.85	1.24	1.33
2	H	79	ASP	C-N	-6.85	1.24	1.33
2	D	100	PRO	CA-CB	-6.85	1.42	1.53
2	F	4	THR	CA-C	-6.85	1.44	1.53
2	F	141	LEU	CA-CB	-6.84	1.41	1.53
2	B	4	THR	N-CA	-6.84	1.34	1.45
1	C	109	LEU	N-CA	6.84	1.55	1.46
2	F	125	PRO	N-CA	-6.83	1.38	1.47
2	D	127	GLN	CA-C	6.83	1.61	1.52
1	G	15	GLY	C-O	-6.83	1.14	1.23
1	G	99	LYS	C-N	6.83	1.43	1.33
2	B	110	LEU	CA-CB	6.82	1.64	1.53
2	B	2	HIS	CE1-NE2	-6.82	1.25	1.32
2	B	77	HIS	CG-ND1	6.82	1.45	1.38
1	E	80	LEU	C-O	6.82	1.33	1.24
2	H	26	GLU	CA-CB	-6.81	1.42	1.53
2	H	47	ASP	CA-C	6.81	1.61	1.52
1	A	31	ARG	CZ-NH1	6.81	1.42	1.32
1	G	40	LYS	C-O	-6.81	1.16	1.24
2	H	50	THR	N-CA	6.80	1.52	1.46
2	F	98	VAL	C-N	6.80	1.43	1.32
2	H	30	ARG	C-O	-6.80	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	23	GLU	CD-OE2	6.79	1.38	1.25
1	G	119	PRO	CA-C	6.79	1.62	1.52
1	C	22	GLY	N-CA	-6.79	1.37	1.45
1	C	76	MET	CA-C	-6.79	1.44	1.52
1	C	104	CYS	CA-C	6.79	1.61	1.52
1	C	122	HIS	CE1-NE2	6.78	1.39	1.32
2	H	57	ASN	CA-CB	-6.78	1.39	1.53
2	F	104	ARG	CD-NE	-6.78	1.36	1.46
2	H	74	GLY	C-N	-6.78	1.25	1.34
2	F	37	TRP	CE2-CZ2	-6.78	1.25	1.39
1	G	47	ASP	C-O	-6.77	1.16	1.24
2	F	43	GLU	C-N	6.76	1.42	1.33
2	B	49	SER	CA-CB	6.76	1.65	1.53
1	C	50	HIS	CD2-NE2	6.76	1.45	1.37
1	G	122	HIS	CA-CB	-6.76	1.42	1.53
1	G	77	PRO	N-CD	6.76	1.57	1.47
2	D	81	LEU	C-N	6.76	1.42	1.33
2	D	144	LYS	CA-C	-6.75	1.42	1.52
2	D	62	ALA	CA-C	-6.75	1.44	1.52
2	B	141	LEU	CB-CG	-6.74	1.40	1.53
1	C	4	PRO	N-CD	6.74	1.57	1.47
1	A	22	GLY	C-N	6.74	1.43	1.33
1	E	112	HIS	C-N	-6.74	1.24	1.33
2	B	3	LEU	C-O	-6.73	1.15	1.23
1	E	2	LEU	CA-C	6.73	1.61	1.52
2	F	28	LEU	CA-C	6.73	1.61	1.52
2	B	71	PHE	C-O	-6.73	1.16	1.24
1	G	87	HIS	CA-C	-6.73	1.43	1.52
2	B	132	LYS	C-N	6.73	1.42	1.33
1	G	78	ASN	CA-CB	-6.73	1.42	1.53
1	C	74	ASP	CG-OD2	-6.72	1.12	1.25
1	G	85	ASP	CG-OD1	6.72	1.38	1.25
1	C	77	PRO	CA-CB	-6.72	1.44	1.53
2	D	30	ARG	CB-CG	-6.72	1.32	1.52
2	H	18	VAL	C-O	-6.71	1.16	1.23
1	C	59	GLY	C-O	-6.71	1.15	1.23
2	F	22	GLU	N-CA	-6.71	1.38	1.46
2	F	73	ASP	CA-C	6.71	1.61	1.52
2	B	106	LEU	C-O	6.71	1.32	1.24
1	A	29	LEU	C-O	6.71	1.32	1.24
2	D	11	VAL	C-O	-6.71	1.16	1.24
1	E	68	ASN	CA-CB	6.71	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	VAL	C-O	-6.71	1.14	1.23
2	D	108	ASN	C-O	6.70	1.32	1.24
1	G	34	LEU	C-O	6.70	1.32	1.24
1	G	102	SER	C-O	-6.70	1.15	1.24
1	E	42	TYR	CG-CD2	-6.70	1.25	1.39
1	A	20	HIS	ND1-CE1	6.70	1.39	1.32
2	B	126	VAL	C-N	-6.69	1.25	1.33
1	C	70	VAL	CA-C	6.69	1.61	1.52
1	E	135	VAL	N-CA	6.69	1.54	1.46
1	E	139	LYS	CD-CE	6.69	1.72	1.52
1	E	105	LEU	CA-C	6.69	1.62	1.52
2	B	78	LEU	CA-CB	-6.69	1.42	1.53
2	D	62	ALA	CA-CB	6.69	1.64	1.53
2	H	11	VAL	CA-C	-6.69	1.44	1.52
2	H	17	LYS	C-O	6.68	1.32	1.24
2	H	78	LEU	CB-CG	-6.68	1.40	1.53
1	E	112	HIS	N-CA	6.68	1.55	1.45
2	D	59	LYS	CG-CD	6.68	1.72	1.52
2	F	15	TRP	C-N	6.67	1.43	1.33
2	H	86	ALA	C-N	6.67	1.43	1.33
2	D	86	ALA	N-CA	-6.66	1.38	1.46
2	F	35	TYR	CZ-OH	-6.66	1.24	1.38
1	G	79	ALA	CA-CB	-6.66	1.45	1.53
1	G	97	ASN	CG-ND2	6.66	1.47	1.33
2	B	117	HIS	CG-ND1	-6.65	1.30	1.38
1	E	23	GLU	N-CA	6.65	1.54	1.46
1	G	45	HIS	N-CA	-6.65	1.37	1.46
2	D	133	VAL	C-N	6.65	1.42	1.33
2	D	95	LYS	CG-CD	6.65	1.72	1.52
2	F	61	LYS	CA-CB	6.64	1.63	1.53
1	E	117	PHE	CG-CD2	6.64	1.52	1.38
2	B	37	TRP	CD2-CE3	-6.63	1.29	1.40
2	B	24	GLY	N-CA	-6.63	1.35	1.45
1	E	11	LYS	C-N	6.63	1.43	1.33
1	G	58	HIS	CG-ND1	-6.63	1.30	1.38
2	D	45	PHE	CE2-CZ	6.63	1.58	1.38
2	D	107	GLY	C-N	-6.63	1.24	1.33
1	A	95	PRO	CA-C	6.62	1.61	1.52
1	E	68	ASN	CG-OD1	6.62	1.36	1.23
2	H	114	LEU	C-O	6.62	1.32	1.24
1	E	27	GLU	N-CA	6.62	1.54	1.46
2	F	113	VAL	C-N	-6.62	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	121	GLU	CD-OE2	6.61	1.38	1.25
2	B	63	HIS	N-CA	-6.61	1.38	1.46
2	D	2	HIS	N-CA	6.60	1.54	1.46
1	G	30	GLU	N-CA	6.60	1.54	1.46
2	D	93	CYS	CA-CB	-6.60	1.42	1.53
1	G	88	ALA	C-N	-6.59	1.23	1.33
2	D	76	ALA	CA-CB	6.59	1.64	1.53
2	D	36	PRO	CA-CB	-6.59	1.44	1.53
2	D	119	GLY	N-CA	6.59	1.55	1.45
2	H	80	ASN	CA-C	6.59	1.62	1.53
1	A	68	ASN	C-N	-6.59	1.24	1.33
2	H	63	HIS	C-O	-6.59	1.16	1.24
2	D	43	GLU	CA-CB	-6.58	1.43	1.53
1	G	107	VAL	CA-CB	6.58	1.62	1.54
1	A	133	SER	C-N	-6.58	1.24	1.33
2	D	79	ASP	CA-C	6.58	1.61	1.52
1	C	49	SER	C-O	6.58	1.33	1.23
1	G	89	HIS	N-CA	6.57	1.54	1.45
2	H	133	VAL	CB-CG1	6.57	1.74	1.52
1	A	3	SER	C-O	-6.57	1.13	1.23
1	C	20	HIS	CA-C	6.57	1.61	1.52
1	C	32	MET	C-N	6.57	1.42	1.34
1	E	80	LEU	C-N	-6.57	1.26	1.33
1	E	43	PHE	N-CA	-6.56	1.40	1.46
1	A	58	HIS	CD2-NE2	-6.55	1.30	1.37
1	E	93	VAL	C-O	6.55	1.31	1.24
2	D	99	ASP	C-O	-6.54	1.15	1.24
1	A	102	SER	C-O	-6.54	1.15	1.24
1	A	11	LYS	N-CA	6.54	1.54	1.46
1	C	26	ALA	C-O	6.54	1.32	1.24
1	E	48	LEU	CA-CB	-6.54	1.44	1.53
1	E	118	THR	C-O	-6.54	1.14	1.23
1	G	19	ALA	N-CA	6.54	1.54	1.46
2	H	56	GLY	N-CA	-6.54	1.35	1.45
2	F	31	LEU	CG-CD1	6.53	1.74	1.52
1	A	36	PHE	N-CA	-6.53	1.39	1.46
1	G	94	ASP	N-CA	6.53	1.55	1.46
1	A	108	THR	CA-CB	6.52	1.64	1.53
2	H	115	ALA	CA-CB	6.52	1.64	1.53
1	C	123	ALA	C-O	-6.52	1.15	1.24
2	H	108	ASN	CB-CG	6.52	1.68	1.52
1	A	128	PHE	CA-CB	6.52	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	38	THR	C-N	6.52	1.42	1.34
2	D	81	LEU	C-O	6.52	1.32	1.24
2	F	132	LYS	C-O	6.52	1.31	1.24
2	H	44	SER	C-N	-6.52	1.25	1.33
2	F	55	MET	SD-CE	6.51	1.95	1.79
1	C	115	ALA	N-CA	-6.51	1.38	1.46
1	A	106	LEU	CA-C	6.51	1.61	1.52
1	E	116	GLU	CB-CG	6.51	1.72	1.52
2	F	27	ALA	CA-C	6.50	1.61	1.52
2	B	78	LEU	N-CA	6.50	1.54	1.46
1	A	57	GLY	N-CA	6.50	1.54	1.45
1	C	140	TYR	C-N	-6.50	1.24	1.33
2	F	30	ARG	C-O	6.50	1.32	1.24
2	F	108	ASN	C-N	-6.50	1.25	1.33
1	G	48	LEU	C-O	6.50	1.32	1.24
2	B	53	ALA	N-CA	6.49	1.54	1.46
2	D	120	LYS	CA-C	-6.49	1.44	1.52
1	E	70	VAL	C-O	6.49	1.32	1.24
2	D	76	ALA	N-CA	-6.49	1.37	1.46
2	B	92	HIS	CB-CG	6.49	1.59	1.50
2	D	106	LEU	CA-C	-6.49	1.44	1.52
1	G	18	GLY	CA-C	6.49	1.61	1.51
1	A	18	GLY	C-O	6.48	1.32	1.23
2	B	50	THR	CB-CG2	6.48	1.74	1.52
1	E	71	ALA	N-CA	6.48	1.54	1.46
2	F	91	LEU	N-CA	-6.48	1.38	1.46
2	F	15	TRP	CA-C	6.48	1.61	1.52
1	A	122	HIS	CA-C	6.48	1.61	1.52
1	A	126	ASP	N-CA	6.48	1.53	1.46
1	C	30	GLU	C-N	-6.48	1.25	1.33
2	B	126	VAL	CA-C	-6.47	1.44	1.52
1	G	19	ALA	CA-C	-6.47	1.43	1.52
1	C	88	ALA	CA-C	6.47	1.61	1.52
1	G	60	LYS	CE-NZ	6.47	1.68	1.49
1	E	92	ARG	CA-C	6.47	1.61	1.52
1	E	126	ASP	C-O	6.47	1.31	1.24
1	A	9	ASN	C-N	-6.46	1.25	1.33
1	C	60	LYS	C-N	6.46	1.42	1.33
2	H	132	LYS	N-CA	6.46	1.54	1.46
2	F	124	PRO	N-CD	6.45	1.56	1.47
1	A	45	HIS	CA-C	-6.45	1.43	1.52
1	C	101	LEU	C-O	-6.45	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	SER	CA-CB	-6.45	1.42	1.53
1	A	134	THR	CA-CB	6.45	1.64	1.53
2	F	40	ARG	NE-CZ	6.45	1.40	1.33
2	H	94	ASP	C-O	6.45	1.31	1.24
1	E	70	VAL	CA-CB	-6.45	1.45	1.54
1	E	99	LYS	C-O	6.45	1.31	1.24
2	B	94	ASP	CA-CB	-6.45	1.43	1.53
2	F	104	ARG	CZ-NH2	6.45	1.41	1.33
2	H	42	PHE	C-O	6.45	1.34	1.23
1	A	81	SER	C-O	6.44	1.32	1.24
2	H	69	GLY	CA-C	6.44	1.60	1.51
2	F	89	SER	CB-OG	6.44	1.55	1.42
2	B	40	ARG	CA-CB	6.44	1.64	1.53
2	H	92	HIS	CE1-NE2	6.44	1.39	1.32
2	B	142	ALA	N-CA	6.43	1.54	1.45
2	F	122	PHE	C-N	-6.43	1.23	1.33
1	E	36	PHE	CE1-CZ	6.42	1.57	1.38
2	H	116	HIS	CE1-NE2	-6.42	1.26	1.32
2	F	95	LYS	CE-NZ	6.42	1.68	1.49
2	F	117	HIS	ND1-CE1	6.42	1.39	1.32
1	C	15	GLY	N-CA	6.41	1.54	1.45
2	F	24	GLY	N-CA	-6.41	1.36	1.45
2	B	128	ALA	N-CA	-6.41	1.38	1.46
1	E	10	VAL	CA-C	-6.41	1.44	1.52
2	H	74	GLY	C-O	6.41	1.31	1.23
1	G	48	LEU	CA-CB	6.40	1.64	1.53
2	B	40	ARG	CZ-NH1	-6.40	1.23	1.32
1	G	78	ASN	CG-ND2	6.40	1.46	1.33
2	D	38	THR	CB-OG1	6.40	1.53	1.43
1	C	138	SER	CA-CB	6.39	1.63	1.53
2	H	36	PRO	N-CA	6.39	1.55	1.47
2	B	105	LEU	C-O	-6.39	1.16	1.24
2	H	104	ARG	CB-CG	6.39	1.71	1.52
2	H	144	LYS	N-CA	6.38	1.54	1.46
2	F	106	LEU	C-O	-6.38	1.16	1.24
2	B	2	HIS	C-N	6.37	1.42	1.33
2	F	9	SER	CA-C	-6.37	1.44	1.52
1	C	121	VAL	CB-CG1	6.37	1.73	1.52
2	H	35	TYR	CG-CD2	6.37	1.52	1.39
2	B	36	PRO	N-CA	-6.37	1.39	1.47
2	B	66	LYS	C-O	6.37	1.32	1.24
2	F	143	HIS	ND1-CE1	6.37	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	4	THR	C-N	-6.37	1.19	1.33
1	G	91	LEU	C-N	-6.36	1.24	1.33
1	A	10	VAL	C-O	-6.36	1.16	1.24
2	B	54	VAL	N-CA	-6.36	1.38	1.46
2	D	102	ASN	CG-ND2	6.36	1.46	1.33
1	C	2	LEU	CA-C	-6.36	1.44	1.52
1	E	18	GLY	C-O	6.36	1.32	1.23
2	F	23	VAL	C-N	-6.36	1.24	1.33
2	B	50	THR	N-CA	-6.35	1.31	1.45
1	C	76	MET	CG-SD	6.35	1.96	1.80
1	G	58	HIS	CA-C	6.35	1.61	1.52
2	B	66	LYS	CA-CB	-6.35	1.42	1.53
1	E	129	LEU	CA-C	-6.35	1.44	1.52
1	A	110	ALA	CA-C	6.35	1.60	1.52
2	B	79	ASP	N-CA	-6.35	1.38	1.46
1	C	116	GLU	CA-CB	6.35	1.63	1.53
2	H	79	ASP	CA-C	6.34	1.60	1.52
2	D	28	LEU	CB-CG	6.34	1.66	1.53
2	H	31	LEU	CB-CG	-6.34	1.40	1.53
1	C	4	PRO	CA-CB	-6.34	1.43	1.53
2	F	76	ALA	C-O	-6.33	1.16	1.24
2	F	87	THR	N-CA	6.33	1.53	1.46
1	C	64	ASP	N-CA	-6.33	1.38	1.46
2	D	68	LEU	N-CA	6.33	1.53	1.46
1	A	90	LYS	CB-CG	6.33	1.71	1.52
1	A	109	LEU	C-O	-6.32	1.16	1.24
1	A	4	PRO	CA-CB	6.32	1.63	1.53
2	B	108	ASN	CG-OD1	6.32	1.35	1.23
1	C	129	LEU	CB-CG	6.32	1.66	1.53
2	B	57	ASN	CG-OD1	6.31	1.35	1.23
2	B	75	LEU	CA-CB	-6.31	1.42	1.53
2	D	18	VAL	N-CA	6.31	1.53	1.46
2	F	47	ASP	CA-CB	6.30	1.60	1.53
2	F	80	ASN	C-N	-6.30	1.25	1.34
1	E	94	ASP	C-N	-6.30	1.27	1.34
2	H	122	PHE	CE1-CZ	6.30	1.57	1.38
2	D	66	LYS	CG-CD	6.29	1.71	1.52
1	G	69	ALA	CA-C	-6.29	1.44	1.52
2	F	90	GLU	C-N	-6.29	1.26	1.33
1	A	62	VAL	CA-C	6.29	1.60	1.52
2	F	92	HIS	CB-CG	-6.29	1.41	1.50
1	G	47	ASP	CG-OD1	6.28	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	143	HIS	CA-C	6.28	1.61	1.52
1	A	119	PRO	N-CA	-6.27	1.39	1.47
2	B	39	GLN	CA-C	6.27	1.61	1.52
1	A	85	ASP	C-N	-6.27	1.25	1.33
1	A	72	HIS	CA-C	-6.26	1.45	1.52
2	D	103	PHE	CB-CG	6.26	1.65	1.50
1	E	1	VAL	C-N	6.26	1.42	1.33
1	A	99	LYS	CA-CB	6.26	1.63	1.53
1	A	38	THR	C-O	-6.26	1.16	1.24
2	H	40	ARG	CD-NE	-6.26	1.37	1.46
1	A	14	TRP	CZ2-CH2	6.26	1.49	1.37
1	G	46	PHE	CA-CB	-6.25	1.44	1.53
1	E	141	ARG	CD-NE	-6.25	1.37	1.46
2	B	33	VAL	CA-C	6.25	1.61	1.52
1	C	60	LYS	CD-CE	6.25	1.71	1.52
1	G	131	SER	N-CA	-6.25	1.39	1.46
2	H	38	THR	CB-CG2	6.25	1.73	1.52
1	G	100	LEU	CB-CG	6.25	1.66	1.53
1	A	101	LEU	CA-CB	-6.24	1.43	1.53
1	G	89	HIS	ND1-CE1	6.24	1.38	1.32
1	G	59	GLY	CA-C	6.24	1.59	1.52
1	E	48	LEU	N-CA	6.24	1.53	1.46
1	C	45	HIS	CE1-NE2	-6.24	1.26	1.32
1	C	58	HIS	CG-CD2	-6.24	1.28	1.35
2	B	141	LEU	N-CA	6.23	1.53	1.46
1	A	93	VAL	C-O	-6.23	1.16	1.24
1	C	91	LEU	CA-C	-6.23	1.44	1.52
2	D	79	ASP	N-CA	6.23	1.54	1.46
2	B	89	SER	CA-C	6.22	1.60	1.52
2	B	146	HIS	CG-ND1	-6.22	1.31	1.38
1	G	96	VAL	CA-CB	6.22	1.62	1.54
2	B	103	PHE	CE1-CZ	6.22	1.57	1.38
2	H	73	ASP	CG-OD2	6.22	1.37	1.25
2	B	18	VAL	N-CA	6.22	1.54	1.46
2	F	45	PHE	N-CA	6.22	1.59	1.46
2	H	60	VAL	CB-CG1	6.21	1.73	1.52
1	E	112	HIS	C-O	6.21	1.32	1.24
1	E	8	THR	C-N	6.20	1.42	1.33
1	A	76	MET	SD-CE	6.20	1.95	1.79
2	D	94	ASP	C-N	-6.20	1.25	1.33
2	H	128	ALA	CA-CB	6.20	1.63	1.53
2	F	85	PHE	CA-CB	6.19	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	99	ASP	CB-CG	6.19	1.67	1.52
2	D	130	TYR	CA-C	6.19	1.61	1.52
1	E	106	LEU	N-CA	6.19	1.54	1.46
2	F	97	HIS	CE1-NE2	-6.19	1.26	1.32
2	D	45	PHE	CA-C	-6.19	1.44	1.52
1	A	24	TYR	CB-CG	6.18	1.65	1.51
2	H	33	VAL	C-N	6.18	1.41	1.33
1	C	26	ALA	CA-CB	-6.17	1.43	1.53
2	F	26	GLU	C-O	-6.17	1.16	1.24
2	F	104	ARG	CA-CB	-6.17	1.43	1.53
2	B	79	ASP	CA-C	6.17	1.61	1.52
2	F	73	ASP	C-N	-6.17	1.23	1.33
1	E	13	ALA	C-N	-6.17	1.25	1.33
2	D	40	ARG	NE-CZ	-6.17	1.26	1.33
1	C	116	GLU	CA-C	6.16	1.60	1.52
1	C	130	ALA	C-N	-6.16	1.25	1.33
2	D	145	TYR	CG-CD1	6.16	1.52	1.39
2	H	26	GLU	C-O	-6.16	1.17	1.24
2	B	126	VAL	C-O	6.16	1.31	1.24
2	F	2	HIS	CE1-NE2	6.16	1.38	1.32
2	H	114	LEU	CA-C	6.15	1.61	1.52
1	A	100	LEU	CA-CB	6.15	1.62	1.53
2	B	1	VAL	C-N	6.15	1.41	1.33
2	D	131	GLN	CA-CB	6.15	1.63	1.53
1	A	97	ASN	CG-ND2	6.15	1.46	1.33
1	E	56	LYS	CA-CB	-6.15	1.43	1.53
1	A	17	VAL	CA-C	6.15	1.60	1.52
2	F	143	HIS	CG-ND1	6.14	1.45	1.38
1	C	90	LYS	CB-CG	6.14	1.70	1.52
1	E	95	PRO	CA-CB	6.14	1.62	1.53
1	G	56	LYS	C-N	-6.14	1.26	1.33
2	B	83	GLY	C-N	-6.13	1.24	1.33
2	F	92	HIS	CG-CD2	6.13	1.42	1.35
1	E	64	ASP	CG-OD1	-6.13	1.13	1.25
1	A	113	LEU	CB-CG	6.13	1.65	1.53
1	G	109	LEU	CA-CB	6.13	1.63	1.53
2	B	104	ARG	CB-CG	6.12	1.70	1.52
2	H	65	LYS	CA-CB	-6.12	1.42	1.53
1	E	79	ALA	CA-CB	-6.12	1.43	1.53
1	C	86	LEU	C-N	6.11	1.42	1.33
1	G	84	SER	C-N	-6.11	1.26	1.33
1	G	93	VAL	N-CA	6.11	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	77	HIS	CA-C	-6.11	1.44	1.52
2	H	6	VAL	CA-C	6.11	1.60	1.52
2	B	132	LYS	C-O	-6.10	1.17	1.24
2	B	65	LYS	CB-CG	6.10	1.70	1.52
1	A	62	VAL	CA-CB	-6.10	1.47	1.54
2	F	7	GLU	CA-C	6.10	1.60	1.52
1	G	107	VAL	C-O	6.10	1.31	1.24
2	B	76	ALA	C-O	6.10	1.32	1.23
2	B	82	LYS	C-O	6.09	1.31	1.24
2	B	27	ALA	CA-C	-6.09	1.45	1.52
2	B	77	HIS	CE1-NE2	-6.09	1.26	1.32
2	F	88	LEU	CG-CD1	6.08	1.72	1.52
1	A	28	ALA	C-O	-6.08	1.16	1.24
1	A	31	ARG	NE-CZ	-6.08	1.26	1.33
2	D	136	GLY	N-CA	-6.08	1.38	1.45
1	E	133	SER	N-CA	6.08	1.53	1.46
1	G	75	ASP	CA-C	6.08	1.62	1.53
1	A	127	LYS	CB-CG	-6.08	1.34	1.52
2	B	51	PRO	N-CA	6.08	1.55	1.47
1	G	73	VAL	CA-C	-6.08	1.45	1.52
1	A	99	LYS	CB-CG	-6.08	1.34	1.52
1	C	109	LEU	C-N	-6.08	1.25	1.33
1	C	97	ASN	CG-ND2	-6.07	1.20	1.33
1	C	110	ALA	CA-C	6.07	1.60	1.52
1	G	16	LYS	CA-CB	6.07	1.63	1.53
2	B	136	GLY	C-O	-6.06	1.15	1.24
1	E	56	LYS	C-O	6.06	1.31	1.24
2	D	29	GLY	C-N	6.06	1.42	1.33
1	C	45	HIS	N-CA	-6.05	1.38	1.46
1	G	49	SER	CB-OG	6.05	1.54	1.42
1	G	45	HIS	CG-CD2	-6.04	1.29	1.35
1	C	53	ALA	C-N	-6.04	1.26	1.33
2	D	3	LEU	CA-C	6.04	1.61	1.53
2	D	18	VAL	C-O	6.04	1.30	1.24
2	H	11	VAL	CA-CB	6.04	1.61	1.54
2	H	96	LEU	C-O	6.04	1.31	1.24
2	B	24	GLY	CA-C	-6.03	1.43	1.51
1	G	90	LYS	C-O	6.03	1.31	1.24
2	B	85	PHE	C-O	6.03	1.31	1.24
2	H	63	HIS	CG-CD2	-6.03	1.29	1.35
1	C	34	LEU	CA-CB	6.03	1.63	1.53
1	E	49	SER	N-CA	6.03	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	59	GLY	C-O	-6.02	1.16	1.23
2	B	77	HIS	C-N	-6.02	1.25	1.33
1	G	117	PHE	N-CA	-6.02	1.38	1.46
1	C	28	ALA	CA-C	6.01	1.60	1.52
2	D	19	ASN	CA-C	6.01	1.60	1.52
1	E	44	PRO	CG-CD	6.01	1.71	1.50
1	C	38	THR	CA-C	-6.01	1.44	1.52
1	G	140	TYR	N-CA	-6.01	1.38	1.46
2	F	26	GLU	N-CA	6.00	1.53	1.46
2	B	32	LEU	CA-C	-6.00	1.45	1.52
2	H	99	ASP	CG-OD2	6.00	1.36	1.25
1	C	58	HIS	CE1-NE2	-6.00	1.26	1.32
2	F	129	ALA	CA-CB	-6.00	1.43	1.53
1	C	48	LEU	N-CA	-6.00	1.39	1.46
2	F	57	ASN	CA-C	-5.99	1.45	1.52
1	C	113	LEU	C-O	5.99	1.30	1.24
2	D	120	LYS	CE-NZ	5.99	1.67	1.49
2	B	71	PHE	C-N	5.99	1.42	1.34
2	B	39	GLN	CA-CB	-5.98	1.44	1.53
2	F	131	GLN	C-N	5.97	1.41	1.33
1	A	47	ASP	C-N	5.97	1.42	1.33
2	H	126	VAL	CA-C	5.97	1.60	1.53
1	A	45	HIS	C-O	-5.97	1.15	1.23
1	A	8	THR	C-O	5.97	1.32	1.24
1	G	43	PHE	N-CA	5.97	1.52	1.46
1	G	43	PHE	CA-CB	5.96	1.59	1.53
2	H	55	MET	N-CA	-5.96	1.38	1.46
2	D	130	TYR	CE2-CZ	5.96	1.52	1.38
1	G	128	PHE	CA-C	5.96	1.60	1.52
2	H	146	HIS	ND1-CE1	-5.96	1.26	1.32
1	A	61	LYS	C-N	5.95	1.41	1.33
2	B	116	HIS	CA-CB	-5.95	1.43	1.53
2	D	59	LYS	CE-NZ	5.95	1.67	1.49
2	D	102	ASN	CA-C	5.95	1.60	1.52
1	C	81	SER	CB-OG	5.95	1.54	1.42
2	H	110	LEU	CA-C	5.95	1.60	1.52
2	D	75	LEU	CB-CG	5.94	1.65	1.53
1	E	90	LYS	N-CA	5.94	1.53	1.46
2	F	117	HIS	N-CA	5.94	1.53	1.46
1	G	66	LEU	CB-CG	5.94	1.65	1.53
2	H	117	HIS	CE1-NE2	5.94	1.38	1.32
2	B	31	LEU	N-CA	5.94	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	LEU	CB-CG	-5.93	1.41	1.53
2	D	5	PRO	N-CD	-5.93	1.39	1.47
1	E	3	SER	CB-OG	5.93	1.54	1.42
2	D	3	LEU	N-CA	5.93	1.54	1.46
1	A	111	ALA	N-CA	5.93	1.53	1.46
2	F	93	CYS	C-N	-5.93	1.26	1.33
2	H	85	PHE	C-N	-5.93	1.23	1.33
1	E	20	HIS	ND1-CE1	-5.93	1.26	1.32
2	H	70	ALA	CA-C	5.93	1.60	1.52
2	H	78	LEU	CA-C	5.92	1.62	1.52
2	D	128	ALA	C-O	-5.92	1.17	1.24
1	E	19	ALA	CA-C	-5.92	1.44	1.52
1	A	24	TYR	N-CA	5.92	1.53	1.46
1	A	93	VAL	C-N	5.92	1.43	1.33
2	B	47	ASP	CB-CG	-5.92	1.37	1.52
2	D	21	ASP	C-O	5.92	1.30	1.24
2	F	131	GLN	CA-CB	-5.92	1.43	1.53
1	G	141	ARG	C-OXT	-5.92	1.11	1.23
1	C	87	HIS	CG-CD2	-5.92	1.29	1.35
1	A	138	SER	C-O	5.91	1.30	1.24
2	D	101	GLU	N-CA	-5.91	1.38	1.46
1	G	17	VAL	N-CA	5.91	1.54	1.46
1	C	14	TRP	CD1-NE1	5.91	1.50	1.37
2	D	51	PRO	N-CA	5.91	1.54	1.47
2	D	94	ASP	CA-C	-5.91	1.44	1.52
2	F	38	THR	N-CA	-5.91	1.39	1.46
2	F	94	ASP	N-CA	5.91	1.54	1.46
1	G	88	ALA	C-O	5.90	1.31	1.24
2	B	14	LEU	C-O	5.90	1.30	1.24
2	D	60	VAL	N-CA	-5.90	1.39	1.46
1	C	141	ARG	NE-CZ	5.90	1.39	1.33
1	E	120	ALA	CA-C	-5.90	1.44	1.52
1	G	118	THR	CB-CG2	5.90	1.72	1.52
2	F	31	LEU	CA-CB	5.90	1.62	1.53
2	H	38	THR	CA-CB	5.90	1.62	1.53
2	B	83	GLY	CA-C	-5.89	1.45	1.52
1	G	27	GLU	CA-C	5.89	1.60	1.52
1	G	70	VAL	C-O	-5.89	1.16	1.24
2	H	41	PHE	CD2-CE2	5.89	1.56	1.38
1	C	7	LYS	C-O	5.89	1.30	1.24
2	B	31	LEU	CG-CD2	5.88	1.72	1.52
2	B	37	TRP	CA-C	-5.88	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	30	GLU	CA-CB	-5.88	1.44	1.53
2	H	120	LYS	CE-NZ	5.88	1.67	1.49
1	E	35	SER	C-N	5.88	1.40	1.33
1	E	117	PHE	CA-C	-5.88	1.46	1.53
1	C	84	SER	CB-OG	5.88	1.53	1.42
1	A	92	ARG	C-N	5.87	1.44	1.33
2	B	131	GLN	CA-CB	5.87	1.63	1.53
1	C	126	ASP	C-O	-5.87	1.16	1.24
1	G	45	HIS	C-O	5.87	1.31	1.24
1	C	8	THR	CA-C	5.85	1.60	1.52
1	C	117	PHE	C-O	5.85	1.31	1.24
2	F	122	PHE	CA-CB	5.85	1.61	1.52
1	E	125	LEU	CG-CD2	5.85	1.71	1.52
2	B	97	HIS	CA-C	5.85	1.60	1.52
2	H	140	ALA	C-N	-5.85	1.26	1.33
2	D	121	GLU	C-O	-5.84	1.16	1.24
1	A	75	ASP	CA-CB	5.84	1.61	1.53
2	F	143	HIS	CG-CD2	-5.84	1.29	1.35
2	B	77	HIS	CG-CD2	-5.84	1.29	1.35
2	D	34	VAL	CA-CB	-5.84	1.46	1.54
2	D	111	VAL	C-N	-5.84	1.26	1.33
2	F	48	LEU	C-O	-5.84	1.15	1.24
2	H	3	LEU	N-CA	-5.84	1.39	1.45
2	B	130	TYR	CG-CD1	5.83	1.51	1.39
1	A	69	ALA	C-O	-5.83	1.17	1.24
2	F	23	VAL	CA-C	-5.83	1.44	1.52
2	D	52	ASP	CG-OD2	5.83	1.36	1.25
2	D	77	HIS	N-CA	5.83	1.55	1.46
2	F	59	LYS	CA-C	-5.83	1.45	1.52
1	C	16	LYS	CD-CE	5.83	1.70	1.52
1	C	96	VAL	CB-CG1	-5.82	1.33	1.52
2	H	4	THR	C-O	5.82	1.31	1.24
2	B	104	ARG	C-O	5.82	1.31	1.24
2	F	15	TRP	NE1-CE2	-5.82	1.31	1.37
2	B	57	ASN	CG-ND2	5.82	1.45	1.33
1	C	82	ALA	C-N	-5.81	1.25	1.33
1	C	123	ALA	C-N	-5.81	1.26	1.33
2	D	28	LEU	C-N	-5.81	1.25	1.33
1	E	27	GLU	C-N	-5.80	1.26	1.33
1	C	51	GLY	CA-C	-5.80	1.44	1.51
2	F	103	PHE	N-CA	5.80	1.53	1.46
1	E	121	VAL	CB-CG2	-5.80	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	139	LYS	C-N	-5.80	1.25	1.33
1	G	70	VAL	CA-CB	-5.80	1.47	1.54
2	H	95	LYS	CA-CB	5.80	1.63	1.53
2	D	144	LYS	CA-CB	5.79	1.61	1.53
2	H	125	PRO	N-CA	5.79	1.54	1.47
1	A	141	ARG	CA-C	-5.78	1.40	1.52
1	E	113	LEU	CB-CG	-5.78	1.41	1.53
1	A	4	PRO	CA-C	5.78	1.60	1.52
2	H	61	LYS	CB-CG	5.78	1.69	1.52
1	A	48	LEU	CB-CG	5.78	1.65	1.53
2	D	96	LEU	CA-C	-5.78	1.44	1.52
2	H	143	HIS	CE1-NE2	-5.78	1.26	1.32
2	B	67	VAL	CA-CB	-5.78	1.47	1.54
1	E	33	PHE	N-CA	5.78	1.53	1.46
2	F	4	THR	C-O	5.78	1.31	1.23
2	F	82	LYS	N-CA	-5.77	1.38	1.46
2	B	85	PHE	CA-CB	5.77	1.61	1.53
1	E	69	ALA	CA-CB	-5.76	1.43	1.53
2	D	5	PRO	CA-CB	-5.76	1.44	1.53
1	E	113	LEU	CG-CD2	5.76	1.71	1.52
2	F	61	LYS	C-N	5.76	1.41	1.33
1	A	65	ALA	CA-CB	-5.76	1.43	1.53
2	B	68	LEU	N-CA	5.75	1.53	1.46
1	E	56	LYS	CE-NZ	5.75	1.66	1.49
2	B	83	GLY	N-CA	5.75	1.53	1.45
1	C	7	LYS	CA-CB	5.75	1.62	1.53
2	F	27	ALA	C-O	5.75	1.30	1.24
1	G	28	ALA	C-O	-5.75	1.16	1.24
2	F	132	LYS	CA-C	5.75	1.60	1.52
2	F	36	PRO	CA-CB	-5.75	1.45	1.53
2	D	51	PRO	N-CD	5.74	1.55	1.47
1	G	87	HIS	N-CA	5.74	1.53	1.46
2	B	122	PHE	CA-C	5.74	1.59	1.53
1	C	106	LEU	C-O	-5.74	1.16	1.24
2	H	42	PHE	CA-C	-5.74	1.45	1.53
2	H	73	ASP	N-CA	5.74	1.54	1.46
1	E	64	ASP	C-O	5.73	1.30	1.24
1	A	136	LEU	CA-C	-5.73	1.44	1.52
1	C	132	VAL	N-CA	5.73	1.53	1.46
2	H	93	CYS	C-N	5.72	1.41	1.33
2	B	84	THR	N-CA	5.72	1.53	1.46
2	D	143	HIS	C-N	5.72	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	118	PHE	CA-CB	5.72	1.64	1.53
2	D	143	HIS	C-O	5.72	1.31	1.24
2	H	82	LYS	CB-CG	5.71	1.69	1.52
2	D	37	TRP	C-O	5.71	1.31	1.24
2	D	42	PHE	C-O	5.71	1.31	1.23
1	G	91	LEU	CG-CD2	-5.71	1.33	1.52
1	C	116	GLU	CD-OE1	5.71	1.36	1.25
2	F	45	PHE	CG-CD1	-5.71	1.26	1.38
2	H	65	LYS	CA-C	5.71	1.60	1.52
1	A	91	LEU	CA-C	-5.71	1.44	1.52
1	C	68	ASN	C-N	-5.71	1.26	1.33
2	D	146	HIS	CA-CB	5.70	1.64	1.53
1	E	36	PHE	CG-CD1	-5.70	1.26	1.38
1	A	2	LEU	C-O	5.70	1.30	1.24
2	D	108	ASN	N-CA	-5.70	1.38	1.46
1	C	79	ALA	CA-C	-5.69	1.45	1.52
1	A	67	THR	CA-CB	5.69	1.62	1.53
1	C	46	PHE	CA-C	-5.69	1.45	1.52
1	E	116	GLU	CA-CB	5.69	1.62	1.54
2	B	87	THR	C-N	-5.69	1.26	1.33
2	H	125	PRO	C-N	5.69	1.41	1.33
1	G	41	THR	CA-CB	5.69	1.63	1.53
1	A	133	SER	N-CA	5.68	1.53	1.46
1	A	118	THR	N-CA	5.68	1.54	1.45
1	C	27	GLU	C-N	5.68	1.41	1.33
1	E	111	ALA	N-CA	-5.68	1.38	1.46
1	G	136	LEU	CB-CG	5.68	1.64	1.53
2	B	42	PHE	CG-CD2	5.68	1.50	1.38
2	D	82	LYS	C-N	-5.68	1.25	1.33
2	D	33	VAL	CA-C	5.67	1.58	1.52
1	G	126	ASP	CB-CG	5.67	1.66	1.52
2	F	103	PHE	CA-C	-5.67	1.45	1.52
2	H	77	HIS	ND1-CE1	-5.67	1.26	1.32
2	D	32	LEU	C-N	5.67	1.38	1.33
1	G	58	HIS	CE1-NE2	-5.67	1.26	1.32
2	B	99	ASP	CA-C	5.67	1.58	1.52
1	E	13	ALA	C-O	5.67	1.30	1.24
1	E	5	ALA	CA-CB	-5.67	1.44	1.53
1	G	50	HIS	ND1-CE1	5.67	1.38	1.32
2	B	101	GLU	CD-OE1	-5.66	1.14	1.25
1	E	67	THR	CB-OG1	-5.66	1.34	1.43
1	A	131	SER	CB-OG	5.66	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	LYS	C-N	5.66	1.42	1.33
1	E	20	HIS	CA-CB	-5.66	1.43	1.53
2	H	146	HIS	CG-ND1	-5.65	1.32	1.38
1	G	138	SER	CA-C	-5.65	1.44	1.52
2	H	98	VAL	N-CA	5.65	1.53	1.46
2	H	109	VAL	CA-CB	-5.65	1.48	1.54
2	F	144	LYS	N-CA	5.64	1.52	1.46
2	H	123	THR	C-O	-5.64	1.15	1.23
2	F	29	GLY	CA-C	-5.64	1.46	1.52
1	A	24	TYR	CZ-OH	5.63	1.49	1.38
1	A	44	PRO	C-O	5.63	1.31	1.24
1	E	94	ASP	N-CA	5.63	1.54	1.46
1	A	51	GLY	N-CA	5.63	1.53	1.45
2	B	92	HIS	CG-CD2	-5.63	1.29	1.35
2	F	22	GLU	CB-CG	5.63	1.69	1.52
1	E	20	HIS	C-O	-5.62	1.16	1.23
1	C	43	PHE	C-N	-5.62	1.27	1.33
1	A	89	HIS	C-O	5.62	1.31	1.23
1	C	97	ASN	CA-CB	5.61	1.62	1.53
2	H	8	LYS	CA-CB	-5.61	1.44	1.53
2	D	124	PRO	CA-C	-5.61	1.47	1.52
2	H	5	PRO	CA-CB	5.61	1.61	1.53
1	G	60	LYS	C-O	-5.61	1.16	1.24
2	H	25	GLY	C-O	5.61	1.30	1.23
1	A	83	LEU	C-O	5.60	1.31	1.24
2	B	135	ALA	N-CA	5.60	1.52	1.46
2	B	77	HIS	C-O	-5.60	1.15	1.23
1	A	60	LYS	N-CA	-5.60	1.39	1.46
2	H	33	VAL	CA-C	-5.60	1.45	1.52
2	D	111	VAL	N-CA	5.59	1.53	1.46
1	G	141	ARG	CA-CB	-5.59	1.42	1.53
2	B	40	ARG	C-O	5.59	1.31	1.24
1	E	45	HIS	ND1-CE1	5.59	1.38	1.32
2	B	48	LEU	CA-C	5.59	1.60	1.53
2	D	37	TRP	CD2-CE2	5.59	1.50	1.41
1	C	139	LYS	CE-NZ	5.58	1.66	1.49
2	D	53	ALA	N-CA	5.58	1.52	1.46
1	C	56	LYS	CA-CB	-5.58	1.44	1.53
1	A	5	ALA	C-O	5.58	1.31	1.24
1	C	118	THR	CB-CG2	5.58	1.71	1.52
2	H	15	TRP	CE2-CZ2	-5.58	1.28	1.39
1	E	131	SER	C-N	5.58	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	27	GLU	C-O	-5.57	1.17	1.24
2	H	102	ASN	CA-C	5.57	1.59	1.52
2	B	12	THR	CB-CG2	5.57	1.71	1.52
2	B	100	PRO	CA-CB	5.57	1.61	1.53
1	G	11	LYS	N-CA	-5.57	1.38	1.46
2	F	15	TRP	N-CA	-5.57	1.39	1.46
1	C	122	HIS	CA-CB	-5.56	1.44	1.53
2	B	23	VAL	CA-CB	5.56	1.62	1.54
1	C	35	SER	N-CA	5.56	1.53	1.46
2	D	26	GLU	N-CA	5.56	1.53	1.46
2	D	32	LEU	N-CA	5.55	1.53	1.46
2	D	59	LYS	N-CA	5.55	1.53	1.46
2	F	52	ASP	C-N	5.55	1.41	1.33
1	A	56	LYS	CA-C	5.55	1.60	1.52
2	B	94	ASP	C-O	5.55	1.30	1.24
2	D	17	LYS	N-CA	5.55	1.53	1.46
2	H	57	ASN	CG-OD1	-5.55	1.13	1.23
1	A	33	PHE	C-N	-5.55	1.25	1.33
1	A	96	VAL	CA-C	-5.55	1.44	1.52
2	F	93	CYS	CB-SG	5.55	1.99	1.81
2	H	13	ALA	CA-CB	5.55	1.62	1.53
1	C	38	THR	C-N	-5.55	1.25	1.33
2	F	135	ALA	CA-CB	5.55	1.62	1.53
2	B	135	ALA	C-N	5.54	1.41	1.33
1	E	52	SER	C-N	-5.54	1.26	1.33
1	G	10	VAL	N-CA	5.54	1.53	1.46
1	G	50	HIS	CA-C	5.54	1.60	1.52
2	H	97	HIS	C-N	5.54	1.40	1.33
2	F	100	PRO	CG-CD	5.54	1.69	1.50
2	H	67	VAL	C-N	5.53	1.41	1.33
2	B	36	PRO	N-CD	5.53	1.55	1.47
2	H	92	HIS	C-N	-5.53	1.25	1.33
1	A	36	PHE	CA-C	5.53	1.58	1.52
2	F	104	ARG	C-O	5.53	1.30	1.24
2	H	32	LEU	CA-C	5.53	1.60	1.52
2	H	141	LEU	CA-CB	5.53	1.61	1.53
2	D	27	ALA	CA-C	-5.52	1.45	1.52
2	B	135	ALA	CA-CB	5.52	1.62	1.53
2	D	55	MET	CA-CB	-5.52	1.43	1.53
1	E	25	GLY	CA-C	-5.52	1.45	1.52
1	G	56	LYS	CD-CE	-5.52	1.35	1.52
1	C	130	ALA	CA-C	5.52	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	118	PHE	CG-CD1	5.52	1.50	1.38
2	B	106	LEU	CG-CD2	5.51	1.70	1.52
1	G	140	TYR	CZ-OH	-5.51	1.26	1.38
2	D	105	LEU	C-N	-5.51	1.25	1.33
1	A	116	GLU	CD-OE2	5.51	1.35	1.25
2	H	84	THR	CA-C	-5.51	1.45	1.52
1	A	32	MET	CA-C	5.51	1.59	1.52
1	G	51	GLY	C-N	-5.50	1.25	1.33
2	B	5	PRO	CA-C	-5.50	1.44	1.52
1	C	108	THR	CA-CB	5.50	1.62	1.53
2	F	37	TRP	CA-C	-5.50	1.45	1.52
2	H	121	GLU	CB-CG	5.50	1.69	1.52
2	B	4	THR	C-N	-5.50	1.26	1.33
2	H	87	THR	C-N	-5.49	1.26	1.33
1	A	1	VAL	N-CA	5.49	1.56	1.46
1	A	108	THR	C-N	-5.49	1.26	1.34
2	F	47	ASP	N-CA	5.49	1.53	1.46
2	B	73	ASP	CA-C	5.49	1.60	1.52
1	G	114	PRO	CG-CD	5.49	1.69	1.50
1	E	140	TYR	CA-CB	5.48	1.62	1.53
2	H	52	ASP	C-O	5.48	1.31	1.24
2	F	24	GLY	CA-C	-5.48	1.44	1.51
2	H	141	LEU	CA-C	5.48	1.59	1.52
1	C	43	PHE	C-O	-5.47	1.17	1.23
2	D	113	VAL	CA-C	5.47	1.59	1.52
2	D	137	VAL	CA-CB	-5.47	1.47	1.54
1	G	17	VAL	CA-CB	-5.47	1.46	1.54
2	B	90	GLU	CG-CD	5.47	1.65	1.52
1	G	21	ALA	C-N	5.47	1.41	1.33
2	B	37	TRP	CE3-CZ3	5.47	1.55	1.38
2	D	139	ASN	CA-C	-5.46	1.45	1.52
2	H	5	PRO	CG-CD	5.46	1.69	1.50
2	B	94	ASP	N-CA	5.46	1.52	1.46
1	E	33	PHE	CA-CB	5.46	1.61	1.53
1	G	44	PRO	CG-CD	-5.46	1.32	1.50
2	H	5	PRO	C-O	-5.46	1.16	1.24
1	C	64	ASP	CB-CG	5.46	1.65	1.52
1	E	80	LEU	CB-CG	-5.45	1.42	1.53
1	A	112	HIS	CG-ND1	-5.45	1.32	1.38
1	A	118	THR	C-O	5.45	1.30	1.23
1	E	131	SER	N-CA	-5.45	1.39	1.46
1	A	78	ASN	C-N	5.45	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	19	ASN	CA-CB	-5.44	1.46	1.53
2	D	42	PHE	CA-C	5.44	1.60	1.53
2	D	93	CYS	C-N	-5.44	1.26	1.33
1	G	42	TYR	C-O	5.44	1.31	1.24
1	A	60	LYS	CG-CD	5.44	1.68	1.52
2	F	106	LEU	CG-CD2	5.44	1.70	1.52
1	A	42	TYR	CG-CD2	5.44	1.50	1.39
1	E	78	ASN	C-O	5.44	1.30	1.24
1	G	84	SER	CA-CB	-5.44	1.44	1.53
2	F	75	LEU	CA-C	-5.44	1.45	1.52
1	A	104	CYS	C-N	-5.43	1.26	1.33
2	B	61	LYS	C-N	-5.43	1.27	1.33
2	F	2	HIS	CG-CD2	5.43	1.41	1.35
2	B	77	HIS	CA-CB	-5.43	1.37	1.53
2	D	78	LEU	CB-CG	-5.43	1.42	1.53
2	D	96	LEU	CA-CB	5.43	1.62	1.53
1	C	34	LEU	N-CA	5.43	1.53	1.46
2	B	65	LYS	CA-CB	5.43	1.61	1.53
2	D	139	ASN	CG-OD1	5.43	1.33	1.23
2	F	87	THR	C-O	-5.43	1.17	1.24
2	F	121	GLU	C-O	5.43	1.30	1.24
1	C	141	ARG	C-O	5.42	1.34	1.23
2	D	67	VAL	C-O	5.42	1.30	1.24
1	E	129	LEU	N-CA	-5.42	1.39	1.46
1	G	109	LEU	CG-CD2	-5.42	1.34	1.52
1	C	139	LYS	N-CA	5.42	1.52	1.46
2	F	92	HIS	N-CA	-5.42	1.39	1.46
2	B	85	PHE	CG-CD1	5.42	1.50	1.38
1	E	60	LYS	N-CA	5.42	1.53	1.46
1	E	98	PHE	C-N	-5.42	1.27	1.33
1	G	116	GLU	CD-OE1	-5.42	1.15	1.25
2	H	73	ASP	CA-CB	5.42	1.62	1.53
2	D	66	LYS	CA-CB	-5.42	1.44	1.53
2	B	122	PHE	CE2-CZ	5.42	1.54	1.38
1	E	81	SER	CA-CB	5.42	1.62	1.53
1	E	118	THR	CB-OG1	5.42	1.52	1.43
1	A	72	HIS	CA-CB	5.42	1.61	1.53
2	F	44	SER	C-O	-5.41	1.15	1.23
1	E	103	HIS	ND1-CE1	-5.41	1.27	1.32
1	A	130	ALA	CA-CB	5.41	1.62	1.53
1	C	139	LYS	CA-C	-5.41	1.44	1.52
1	A	103	HIS	C-N	5.41	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	ARG	N-CA	-5.40	1.39	1.46
2	F	39	GLN	CA-C	5.40	1.60	1.52
1	C	104	CYS	CA-CB	-5.40	1.44	1.53
2	D	141	LEU	N-CA	5.40	1.53	1.46
1	C	134	THR	CA-C	5.39	1.59	1.53
1	E	83	LEU	C-O	5.39	1.31	1.24
1	G	2	LEU	CA-CB	5.39	1.61	1.53
1	E	98	PHE	N-CA	5.39	1.52	1.46
1	A	20	HIS	C-N	-5.39	1.26	1.33
2	B	99	ASP	C-N	-5.39	1.28	1.34
2	D	98	VAL	CA-C	5.39	1.59	1.52
2	D	142	ALA	CA-C	-5.38	1.45	1.52
1	G	106	LEU	C-N	-5.38	1.27	1.33
2	H	112	CYS	CB-SG	-5.38	1.63	1.81
2	H	31	LEU	C-O	5.38	1.30	1.24
2	H	86	ALA	CA-C	5.38	1.59	1.52
1	E	89	HIS	N-CA	5.38	1.53	1.46
2	H	126	VAL	CA-CB	-5.38	1.48	1.54
1	E	30	GLU	C-N	-5.38	1.27	1.33
1	A	50	HIS	ND1-CE1	5.37	1.38	1.32
2	D	72	SER	CA-C	5.37	1.59	1.52
1	G	20	HIS	ND1-CE1	5.37	1.38	1.32
1	A	6	ASP	C-O	-5.37	1.17	1.24
1	C	138	SER	C-O	5.37	1.30	1.24
1	A	32	MET	CG-SD	5.37	1.94	1.80
1	C	16	LYS	C-N	-5.37	1.26	1.33
1	C	41	THR	CA-CB	5.36	1.62	1.53
1	G	77	PRO	C-O	5.36	1.30	1.24
1	E	16	LYS	CA-C	-5.36	1.45	1.52
1	G	85	ASP	C-O	5.36	1.30	1.24
1	A	122	HIS	C-N	5.36	1.41	1.33
1	E	83	LEU	CA-CB	5.35	1.62	1.53
1	E	86	LEU	CA-CB	-5.35	1.45	1.53
2	F	15	TRP	CD2-CE3	5.35	1.48	1.40
1	G	62	VAL	CB-CG1	5.35	1.70	1.52
1	C	20	HIS	C-N	-5.35	1.26	1.33
1	C	127	LYS	N-CA	-5.35	1.40	1.46
2	D	112	CYS	CA-C	5.35	1.59	1.52
1	G	124	SER	CB-OG	5.35	1.52	1.42
2	B	19	ASN	C-N	-5.35	1.26	1.33
2	D	44	SER	CB-OG	5.34	1.52	1.42
2	D	87	THR	CA-C	5.34	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	TYR	CD1-CE1	-5.34	1.22	1.38
2	D	18	VAL	CA-C	-5.33	1.46	1.52
1	A	134	THR	C-O	5.33	1.30	1.24
2	D	110	LEU	CA-CB	5.33	1.62	1.53
1	A	118	THR	CB-OG1	5.33	1.52	1.43
2	F	101	GLU	CD-OE1	5.33	1.35	1.25
2	H	71	PHE	CA-CB	5.33	1.61	1.53
1	C	52	SER	C-O	5.32	1.30	1.24
2	B	59	LYS	CE-NZ	5.32	1.65	1.49
1	E	126	ASP	CG-OD2	5.32	1.35	1.25
2	B	26	GLU	N-CA	-5.32	1.39	1.46
2	D	37	TRP	CZ3-CH2	5.32	1.53	1.40
2	F	45	PHE	CA-CB	-5.32	1.45	1.53
2	F	138	ALA	CA-CB	5.32	1.61	1.53
1	G	20	HIS	C-N	5.32	1.40	1.33
1	G	105	LEU	CA-C	5.31	1.59	1.52
2	B	11	VAL	CA-CB	-5.31	1.47	1.54
2	D	92	HIS	CG-CD2	-5.31	1.30	1.35
1	E	1	VAL	CA-CB	5.31	1.68	1.54
2	H	107	GLY	CA-C	-5.31	1.44	1.51
1	A	68	ASN	CA-C	5.31	1.59	1.52
1	E	109	LEU	CA-CB	5.31	1.62	1.53
2	F	112	CYS	CA-CB	5.31	1.61	1.53
1	C	28	ALA	N-CA	5.31	1.53	1.46
2	B	58	PRO	CG-CD	5.31	1.68	1.50
2	D	35	TYR	CD1-CE1	5.30	1.54	1.38
2	F	79	ASP	CA-C	-5.30	1.45	1.52
1	E	126	ASP	C-N	-5.29	1.25	1.33
2	B	30	ARG	CZ-NH2	-5.29	1.26	1.33
1	G	70	VAL	CB-CG1	5.29	1.70	1.52
2	B	41	PHE	C-N	-5.28	1.25	1.33
2	D	51	PRO	CA-CB	-5.28	1.46	1.53
1	A	66	LEU	C-O	5.28	1.30	1.24
1	A	123	ALA	CA-CB	5.28	1.62	1.53
2	F	73	ASP	CG-OD1	-5.28	1.15	1.25
2	B	107	GLY	N-CA	5.28	1.52	1.45
2	B	145	TYR	CZ-OH	5.27	1.49	1.38
1	C	96	VAL	CA-C	5.27	1.60	1.52
2	B	51	PRO	CA-CB	-5.27	1.46	1.53
2	F	100	PRO	N-CD	5.27	1.55	1.47
1	A	3	SER	CA-C	5.27	1.59	1.52
1	C	95	PRO	C-N	5.27	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	46	GLY	CA-C	-5.27	1.46	1.52
1	A	107	VAL	N-CA	-5.27	1.40	1.46
2	D	105	LEU	CG-CD1	5.27	1.70	1.52
2	F	2	HIS	C-O	5.27	1.30	1.24
1	G	106	LEU	C-O	5.27	1.30	1.24
2	B	15	TRP	C-N	5.26	1.42	1.33
2	D	88	LEU	N-CA	5.26	1.53	1.46
2	F	20	VAL	CA-CB	5.26	1.62	1.54
2	H	103	PHE	C-N	-5.26	1.27	1.33
2	D	27	ALA	N-CA	5.25	1.52	1.46
2	B	16	GLY	N-CA	5.25	1.53	1.45
2	D	138	ALA	N-CA	-5.25	1.40	1.46
2	H	72	SER	CA-C	-5.25	1.45	1.52
2	B	71	PHE	CG-CD1	-5.25	1.27	1.38
1	E	19	ALA	C-O	5.25	1.30	1.24
1	E	64	ASP	C-N	5.25	1.40	1.33
1	C	58	HIS	C-O	5.24	1.30	1.24
1	E	54	GLN	CA-CB	5.24	1.61	1.53
1	G	138	SER	N-CA	5.24	1.53	1.46
2	H	146	HIS	CE1-NE2	5.24	1.37	1.32
1	G	116	GLU	CA-CB	-5.24	1.43	1.54
2	D	64	GLY	CA-C	5.24	1.57	1.52
2	H	12	THR	CB-OG1	5.24	1.52	1.43
1	C	139	LYS	CA-CB	5.24	1.61	1.53
2	F	102	ASN	C-O	5.24	1.30	1.24
1	C	3	SER	C-N	-5.23	1.27	1.34
1	C	56	LYS	C-O	-5.23	1.18	1.24
2	D	77	HIS	CE1-NE2	5.23	1.37	1.32
1	E	25	GLY	C-O	5.23	1.30	1.23
2	F	63	HIS	ND1-CE1	-5.23	1.27	1.32
1	E	36	PHE	C-O	5.22	1.29	1.24
1	G	135	VAL	N-CA	-5.22	1.40	1.46
1	G	20	HIS	CG-ND1	5.21	1.44	1.38
2	H	129	ALA	CA-C	5.21	1.59	1.52
1	E	123	ALA	N-CA	-5.21	1.39	1.46
2	F	19	ASN	CA-CB	-5.21	1.46	1.53
2	F	118	PHE	CA-C	5.21	1.60	1.52
2	D	63	HIS	N-CA	5.21	1.52	1.46
2	D	37	TRP	CZ2-CH2	-5.20	1.27	1.37
2	H	18	VAL	N-CA	-5.20	1.40	1.46
2	H	34	VAL	CB-CG2	5.20	1.69	1.52
2	H	45	PHE	CE2-CZ	5.20	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	50	THR	CA-C	-5.20	1.46	1.52
1	G	139	LYS	C-O	5.20	1.31	1.23
2	H	71	PHE	C-N	-5.20	1.27	1.33
2	F	100	PRO	N-CA	-5.20	1.40	1.47
2	B	10	ALA	C-N	-5.19	1.26	1.33
1	E	24	TYR	CG-CD1	-5.19	1.28	1.39
1	G	87	HIS	C-O	-5.19	1.18	1.24
2	B	97	HIS	N-CA	5.19	1.52	1.46
2	D	79	ASP	CB-CG	5.19	1.65	1.52
1	C	54	GLN	N-CA	-5.19	1.40	1.46
1	C	126	ASP	N-CA	5.19	1.52	1.46
1	G	61	LYS	CE-NZ	-5.19	1.33	1.49
1	A	78	ASN	CA-C	5.19	1.59	1.52
1	A	98	PHE	CA-CB	5.18	1.61	1.53
1	C	18	GLY	C-O	5.18	1.30	1.23
2	D	71	PHE	CA-C	5.18	1.59	1.52
1	A	140	TYR	CE1-CZ	5.18	1.50	1.38
2	B	13	ALA	N-CA	5.18	1.52	1.46
1	C	32	MET	CB-CG	5.18	1.68	1.52
1	C	94	ASP	CA-CB	5.18	1.60	1.53
1	C	122	HIS	CG-CD2	-5.18	1.30	1.35
2	H	51	PRO	CA-CB	-5.18	1.46	1.53
1	A	25	GLY	C-O	-5.17	1.17	1.23
1	A	29	LEU	CB-CG	5.17	1.63	1.53
1	G	91	LEU	CA-C	-5.17	1.45	1.52
2	H	75	LEU	C-O	-5.17	1.17	1.24
1	C	1	VAL	CA-CB	5.17	1.68	1.54
1	A	2	LEU	CG-CD2	5.17	1.69	1.52
1	A	108	THR	CA-C	5.17	1.59	1.52
2	B	103	PHE	C-N	5.17	1.41	1.34
1	C	98	PHE	CA-CB	5.17	1.61	1.53
1	E	119	PRO	CA-CB	5.17	1.61	1.53
2	D	66	LYS	CA-C	-5.17	1.45	1.52
2	H	111	VAL	N-CA	5.17	1.52	1.46
2	D	139	ASN	CA-CB	5.16	1.62	1.53
2	H	2	HIS	CG-CD2	-5.16	1.30	1.35
1	A	10	VAL	N-CA	-5.16	1.40	1.46
2	H	136	GLY	N-CA	-5.16	1.37	1.45
2	B	15	TRP	CD2-CE2	5.16	1.50	1.41
2	D	85	PHE	CE2-CZ	5.16	1.54	1.38
2	F	121	GLU	CA-C	5.16	1.59	1.52
1	A	20	HIS	CG-ND1	-5.16	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	LYS	CA-CB	-5.16	1.47	1.53
2	B	31	LEU	CA-C	5.16	1.59	1.52
2	B	80	ASN	CA-C	5.16	1.59	1.52
1	E	31	ARG	CZ-NH1	5.16	1.40	1.32
1	G	110	ALA	CA-CB	5.16	1.61	1.53
2	H	97	HIS	CG-CD2	-5.16	1.30	1.35
2	B	121	GLU	CG-CD	5.15	1.65	1.52
1	C	47	ASP	CG-OD2	5.15	1.35	1.25
2	H	136	GLY	CA-C	5.15	1.59	1.51
2	D	135	ALA	N-CA	-5.15	1.40	1.46
1	E	122	HIS	CB-CG	-5.14	1.43	1.50
2	D	1	VAL	C-O	5.14	1.33	1.23
2	H	37	TRP	CA-CB	-5.14	1.45	1.53
1	C	46	PHE	CB-CG	-5.14	1.38	1.50
2	F	71	PHE	C-N	5.13	1.40	1.33
1	A	31	ARG	CD-NE	-5.13	1.39	1.46
1	A	46	PHE	CG-CD1	5.13	1.49	1.38
2	F	130	TYR	C-N	-5.13	1.25	1.33
2	B	66	LYS	N-CA	5.13	1.52	1.46
2	F	38	THR	C-N	5.13	1.40	1.34
2	H	120	LYS	C-O	5.12	1.31	1.24
2	B	59	LYS	CB-CG	5.12	1.67	1.52
2	D	36	PRO	N-CD	-5.12	1.40	1.47
2	H	143	HIS	CA-CB	5.12	1.61	1.53
2	H	52	ASP	CB-CG	5.12	1.64	1.52
1	A	4	PRO	N-CA	-5.11	1.40	1.47
2	B	33	VAL	C-O	-5.11	1.18	1.23
1	E	73	VAL	C-O	-5.11	1.18	1.24
2	H	100	PRO	N-CD	-5.11	1.40	1.47
1	A	4	PRO	N-CD	5.11	1.54	1.47
2	B	127	GLN	C-N	-5.11	1.27	1.33
2	B	66	LYS	CG-CD	-5.11	1.37	1.52
2	F	66	LYS	CD-CE	5.11	1.67	1.52
2	F	139	ASN	N-CA	5.11	1.52	1.46
1	G	90	LYS	CB-CG	5.10	1.67	1.52
1	E	72	HIS	CB-CG	-5.10	1.43	1.50
2	F	68	LEU	C-O	5.10	1.29	1.24
2	H	121	GLU	C-N	5.10	1.40	1.33
1	A	115	ALA	C-N	5.09	1.42	1.33
2	F	86	ALA	N-CA	-5.09	1.39	1.46
2	H	129	ALA	C-N	-5.09	1.26	1.33
1	E	17	VAL	CA-CB	5.09	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	53	ALA	CA-C	5.09	1.59	1.52
2	F	42	PHE	CA-CB	5.09	1.60	1.53
2	H	45	PHE	CD2-CE2	-5.09	1.23	1.38
1	G	4	PRO	CA-C	5.09	1.59	1.52
1	A	77	PRO	CB-CG	5.08	1.75	1.49
1	A	120	ALA	CA-C	5.08	1.59	1.52
2	H	121	GLU	C-O	5.08	1.30	1.24
2	F	39	GLN	C-N	-5.08	1.26	1.33
1	E	81	SER	C-N	-5.08	1.26	1.34
1	G	91	LEU	CG-CD1	5.08	1.69	1.52
2	B	125	PRO	N-CA	5.07	1.53	1.47
2	F	37	TRP	CD2-CE3	-5.07	1.32	1.40
1	G	134	THR	C-O	5.07	1.30	1.24
1	G	17	VAL	C-O	-5.07	1.17	1.23
1	E	56	LYS	C-N	5.07	1.39	1.33
1	G	53	ALA	CA-C	-5.07	1.45	1.52
2	H	63	HIS	CG-ND1	5.07	1.43	1.38
2	B	124	PRO	CA-CB	5.06	1.60	1.54
1	A	58	HIS	C-N	-5.06	1.27	1.33
2	H	139	ASN	C-N	5.06	1.40	1.33
2	F	59	LYS	N-CA	5.06	1.52	1.46
2	B	104	ARG	NE-CZ	5.05	1.38	1.33
1	G	31	ARG	CZ-NH2	-5.05	1.26	1.33
1	C	50	HIS	ND1-CE1	-5.05	1.27	1.32
2	D	96	LEU	C-O	-5.05	1.17	1.24
1	G	27	GLU	C-N	5.05	1.40	1.33
2	B	129	ALA	C-N	-5.05	1.25	1.33
1	E	51	GLY	CA-C	5.05	1.58	1.51
2	F	21	ASP	CG-OD2	-5.05	1.15	1.25
1	G	39	THR	C-N	5.05	1.40	1.33
2	H	59	LYS	CB-CG	5.05	1.67	1.52
1	A	72	HIS	CG-ND1	5.05	1.43	1.38
1	E	46	PHE	CA-CB	5.04	1.65	1.53
1	E	92	ARG	CD-NE	5.04	1.53	1.46
1	G	108	THR	N-CA	-5.04	1.40	1.46
2	H	24	GLY	N-CA	5.04	1.51	1.45
2	B	105	LEU	CB-CG	-5.04	1.43	1.53
2	D	40	ARG	CZ-NH2	5.04	1.40	1.33
1	A	74	ASP	CG-OD1	5.04	1.34	1.25
1	C	31	ARG	NE-CZ	5.04	1.38	1.33
1	E	91	LEU	C-N	-5.04	1.26	1.33
2	H	133	VAL	C-O	5.03	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	8	THR	CA-C	-5.03	1.46	1.52
2	F	111	VAL	C-N	-5.03	1.27	1.33
2	D	95	LYS	C-N	5.03	1.41	1.33
2	B	27	ALA	C-O	-5.03	1.18	1.24
2	F	38	THR	CB-CG2	5.03	1.69	1.52
1	G	9	ASN	C-N	5.03	1.40	1.33
1	A	74	ASP	CA-CB	5.02	1.61	1.53
2	H	120	LYS	C-N	-5.02	1.25	1.33
2	B	141	LEU	C-N	5.02	1.42	1.33
1	E	68	ASN	CA-C	5.02	1.59	1.52
1	E	139	LYS	CE-NZ	5.02	1.64	1.49
2	F	50	THR	N-CA	5.02	1.51	1.46
1	G	101	LEU	CG-CD2	-5.02	1.35	1.52
1	G	11	LYS	C-N	-5.02	1.27	1.33
1	E	68	ASN	CG-ND2	5.01	1.43	1.33
2	H	104	ARG	N-CA	-5.01	1.40	1.46
2	F	45	PHE	C-N	-5.01	1.26	1.33
1	A	24	TYR	CA-C	5.01	1.59	1.52
1	G	138	SER	CB-OG	5.01	1.52	1.42
2	B	5	PRO	N-CD	-5.00	1.40	1.47
2	F	139	ASN	CA-C	-5.00	1.45	1.52
2	B	42	PHE	CA-C	-5.00	1.44	1.52
1	C	16	LYS	CA-C	5.00	1.59	1.52
1	E	120	ALA	CA-CB	5.00	1.62	1.53
1	G	95	PRO	N-CA	-5.00	1.41	1.47
1	A	50	HIS	CA-C	5.00	1.59	1.52
1	A	82	ALA	C-N	-5.00	1.27	1.34
1	C	128	PHE	C-O	-5.00	1.18	1.24
1	G	75	ASP	N-CA	5.00	1.55	1.47

All (5500) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	47	ASP	CA-CB-CG	55.17	167.77	112.60
1	E	31	ARG	NE-CZ-NH1	50.69	172.19	121.50
2	B	45	PHE	CA-CB-CG	46.21	160.01	113.80
1	E	10	VAL	CA-C-N	43.85	177.45	120.44
1	E	10	VAL	C-N-CA	43.85	177.45	120.44
1	E	31	ARG	NE-CZ-NH2	-43.54	80.01	119.20
2	B	80	ASN	OD1-CG-ND2	42.36	164.96	122.60
1	G	85	ASP	CA-CB-CG	41.00	153.60	112.60
1	A	122	HIS	CA-CB-CG	40.43	154.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	40	ARG	CD-NE-CZ	39.05	179.07	124.40
1	C	58	HIS	CA-C-N	39.04	162.49	119.94
1	C	58	HIS	C-N-CA	39.04	162.49	119.94
1	A	62	VAL	N-CA-CB	38.24	152.30	110.62
1	C	75	ASP	CA-CB-CG	-37.54	75.06	112.60
2	H	140	ALA	CA-C-N	37.41	169.08	120.44
2	H	140	ALA	C-N-CA	37.41	169.08	120.44
1	C	35	SER	CA-C-N	37.25	163.94	122.59
1	C	35	SER	C-N-CA	37.25	163.94	122.59
2	B	40	ARG	CD-NE-CZ	37.19	176.46	124.40
1	C	37	PRO	CA-C-N	36.43	175.69	120.31
1	C	37	PRO	C-N-CA	36.43	175.69	120.31
1	A	100	LEU	CA-C-N	36.01	179.21	120.88
1	A	100	LEU	C-N-CA	36.01	179.21	120.88
2	H	99	ASP	CA-CB-CG	35.98	148.58	112.60
2	D	87	THR	O-C-N	35.40	160.26	122.03
2	F	16	GLY	CA-C-N	35.11	179.36	120.72
2	F	16	GLY	C-N-CA	35.11	179.36	120.72
1	G	23	GLU	CA-C-N	34.63	169.46	120.29
1	G	23	GLU	C-N-CA	34.63	169.46	120.29
1	G	141	ARG	NE-CZ-NH2	-34.21	88.41	119.20
2	F	83	GLY	CA-C-N	33.77	177.10	120.71
2	F	83	GLY	C-N-CA	33.77	177.10	120.71
1	E	122	HIS	CA-CB-CG	33.47	147.27	113.80
2	F	79	ASP	CA-CB-CG	33.46	146.06	112.60
1	E	97	ASN	OD1-CG-ND2	-32.71	89.89	122.60
1	C	110	ALA	CA-C-N	31.89	173.67	122.65
1	C	110	ALA	C-N-CA	31.89	173.67	122.65
1	A	129	LEU	CA-C-N	31.62	171.46	121.19
1	A	129	LEU	C-N-CA	31.62	171.46	121.19
2	B	19	ASN	CA-CB-CG	31.46	144.06	112.60
1	G	107	VAL	CA-C-N	31.36	161.21	120.44
1	G	107	VAL	C-N-CA	31.36	161.21	120.44
1	C	89	HIS	CA-CB-CG	-31.32	82.48	113.80
2	H	108	ASN	OD1-CG-ND2	30.88	153.48	122.60
1	C	70	VAL	O-C-N	30.53	151.83	121.91
1	E	58	HIS	CA-C-N	30.43	154.38	119.99
1	E	58	HIS	C-N-CA	30.43	154.38	119.99
2	H	75	LEU	CA-C-N	30.31	160.66	120.65
2	H	75	LEU	C-N-CA	30.31	160.66	120.65
1	C	43	PHE	O-C-N	30.22	149.27	121.17
1	A	35	SER	CA-C-N	29.97	150.24	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	SER	C-N-CA	29.97	150.24	122.37
2	B	72	SER	CA-C-O	-29.70	86.54	120.10
1	C	28	ALA	CA-C-N	29.70	159.04	120.44
1	C	28	ALA	C-N-CA	29.70	159.04	120.44
1	C	94	ASP	CA-C-O	29.63	150.99	120.17
1	G	32	MET	CA-C-N	29.57	161.89	120.79
1	G	32	MET	C-N-CA	29.57	161.89	120.79
1	A	62	VAL	CA-C-O	-29.56	89.66	121.29
2	H	127	GLN	OE1-CD-NE2	-29.34	93.26	122.60
2	B	19	ASN	OD1-CG-ND2	-29.15	93.45	122.60
1	G	37	PRO	CA-C-N	29.10	172.07	121.14
1	G	37	PRO	C-N-CA	29.10	172.07	121.14
2	F	23	VAL	CA-C-N	28.98	178.20	121.41
2	F	23	VAL	C-N-CA	28.98	178.20	121.41
2	F	97	HIS	CA-C-N	28.93	158.88	122.43
2	F	97	HIS	C-N-CA	28.93	158.88	122.43
1	E	72	HIS	CA-CB-CG	28.63	142.43	113.80
2	B	139	ASN	OD1-CG-ND2	28.55	151.15	122.60
2	B	35	TYR	O-C-N	28.52	147.28	121.32
1	E	138	SER	CA-CB-OG	28.52	168.13	111.10
2	F	30	ARG	NE-CZ-NH1	-28.49	93.01	121.50
1	E	98	PHE	CA-C-O	28.14	150.24	120.42
2	F	134	VAL	CA-C-N	28.04	157.66	120.65
2	F	134	VAL	C-N-CA	28.04	157.66	120.65
2	H	127	GLN	CA-C-N	27.91	162.68	120.82
2	H	127	GLN	C-N-CA	27.91	162.68	120.82
1	E	109	LEU	CA-C-N	27.86	174.74	121.54
1	E	109	LEU	C-N-CA	27.86	174.74	121.54
1	C	40	LYS	CA-C-N	27.82	160.34	120.28
1	C	40	LYS	C-N-CA	27.82	160.34	120.28
1	A	70	VAL	CA-C-O	-27.73	92.11	120.95
1	G	130	ALA	CA-C-N	27.39	157.88	120.63
1	G	130	ALA	C-N-CA	27.39	157.88	120.63
1	C	135	VAL	CA-C-N	27.38	156.97	120.28
1	C	135	VAL	C-N-CA	27.38	156.97	120.28
1	E	25	GLY	O-C-N	27.36	148.71	122.17
1	G	27	GLU	CB-CG-CD	27.18	158.81	112.60
1	G	54	GLN	OE1-CD-NE2	27.15	149.75	122.60
1	A	9	ASN	CA-CB-CG	27.11	139.71	112.60
1	E	121	VAL	CA-C-N	27.10	157.30	120.44
1	E	121	VAL	C-N-CA	27.10	157.30	120.44
1	E	6	ASP	CA-CB-CG	26.99	139.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	19	ASN	CA-CB-CG	26.88	139.48	112.60
2	F	135	ALA	CA-C-N	26.81	173.95	121.41
2	F	135	ALA	C-N-CA	26.81	173.95	121.41
1	C	115	ALA	CA-C-N	26.76	156.67	120.54
1	C	115	ALA	C-N-CA	26.76	156.67	120.54
2	F	23	VAL	O-C-N	-26.74	91.58	121.80
1	C	105	LEU	CA-C-N	26.71	172.56	121.54
1	C	105	LEU	C-N-CA	26.71	172.56	121.54
1	G	141	ARG	NH1-CZ-NH2	26.68	153.98	119.30
2	H	40	ARG	NE-CZ-NH2	-26.65	95.21	119.20
1	G	35	SER	CA-C-O	26.58	150.37	119.27
2	D	121	GLU	CA-CB-CG	26.21	166.53	114.10
1	C	64	ASP	CA-CB-CG	-26.14	86.46	112.60
2	F	51	PRO	CA-C-N	26.11	156.14	120.63
2	F	51	PRO	C-N-CA	26.11	156.14	120.63
2	D	112	CYS	CA-C-O	-26.09	93.40	120.80
2	B	118	PHE	N-CA-C	26.03	145.50	113.23
2	H	117	HIS	CA-C-N	25.74	169.94	122.06
2	H	117	HIS	C-N-CA	25.74	169.94	122.06
1	C	126	ASP	CA-C-N	25.70	153.86	120.44
1	C	126	ASP	C-N-CA	25.70	153.86	120.44
2	H	110	LEU	CA-C-O	25.70	149.52	119.97
1	G	141	ARG	CA-CB-CG	25.67	165.44	114.10
2	H	3	LEU	O-C-N	25.61	152.55	123.10
2	D	45	PHE	CA-CB-CG	-25.58	88.22	113.80
1	A	109	LEU	CA-C-N	25.45	153.53	120.44
1	A	109	LEU	C-N-CA	25.45	153.53	120.44
2	H	39	GLN	OE1-CD-NE2	-25.11	97.49	122.60
1	E	102	SER	CA-C-O	-25.09	93.83	120.42
1	C	56	LYS	O-C-N	25.08	148.12	122.03
2	B	110	LEU	CA-C-O	-25.06	91.78	120.10
2	F	109	VAL	CA-C-O	24.91	147.15	120.25
2	H	15	TRP	CA-C-N	24.88	170.18	121.41
2	H	15	TRP	C-N-CA	24.88	170.18	121.41
1	A	106	LEU	CA-C-N	24.84	152.64	120.60
1	A	106	LEU	C-N-CA	24.84	152.64	120.60
2	H	38	THR	CA-CB-OG1	24.80	146.81	109.60
1	G	63	ALA	CA-C-N	24.79	153.37	120.65
1	G	63	ALA	C-N-CA	24.79	153.37	120.65
1	C	9	ASN	CA-CB-CG	-24.72	87.88	112.60
1	C	67	THR	CA-C-O	24.68	147.99	120.10
2	H	115	ALA	CA-C-N	24.65	155.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	115	ALA	C-N-CA	24.65	155.78	120.28
1	E	50	HIS	CA-C-O	-24.63	96.32	120.95
2	F	116	HIS	CB-CG-CD2	-24.57	99.26	131.20
1	A	116	GLU	CB-CG-CD	24.52	154.29	112.60
1	E	42	TYR	CB-CG-CD2	24.51	157.56	120.80
2	B	16	GLY	CA-C-O	24.50	145.44	120.45
1	G	126	ASP	CA-CB-CG	-24.38	88.22	112.60
2	F	60	VAL	CA-C-O	24.36	146.67	120.85
2	D	14	LEU	CA-C-O	24.36	150.71	119.05
1	G	105	LEU	CA-C-O	24.36	146.57	121.00
2	H	55	MET	CA-C-N	24.30	169.05	121.41
2	H	55	MET	C-N-CA	24.30	169.05	121.41
2	D	129	ALA	CA-C-O	24.27	146.52	120.55
1	A	70	VAL	CA-C-N	24.23	161.19	120.72
1	A	70	VAL	C-N-CA	24.23	161.19	120.72
1	C	9	ASN	OD1-CG-ND2	24.23	146.83	122.60
2	F	57	ASN	OD1-CG-ND2	-24.22	98.38	122.60
2	B	128	ALA	O-C-N	24.21	149.95	122.11
1	G	58	HIS	CA-C-N	24.20	146.84	119.98
1	G	58	HIS	C-N-CA	24.20	146.84	119.98
1	G	112	HIS	CA-CB-CG	-24.18	89.62	113.80
2	D	134	VAL	CA-C-N	24.15	152.64	120.28
2	D	134	VAL	C-N-CA	24.15	152.64	120.28
1	E	90	LYS	CA-C-O	23.83	155.66	120.16
2	D	50	THR	O-C-N	23.73	140.34	121.83
2	F	118	PHE	O-C-N	23.70	151.51	122.35
1	E	82	ALA	O-C-N	23.69	151.41	122.27
1	E	72	HIS	CA-C-N	23.67	164.58	121.97
1	E	72	HIS	C-N-CA	23.67	164.58	121.97
2	B	140	ALA	CA-C-O	-23.67	95.33	120.42
1	E	113	LEU	O-C-N	23.64	142.83	121.32
1	G	50	HIS	CA-C-O	-23.60	86.77	120.51
2	H	103	PHE	CA-CB-CG	23.59	137.39	113.80
1	E	82	ALA	CA-C-O	-23.57	92.87	119.97
1	C	99	LYS	O-C-N	23.55	152.94	122.33
1	G	50	HIS	CA-CB-CG	-23.54	90.26	113.80
1	C	68	ASN	CA-C-N	23.53	152.63	120.63
1	C	68	ASN	C-N-CA	23.53	152.63	120.63
2	F	39	GLN	OE1-CD-NE2	23.53	146.13	122.60
1	C	27	GLU	CA-C-O	23.51	149.61	119.05
2	H	43	GLU	CB-CG-CD	23.45	152.46	112.60
1	C	12	ALA	CA-C-O	-23.37	95.65	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	77	HIS	CB-CG-ND1	23.37	157.75	122.70
2	F	132	LYS	CA-C-O	-23.35	96.65	120.70
2	D	113	VAL	O-C-N	23.35	151.76	122.57
1	G	55	VAL	O-C-N	23.31	153.75	121.82
1	C	58	HIS	CA-CB-CG	-23.29	90.51	113.80
1	C	21	ALA	CA-C-N	23.15	149.62	120.22
1	C	21	ALA	C-N-CA	23.15	149.62	120.22
1	G	131	SER	CA-C-O	-23.11	97.10	120.90
2	B	104	ARG	CA-C-N	23.06	150.42	120.44
2	B	104	ARG	C-N-CA	23.06	150.42	120.44
2	H	135	ALA	CA-C-N	23.03	166.54	121.41
2	H	135	ALA	C-N-CA	23.03	166.54	121.41
1	G	47	ASP	CA-CB-CG	-23.01	89.59	112.60
2	H	11	VAL	O-C-N	22.75	152.51	122.26
2	D	126	VAL	CA-C-O	22.74	138.91	118.90
2	H	45	PHE	CA-C-N	22.73	141.18	121.86
2	H	45	PHE	C-N-CA	22.73	141.18	121.86
1	E	31	ARG	CD-NE-CZ	22.69	156.16	124.40
2	B	115	ALA	O-C-N	22.65	146.32	122.08
2	H	138	ALA	CA-C-N	22.65	152.45	120.29
2	H	138	ALA	C-N-CA	22.65	152.45	120.29
2	H	131	GLN	OE1-CD-NE2	-22.61	99.99	122.60
2	F	118	PHE	CA-CB-CG	22.57	136.37	113.80
2	H	98	VAL	CA-C-O	-22.55	95.33	121.04
1	C	56	LYS	N-CA-CB	22.54	142.82	109.91
2	F	63	HIS	CA-CB-CG	22.52	136.32	113.80
2	D	107	GLY	O-C-N	22.52	144.01	122.17
2	H	90	GLU	CA-C-N	22.52	159.08	120.58
2	H	90	GLU	C-N-CA	22.52	159.08	120.58
2	D	10	ALA	CA-C-N	22.46	162.40	121.97
2	D	10	ALA	C-N-CA	22.46	162.40	121.97
1	C	30	GLU	CA-C-O	-22.36	97.67	120.70
1	A	127	LYS	CA-CB-CG	22.34	158.79	114.10
2	H	63	HIS	N-CA-CB	22.33	143.77	109.82
1	G	50	HIS	O-C-N	22.27	152.21	122.59
2	B	47	ASP	CA-CB-CG	22.24	134.84	112.60
1	C	94	ASP	CA-C-N	22.22	145.25	119.47
1	C	94	ASP	C-N-CA	22.22	145.25	119.47
2	D	43	GLU	CA-C-N	22.19	160.51	122.79
2	D	43	GLU	C-N-CA	22.19	160.51	122.79
2	F	33	VAL	CA-C-O	22.14	143.17	119.92
2	B	131	GLN	OE1-CD-NE2	22.12	144.72	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	ALA	CA-C-O	-22.10	97.61	120.82
2	F	9	SER	CA-C-O	22.10	146.87	121.02
2	H	101	GLU	CA-C-N	22.09	150.67	120.63
2	H	101	GLU	C-N-CA	22.09	150.67	120.63
1	A	31	ARG	CD-NE-CZ	22.08	155.31	124.40
2	D	90	GLU	CA-C-N	22.02	149.06	120.44
2	D	90	GLU	C-N-CA	22.02	149.06	120.44
1	C	5	ALA	CA-C-O	21.96	144.40	120.90
1	A	107	VAL	CA-C-O	-21.94	98.45	121.27
2	F	91	LEU	CA-C-O	-21.94	97.42	120.90
1	C	31	ARG	CD-NE-CZ	-21.93	93.69	124.40
2	F	132	LYS	O-C-N	21.85	145.69	122.09
2	F	23	VAL	CA-C-O	-21.77	96.95	120.47
1	G	82	ALA	CA-C-N	21.75	152.13	120.38
1	G	82	ALA	C-N-CA	21.75	152.13	120.38
1	E	10	VAL	CA-C-O	-21.74	97.44	120.71
1	G	113	LEU	N-CA-CB	-21.71	84.17	111.09
1	C	111	ALA	CA-C-N	21.69	156.06	120.70
1	C	111	ALA	C-N-CA	21.69	156.06	120.70
1	C	138	SER	O-C-N	-21.66	99.16	122.12
1	G	58	HIS	CA-CB-CG	21.63	135.43	113.80
1	C	119	PRO	CA-C-O	21.62	147.62	118.86
1	E	4	PRO	CA-C-O	-21.58	91.71	118.90
2	B	43	GLU	CB-CG-CD	21.57	149.27	112.60
1	E	54	GLN	O-C-N	-21.48	99.10	122.08
2	H	30	ARG	CB-CG-CD	21.47	160.69	111.30
2	F	33	VAL	CA-C-N	21.33	147.86	120.56
2	F	33	VAL	C-N-CA	21.33	147.86	120.56
1	E	81	SER	CA-C-O	-21.26	96.14	121.02
1	G	82	ALA	O-C-N	-21.25	94.33	122.59
1	E	42	TYR	CB-CG-CD1	-21.22	88.97	120.80
2	H	98	VAL	N-CA-C	21.16	135.74	109.30
1	E	106	LEU	CA-C-N	21.11	159.96	121.97
1	E	106	LEU	C-N-CA	21.11	159.96	121.97
1	E	116	GLU	O-C-N	21.07	143.89	122.19
1	A	132	VAL	CA-C-O	-21.06	98.85	121.17
1	C	132	VAL	N-CA-C	-21.06	89.88	110.30
2	F	102	ASN	CA-CB-CG	20.99	133.59	112.60
2	B	145	TYR	CA-C-O	-20.99	97.33	121.47
2	B	2	HIS	CA-C-O	20.97	142.65	120.63
1	C	72	HIS	CA-C-N	20.97	159.71	121.97
1	C	72	HIS	C-N-CA	20.97	159.71	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	91	LEU	N-CA-CB	20.95	140.39	110.01
1	C	126	ASP	O-C-N	-20.94	94.74	122.59
2	B	61	LYS	CA-C-N	20.93	149.88	120.79
2	B	61	LYS	C-N-CA	20.93	149.88	120.79
2	F	94	ASP	CA-CB-CG	20.87	133.47	112.60
2	F	59	LYS	N-CA-C	-20.87	88.53	111.28
1	E	130	ALA	CA-C-O	20.86	142.72	120.82
1	C	94	ASP	O-C-N	-20.82	99.85	121.30
1	G	131	SER	N-CA-C	-20.79	87.95	111.03
1	G	87	HIS	CA-C-O	-20.78	98.19	120.63
2	F	9	SER	CA-C-N	20.75	149.63	120.79
2	F	9	SER	C-N-CA	20.75	149.63	120.79
1	E	78	ASN	CA-C-N	20.70	147.35	120.44
1	E	78	ASN	C-N-CA	20.70	147.35	120.44
2	B	112	CYS	CA-C-O	-20.62	99.15	120.80
1	C	47	ASP	CA-CB-CG	20.60	133.20	112.60
1	G	55	VAL	CA-C-O	-20.59	98.02	120.25
1	G	127	LYS	O-C-N	20.58	145.66	122.20
2	H	63	HIS	O-C-N	20.46	143.97	122.08
2	D	84	THR	N-CA-C	20.30	135.05	111.71
2	H	84	THR	O-C-N	-20.25	100.41	122.08
1	E	90	LYS	O-C-N	-20.18	95.68	121.92
2	F	27	ALA	CA-C-N	20.17	148.06	120.63
2	F	27	ALA	C-N-CA	20.17	148.06	120.63
1	E	51	GLY	CA-C-O	-20.16	95.87	119.06
2	B	38	THR	CB-CA-C	20.15	146.29	110.01
1	C	103	HIS	CB-CG-CD2	20.11	157.35	131.20
1	E	30	GLU	O-C-N	20.07	142.96	122.09
1	A	109	LEU	O-C-N	-20.04	97.63	122.27
1	G	46	PHE	CA-CB-CG	20.01	133.81	113.80
2	F	33	VAL	O-C-N	-20.00	92.04	122.04
1	G	114	PRO	CA-C-N	-20.00	96.23	123.03
1	G	114	PRO	C-N-CA	-20.00	96.23	123.03
2	F	79	ASP	CA-C-O	-19.98	97.17	119.14
1	C	71	ALA	CA-C-O	19.97	145.01	119.05
1	C	129	LEU	N-CA-CB	-19.97	77.25	110.39
2	H	45	PHE	CA-CB-CG	19.95	133.75	113.80
2	F	60	VAL	O-C-N	-19.93	101.31	121.83
1	G	23	GLU	CA-C-O	-19.91	99.44	120.55
1	C	67	THR	O-C-N	-19.86	98.98	122.22
2	H	129	ALA	CA-C-N	19.85	154.43	120.68
2	H	129	ALA	C-N-CA	19.85	154.43	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	9	ASN	O-C-N	19.80	142.68	122.09
2	F	131	GLN	OE1-CD-NE2	-19.75	102.85	122.60
1	C	57	GLY	CA-C-N	19.74	147.47	120.63
1	C	57	GLY	C-N-CA	19.74	147.47	120.63
2	F	104	ARG	CA-C-O	19.69	141.49	120.82
2	B	41	PHE	CA-CB-CG	19.69	133.49	113.80
1	A	67	THR	CA-CB-OG1	-19.68	80.08	109.60
2	F	82	LYS	O-C-N	19.64	148.71	122.59
2	F	100	PRO	O-C-N	-19.59	99.71	122.24
1	C	46	PHE	CA-CB-CG	19.59	133.38	113.80
1	E	70	VAL	O-C-N	19.57	148.62	121.82
1	E	11	LYS	CA-C-O	19.54	141.33	120.82
1	A	103	HIS	CA-CB-CG	-19.42	94.38	113.80
2	B	114	LEU	O-C-N	19.41	144.27	122.15
1	C	78	ASN	CB-CG-ND2	-19.39	87.32	116.40
1	C	54	GLN	O-C-N	19.38	142.03	122.07
1	G	6	ASP	CA-CB-CG	19.38	131.98	112.60
1	C	74	ASP	CA-C-O	19.37	141.94	119.67
1	E	75	ASP	CA-C-O	19.35	143.46	121.78
1	A	109	LEU	CA-C-O	19.34	142.22	119.97
1	E	24	TYR	CA-C-O	19.34	141.05	120.55
2	F	108	ASN	OD1-CG-ND2	-19.34	103.27	122.60
1	A	58	HIS	CA-C-O	19.33	142.57	120.92
1	C	120	ALA	N-CA-C	-19.33	89.90	110.97
2	F	45	PHE	CA-CB-CG	19.33	133.13	113.80
2	B	118	PHE	CA-C-N	19.26	152.79	120.25
2	B	118	PHE	C-N-CA	19.26	152.79	120.25
1	E	74	ASP	CA-CB-CG	19.24	131.84	112.60
2	B	65	LYS	CA-C-O	19.21	140.92	120.55
2	D	131	GLN	CA-C-O	-19.21	100.06	120.42
2	D	74	GLY	CA-C-O	-19.18	96.86	119.50
2	D	31	LEU	CA-C-N	19.17	147.89	120.28
2	D	31	LEU	C-N-CA	19.17	147.89	120.28
1	G	37	PRO	O-C-N	-19.17	96.76	122.64
1	C	31	ARG	NE-CZ-NH2	-19.17	101.95	119.20
2	H	102	ASN	O-C-N	19.15	142.71	122.03
2	F	111	VAL	CA-C-O	19.11	140.89	120.25
2	B	11	VAL	CA-C-N	19.10	146.32	120.54
2	B	11	VAL	C-N-CA	19.10	146.32	120.54
2	F	116	HIS	CB-CG-ND1	19.09	151.34	122.70
2	H	59	LYS	N-CA-C	-19.09	87.89	112.90
2	H	131	GLN	N-CA-CB	19.09	141.51	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	60	LYS	CB-CG-CD	19.09	155.20	111.30
2	D	82	LYS	CA-C-O	19.05	140.75	120.55
2	D	30	ARG	CD-NE-CZ	19.03	151.04	124.40
2	B	108	ASN	CA-C-N	19.02	144.09	120.88
2	B	108	ASN	C-N-CA	19.02	144.09	120.88
1	C	129	LEU	CB-CA-C	19.00	150.01	110.31
1	A	52	SER	CA-C-N	18.98	148.09	120.38
1	A	52	SER	C-N-CA	18.98	148.09	120.38
2	B	7	GLU	O-C-N	-18.89	101.97	122.38
1	G	125	LEU	CA-C-O	-18.86	98.28	119.97
2	D	77	HIS	ND1-CG-CD2	-18.85	87.25	106.10
2	B	139	ASN	O-C-N	18.84	142.09	122.12
2	F	8	LYS	CA-C-O	-18.80	100.49	120.42
2	H	129	ALA	CA-C-O	-18.80	100.49	120.42
1	E	116	GLU	CG-CD-OE1	18.78	161.59	118.40
1	A	140	TYR	CA-C-O	18.77	142.96	120.62
2	F	31	LEU	CA-C-O	18.76	141.06	120.24
2	H	61	LYS	CA-C-N	18.75	152.64	120.58
2	H	61	LYS	C-N-CA	18.75	152.64	120.58
1	G	87	HIS	CA-CB-CG	-18.73	95.07	113.80
2	H	38	THR	CA-C-O	18.72	141.02	120.24
2	D	21	ASP	CA-CB-CG	-18.71	93.89	112.60
1	G	23	GLU	N-CA-C	18.68	131.64	111.28
2	D	57	ASN	OD1-CG-ND2	18.67	141.27	122.60
2	D	100	PRO	CB-CA-C	18.67	143.14	111.21
1	G	113	LEU	CA-C-N	18.67	143.18	119.84
1	G	113	LEU	C-N-CA	18.67	143.18	119.84
2	B	104	ARG	NE-CZ-NH2	18.67	136.00	119.20
2	H	103	PHE	CB-CA-C	18.65	142.38	110.68
1	E	33	PHE	O-C-N	-18.63	102.37	122.12
2	B	67	VAL	CA-C-O	-18.58	101.48	121.17
2	D	86	ALA	CA-C-O	18.58	140.43	120.55
1	C	141	ARG	CA-CB-CG	18.55	151.19	114.10
1	G	108	THR	O-C-N	18.54	141.16	122.07
1	G	134	THR	CA-C-N	18.53	143.86	120.70
1	G	134	THR	C-N-CA	18.53	143.86	120.70
2	B	7	GLU	CA-C-O	18.52	141.08	120.71
1	G	102	SER	N-CA-C	-18.50	90.44	111.71
1	C	45	HIS	CA-CB-CG	-18.47	95.33	113.80
1	G	117	PHE	CA-CB-CG	-18.47	95.33	113.80
1	G	8	THR	CA-C-N	18.47	144.45	120.44
1	G	8	THR	C-N-CA	18.47	144.45	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	78	ASN	CB-CG-ND2	-18.43	88.76	116.40
2	H	19	ASN	CA-C-N	18.40	144.87	120.77
2	H	19	ASN	C-N-CA	18.40	144.87	120.77
2	B	23	VAL	CA-C-N	18.39	157.46	121.41
2	B	23	VAL	C-N-CA	18.39	157.46	121.41
2	D	117	HIS	CB-CG-ND1	-18.38	95.14	122.70
2	H	30	ARG	CA-C-O	-18.36	99.35	120.10
2	D	39	GLN	CA-C-O	18.36	140.77	120.20
1	E	85	ASP	CA-C-O	-18.36	100.81	120.63
1	A	101	LEU	CA-C-O	-18.35	101.53	120.80
2	F	144	LYS	CA-C-O	-18.34	96.49	120.15
2	D	34	VAL	CB-CA-C	18.32	137.49	111.65
1	G	83	LEU	CA-C-N	18.31	144.82	120.65
1	G	83	LEU	C-N-CA	18.31	144.82	120.65
2	D	99	ASP	O-C-N	18.30	142.36	121.32
1	C	83	LEU	CA-C-O	18.27	140.97	119.60
1	G	91	LEU	CA-C-N	18.26	156.42	121.54
1	G	91	LEU	C-N-CA	18.26	156.42	121.54
2	H	146	HIS	CA-CB-CG	-18.25	95.55	113.80
1	A	130	ALA	O-C-N	18.24	144.27	122.20
1	C	141	ARG	CD-NE-CZ	-18.24	98.87	124.40
2	D	146	HIS	CA-CB-CG	-18.24	95.56	113.80
1	G	21	ALA	O-C-N	18.24	144.26	122.20
1	G	127	LYS	CA-C-O	-18.20	99.81	120.20
1	E	32	MET	CA-C-O	-18.19	101.06	121.07
1	G	101	LEU	CA-C-O	18.18	139.69	120.42
1	E	131	SER	CA-C-O	18.18	140.35	120.90
2	D	101	GLU	N-CA-C	-18.17	90.37	112.54
1	C	84	SER	O-C-N	18.14	140.76	122.07
1	E	31	ARG	CB-CA-C	18.14	138.90	110.96
2	D	108	ASN	OD1-CG-ND2	-18.14	104.46	122.60
2	D	80	ASN	CA-CB-CG	-18.09	94.51	112.60
2	D	113	VAL	CA-C-O	-18.09	98.17	120.78
1	G	131	SER	N-CA-CB	18.08	136.20	109.98
2	D	23	VAL	N-CA-CB	18.06	135.10	110.54
1	A	92	ARG	CA-C-O	18.04	142.76	121.84
1	G	16	LYS	N-CA-C	18.02	134.63	113.19
2	D	71	PHE	CA-C-N	18.01	155.94	121.54
2	D	71	PHE	C-N-CA	18.01	155.94	121.54
2	H	89	SER	N-CA-CB	18.00	140.91	110.49
1	C	50	HIS	CB-CG-CD2	-17.98	107.83	131.20
2	D	74	GLY	N-CA-C	-17.98	92.41	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	54	GLN	CB-CA-C	17.98	139.50	110.92
2	F	118	PHE	CA-C-O	-17.98	98.39	119.78
1	G	125	LEU	O-C-N	17.96	144.36	122.27
1	A	58	HIS	CE1-NE2-CD2	17.88	126.88	109.00
2	F	40	ARG	NE-CZ-NH2	-17.88	103.11	119.20
2	H	130	TYR	CA-C-O	17.83	140.83	119.79
1	C	131	SER	CA-CB-OG	17.81	146.73	111.10
2	B	139	ASN	CA-CB-CG	-17.80	94.80	112.60
1	C	53	ALA	CA-C-N	17.80	143.59	120.44
1	C	53	ALA	C-N-CA	17.80	143.59	120.44
1	C	50	HIS	CB-CA-C	17.77	136.92	110.26
2	D	25	GLY	CA-C-O	17.75	142.09	119.01
2	H	142	ALA	CA-C-N	17.75	147.44	120.82
2	H	142	ALA	C-N-CA	17.75	147.44	120.82
1	E	138	SER	CA-C-O	-17.72	101.63	120.42
1	A	113	LEU	O-C-N	17.70	135.56	121.23
1	G	134	THR	CA-CB-CG2	17.69	140.57	110.50
2	F	142	ALA	CA-C-O	17.68	138.50	119.05
2	D	22	GLU	CA-CB-CG	17.66	149.43	114.10
2	D	108	ASN	CB-CG-OD1	17.64	156.08	120.80
1	A	97	ASN	CA-CB-CG	17.63	130.23	112.60
1	G	39	THR	CA-C-O	17.63	140.16	119.18
2	H	90	GLU	CA-C-O	-17.63	100.18	120.10
1	G	64	ASP	N-CA-C	-17.62	91.77	110.97
1	E	61	LYS	CA-CB-CG	17.61	149.31	114.10
1	G	83	LEU	CA-CB-CG	17.59	177.88	116.30
2	D	20	VAL	CA-C-N	17.57	144.27	120.54
2	D	20	VAL	C-N-CA	17.57	144.27	120.54
2	F	108	ASN	CA-C-O	-17.55	97.54	119.31
1	A	61	LYS	O-C-N	17.54	141.04	122.09
1	E	38	THR	O-C-N	17.47	140.26	122.09
1	E	141	ARG	CA-CB-CG	17.47	149.04	114.10
2	F	43	GLU	CA-C-O	17.47	141.95	121.34
1	C	139	LYS	N-CA-CB	-17.44	86.50	110.56
1	G	40	LYS	CA-C-N	17.42	154.81	121.54
1	G	40	LYS	C-N-CA	17.42	154.81	121.54
2	D	117	HIS	CB-CG-CD2	17.42	153.84	131.20
2	B	57	ASN	CA-C-N	17.39	137.81	118.85
2	B	57	ASN	C-N-CA	17.39	137.81	118.85
2	D	6	VAL	CA-C-N	17.38	143.59	120.65
2	D	6	VAL	C-N-CA	17.38	143.59	120.65
1	E	72	HIS	ND1-CE1-NE2	17.37	125.77	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	36	PHE	CA-CB-CG	17.35	131.15	113.80
2	F	63	HIS	CA-C-N	-17.29	100.98	120.00
2	F	63	HIS	C-N-CA	-17.29	100.98	120.00
2	D	87	THR	CA-C-N	-17.29	92.94	120.60
2	D	87	THR	C-N-CA	-17.29	92.94	120.60
2	H	66	LYS	CA-C-N	17.27	141.79	120.72
2	H	66	LYS	C-N-CA	17.27	141.79	120.72
2	B	44	SER	CA-C-O	17.25	140.70	119.31
2	D	91	LEU	CA-C-O	-17.21	102.75	120.82
1	C	20	HIS	CB-CG-CD2	17.19	153.54	131.20
1	G	7	LYS	CA-C-N	-17.17	95.90	120.29
1	G	7	LYS	C-N-CA	-17.17	95.90	120.29
1	E	33	PHE	CB-CG-CD2	17.16	149.86	120.70
1	E	45	HIS	CA-C-N	17.16	149.75	122.81
1	E	45	HIS	C-N-CA	17.16	149.75	122.81
2	D	128	ALA	CA-C-N	17.09	149.26	120.71
2	D	128	ALA	C-N-CA	17.09	149.26	120.71
1	A	56	LYS	CA-C-O	-17.07	102.28	120.55
1	E	122	HIS	N-CA-C	-17.07	92.71	111.14
1	E	136	LEU	CA-C-N	-17.07	95.70	122.49
1	E	136	LEU	C-N-CA	-17.07	95.70	122.49
1	E	65	ALA	CA-C-N	17.04	143.55	120.54
1	E	65	ALA	C-N-CA	17.04	143.55	120.54
2	F	91	LEU	O-C-N	16.98	139.75	122.09
1	A	107	VAL	CB-CA-C	16.98	133.62	111.88
1	A	101	LEU	O-C-N	16.93	141.74	122.11
1	C	72	HIS	CA-C-O	-16.90	99.50	119.95
1	A	66	LEU	O-C-N	16.87	144.16	122.23
2	D	101	GLU	CA-CB-CG	16.87	147.84	114.10
2	B	128	ALA	CA-C-O	-16.86	102.03	120.92
2	B	98	VAL	O-C-N	16.85	141.90	122.69
1	G	128	PHE	CA-C-N	16.85	147.56	120.60
1	G	128	PHE	C-N-CA	16.85	147.56	120.60
2	H	146	HIS	CB-CG-CD2	16.85	153.10	131.20
2	B	146	HIS	CA-CB-CG	-16.83	96.97	113.80
2	H	6	VAL	CA-C-O	16.82	139.13	120.46
1	E	124	SER	N-CA-C	-16.80	93.04	111.36
1	A	23	GLU	O-C-N	16.80	144.87	122.36
2	H	87	THR	N-CA-CB	16.79	138.86	110.49
2	H	123	THR	N-CA-CB	16.79	132.95	110.29
1	E	41	THR	N-CA-CB	16.78	138.85	110.49
2	D	28	LEU	N-CA-CB	16.77	134.93	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	98	VAL	CB-CA-C	16.77	135.81	110.83
1	C	29	LEU	N-CA-C	-16.76	93.14	111.07
1	C	103	HIS	CB-CG-ND1	-16.75	97.57	122.70
2	B	19	ASN	N-CA-CB	16.75	138.01	110.37
2	D	121	GLU	CA-C-O	16.73	139.21	119.97
1	A	134	THR	CA-C-O	16.73	144.43	120.51
2	H	59	LYS	CB-CA-C	16.72	143.29	109.67
1	C	87	HIS	CB-CG-CD2	16.72	152.94	131.20
2	F	40	ARG	NE-CZ-NH1	16.72	138.22	121.50
1	E	120	ALA	N-CA-C	16.72	133.41	113.18
2	D	97	HIS	CA-C-N	-16.70	102.48	123.19
2	D	97	HIS	C-N-CA	-16.70	102.48	123.19
1	E	36	PHE	CA-CB-CG	16.67	130.47	113.80
2	D	54	VAL	CA-C-O	16.65	141.59	120.78
1	G	11	LYS	CA-C-N	16.64	143.07	120.44
1	G	11	LYS	C-N-CA	16.64	143.07	120.44
2	D	117	HIS	CA-CB-CG	-16.63	97.17	113.80
1	A	104	CYS	CA-C-N	16.63	148.47	120.71
1	A	104	CYS	C-N-CA	16.63	148.47	120.71
2	H	13	ALA	CA-C-O	-16.61	103.79	120.90
2	B	39	GLN	CB-CA-C	16.58	138.87	110.68
1	G	55	VAL	CA-C-N	-16.58	95.11	120.31
1	G	55	VAL	C-N-CA	-16.58	95.11	120.31
2	B	129	ALA	O-C-N	-16.57	98.24	122.43
2	D	138	ALA	CA-C-O	16.57	138.63	120.90
1	G	106	LEU	CA-C-N	16.56	141.43	120.56
1	G	106	LEU	C-N-CA	16.56	141.43	120.56
1	C	124	SER	CA-C-N	16.53	153.12	121.54
1	C	124	SER	C-N-CA	16.53	153.12	121.54
1	E	84	SER	N-CA-C	-16.52	91.37	111.69
2	B	143	HIS	CB-CG-ND1	16.50	147.45	122.70
1	C	141	ARG	NE-CZ-NH1	16.50	138.00	121.50
2	B	63	HIS	CA-CB-CG	-16.49	97.31	113.80
1	A	117	PHE	CA-CB-CG	-16.48	97.32	113.80
2	B	73	ASP	CA-CB-CG	-16.48	96.12	112.60
2	B	104	ARG	O-C-N	-16.46	102.02	122.27
2	H	28	LEU	N-CA-C	-16.46	93.42	111.36
1	E	122	HIS	CA-C-O	-16.46	103.75	120.70
1	C	26	ALA	CA-C-O	-16.45	100.38	119.79
1	A	52	SER	N-CA-CB	16.44	135.03	109.71
2	D	120	LYS	CB-CG-CD	16.40	149.03	111.30
2	B	90	GLU	CA-C-O	-16.40	101.83	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	94	ASP	CA-CB-CG	-16.37	96.23	112.60
2	B	95	LYS	CA-C-N	16.37	147.39	120.88
2	B	95	LYS	C-N-CA	16.37	147.39	120.88
2	D	70	ALA	CA-C-N	16.36	142.88	120.63
2	D	70	ALA	C-N-CA	16.36	142.88	120.63
2	F	96	LEU	CB-CA-C	16.35	140.62	110.70
2	B	10	ALA	CA-C-O	16.33	137.86	120.55
2	B	17	LYS	CA-C-O	-16.32	103.09	120.55
2	D	47	ASP	O-C-N	16.31	143.09	123.02
2	F	59	LYS	CB-CA-C	16.31	137.86	110.79
1	G	53	ALA	CA-C-O	-16.31	98.55	119.10
1	C	31	ARG	NE-CZ-NH1	16.30	137.80	121.50
1	C	126	ASP	CA-C-O	16.30	143.82	120.51
2	B	43	GLU	CA-CB-CG	16.30	146.69	114.10
2	D	77	HIS	N-CA-CB	-16.29	72.48	111.74
2	D	127	GLN	CA-C-N	16.29	143.42	120.29
2	D	127	GLN	C-N-CA	16.29	143.42	120.29
2	D	133	VAL	O-C-N	16.29	138.84	121.90
1	G	90	LYS	N-CA-CB	16.29	138.01	110.49
2	H	139	ASN	CB-CG-OD1	16.28	153.37	120.80
2	B	9	SER	N-CA-CB	16.26	133.65	109.91
2	H	64	GLY	CA-C-O	-16.25	104.02	120.75
2	D	115	ALA	CA-C-O	16.25	138.94	121.07
1	E	73	VAL	CA-C-O	16.24	141.08	120.78
1	A	107	VAL	N-CA-C	-16.23	93.32	110.36
2	H	20	VAL	CB-CA-C	-16.20	90.97	111.70
1	E	5	ALA	N-CA-CB	16.20	135.24	110.30
1	C	98	PHE	CA-CB-CG	-16.19	97.61	113.80
1	C	55	VAL	CB-CA-C	-16.19	89.88	112.22
1	G	78	ASN	OD1-CG-ND2	16.19	138.79	122.60
1	A	58	HIS	CA-C-N	16.18	137.90	119.94
1	A	58	HIS	C-N-CA	16.18	137.90	119.94
2	H	133	VAL	O-C-N	16.17	138.72	121.90
2	F	60	VAL	N-CA-C	16.17	127.05	110.72
2	F	30	ARG	NH1-CZ-NH2	16.16	140.31	119.30
2	D	52	ASP	CA-C-O	16.16	137.68	120.55
1	C	31	ARG	N-CA-CB	16.15	137.20	110.39
2	F	29	GLY	CA-C-O	16.14	138.43	121.00
1	G	75	ASP	O-C-N	16.14	151.82	122.44
1	C	69	ALA	O-C-N	16.13	139.45	122.03
1	A	77	PRO	O-C-N	16.13	139.60	122.18
1	C	61	LYS	CA-CB-CG	16.11	146.32	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	8	THR	N-CA-C	16.10	128.91	111.36
2	D	20	VAL	CA-C-O	-16.09	100.66	120.78
1	C	93	VAL	CA-C-N	-16.09	98.02	120.39
1	C	93	VAL	C-N-CA	-16.09	98.02	120.39
1	A	92	ARG	NE-CZ-NH1	-16.09	105.41	121.50
1	G	35	SER	O-C-N	-16.07	100.45	122.46
1	G	20	HIS	CA-CB-CG	-16.06	97.74	113.80
2	H	63	HIS	CA-C-O	-16.04	103.43	121.07
2	B	135	ALA	CB-CA-C	16.01	135.77	110.95
1	G	55	VAL	N-CA-C	-15.99	90.01	111.44
2	H	50	THR	N-CA-CB	-15.98	96.25	111.27
2	F	42	PHE	CB-CG-CD2	15.97	147.85	120.70
2	H	29	GLY	CA-C-O	15.96	148.35	120.57
1	A	103	HIS	CE1-NE2-CD2	15.94	124.94	109.00
1	E	70	VAL	CA-C-O	-15.93	103.05	120.25
2	D	98	VAL	N-CA-CB	-15.93	89.59	111.25
1	G	7	LYS	CB-CG-CD	15.93	147.94	111.30
2	B	103	PHE	CA-C-N	-15.91	96.12	120.31
2	B	103	PHE	C-N-CA	-15.91	96.12	120.31
2	F	79	ASP	O-C-N	15.90	143.79	122.49
2	D	84	THR	CA-CB-OG1	-15.89	85.76	109.60
2	B	20	VAL	CA-C-O	-15.88	102.07	120.96
2	D	79	ASP	CA-C-O	15.84	138.19	119.97
1	C	62	VAL	CA-CB-CG2	15.84	137.33	110.40
1	G	61	LYS	CB-CA-C	15.83	137.77	110.85
2	H	104	ARG	NE-CZ-NH1	15.83	137.33	121.50
2	B	113	VAL	CA-C-N	15.83	142.76	120.29
2	B	113	VAL	C-N-CA	15.83	142.76	120.29
1	G	69	ALA	N-CA-CB	-15.81	86.64	110.20
1	C	131	SER	CA-C-O	15.80	137.78	120.24
2	D	108	ASN	CA-C-O	-15.80	99.72	119.31
2	B	127	GLN	CA-CB-CG	-15.79	82.53	114.10
2	D	96	LEU	CA-C-N	15.78	145.56	122.36
2	D	96	LEU	C-N-CA	15.78	145.56	122.36
1	E	70	VAL	N-CA-C	-15.78	90.29	111.44
1	C	61	LYS	O-C-N	15.77	140.13	122.15
2	H	88	LEU	CA-C-O	-15.76	97.97	120.51
1	C	20	HIS	CA-C-N	15.74	151.60	121.54
1	C	20	HIS	C-N-CA	15.74	151.60	121.54
1	C	141	ARG	CG-CD-NE	-15.73	77.39	112.00
2	F	67	VAL	CB-CA-C	15.73	137.08	111.29
1	E	98	PHE	O-C-N	-15.71	104.24	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	57	ASN	CA-C-O	15.71	134.91	119.51
1	E	123	ALA	O-C-N	15.68	143.44	122.59
2	B	63	HIS	CA-C-N	15.67	137.34	119.94
2	B	63	HIS	C-N-CA	15.67	137.34	119.94
2	H	20	VAL	O-C-N	15.66	138.88	121.96
2	H	113	VAL	CA-C-O	-15.65	104.67	120.95
2	F	136	GLY	O-C-N	15.65	143.04	122.70
2	H	108	ASN	CB-CG-ND2	-15.65	92.93	116.40
1	A	72	HIS	CA-CB-CG	-15.63	98.17	113.80
2	H	62	ALA	O-C-N	15.62	142.53	122.23
1	A	125	LEU	CA-C-O	15.62	136.97	120.42
1	E	36	PHE	CA-C-O	15.61	138.64	121.00
1	G	114	PRO	O-C-N	15.61	143.71	122.64
2	H	44	SER	CA-C-N	15.60	146.78	120.72
2	H	44	SER	C-N-CA	15.60	146.78	120.72
2	H	39	GLN	N-CA-CB	-15.59	84.14	110.49
1	G	36	PHE	CA-C-O	15.59	138.42	121.28
2	H	102	ASN	CA-C-O	-15.54	104.89	120.90
2	B	94	ASP	N-CA-C	15.54	128.22	111.28
2	F	97	HIS	CB-CG-ND1	15.53	145.99	122.70
2	D	137	VAL	CA-C-N	15.52	141.49	120.54
2	D	137	VAL	C-N-CA	15.52	141.49	120.54
2	D	84	THR	CA-C-N	15.51	148.07	122.79
2	D	84	THR	C-N-CA	15.51	148.07	122.79
2	B	72	SER	O-C-N	15.50	140.36	122.22
1	E	122	HIS	CA-C-N	15.49	151.14	121.54
1	E	122	HIS	C-N-CA	15.49	151.14	121.54
1	A	61	LYS	CA-C-N	-15.49	101.34	120.70
1	A	61	LYS	C-N-CA	-15.49	101.34	120.70
1	C	10	VAL	CA-C-N	15.49	141.45	120.54
1	C	10	VAL	C-N-CA	15.49	141.45	120.54
2	D	38	THR	N-CA-C	-15.49	94.44	113.18
1	A	136	LEU	O-C-N	-15.48	104.55	122.20
1	G	32	MET	CA-C-O	15.46	138.08	121.07
2	H	111	VAL	CB-CA-C	15.46	133.01	112.14
1	C	116	GLU	CA-C-N	15.45	151.05	121.54
1	C	116	GLU	C-N-CA	15.45	151.05	121.54
1	C	61	LYS	CA-C-O	-15.39	104.11	120.42
1	G	96	VAL	O-C-N	15.38	136.79	121.87
1	C	41	THR	CA-CB-OG1	-15.37	86.55	109.60
1	E	15	GLY	CA-C-O	15.36	147.29	120.57
2	F	8	LYS	O-C-N	15.34	139.63	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	73	ASP	CA-CB-CG	-15.32	97.28	112.60
2	D	10	ALA	O-C-N	-15.31	106.30	122.07
2	B	144	LYS	CA-CB-CG	15.31	144.72	114.10
2	B	101	GLU	O-C-N	15.28	141.07	122.27
2	B	126	VAL	CA-CB-CG2	-15.27	84.45	110.40
2	D	86	ALA	N-CA-CB	-15.26	87.54	110.13
1	E	90	LYS	CA-C-N	15.26	146.19	120.71
1	E	90	LYS	C-N-CA	15.26	146.19	120.71
1	C	81	SER	CA-C-N	15.26	142.25	120.28
1	C	81	SER	C-N-CA	15.26	142.25	120.28
1	C	113	LEU	N-CA-CB	-15.26	92.17	111.09
2	B	42	PHE	N-CA-C	15.25	130.40	110.88
1	E	38	THR	CA-C-O	-15.24	104.59	120.90
2	H	139	ASN	OD1-CG-ND2	-15.22	107.38	122.60
1	A	105	LEU	O-C-N	15.18	140.54	122.17
1	C	18	GLY	O-C-N	15.17	142.41	122.70
2	H	87	THR	CA-C-O	-15.17	98.82	120.51
1	E	89	HIS	CA-C-O	-15.16	101.28	119.32
2	B	72	SER	CA-CB-OG	15.15	141.40	111.10
2	D	101	GLU	N-CA-CB	15.15	135.54	110.39
2	D	67	VAL	CA-C-O	-15.15	104.79	120.85
2	D	118	PHE	CA-CB-CG	15.15	128.95	113.80
2	D	99	ASP	N-CA-CB	15.13	137.31	110.37
1	E	102	SER	O-C-N	15.13	139.40	122.15
2	B	19	ASN	O-C-N	15.10	141.02	123.05
2	F	25	GLY	O-C-N	15.10	140.35	122.84
2	F	112	CYS	CA-C-N	15.08	139.56	120.56
2	F	112	CYS	C-N-CA	15.08	139.56	120.56
2	H	111	VAL	CA-C-O	-15.05	105.29	120.95
2	B	7	GLU	CA-C-N	15.05	140.45	120.28
2	B	7	GLU	C-N-CA	15.05	140.45	120.28
1	A	126	ASP	CB-CA-C	15.01	134.79	110.92
2	D	22	GLU	N-CA-C	-15.01	93.24	112.90
1	G	97	ASN	CA-C-O	15.00	137.91	119.31
2	H	45	PHE	N-CA-C	15.00	130.84	112.54
2	F	39	GLN	CG-CD-NE2	-14.99	93.92	116.40
1	A	38	THR	O-C-N	14.98	138.00	122.12
2	F	109	VAL	CB-CA-C	14.97	136.56	112.16
2	F	139	ASN	OD1-CG-ND2	-14.97	107.63	122.60
1	A	112	HIS	CA-C-N	14.96	139.31	122.85
1	A	112	HIS	C-N-CA	14.96	139.31	122.85
2	F	137	VAL	N-CA-C	-14.96	96.31	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	69	GLY	O-C-N	14.96	139.58	122.68
1	C	81	SER	CA-CB-OG	-14.95	81.20	111.10
2	D	116	HIS	ND1-CE1-NE2	14.95	123.35	108.40
1	C	20	HIS	CB-CG-ND1	-14.93	100.30	122.70
1	E	7	LYS	N-CA-CB	14.93	131.66	110.01
2	F	102	ASN	OD1-CG-ND2	-14.93	107.67	122.60
1	E	104	CYS	CB-CA-C	-14.93	87.19	110.92
2	B	144	LYS	CA-C-N	14.92	146.16	121.39
2	B	144	LYS	C-N-CA	14.92	146.16	121.39
1	G	137	THR	CA-CB-OG1	-14.91	87.23	109.60
2	H	91	LEU	CA-C-O	14.91	136.79	120.24
1	E	15	GLY	O-C-N	-14.91	103.32	122.70
1	A	100	LEU	CA-C-O	-14.90	104.75	120.55
1	C	6	ASP	CA-CB-CG	-14.90	97.70	112.60
2	D	131	GLN	CA-C-N	14.90	148.94	121.52
2	D	131	GLN	C-N-CA	14.90	148.94	121.52
1	E	10	VAL	O-C-N	-14.89	102.18	121.84
1	G	33	PHE	CA-C-O	-14.89	104.69	121.07
1	C	63	ALA	O-C-N	14.89	137.40	122.07
1	C	117	PHE	CA-C-O	14.89	141.80	120.51
1	G	50	HIS	CA-C-N	14.88	150.58	121.41
1	G	50	HIS	C-N-CA	14.88	150.58	121.41
1	A	4	PRO	CA-C-O	14.87	143.06	119.86
2	H	136	GLY	CA-C-N	14.86	139.59	120.56
2	H	136	GLY	C-N-CA	14.86	139.59	120.56
1	C	67	THR	CA-CB-OG1	14.85	131.88	109.60
2	D	120	LYS	O-C-N	-14.85	104.01	122.27
2	H	131	GLN	N-CA-C	-14.85	94.48	112.89
2	D	130	TYR	N-CA-CB	14.84	133.07	110.22
1	C	72	HIS	CB-CG-ND1	14.83	144.95	122.70
2	D	13	ALA	N-CA-CB	14.83	135.25	110.33
2	H	47	ASP	O-C-N	14.82	141.25	123.02
1	G	103	HIS	N-CA-CB	14.81	132.32	110.26
1	A	95	PRO	CA-C-N	14.80	144.58	120.30
1	A	95	PRO	C-N-CA	14.80	144.58	120.30
2	F	97	HIS	CB-CG-CD2	-14.80	111.96	131.20
1	A	132	VAL	CA-CB-CG1	14.79	135.55	110.40
2	F	129	ALA	N-CA-C	-14.79	95.24	111.36
1	A	58	HIS	CA-CB-CG	-14.79	99.01	113.80
2	F	80	ASN	CA-C-N	14.79	142.79	120.31
2	F	80	ASN	C-N-CA	14.79	142.79	120.31
2	H	12	THR	CA-C-O	-14.79	101.96	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	LEU	CB-CA-C	14.78	139.14	110.46
2	H	84	THR	N-CA-C	14.79	129.06	111.02
1	G	126	ASP	CA-C-N	14.78	141.96	120.38
1	G	126	ASP	C-N-CA	14.78	141.96	120.38
2	F	53	ALA	N-CA-C	-14.77	95.27	111.07
1	A	97	ASN	OD1-CG-ND2	-14.76	107.84	122.60
1	C	9	ASN	CA-C-O	-14.76	105.11	120.90
1	C	41	THR	O-C-N	14.75	139.48	122.22
1	E	96	VAL	O-C-N	14.74	136.76	121.87
2	B	62	ALA	N-CA-C	14.74	129.00	111.02
1	E	19	ALA	CA-C-O	-14.73	102.25	119.78
2	F	139	ASN	CA-C-O	14.71	136.73	120.10
2	B	28	LEU	N-CA-C	-14.71	93.69	112.23
1	G	115	ALA	CB-CA-C	14.71	133.48	111.85
1	A	138	SER	O-C-N	-14.68	105.23	122.11
2	B	136	GLY	CA-C-N	-14.68	102.81	120.72
2	B	136	GLY	C-N-CA	-14.68	102.81	120.72
1	G	61	LYS	N-CA-C	-14.67	95.37	111.36
1	G	76	MET	CA-CB-CG	14.64	143.38	114.10
1	E	109	LEU	CA-C-O	-14.62	103.58	120.10
2	H	34	VAL	O-C-N	14.62	140.91	121.90
1	C	38	THR	CA-CB-OG1	14.62	131.53	109.60
2	D	118	PHE	O-C-N	-14.62	102.43	122.46
1	A	132	VAL	N-CA-CB	14.61	127.65	110.55
2	F	44	SER	N-CA-C	-14.61	95.14	113.55
2	H	34	VAL	CA-C-O	-14.60	103.58	120.96
1	E	118	THR	N-CA-CB	-14.60	90.58	109.55
2	H	133	VAL	CA-C-O	-14.59	104.85	121.05
2	B	38	THR	OG1-CB-CG2	-14.58	80.15	109.30
1	C	107	VAL	CA-C-O	-14.58	105.79	120.95
1	A	58	HIS	CB-CG-CD2	-14.57	112.26	131.20
2	B	19	ASN	CB-CG-ND2	14.56	138.24	116.40
1	C	72	HIS	CB-CG-CD2	-14.56	112.28	131.20
2	D	33	VAL	CB-CA-C	-14.54	94.82	111.55
1	A	101	LEU	N-CA-CB	14.53	131.43	110.07
2	F	55	MET	O-C-N	-14.53	103.65	122.39
2	H	80	ASN	CA-CB-CG	14.52	127.12	112.60
1	C	1	VAL	CB-CA-C	-14.51	83.82	111.40
2	F	66	LYS	CA-C-O	14.50	136.05	120.82
2	D	89	SER	CA-C-O	14.50	136.24	119.27
2	B	110	LEU	O-C-N	14.50	139.18	122.22
1	E	45	HIS	CB-CG-CD2	14.49	150.03	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	70	ALA	CA-C-O	14.49	137.97	121.02
1	A	5	ALA	CA-C-O	14.48	136.88	119.79
1	C	22	GLY	CA-C-O	14.48	136.23	120.30
1	G	54	GLN	CA-C-O	14.48	136.54	119.60
2	F	35	TYR	N-CA-CB	14.48	136.14	110.37
2	B	139	ASN	CA-C-O	-14.48	105.00	120.63
1	A	52	SER	CA-C-O	14.47	137.36	120.58
1	G	118	THR	O-C-N	-14.47	109.52	121.38
2	D	8	LYS	CA-C-N	14.47	152.45	121.64
2	D	8	LYS	C-N-CA	14.47	152.45	121.64
2	B	103	PHE	O-C-N	14.45	137.44	122.12
1	G	105	LEU	O-C-N	-14.45	107.00	122.03
1	A	136	LEU	N-CA-C	-14.43	93.28	111.75
2	H	39	GLN	CA-C-O	14.43	141.15	120.51
1	E	89	HIS	CB-CG-CD2	14.42	149.95	131.20
1	A	50	HIS	CA-CB-CG	14.42	128.22	113.80
2	F	39	GLN	CA-CB-CG	14.41	142.91	114.10
2	B	78	LEU	CA-C-N	14.40	141.02	120.28
2	B	78	LEU	C-N-CA	14.40	141.02	120.28
2	D	23	VAL	CA-C-O	-14.40	105.97	120.95
2	F	95	LYS	CA-C-N	14.38	145.17	120.58
2	F	95	LYS	C-N-CA	14.38	145.17	120.58
1	G	53	ALA	CA-C-N	14.38	147.98	121.52
1	G	53	ALA	C-N-CA	14.38	147.98	121.52
1	E	129	LEU	CA-C-O	14.37	135.79	120.55
1	G	23	GLU	CG-CD-OE1	14.36	151.44	118.40
1	G	92	ARG	CD-NE-CZ	14.35	144.49	124.40
2	F	123	THR	N-CA-CB	-14.34	92.24	109.59
2	H	84	THR	CA-CB-OG1	-14.33	88.10	109.60
2	F	42	PHE	CB-CG-CD1	-14.33	96.34	120.70
1	C	70	VAL	CA-C-O	-14.32	105.99	121.17
2	F	61	LYS	N-CA-CB	-14.32	89.07	110.12
2	F	143	HIS	CG-CD2-NE2	14.32	121.52	107.20
2	F	103	PHE	CA-C-O	14.31	135.59	120.42
1	C	141	ARG	CB-CG-CD	14.31	144.20	111.30
1	C	44	PRO	CA-C-O	-14.30	98.74	119.18
2	D	85	PHE	CA-C-N	14.29	144.58	120.71
2	D	85	PHE	C-N-CA	14.29	144.58	120.71
2	H	127	GLN	CG-CD-NE2	14.29	137.84	116.40
1	G	44	PRO	N-CD-CG	14.28	124.63	103.20
2	F	77	HIS	CA-C-N	14.28	148.82	121.54
2	F	77	HIS	C-N-CA	14.28	148.82	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	14	LEU	CA-C-O	-14.28	105.37	121.07
2	D	105	LEU	CA-C-O	-14.27	102.95	119.79
1	E	113	LEU	CA-C-O	-14.27	102.76	120.74
2	H	109	VAL	CA-C-O	-14.23	101.78	119.43
2	F	117	HIS	N-CA-C	14.22	126.50	111.14
1	E	35	SER	CA-C-N	-14.22	104.93	122.42
1	E	35	SER	C-N-CA	-14.22	104.93	122.42
2	B	101	GLU	CB-CG-CD	14.21	136.76	112.60
1	G	112	HIS	CB-CG-ND1	-14.21	101.38	122.70
1	E	79	ALA	CA-C-O	14.20	135.73	120.82
1	C	97	ASN	CA-CB-CG	-14.20	98.40	112.60
1	C	107	VAL	O-C-N	-14.19	108.10	121.87
2	F	90	GLU	OE1-CD-OE2	14.19	156.96	122.90
2	B	104	ARG	CB-CA-C	14.18	137.89	110.67
1	C	81	SER	CB-CA-C	-14.18	82.21	110.42
2	H	33	VAL	CA-C-O	14.16	136.18	120.46
2	D	25	GLY	O-C-N	-14.16	106.42	122.84
2	B	108	ASN	CA-C-O	14.15	136.78	119.38
2	D	104	ARG	CA-CB-CG	-14.14	85.81	114.10
1	C	1	VAL	N-CA-CB	-14.13	87.48	111.50
2	H	113	VAL	N-CA-C	-14.13	96.21	110.62
1	E	116	GLU	N-CA-C	-14.12	93.91	114.39
2	F	133	VAL	CA-CB-CG1	14.12	134.40	110.40
1	E	119	PRO	CA-C-O	-14.11	96.00	119.84
1	A	122	HIS	CB-CG-ND1	14.11	143.86	122.70
2	D	125	PRO	N-CA-C	14.10	131.12	114.20
1	E	25	GLY	CA-C-O	-14.10	106.98	120.80
2	D	47	ASP	CA-C-O	-14.10	104.14	120.49
2	D	20	VAL	N-CA-CB	14.09	134.48	111.23
2	F	49	SER	O-C-N	14.08	141.29	122.43
1	C	137	THR	CA-C-O	-14.06	102.44	119.18
2	D	55	MET	CA-C-N	14.06	148.97	121.41
2	D	55	MET	C-N-CA	14.06	148.97	121.41
2	F	85	PHE	CA-CB-CG	14.06	127.86	113.80
1	G	93	VAL	CA-CB-CG1	14.06	134.30	110.40
1	A	3	SER	N-CA-CB	14.05	126.59	109.59
2	B	15	TRP	N-CA-CB	-14.05	86.43	110.32
1	A	112	HIS	O-C-N	-14.05	107.72	122.19
2	D	140	ALA	N-CA-CB	14.03	131.37	110.33
2	F	83	GLY	O-C-N	-14.02	102.91	122.68
2	B	102	ASN	CA-CB-CG	14.01	126.61	112.60
1	G	58	HIS	CB-CG-ND1	14.01	143.71	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	PRO	CB-CA-C	14.01	134.67	111.56
2	F	77	HIS	O-C-N	-13.97	103.09	121.95
1	G	68	ASN	N-CA-C	-13.95	95.66	111.71
2	F	137	VAL	CA-C-O	-13.95	104.36	120.96
1	C	140	TYR	O-C-N	-13.93	107.60	122.09
2	H	145	TYR	CA-C-O	-13.92	104.82	120.69
1	G	124	SER	CA-C-N	-13.92	99.16	120.31
1	G	124	SER	C-N-CA	-13.92	99.16	120.31
1	G	11	LYS	O-C-N	-13.91	103.78	122.43
1	A	26	ALA	CA-C-O	-13.91	103.32	119.60
2	H	20	VAL	N-CA-CB	13.91	125.23	110.62
1	C	55	VAL	CA-C-N	13.91	139.01	120.65
1	C	55	VAL	C-N-CA	13.91	139.01	120.65
2	H	44	SER	N-CA-C	-13.91	95.64	113.72
2	B	26	GLU	N-CA-C	13.90	126.51	111.36
1	A	56	LYS	N-CA-C	-13.90	94.44	111.40
1	C	119	PRO	O-C-N	-13.90	103.06	122.38
2	H	131	GLN	CB-CG-CD	13.89	136.22	112.60
2	B	132	LYS	O-C-N	13.89	136.38	122.07
2	F	106	LEU	CA-C-O	13.89	135.80	120.10
2	B	38	THR	CA-C-N	13.89	139.41	120.38
2	B	38	THR	C-N-CA	13.89	139.41	120.38
1	E	31	ARG	CA-C-N	13.89	140.09	120.79
1	E	31	ARG	C-N-CA	13.89	140.09	120.79
1	G	31	ARG	CA-C-O	-13.89	104.00	119.97
2	B	92	HIS	N-CA-CB	13.88	130.53	110.12
1	C	133	SER	CA-C-O	-13.88	101.01	119.05
2	B	90	GLU	N-CA-CB	13.87	133.30	109.72
1	G	126	ASP	CB-CG-OD1	13.87	150.30	118.40
1	A	95	PRO	N-CA-CB	13.86	117.81	103.25
2	F	47	ASP	CA-CB-CG	-13.85	98.75	112.60
1	A	104	CYS	N-CA-C	13.84	129.27	112.38
1	A	137	THR	CA-C-N	13.84	141.58	120.82
1	A	137	THR	C-N-CA	13.84	141.58	120.82
2	B	37	TRP	CA-C-O	-13.83	102.54	119.28
2	B	126	VAL	CA-CB-CG1	13.82	133.90	110.40
2	F	137	VAL	CA-C-N	13.82	139.43	120.63
2	F	137	VAL	C-N-CA	13.82	139.43	120.63
1	C	13	ALA	N-CA-CB	-13.82	88.77	110.46
1	C	31	ARG	CG-CD-NE	13.81	142.38	112.00
2	B	115	ALA	CB-CA-C	-13.79	89.00	110.92
2	D	136	GLY	CA-C-N	-13.79	100.84	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	136	GLY	C-N-CA	-13.79	100.84	120.42
2	F	22	GLU	CA-C-N	-13.79	97.69	120.30
2	F	22	GLU	C-N-CA	-13.79	97.69	120.30
1	C	113	LEU	O-C-N	-13.77	109.47	121.17
1	G	85	ASP	N-CA-C	-13.76	96.35	111.07
1	C	69	ALA	N-CA-CB	13.75	129.92	109.98
2	B	32	LEU	CA-C-O	13.75	135.13	120.55
1	C	29	LEU	CA-C-N	-13.75	101.74	120.44
1	C	29	LEU	C-N-CA	-13.75	101.74	120.44
1	A	140	TYR	CA-CB-CG	13.75	138.65	113.90
1	C	76	MET	O-C-N	-13.74	105.52	121.32
1	C	39	THR	CA-CB-OG1	-13.73	89.01	109.60
1	G	123	ALA	N-CA-C	-13.73	96.40	111.36
2	H	111	VAL	O-C-N	13.73	135.19	121.87
1	A	37	PRO	N-CA-CB	-13.73	88.84	103.25
2	B	72	SER	N-CA-CB	13.72	131.36	110.22
2	D	101	GLU	OE1-CD-OE2	13.72	155.83	122.90
2	B	52	ASP	N-CA-CB	13.71	131.43	110.19
2	H	9	SER	CA-C-O	13.69	136.29	119.31
2	H	105	LEU	CA-C-O	-13.70	103.25	119.27
2	H	12	THR	CA-CB-CG2	13.68	133.75	110.50
1	E	27	GLU	CA-CB-CG	13.67	141.44	114.10
2	H	133	VAL	CA-CB-CG1	-13.67	87.17	110.40
2	D	43	GLU	CB-CA-C	13.66	130.13	111.14
1	G	20	HIS	N-CA-CB	13.65	130.27	110.47
2	B	104	ARG	NE-CZ-NH1	-13.65	107.85	121.50
2	B	125	PRO	O-C-N	-13.65	103.58	122.55
2	H	104	ARG	CA-C-O	13.65	136.08	121.07
1	C	8	THR	CA-C-N	13.63	138.94	120.54
1	C	8	THR	C-N-CA	13.63	138.94	120.54
2	F	62	ALA	CB-CA-C	13.63	131.95	110.96
1	E	3	SER	CA-C-O	-13.63	101.49	120.16
1	E	28	ALA	CA-C-N	-13.62	102.15	120.54
1	E	28	ALA	C-N-CA	-13.62	102.15	120.54
1	C	9	ASN	CB-CG-OD1	-13.62	93.57	120.80
1	G	64	ASP	O-C-N	13.62	136.19	122.03
1	A	67	THR	OG1-CB-CG2	13.61	136.52	109.30
2	D	107	GLY	CA-C-O	-13.61	107.46	120.80
1	E	127	LYS	CA-C-O	-13.60	102.44	119.31
2	H	137	VAL	N-CA-CB	13.60	127.98	110.57
2	F	113	VAL	CB-CA-C	13.60	129.37	111.97
2	F	4	THR	CA-C-O	-13.59	106.64	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	47	ASP	N-CA-CB	13.59	132.02	109.87
1	E	36	PHE	CB-CA-C	13.58	131.80	111.02
2	F	90	GLU	CB-CA-C	-13.58	88.29	110.84
1	E	122	HIS	N-CA-CB	13.58	129.75	110.07
1	A	6	ASP	CA-C-N	13.57	138.08	120.44
1	A	6	ASP	C-N-CA	13.57	138.08	120.44
1	A	7	LYS	CA-C-O	-13.56	106.58	120.82
2	D	129	ALA	N-CA-C	-13.56	94.85	111.40
1	A	34	LEU	CA-C-O	-13.56	103.74	119.60
1	A	42	TYR	CG-CD1-CE1	13.56	141.53	121.20
2	B	24	GLY	O-C-N	-13.54	105.09	122.70
2	H	142	ALA	O-C-N	-13.53	104.69	122.42
2	D	60	VAL	CB-CA-C	13.53	129.76	112.04
1	E	140	TYR	CA-CB-CG	13.53	138.25	113.90
1	A	41	THR	CA-C-O	13.52	135.35	120.20
2	B	132	LYS	N-CA-C	-13.52	96.60	111.07
2	H	17	LYS	CA-C-O	13.52	135.64	119.28
2	D	110	LEU	CA-C-N	13.52	142.18	120.55
2	D	110	LEU	C-N-CA	13.52	142.18	120.55
2	B	52	ASP	OD1-CG-OD2	13.49	155.28	122.90
2	D	130	TYR	CA-C-N	13.49	139.44	120.29
2	D	130	TYR	C-N-CA	13.49	139.44	120.29
1	G	3	SER	O-C-N	13.49	136.83	121.32
1	G	14	TRP	N-CA-C	-13.48	96.18	111.82
2	B	115	ALA	N-CA-CB	13.47	130.30	109.82
1	E	134	THR	CA-CB-OG1	-13.46	89.41	109.60
1	A	110	ALA	CA-C-O	13.46	134.95	120.82
1	C	32	MET	CA-C-N	13.45	139.65	120.28
1	C	32	MET	C-N-CA	13.45	139.65	120.28
1	G	141	ARG	CA-C-O	-13.45	80.65	121.00
2	H	20	VAL	N-CA-C	13.45	124.22	110.23
2	B	53	ALA	N-CA-C	-13.45	95.06	111.33
1	E	136	LEU	O-C-N	13.45	140.45	122.43
2	F	52	ASP	CA-C-O	13.44	134.75	120.90
1	C	102	SER	CA-CB-OG	13.42	137.94	111.10
2	B	89	SER	N-CA-C	-13.40	96.67	111.14
2	B	82	LYS	CB-CA-C	13.39	135.41	110.63
2	F	9	SER	O-C-N	-13.39	106.00	122.20
2	F	72	SER	CA-C-N	13.37	147.07	121.54
2	F	72	SER	C-N-CA	13.37	147.07	121.54
2	B	49	SER	CA-C-N	13.36	155.05	122.31
2	B	49	SER	C-N-CA	13.36	155.05	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	116	GLU	CA-C-N	13.36	147.06	121.54
1	G	116	GLU	C-N-CA	13.36	147.06	121.54
1	C	56	LYS	CA-C-O	-13.35	106.98	121.00
1	E	33	PHE	CB-CG-CD1	-13.35	98.00	120.70
1	A	31	ARG	NE-CZ-NH2	13.34	131.21	119.20
1	C	128	PHE	CA-C-O	-13.34	105.43	120.24
2	H	102	ASN	OD1-CG-ND2	13.34	135.94	122.60
2	D	4	THR	O-C-N	13.32	134.49	121.57
1	A	2	LEU	CA-C-N	-13.32	102.57	122.29
1	A	2	LEU	C-N-CA	-13.32	102.57	122.29
2	B	35	TYR	CA-C-O	-13.31	103.96	120.74
2	B	8	LYS	N-CA-C	-13.31	96.77	111.28
2	H	18	VAL	O-C-N	13.31	139.28	122.77
1	A	24	TYR	CB-CG-CD2	-13.30	100.85	120.80
1	C	50	HIS	CB-CG-ND1	13.29	142.64	122.70
1	E	140	TYR	CB-CA-C	13.29	135.02	110.70
2	H	12	THR	O-C-N	13.29	141.82	122.28
2	B	121	GLU	OE1-CD-OE2	13.29	154.79	122.90
1	A	108	THR	CA-CB-OG1	-13.28	89.68	109.60
1	G	31	ARG	CA-CB-CG	13.28	140.66	114.10
2	D	65	LYS	CA-C-N	-13.26	101.19	120.28
2	D	65	LYS	C-N-CA	-13.26	101.19	120.28
1	E	41	THR	O-C-N	13.26	140.22	122.59
1	A	41	THR	CA-CB-OG1	-13.26	89.72	109.60
2	H	57	ASN	CA-CB-CG	13.26	125.86	112.60
2	B	47	ASP	CB-CG-OD1	13.25	148.88	118.40
1	E	54	GLN	N-CA-CB	-13.25	89.68	109.82
2	B	30	ARG	NE-CZ-NH1	-13.25	108.25	121.50
2	H	106	LEU	O-C-N	13.25	138.56	122.27
2	F	57	ASN	CA-C-O	-13.24	106.38	119.49
2	H	127	GLN	O-C-N	-13.23	105.00	122.59
2	F	35	TYR	CB-CG-CD1	13.22	140.63	120.80
1	E	12	ALA	O-C-N	13.22	138.16	122.17
2	B	14	LEU	O-C-N	13.21	136.22	122.08
1	C	8	THR	CA-CB-CG2	13.21	132.96	110.50
2	D	67	VAL	N-CA-CB	13.21	130.39	110.58
1	C	78	ASN	N-CA-CB	-13.21	88.88	110.40
1	E	114	PRO	CB-CA-C	13.19	133.33	111.56
2	B	118	PHE	CA-CB-CG	-13.18	100.62	113.80
1	C	85	ASP	CA-C-N	13.18	146.72	121.54
1	C	85	ASP	C-N-CA	13.18	146.72	121.54
2	B	115	ALA	CA-C-O	-13.18	106.57	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	58	PRO	O-C-N	-13.18	104.85	122.64
1	G	121	VAL	CA-C-O	13.17	134.81	120.71
2	B	133	VAL	O-C-N	-13.16	108.28	121.83
1	C	67	THR	CA-CB-CG2	-13.16	88.13	110.50
1	E	4	PRO	N-CA-CB	13.16	115.70	103.20
2	B	59	LYS	N-CA-C	-13.15	96.95	111.28
1	A	7	LYS	N-CA-CB	-13.14	90.96	110.01
1	G	89	HIS	CA-CB-CG	13.14	126.94	113.80
1	A	24	TYR	N-CA-CB	13.12	129.81	110.26
1	A	141	ARG	N-CA-CB	-13.12	88.20	110.50
1	G	62	VAL	CA-C-O	-13.12	104.83	120.83
1	E	14	TRP	CA-C-O	13.11	136.09	119.05
2	D	14	LEU	O-C-N	-13.11	104.38	122.46
1	A	19	ALA	O-C-N	-13.10	106.62	122.48
2	H	137	VAL	CA-C-O	13.10	135.59	121.05
2	H	136	GLY	O-C-N	13.07	139.69	122.70
1	G	47	ASP	CA-C-N	13.07	148.08	121.94
1	G	47	ASP	C-N-CA	13.07	148.08	121.94
2	H	101	GLU	CA-C-O	-13.07	105.33	120.10
1	E	72	HIS	CA-C-O	13.05	134.77	121.20
2	H	116	HIS	ND1-CG-CD2	13.05	119.15	106.10
1	C	78	ASN	CB-CG-OD1	13.04	146.89	120.80
2	F	14	LEU	CB-CA-C	13.04	136.97	110.38
2	D	85	PHE	CA-CB-CG	13.03	126.83	113.80
1	C	92	ARG	NE-CZ-NH2	13.02	130.92	119.20
1	C	101	LEU	CA-C-O	-13.02	106.62	120.42
1	G	119	PRO	CA-C-N	13.02	138.22	120.38
1	G	119	PRO	C-N-CA	13.02	138.22	120.38
2	D	84	THR	O-C-N	-13.01	107.00	122.22
2	D	114	LEU	N-CA-C	-13.01	97.10	111.28
2	H	30	ARG	CA-C-N	13.00	138.12	120.44
2	H	30	ARG	C-N-CA	13.00	138.12	120.44
1	C	103	HIS	ND1-CE1-NE2	13.00	121.40	108.40
1	A	101	LEU	N-CA-C	-12.99	94.49	111.24
2	H	60	VAL	CA-CB-CG1	-12.99	88.32	110.40
2	F	8	LYS	N-CA-C	-12.98	97.21	111.36
1	A	103	HIS	ND1-CE1-NE2	-12.98	95.42	108.40
1	E	116	GLU	CA-C-O	-12.98	103.76	118.69
1	G	120	ALA	CA-C-N	12.98	141.32	120.55
1	G	120	ALA	C-N-CA	12.98	141.32	120.55
1	E	127	LYS	O-C-N	12.98	140.37	122.46
2	H	66	LYS	CB-CA-C	-12.97	89.31	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	77	HIS	CG-ND1-CE1	12.97	131.35	109.30
2	F	33	VAL	CA-CB-CG2	12.96	132.43	110.40
2	B	113	VAL	O-C-N	-12.94	108.83	121.90
2	H	92	HIS	CA-C-N	12.94	146.25	121.54
2	H	92	HIS	C-N-CA	12.94	146.25	121.54
1	C	12	ALA	O-C-N	12.94	136.90	122.15
1	A	75	ASP	CA-C-O	-12.93	107.75	121.20
2	F	131	GLN	O-C-N	12.93	140.17	122.46
2	H	133	VAL	CA-C-N	-12.93	99.18	120.64
2	H	133	VAL	C-N-CA	-12.93	99.18	120.64
1	A	89	HIS	CA-C-N	12.92	139.66	121.71
1	A	89	HIS	C-N-CA	12.92	139.66	121.71
1	A	128	PHE	CA-C-N	-12.91	101.45	120.82
1	A	128	PHE	C-N-CA	-12.91	101.45	120.82
2	H	96	LEU	CA-C-N	12.91	146.20	121.54
2	H	96	LEU	C-N-CA	12.91	146.20	121.54
1	E	32	MET	CA-CB-CG	-12.91	88.28	114.10
2	B	79	ASP	CB-CG-OD1	12.91	148.08	118.40
1	E	64	ASP	CA-C-O	-12.91	106.74	120.55
2	H	84	THR	CA-C-O	12.90	135.26	121.07
1	C	77	PRO	CB-CA-C	12.90	130.94	112.11
2	B	109	VAL	CA-CB-CG2	12.89	132.31	110.40
2	F	68	LEU	N-CA-C	12.88	126.57	111.11
2	D	19	ASN	OD1-CG-ND2	12.88	135.48	122.60
1	E	38	THR	N-CA-CB	12.86	129.11	109.94
1	E	72	HIS	CE1-NE2-CD2	-12.86	96.14	109.00
2	D	121	GLU	CB-CG-CD	12.86	134.46	112.60
2	D	89	SER	N-CA-C	12.86	129.17	113.23
2	D	128	ALA	O-C-N	-12.86	107.50	122.15
2	F	105	LEU	O-C-N	-12.84	108.22	122.09
2	B	136	GLY	CA-C-O	12.84	134.80	119.65
1	E	103	HIS	CE1-NE2-CD2	12.83	121.83	109.00
2	H	39	GLN	CB-CA-C	12.83	135.95	110.42
2	F	119	GLY	CA-C-N	12.83	139.81	120.31
2	F	119	GLY	C-N-CA	12.83	139.81	120.31
1	E	45	HIS	CG-CD2-NE2	12.82	120.03	107.20
1	E	64	ASP	CA-C-N	-12.82	103.10	120.28
1	E	64	ASP	C-N-CA	-12.82	103.10	120.28
1	A	18	GLY	CA-C-N	-12.81	101.11	122.11
1	A	18	GLY	C-N-CA	-12.81	101.11	122.11
1	A	89	HIS	CA-C-O	-12.79	102.22	120.13
2	B	106	LEU	CA-C-O	-12.79	102.43	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	100	PRO	CA-C-O	12.79	141.45	119.84
2	B	3	LEU	N-CA-CB	12.78	130.52	110.85
1	G	34	LEU	N-CA-CB	12.77	129.06	110.16
1	G	56	LYS	CA-CB-CG	12.77	139.64	114.10
1	A	60	LYS	CA-C-O	12.77	134.22	120.82
1	C	36	PHE	CA-C-N	12.76	134.27	119.47
1	C	36	PHE	C-N-CA	12.76	134.27	119.47
2	F	59	LYS	O-C-N	-12.76	108.60	122.12
1	G	75	ASP	CA-C-O	-12.76	99.04	121.62
2	B	80	ASN	CB-CG-ND2	-12.75	97.27	116.40
2	F	31	LEU	CA-C-N	12.75	137.75	120.54
2	F	31	LEU	C-N-CA	12.75	137.75	120.54
2	F	48	LEU	CA-C-N	12.74	142.00	120.72
2	F	48	LEU	C-N-CA	12.74	142.00	120.72
1	G	30	GLU	CA-C-N	12.73	139.66	120.31
1	G	30	GLU	C-N-CA	12.73	139.66	120.31
2	B	92	HIS	CB-CG-CD2	12.73	147.74	131.20
1	A	84	SER	CB-CA-C	12.72	132.48	110.85
1	C	40	LYS	N-CA-CB	-12.72	90.05	110.14
1	E	5	ALA	CA-C-N	-12.72	100.98	120.31
1	E	5	ALA	C-N-CA	-12.72	100.98	120.31
2	F	25	GLY	N-CA-C	-12.71	100.69	114.67
2	H	109	VAL	CA-CB-CG2	12.70	131.98	110.40
1	G	111	ALA	CB-CA-C	-12.69	93.50	111.14
2	D	114	LEU	N-CA-CB	12.69	128.77	110.12
1	A	101	LEU	CA-C-N	-12.68	99.54	120.72
1	A	101	LEU	C-N-CA	-12.68	99.54	120.72
2	D	12	THR	CA-CB-OG1	-12.67	90.59	109.60
1	A	58	HIS	CG-CD2-NE2	-12.67	94.53	107.20
1	G	85	ASP	CB-CA-C	12.67	130.77	110.88
1	A	19	ALA	N-CA-CB	-12.66	93.07	110.67
1	E	136	LEU	CA-C-O	-12.66	103.81	119.38
2	D	6	VAL	N-CA-CB	12.65	132.11	111.23
1	A	122	HIS	ND1-CE1-NE2	-12.64	95.76	108.40
1	A	139	LYS	N-CA-CB	-12.64	89.13	110.49
1	A	89	HIS	N-CA-CB	12.64	131.56	110.33
2	D	87	THR	N-CA-C	-12.64	97.00	111.03
1	E	55	VAL	CA-C-N	-12.63	103.36	120.28
1	E	55	VAL	C-N-CA	-12.63	103.36	120.28
1	E	108	THR	CA-C-O	-12.63	107.54	120.80
1	E	52	SER	O-C-N	12.62	137.07	122.94
1	A	48	LEU	CB-CA-C	12.62	135.53	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	57	ASN	CA-CB-CG	12.62	125.22	112.60
2	D	83	GLY	CA-C-N	-12.61	102.13	120.28
2	D	83	GLY	C-N-CA	-12.61	102.13	120.28
1	G	135	VAL	CB-CA-C	-12.59	96.07	111.81
1	A	28	ALA	CA-C-O	12.59	138.51	120.51
2	F	90	GLU	N-CA-CB	12.59	131.12	109.72
1	A	98	PHE	CB-CA-C	12.59	131.68	110.79
2	H	79	ASP	N-CA-CB	12.59	131.47	110.33
1	A	73	VAL	CA-CB-CG1	-12.57	89.02	110.40
2	H	126	VAL	N-CA-C	-12.57	94.92	113.39
1	C	9	ASN	N-CA-CB	12.56	128.66	109.94
2	F	90	GLU	CA-C-N	12.56	137.49	120.54
2	F	90	GLU	C-N-CA	12.56	137.49	120.54
1	C	16	LYS	CG-CD-CE	-12.55	82.42	111.30
2	B	38	THR	CA-CB-CG2	12.54	131.83	110.50
2	B	35	TYR	CB-CG-CD2	12.53	139.60	120.80
1	A	41	THR	CA-CB-CG2	-12.53	89.20	110.50
2	B	1	VAL	CA-CB-CG1	12.53	131.70	110.40
1	A	20	HIS	O-C-N	-12.52	102.37	122.41
2	D	45	PHE	CA-C-O	-12.52	102.77	119.05
2	B	87	THR	CA-C-N	12.52	136.72	120.44
2	B	87	THR	C-N-CA	12.52	136.72	120.44
2	H	104	ARG	NE-CZ-NH2	-12.51	107.94	119.20
1	E	56	LYS	CA-C-O	12.51	133.81	120.55
1	C	40	LYS	O-C-N	-12.50	107.95	122.20
1	C	54	GLN	CA-C-O	-12.49	107.71	120.82
2	F	53	ALA	N-CA-CB	12.49	128.12	110.01
2	F	104	ARG	CD-NE-CZ	12.49	141.88	124.40
1	A	86	LEU	CA-C-O	12.48	135.92	120.31
2	H	97	HIS	CA-C-N	-12.48	104.00	120.98
2	H	97	HIS	C-N-CA	-12.48	104.00	120.98
1	C	102	SER	N-CA-C	12.48	126.43	111.33
1	E	38	THR	CB-CA-C	-12.48	90.84	110.81
2	D	77	HIS	CB-CG-CD2	-12.48	114.98	131.20
1	G	72	HIS	CB-CG-ND1	12.48	141.42	122.70
2	H	42	PHE	N-CA-C	12.48	126.14	108.54
1	A	30	GLU	CB-CA-C	12.48	131.50	110.79
1	C	133	SER	CA-C-N	12.47	148.74	121.80
1	C	133	SER	C-N-CA	12.47	148.74	121.80
1	G	64	ASP	CB-CA-C	12.47	130.17	110.96
2	F	104	ARG	O-C-N	-12.47	109.22	122.07
1	A	121	VAL	CB-CA-C	12.47	128.25	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	125	LEU	CA-C-N	-12.47	103.46	120.79
1	G	125	LEU	C-N-CA	-12.47	103.46	120.79
2	D	104	ARG	NE-CZ-NH2	-12.47	107.98	119.20
1	G	87	HIS	CB-CA-C	-12.46	89.50	110.68
2	D	87	THR	CA-C-O	-12.46	108.07	120.90
2	H	85	PHE	O-C-N	12.46	138.10	122.65
1	C	132	VAL	N-CA-CB	12.46	124.20	110.62
2	F	134	VAL	CA-C-O	-12.46	108.32	121.27
2	B	143	HIS	CB-CG-CD2	-12.45	115.01	131.20
2	F	59	LYS	CB-CG-CD	12.45	139.94	111.30
2	H	63	HIS	N-CA-C	-12.45	95.83	111.02
2	B	2	HIS	O-C-N	-12.45	112.05	123.50
2	H	73	ASP	O-C-N	-12.45	102.50	122.41
1	G	29	LEU	CA-CB-CG	12.45	159.86	116.30
1	E	20	HIS	CG-CD2-NE2	-12.44	94.76	107.20
1	A	75	ASP	CA-C-N	12.44	134.87	120.06
1	A	75	ASP	C-N-CA	12.44	134.87	120.06
1	A	128	PHE	CB-CG-CD2	12.44	141.85	120.70
2	D	130	TYR	O-C-N	12.44	136.78	122.22
2	B	135	ALA	CA-C-O	-12.44	108.09	120.90
1	C	54	GLN	CB-CG-CD	12.44	133.75	112.60
2	B	23	VAL	CA-C-O	12.44	133.88	120.57
2	F	50	THR	O-C-N	12.43	133.03	121.71
1	C	102	SER	CA-C-N	12.42	137.92	120.29
1	C	102	SER	C-N-CA	12.42	137.92	120.29
1	A	29	LEU	CA-C-N	-12.41	103.65	120.28
1	A	29	LEU	C-N-CA	-12.41	103.65	120.28
1	G	72	HIS	CB-CG-CD2	-12.41	115.07	131.20
1	A	72	HIS	CA-C-O	12.40	134.17	119.78
2	F	82	LYS	N-CA-CB	12.40	131.45	110.49
1	G	129	LEU	O-C-N	12.39	138.50	122.39
1	G	94	ASP	N-CA-CB	-12.39	87.55	109.73
2	D	91	LEU	O-C-N	12.38	134.83	122.07
1	G	79	ALA	CB-CA-C	12.38	131.08	111.39
1	A	69	ALA	CB-CA-C	12.38	133.36	110.70
2	B	135	ALA	CA-C-N	12.38	142.03	120.74
2	B	135	ALA	C-N-CA	12.38	142.03	120.74
1	G	27	GLU	CA-C-O	12.38	134.40	119.79
2	H	95	LYS	CA-C-O	-12.38	105.44	119.67
1	E	19	ALA	CA-C-N	-12.38	102.12	122.54
1	E	19	ALA	C-N-CA	-12.38	102.12	122.54
1	G	35	SER	CA-C-N	12.37	136.45	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	35	SER	C-N-CA	12.37	136.45	122.85
1	E	54	GLN	OE1-CD-NE2	12.36	134.96	122.60
2	D	14	LEU	N-CA-CB	-12.36	88.76	110.39
1	G	9	ASN	O-C-N	12.36	134.80	122.07
2	F	11	VAL	CA-CB-CG2	12.36	131.40	110.40
2	F	60	VAL	CA-CB-CG1	12.35	131.40	110.40
2	B	50	THR	CA-CB-OG1	12.34	128.11	109.60
2	D	132	LYS	CA-C-N	-12.34	104.77	120.56
2	D	132	LYS	C-N-CA	-12.34	104.77	120.56
1	G	30	GLU	CB-CG-CD	12.33	133.56	112.60
2	F	79	ASP	N-CA-CB	12.33	128.65	110.53
1	A	58	HIS	N-CA-CB	-12.32	89.70	109.78
1	E	45	HIS	CA-CB-CG	-12.31	101.49	113.80
2	F	104	ARG	NE-CZ-NH1	12.31	133.81	121.50
1	C	69	ALA	CA-C-O	-12.31	108.22	120.90
2	D	26	GLU	O-C-N	12.30	138.31	122.19
2	D	14	LEU	CB-CA-C	12.30	135.26	110.17
2	F	105	LEU	CB-CA-C	12.29	130.31	110.90
2	F	116	HIS	CA-C-N	12.28	137.15	120.44
2	F	116	HIS	C-N-CA	12.28	137.15	120.44
1	E	103	HIS	CG-CD2-NE2	-12.28	94.92	107.20
1	E	105	LEU	CA-C-N	12.27	144.97	121.54
1	E	105	LEU	C-N-CA	12.27	144.97	121.54
2	F	37	TRP	CG-CD1-NE1	12.26	126.14	110.20
1	C	6	ASP	CA-C-N	12.26	137.09	120.54
1	C	6	ASP	C-N-CA	12.26	137.09	120.54
2	B	106	LEU	O-C-N	12.26	139.38	122.46
1	G	67	THR	OG1-CB-CG2	12.25	133.80	109.30
1	A	13	ALA	O-C-N	12.25	136.12	122.15
2	H	103	PHE	CA-C-N	12.25	137.81	120.79
2	H	103	PHE	C-N-CA	12.25	137.81	120.79
1	A	10	VAL	O-C-N	12.24	137.99	121.84
2	B	30	ARG	NE-CZ-NH2	12.24	130.21	119.20
1	A	96	VAL	CA-C-O	12.23	133.68	120.47
1	G	32	MET	CB-CA-C	-12.23	91.48	110.92
2	B	89	SER	N-CA-CB	12.22	127.80	110.07
1	E	89	HIS	CA-CB-CG	12.22	126.02	113.80
1	C	71	ALA	CB-CA-C	12.22	135.09	110.17
2	H	142	ALA	CB-CA-C	12.21	130.91	109.65
2	H	146	HIS	CB-CG-ND1	-12.22	104.38	122.70
2	D	20	VAL	O-C-N	12.21	137.83	122.57
1	A	33	PHE	CA-CB-CG	-12.21	101.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	GLU	N-CA-C	-12.19	98.92	114.04
1	A	26	ALA	O-C-N	12.19	139.67	122.36
2	D	92	HIS	CG-CD2-NE2	12.19	119.39	107.20
1	G	2	LEU	O-C-N	-12.19	108.92	123.19
2	H	97	HIS	CA-CB-CG	-12.19	101.61	113.80
2	F	63	HIS	N-CA-C	-12.19	98.41	113.28
2	B	18	VAL	CA-C-O	12.19	136.01	120.78
1	C	25	GLY	CA-C-N	-12.19	99.96	120.68
1	C	25	GLY	C-N-CA	-12.19	99.96	120.68
1	G	61	LYS	CA-CB-CG	12.19	138.47	114.10
1	C	5	ALA	O-C-N	-12.18	109.42	122.09
2	B	139	ASN	CB-CG-OD1	-12.18	96.45	120.80
2	F	91	LEU	N-CA-CB	12.17	128.08	109.94
2	B	46	GLY	CA-C-O	-12.17	109.10	122.24
2	F	133	VAL	N-CA-CB	-12.16	86.42	111.24
1	A	104	CYS	CA-C-O	-12.16	104.77	119.49
2	D	37	TRP	CH2-CZ2-CE2	12.16	133.31	117.50
1	C	69	ALA	CB-CA-C	-12.16	92.10	110.95
2	D	81	LEU	CA-C-O	12.16	133.74	120.24
1	G	140	TYR	O-C-N	-12.15	107.46	122.17
2	H	93	CYS	CA-C-N	-12.15	103.73	120.38
2	H	93	CYS	C-N-CA	-12.15	103.73	120.38
2	H	61	LYS	CG-CD-CE	12.14	139.22	111.30
1	A	118	THR	CA-CB-OG1	12.13	127.80	109.60
1	A	129	LEU	CA-C-O	-12.13	107.33	120.92
2	B	45	PHE	CA-C-O	-12.13	106.39	120.10
1	E	130	ALA	CA-C-N	12.12	136.91	120.54
1	E	130	ALA	C-N-CA	12.12	136.91	120.54
2	H	133	VAL	CA-CB-CG2	12.12	131.01	110.40
1	G	26	ALA	CA-C-O	-12.12	105.49	119.79
1	A	72	HIS	CA-C-N	12.11	143.77	121.97
1	A	72	HIS	C-N-CA	12.11	143.77	121.97
2	F	47	ASP	CB-CG-OD1	12.11	146.26	118.40
2	B	116	HIS	CA-CB-CG	12.11	125.91	113.80
2	B	62	ALA	N-CA-CB	-12.10	91.42	109.82
2	D	117	HIS	CB-CA-C	-12.10	90.27	110.85
2	H	6	VAL	CA-CB-CG1	12.10	130.98	110.40
1	C	110	ALA	CB-CA-C	-12.10	86.34	110.42
1	C	55	VAL	N-CA-CB	12.09	128.71	110.58
2	B	125	PRO	CA-C-O	12.09	135.70	118.78
1	A	27	GLU	CA-C-O	12.08	133.86	119.97
1	C	3	SER	CA-C-O	-12.08	103.61	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	25	GLY	CA-C-N	12.07	136.13	120.44
2	H	25	GLY	C-N-CA	12.07	136.13	120.44
1	E	45	HIS	CB-CG-ND1	-12.06	104.61	122.70
1	E	73	VAL	N-CA-CB	12.06	131.13	111.23
1	A	73	VAL	CB-CA-C	12.05	131.06	111.29
2	B	99	ASP	O-C-N	12.05	131.55	121.31
1	E	104	CYS	CA-C-O	12.05	134.32	121.07
2	B	19	ASN	CA-C-O	-12.04	108.01	120.54
2	F	118	PHE	CB-CA-C	12.04	130.80	110.94
2	B	127	GLN	N-CA-C	-12.04	95.71	111.24
2	F	124	PRO	CA-C-N	12.03	132.40	119.05
2	F	124	PRO	C-N-CA	12.03	132.40	119.05
1	E	74	ASP	CA-C-O	-12.02	105.82	119.41
1	G	19	ALA	O-C-N	-12.02	105.30	122.36
1	C	121	VAL	CA-CB-CG2	12.01	130.82	110.40
2	H	101	GLU	CG-CD-OE1	12.01	146.03	118.40
1	C	116	GLU	CA-C-O	-12.01	108.05	120.90
1	A	125	LEU	N-CA-CB	-12.01	92.39	110.16
2	B	62	ALA	CB-CA-C	-12.00	91.83	110.92
1	E	70	VAL	CA-C-N	-12.00	97.94	121.94
1	E	70	VAL	C-N-CA	-12.00	97.94	121.94
1	A	134	THR	O-C-N	-12.00	106.63	122.59
1	C	120	ALA	O-C-N	12.00	134.51	122.03
1	E	40	LYS	O-C-N	-11.99	107.52	122.27
2	F	22	GLU	N-CA-CB	11.99	127.90	110.16
1	C	119	PRO	N-CA-C	-11.97	97.55	114.18
1	G	31	ARG	CG-CD-NE	11.96	138.32	112.00
2	F	34	VAL	CA-C-N	11.95	150.97	121.80
2	F	34	VAL	C-N-CA	11.95	150.97	121.80
2	H	90	GLU	N-CA-C	11.95	125.46	111.71
2	B	142	ALA	O-C-N	11.95	136.13	122.27
2	F	109	VAL	O-C-N	-11.94	105.46	121.82
1	E	97	ASN	CB-CG-ND2	11.93	134.30	116.40
1	G	33	PHE	O-C-N	11.93	134.84	122.08
2	H	68	LEU	CB-CA-C	11.93	136.34	110.21
1	A	50	HIS	N-CA-CB	11.91	127.93	109.48
2	B	1	VAL	O-C-N	11.90	142.04	123.00
2	B	21	ASP	CB-CA-C	11.90	132.38	110.36
2	H	74	GLY	CA-C-N	11.90	137.76	120.38
2	H	74	GLY	C-N-CA	11.90	137.76	120.38
1	E	55	VAL	N-CA-C	-11.90	95.57	112.35
1	E	125	LEU	N-CA-CB	11.90	130.15	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	111	VAL	N-CA-C	-11.89	98.04	111.00
2	D	126	VAL	N-CA-C	-11.89	99.50	113.42
2	B	49	SER	CA-C-O	11.89	134.00	119.38
1	A	17	VAL	O-C-N	11.89	138.48	122.31
2	H	117	HIS	N-CA-CB	11.89	130.58	110.49
1	A	114	PRO	N-CD-CG	11.88	121.02	103.20
1	C	96	VAL	CA-C-O	-11.88	107.64	120.47
2	B	84	THR	N-CA-CB	-11.88	91.03	110.40
1	E	7	LYS	CA-C-O	-11.88	108.34	120.82
2	D	35	TYR	O-C-N	11.88	131.91	121.34
1	C	30	GLU	N-CA-CB	11.87	127.28	110.07
2	D	57	ASN	CA-CB-CG	-11.87	100.73	112.60
1	C	63	ALA	CA-C-N	11.86	139.58	120.60
1	C	63	ALA	C-N-CA	11.86	139.58	120.60
2	F	141	LEU	CA-CB-CG	11.86	157.81	116.30
2	H	94	ASP	O-C-N	-11.86	109.55	122.12
1	C	45	HIS	ND1-CG-CD2	11.85	117.95	106.10
1	C	77	PRO	CA-C-N	-11.85	100.39	121.14
1	C	77	PRO	C-N-CA	-11.85	100.39	121.14
1	G	132	VAL	CA-C-O	-11.85	108.29	120.85
2	H	5	PRO	N-CA-CB	11.85	115.69	103.25
1	C	64	ASP	CA-C-N	11.84	144.16	121.54
1	C	64	ASP	C-N-CA	11.84	144.16	121.54
1	E	68	ASN	N-CA-CB	11.84	127.84	110.20
1	G	13	ALA	CB-CA-C	11.84	132.48	110.11
2	B	137	VAL	N-CA-CB	11.83	124.02	110.65
2	H	6	VAL	CA-C-N	-11.83	103.11	120.38
2	H	6	VAL	C-N-CA	-11.83	103.11	120.38
2	D	90	GLU	CG-CD-OE1	11.82	145.58	118.40
1	G	97	ASN	OD1-CG-ND2	-11.82	110.78	122.60
1	C	111	ALA	N-CA-C	11.81	127.45	112.92
2	F	30	ARG	CA-C-O	-11.81	104.85	119.38
1	E	103	HIS	CA-C-O	-11.80	107.91	120.42
1	C	120	ALA	N-CA-CB	11.80	127.14	109.91
2	D	66	LYS	CA-C-N	-11.80	103.67	120.42
2	D	66	LYS	C-N-CA	-11.80	103.67	120.42
2	D	58	PRO	O-C-N	11.79	138.77	122.38
1	E	54	GLN	CA-C-N	11.79	139.10	120.82
1	E	54	GLN	C-N-CA	11.79	139.10	120.82
1	C	96	VAL	O-C-N	11.79	135.12	121.80
1	G	16	LYS	CG-CD-CE	11.79	138.41	111.30
1	G	11	LYS	CB-CG-CD	11.79	138.41	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	78	ASN	O-C-N	11.78	135.58	122.15
1	C	89	HIS	ND1-CG-CD2	11.78	117.88	106.10
2	B	79	ASP	CA-C-N	11.77	144.03	121.54
2	B	79	ASP	C-N-CA	11.77	144.03	121.54
2	F	68	LEU	CB-CA-C	-11.77	91.97	110.81
2	F	57	ASN	CB-CG-ND2	11.77	134.06	116.40
1	A	80	LEU	CA-C-N	-11.77	103.34	120.28
1	A	80	LEU	C-N-CA	-11.77	103.34	120.28
1	C	89	HIS	CG-CD2-NE2	-11.77	95.43	107.20
1	A	122	HIS	CB-CG-CD2	-11.76	115.92	131.20
1	E	101	LEU	CA-C-N	11.75	136.98	120.29
1	E	101	LEU	C-N-CA	11.75	136.98	120.29
1	G	86	LEU	N-CA-CB	11.75	130.34	110.49
1	G	129	LEU	N-CA-C	11.75	126.71	112.38
2	B	113	VAL	CG1-CB-CG2	11.74	136.63	110.80
1	G	136	LEU	CA-C-O	-11.73	104.95	119.38
1	C	31	ARG	CB-CA-C	-11.73	85.79	110.31
1	A	55	VAL	CA-C-N	11.70	140.25	120.71
1	A	55	VAL	C-N-CA	11.70	140.25	120.71
1	C	137	THR	N-CA-C	-11.70	99.00	113.28
1	A	59	GLY	O-C-N	11.70	133.41	122.18
2	B	143	HIS	N-CA-CB	11.70	130.26	110.49
1	E	137	THR	CA-C-N	11.70	136.90	120.29
1	E	137	THR	C-N-CA	11.70	136.90	120.29
2	H	85	PHE	CB-CG-CD2	11.70	140.58	120.70
2	H	57	ASN	CB-CG-ND2	11.69	133.93	116.40
2	B	34	VAL	CA-C-O	11.68	133.55	121.17
1	E	36	PHE	O-C-N	-11.68	111.93	121.27
2	B	40	ARG	N-CA-CB	-11.67	90.76	110.49
1	E	49	SER	N-CA-CB	-11.67	92.88	110.04
2	B	73	ASP	CA-C-N	11.67	144.28	121.41
2	B	73	ASP	C-N-CA	11.67	144.28	121.41
1	E	59	GLY	O-C-N	-11.67	110.58	122.13
2	D	76	ALA	CB-CA-C	-11.66	85.61	109.99
2	H	85	PHE	CA-C-O	-11.65	105.66	121.86
1	A	128	PHE	CB-CG-CD1	-11.65	100.90	120.70
2	D	117	HIS	ND1-CE1-NE2	-11.65	96.75	108.40
1	G	94	ASP	CB-CA-C	11.63	127.89	109.62
2	F	24	GLY	CA-C-O	-11.63	100.33	120.57
1	C	12	ALA	CA-C-N	-11.61	100.47	122.06
1	C	12	ALA	C-N-CA	-11.61	100.47	122.06
1	G	97	ASN	CA-CB-CG	11.61	124.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	123	THR	CA-C-N	11.61	132.34	120.38
2	H	123	THR	C-N-CA	11.61	132.34	120.38
2	H	47	ASP	CA-C-N	11.61	140.09	121.99
2	H	47	ASP	C-N-CA	11.61	140.09	121.99
1	A	108	THR	CA-CB-CG2	11.60	130.22	110.50
1	G	32	MET	N-CA-CB	11.59	127.44	109.82
2	H	26	GLU	CB-CG-CD	11.59	132.31	112.60
2	B	86	ALA	CB-CA-C	-11.59	91.14	110.85
1	A	76	MET	CA-CB-CG	-11.59	90.93	114.10
2	B	65	LYS	CB-CA-C	11.59	130.02	110.79
2	F	8	LYS	CB-CA-C	11.58	130.53	110.85
2	H	49	SER	N-CA-CB	-11.57	90.05	110.42
1	A	38	THR	N-CA-C	11.57	123.89	111.28
2	B	128	ALA	CB-CA-C	-11.57	91.54	110.74
1	E	53	ALA	O-C-N	11.57	137.43	122.39
2	F	62	ALA	N-CA-CB	-11.57	93.02	109.91
1	A	121	VAL	CA-C-O	-11.56	106.72	120.83
2	D	118	PHE	CB-CA-C	11.56	133.01	109.55
1	E	41	THR	CA-CB-CG2	11.56	130.15	110.50
1	G	52	SER	CA-C-O	11.56	137.04	120.51
1	E	116	GLU	CG-CD-OE2	-11.54	91.85	118.40
2	F	101	GLU	CA-C-O	11.54	137.01	120.51
1	A	104	CYS	CA-CB-SG	-11.53	87.89	114.40
1	C	92	ARG	CD-NE-CZ	-11.53	108.26	124.40
1	G	38	THR	CA-CB-OG1	11.53	126.89	109.60
1	G	58	HIS	CA-C-O	-11.53	105.20	119.38
2	H	139	ASN	CB-CG-ND2	-11.52	99.11	116.40
1	C	71	ALA	CA-C-N	-11.52	104.41	122.49
1	C	71	ALA	C-N-CA	-11.52	104.41	122.49
1	E	85	ASP	O-C-N	11.52	134.33	122.12
2	B	61	LYS	O-C-N	-11.52	108.26	122.20
2	B	80	ASN	CB-CG-OD1	-11.51	97.77	120.80
1	G	29	LEU	CB-CA-C	11.51	130.25	110.68
1	C	36	PHE	CB-CG-CD2	11.51	140.26	120.70
1	G	89	HIS	CB-CG-CD2	11.51	146.16	131.20
1	E	120	ALA	CA-C-N	11.50	139.97	121.34
1	E	120	ALA	C-N-CA	11.50	139.97	121.34
2	D	27	ALA	CA-C-O	11.50	132.90	120.82
1	A	61	LYS	N-CA-C	-11.49	98.73	111.14
1	A	21	ALA	N-CA-CB	-11.49	91.08	110.49
1	G	59	GLY	N-CA-C	11.49	126.51	112.73
2	H	122	PHE	O-C-N	11.48	137.26	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	24	TYR	CB-CG-CD1	11.48	138.02	120.80
2	B	134	VAL	CA-C-O	11.48	133.97	119.39
2	F	55	MET	CB-CA-C	11.48	130.80	110.37
2	D	70	ALA	O-C-N	11.47	137.31	122.39
1	C	122	HIS	O-C-N	-11.47	109.96	122.12
2	D	12	THR	CA-CB-CG2	11.47	130.00	110.50
1	E	68	ASN	CB-CG-ND2	11.47	133.60	116.40
2	F	102	ASN	CA-C-N	11.46	136.57	120.29
2	F	102	ASN	C-N-CA	11.46	136.57	120.29
1	G	124	SER	CB-CA-C	11.46	130.34	110.85
1	C	16	LYS	CB-CG-CD	-11.45	84.97	111.30
2	H	79	ASP	N-CA-C	-11.45	97.45	112.68
1	C	56	LYS	CG-CD-CE	11.45	137.63	111.30
2	D	93	CYS	N-CA-CB	11.45	129.84	110.49
1	C	101	LEU	O-C-N	11.44	135.20	122.15
1	E	58	HIS	CA-C-O	11.45	133.74	120.92
2	D	75	LEU	CB-CA-C	11.44	132.46	110.27
2	B	47	ASP	OD1-CG-OD2	-11.44	95.45	122.90
1	G	129	LEU	CB-CA-C	-11.44	86.19	110.32
2	B	77	HIS	O-C-N	11.44	136.83	122.65
1	G	62	VAL	N-CA-C	-11.42	100.83	111.45
1	C	107	VAL	CA-C-N	11.41	140.10	120.58
1	C	107	VAL	C-N-CA	11.41	140.10	120.58
2	F	137	VAL	N-CA-CB	11.41	126.95	110.52
2	H	79	ASP	CB-CG-OD1	11.41	144.63	118.40
2	D	30	ARG	CB-CG-CD	11.40	137.53	111.30
2	B	44	SER	CB-CA-C	11.40	133.82	109.99
2	B	86	ALA	N-CA-C	11.40	123.78	111.36
1	C	40	LYS	CB-CG-CD	-11.40	85.09	111.30
1	E	106	LEU	CB-CA-C	11.39	133.08	110.42
2	F	69	GLY	N-CA-C	-11.39	100.38	114.16
2	D	120	LYS	CA-C-N	11.38	137.60	120.31
2	D	120	LYS	C-N-CA	11.38	137.60	120.31
2	H	50	THR	CA-CB-OG1	-11.37	92.54	109.60
1	E	5	ALA	O-C-N	11.37	137.56	122.33
2	D	42	PHE	CE1-CZ-CE2	11.36	140.45	120.00
1	G	33	PHE	N-CA-CB	11.35	127.06	109.82
1	E	11	LYS	CA-C-N	11.34	139.65	120.71
1	E	11	LYS	C-N-CA	11.34	139.65	120.71
2	D	76	ALA	O-C-N	11.34	138.11	122.46
2	D	106	LEU	CB-CA-C	11.34	131.54	110.11
2	F	120	LYS	CA-C-O	-11.33	106.94	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	108	ASN	CB-CG-ND2	-11.33	99.40	116.40
2	B	3	LEU	CA-C-O	11.32	135.26	121.56
2	H	12	THR	CA-C-N	11.32	136.03	120.63
2	H	12	THR	C-N-CA	11.32	136.03	120.63
1	G	63	ALA	CA-C-O	-11.32	104.62	119.11
1	A	34	LEU	CB-CG-CD2	-11.32	76.75	110.70
1	E	86	LEU	CA-C-O	11.32	133.81	120.00
2	D	4	THR	CA-C-O	-11.31	106.95	120.41
2	B	91	LEU	CA-C-O	-11.30	105.73	119.18
1	G	122	HIS	CA-C-O	-11.30	108.95	120.82
2	D	100	PRO	N-CA-CB	-11.30	91.89	103.19
2	D	53	ALA	N-CA-CB	11.30	126.36	109.98
2	F	111	VAL	CB-CA-C	-11.30	93.75	112.16
2	F	133	VAL	CA-CB-CG2	-11.30	91.20	110.40
2	H	32	LEU	CA-C-O	11.30	132.85	120.20
2	B	19	ASN	N-CA-C	-11.29	88.90	108.20
2	D	65	LYS	CB-CA-C	11.29	128.87	110.81
1	E	87	HIS	CA-C-N	11.29	143.10	121.54
1	E	87	HIS	C-N-CA	11.29	143.10	121.54
1	A	83	LEU	CB-CA-C	11.29	132.34	110.67
2	H	44	SER	N-CA-CB	11.29	127.24	110.65
1	G	17	VAL	N-CA-C	-11.28	99.62	111.58
2	D	30	ARG	CA-CB-CG	11.28	136.65	114.10
2	D	86	ALA	CB-CA-C	11.27	129.73	110.79
2	D	43	GLU	N-CA-CB	-11.27	94.11	110.79
2	D	88	LEU	CA-C-O	-11.27	105.86	119.49
1	A	121	VAL	CA-CB-CG2	-11.26	91.25	110.40
2	H	105	LEU	N-CA-CB	11.26	128.01	110.44
1	C	141	ARG	NH1-CZ-NH2	-11.26	104.66	119.30
2	F	53	ALA	CB-CA-C	-11.25	93.21	110.88
2	F	70	ALA	CB-CA-C	11.24	129.50	110.84
1	A	6	ASP	CA-C-O	11.23	132.91	120.90
1	G	54	GLN	N-CA-C	11.21	127.58	112.90
2	F	101	GLU	CG-CD-OE1	11.21	144.18	118.40
1	G	98	PHE	CB-CA-C	11.21	129.73	110.68
2	H	10	ALA	O-C-N	11.19	133.67	122.03
1	E	4	PRO	N-CA-C	-11.19	99.17	114.27
2	B	80	ASN	O-C-N	-11.18	107.72	122.59
2	B	30	ARG	CG-CD-NE	11.18	136.59	112.00
2	H	124	PRO	N-CA-CB	11.18	113.92	103.08
2	D	131	GLN	CB-CG-CD	-11.17	93.61	112.60
1	E	56	LYS	CA-C-N	11.17	132.12	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	56	LYS	C-N-CA	11.17	132.12	119.94
2	H	4	THR	CA-CB-CG2	-11.16	91.52	110.50
1	G	12	ALA	CA-C-O	11.16	132.19	120.70
1	A	47	ASP	N-CA-C	-11.16	89.12	108.20
2	F	113	VAL	O-C-N	-11.16	110.98	121.91
2	F	84	THR	N-CA-C	-11.15	97.80	111.40
2	F	122	PHE	CA-C-N	11.15	138.79	122.29
2	F	122	PHE	C-N-CA	11.15	138.79	122.29
1	G	101	LEU	CD1-CG-CD2	11.14	135.30	110.80
1	E	54	GLN	CB-CG-CD	11.13	131.53	112.60
1	E	56	LYS	O-C-N	-11.13	110.32	122.12
2	F	44	SER	N-CA-CB	11.13	126.55	110.40
2	D	30	ARG	CA-C-O	-11.13	104.86	119.11
2	F	101	GLU	CA-CB-CG	-11.13	91.84	114.10
2	D	86	ALA	O-C-N	-11.13	108.71	122.17
1	E	100	LEU	CB-CA-C	11.12	131.05	110.70
2	F	97	HIS	CA-CB-CG	11.12	124.92	113.80
1	G	103	HIS	CG-ND1-CE1	11.11	128.19	109.30
1	C	132	VAL	O-C-N	11.11	133.38	121.94
1	E	137	THR	O-C-N	11.10	136.66	122.22
1	C	11	LYS	CA-C-N	11.09	136.04	120.29
1	C	11	LYS	C-N-CA	11.09	136.04	120.29
2	D	89	SER	O-C-N	-11.09	107.27	122.46
2	D	72	SER	CA-C-O	11.09	136.36	120.51
2	F	77	HIS	CA-CB-CG	-11.09	102.71	113.80
1	G	18	GLY	O-C-N	11.08	137.10	122.70
2	D	105	LEU	N-CA-CB	11.08	127.36	110.30
1	C	53	ALA	O-C-N	-11.07	108.65	122.27
2	H	81	LEU	N-CA-CB	11.07	126.34	110.07
2	F	77	HIS	CE1-NE2-CD2	11.07	120.07	109.00
2	F	139	ASN	O-C-N	-11.07	109.27	122.22
1	E	40	LYS	CA-C-N	11.06	142.67	121.54
1	E	40	LYS	C-N-CA	11.06	142.67	121.54
2	B	108	ASN	CA-CB-CG	11.06	123.66	112.60
2	F	70	ALA	O-C-N	-11.05	108.82	122.20
2	B	11	VAL	CA-C-O	11.05	134.60	120.78
2	B	86	ALA	O-C-N	-11.05	109.55	122.15
2	H	55	MET	O-C-N	-11.05	108.02	122.39
2	F	37	TRP	CB-CG-CD2	11.05	142.26	126.80
2	B	82	LYS	CA-C-N	11.04	132.19	119.94
2	B	82	LYS	C-N-CA	11.04	132.19	119.94
2	F	126	VAL	CA-C-O	-11.04	109.15	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	36	PRO	N-CA-CB	11.03	114.83	103.25
1	A	49	SER	CA-C-N	-11.03	105.28	121.05
1	A	49	SER	C-N-CA	-11.03	105.28	121.05
2	F	143	HIS	CA-CB-CG	-11.03	102.77	113.80
1	G	117	PHE	CA-C-N	11.02	136.59	120.83
1	G	117	PHE	C-N-CA	11.02	136.59	120.83
2	D	8	LYS	CB-CG-CD	-11.02	85.95	111.30
1	G	14	TRP	CB-CG-CD2	-11.02	111.37	126.80
2	B	70	ALA	CA-C-O	11.01	132.24	120.90
1	E	63	ALA	O-C-N	11.01	133.79	122.12
2	F	54	VAL	CA-CB-CG1	-11.01	91.69	110.40
1	A	97	ASN	CB-CG-ND2	11.00	132.90	116.40
1	G	68	ASN	O-C-N	11.00	135.09	122.22
2	F	141	LEU	CA-C-O	-11.00	104.75	119.05
1	A	62	VAL	CB-CA-C	-11.00	98.06	111.81
2	B	4	THR	CA-C-O	11.00	131.96	120.63
1	G	89	HIS	CB-CG-ND1	-11.00	106.21	122.70
2	H	75	LEU	N-CA-C	-10.99	97.68	111.75
2	B	118	PHE	N-CA-CB	-10.99	93.29	110.44
1	E	20	HIS	CB-CG-ND1	-10.99	106.22	122.70
1	C	106	LEU	CD1-CG-CD2	10.99	134.97	110.80
2	D	2	HIS	CB-CG-CD2	10.98	145.47	131.20
1	C	108	THR	CA-CB-CG2	10.98	129.16	110.50
1	C	63	ALA	CB-CA-C	-10.97	93.65	110.88
1	E	110	ALA	N-CA-CB	-10.97	91.95	110.49
2	H	113	VAL	O-C-N	10.97	132.51	121.87
1	C	42	TYR	CA-C-O	-10.97	106.13	119.18
2	D	42	PHE	CA-CB-CG	-10.97	102.83	113.80
2	F	88	LEU	CD1-CG-CD2	10.97	134.94	110.80
1	E	86	LEU	N-CA-CB	-10.97	93.92	110.26
1	G	141	ARG	CG-CD-NE	10.97	136.12	112.00
2	B	67	VAL	O-C-N	10.96	132.65	121.91
2	H	82	LYS	CA-C-N	-10.96	99.93	121.41
2	H	82	LYS	C-N-CA	-10.96	99.93	121.41
2	H	112	CYS	CA-C-O	-10.95	106.78	119.60
1	C	43	PHE	CA-C-N	-10.95	108.39	119.56
1	C	43	PHE	C-N-CA	-10.95	108.39	119.56
2	F	82	LYS	CA-C-O	-10.94	104.86	120.51
1	C	64	ASP	CB-CG-OD1	-10.93	93.25	118.40
1	C	62	VAL	CB-CA-C	10.93	126.88	112.24
1	E	52	SER	CB-CA-C	-10.93	90.71	109.83
1	A	125	LEU	CB-CA-C	10.92	129.42	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	108	ASN	CA-C-N	-10.92	104.19	121.34
2	D	108	ASN	C-N-CA	-10.92	104.19	121.34
1	C	68	ASN	N-CA-CB	10.92	126.17	110.12
1	E	135	VAL	CB-CA-C	10.92	125.94	111.97
1	E	103	HIS	ND1-CE1-NE2	-10.91	97.49	108.40
1	E	58	HIS	N-CA-CB	10.91	127.56	109.78
1	A	137	THR	CA-C-O	10.90	132.51	119.97
1	G	134	THR	O-C-N	-10.90	110.56	122.12
2	D	92	HIS	CA-C-O	10.90	132.65	119.79
1	E	126	ASP	CA-C-O	-10.90	109.37	120.82
1	G	40	LYS	O-C-N	-10.90	110.42	122.08
2	H	1	VAL	CA-C-O	-10.90	102.28	120.80
1	G	68	ASN	CB-CG-ND2	-10.89	100.06	116.40
2	H	95	LYS	CA-C-N	10.89	142.33	121.54
2	H	95	LYS	C-N-CA	10.89	142.33	121.54
2	B	54	VAL	CA-C-O	-10.88	108.97	121.05
1	G	132	VAL	O-C-N	10.88	133.04	121.83
2	D	117	HIS	CE1-NE2-CD2	10.88	119.88	109.00
1	G	24	TYR	N-CA-C	-10.87	99.51	111.36
2	F	90	GLU	N-CA-C	-10.87	93.54	111.37
1	G	8	THR	OG1-CB-CG2	10.86	131.02	109.30
1	G	60	LYS	N-CA-C	-10.86	100.17	113.41
1	C	6	ASP	N-CA-C	10.85	124.13	111.11
2	D	78	LEU	CB-CA-C	10.85	129.30	110.85
2	F	59	LYS	CA-CB-CG	10.85	135.81	114.10
1	C	85	ASP	CA-C-O	10.85	132.36	120.10
2	F	36	PRO	N-CA-CB	-10.85	91.86	103.25
2	B	79	ASP	CB-CG-OD2	-10.84	93.47	118.40
2	H	63	HIS	CB-CG-CD2	10.84	145.29	131.20
2	D	139	ASN	CA-C-O	-10.83	105.88	119.31
1	E	61	LYS	O-C-N	10.83	136.84	122.33
1	E	134	THR	N-CA-CB	10.83	126.19	110.16
2	F	24	GLY	O-C-N	10.83	136.78	122.70
2	F	116	HIS	N-CA-C	-10.83	99.48	111.28
2	D	18	VAL	CA-C-O	-10.82	107.99	120.65
2	H	33	VAL	CA-CB-CG1	10.82	128.80	110.40
2	H	104	ARG	O-C-N	-10.81	110.51	122.08
1	G	140	TYR	CA-CB-CG	10.81	133.36	113.90
1	E	19	ALA	N-CA-C	-10.80	100.40	112.72
2	H	108	ASN	CA-C-N	-10.80	103.27	121.09
2	H	108	ASN	C-N-CA	-10.80	103.27	121.09
2	F	50	THR	CB-CA-C	10.80	124.47	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	90	LYS	CD-CE-NZ	10.79	146.44	111.90
1	E	1	VAL	CB-CA-C	-10.79	90.91	111.40
2	F	122	PHE	CA-CB-CG	10.79	124.59	113.80
2	H	40	ARG	CD-NE-CZ	-10.79	109.30	124.40
1	A	84	SER	CA-C-N	10.78	138.73	120.72
1	A	84	SER	C-N-CA	10.78	138.73	120.72
1	E	108	THR	O-C-N	10.78	134.62	122.11
2	B	18	VAL	CA-CB-CG2	10.78	128.72	110.40
2	D	6	VAL	CA-CB-CG2	10.78	128.72	110.40
1	A	116	GLU	CB-CA-C	10.76	128.30	109.15
2	F	47	ASP	CA-C-N	10.76	140.10	122.14
2	F	47	ASP	C-N-CA	10.76	140.10	122.14
1	G	92	ARG	CG-CD-NE	10.75	135.66	112.00
2	B	99	ASP	N-CA-CB	10.75	126.67	109.90
1	C	140	TYR	CA-C-N	10.75	141.05	121.70
1	C	140	TYR	C-N-CA	10.75	141.05	121.70
2	B	79	ASP	CA-C-O	-10.75	107.95	120.10
1	C	84	SER	N-CA-C	-10.74	99.57	111.07
1	E	117	PHE	CA-C-O	10.74	134.27	122.13
1	G	67	THR	CA-C-O	10.74	132.63	119.31
1	C	87	HIS	CA-CB-CG	-10.74	103.06	113.80
1	C	17	VAL	O-C-N	10.74	135.99	122.57
1	G	104	CYS	CA-C-O	-10.73	107.63	119.97
1	E	78	ASN	N-CA-C	10.73	124.89	111.69
2	F	123	THR	CA-C-N	10.73	131.43	120.38
2	F	123	THR	C-N-CA	10.73	131.43	120.38
2	B	103	PHE	N-CA-C	-10.73	98.35	111.33
2	F	15	TRP	O-C-N	10.73	134.77	122.22
1	G	120	ALA	O-C-N	-10.72	110.75	122.12
1	G	7	LYS	CA-C-O	10.72	133.56	121.02
1	G	84	SER	N-CA-C	-10.72	99.28	110.97
2	D	112	CYS	N-CA-CB	10.72	125.83	110.07
2	F	127	GLN	CA-C-O	10.72	132.07	120.82
1	G	14	TRP	CB-CA-C	-10.72	90.09	110.67
2	B	112	CYS	N-CA-CB	10.71	125.82	110.07
2	D	19	ASN	CB-CA-C	-10.71	93.64	110.78
1	E	98	PHE	CA-CB-CG	-10.71	103.09	113.80
2	H	86	ALA	N-CA-C	-10.71	100.76	114.04
2	H	146	HIS	ND1-CE1-NE2	-10.71	97.69	108.40
2	B	89	SER	CB-CA-C	-10.70	93.99	110.90
1	A	10	VAL	CB-CA-C	10.69	126.56	112.24
2	B	124	PRO	CA-C-O	-10.69	105.07	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	32	MET	N-CA-CB	10.68	126.05	109.82
1	E	137	THR	CA-C-O	-10.68	107.03	119.95
1	C	23	GLU	N-CA-C	-10.68	96.67	112.04
2	F	129	ALA	CB-CA-C	10.66	128.98	110.85
2	F	135	ALA	CA-C-O	-10.66	109.80	121.00
1	C	137	THR	O-C-N	10.66	137.55	122.41
2	F	26	GLU	CA-C-N	10.66	135.61	120.79
2	F	26	GLU	C-N-CA	10.66	135.61	120.79
2	B	112	CYS	N-CA-C	-10.66	97.49	111.24
2	H	121	GLU	CA-CB-CG	-10.66	92.78	114.10
1	G	14	TRP	CA-CB-CG	-10.66	93.35	113.60
2	B	1	VAL	CA-C-N	-10.65	105.39	121.26
2	B	1	VAL	C-N-CA	-10.65	105.39	121.26
2	F	17	LYS	N-CA-CB	-10.64	92.72	110.39
1	A	27	GLU	CB-CA-C	10.63	131.08	110.67
1	A	30	GLU	CA-C-N	10.62	134.93	120.38
1	A	30	GLU	C-N-CA	10.62	134.93	120.38
2	H	57	ASN	OD1-CG-ND2	-10.61	111.99	122.60
2	B	98	VAL	CA-CB-CG1	10.61	128.43	110.40
1	C	68	ASN	CB-CG-ND2	10.60	132.30	116.40
1	C	89	HIS	O-C-N	10.60	137.41	122.36
2	H	31	LEU	N-CA-C	-10.60	99.69	111.14
1	G	133	SER	CA-CB-OG	10.60	132.30	111.10
2	D	12	THR	CA-C-O	-10.60	105.27	119.05
1	E	96	VAL	N-CA-C	-10.59	97.81	111.05
1	A	116	GLU	CA-C-N	10.59	138.54	122.23
1	A	116	GLU	C-N-CA	10.59	138.54	122.23
1	C	10	VAL	N-CA-CB	-10.59	97.93	110.64
1	E	32	MET	O-C-N	10.58	133.40	122.08
1	E	74	ASP	CB-CA-C	10.58	127.75	109.24
2	B	98	VAL	CB-CA-C	10.57	127.28	111.31
1	G	58	HIS	CE1-NE2-CD2	-10.57	98.43	109.00
1	G	122	HIS	N-CA-C	-10.57	99.76	111.07
1	E	97	ASN	CA-CB-CG	10.57	123.17	112.60
2	F	122	PHE	CA-C-O	-10.57	109.62	122.41
2	D	112	CYS	O-C-N	10.57	134.37	122.11
2	F	53	ALA	CA-C-N	-10.57	102.97	120.30
2	F	53	ALA	C-N-CA	-10.57	102.97	120.30
2	H	105	LEU	O-C-N	10.57	136.94	122.46
1	A	73	VAL	CA-CB-CG2	10.55	128.34	110.40
1	G	112	HIS	CB-CG-CD2	10.55	144.92	131.20
1	E	31	ARG	NH1-CZ-NH2	-10.55	105.59	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	17	LYS	N-CA-C	10.55	125.41	112.54
2	B	82	LYS	CA-C-O	10.54	132.01	120.10
2	B	11	VAL	O-C-N	-10.54	109.40	122.57
2	D	121	GLU	N-CA-CB	10.53	126.61	110.28
2	F	44	SER	O-C-N	10.53	137.93	122.13
2	H	9	SER	CA-CB-OG	-10.53	90.04	111.10
1	A	3	SER	CA-C-N	10.53	130.74	119.05
1	A	3	SER	C-N-CA	10.53	130.74	119.05
2	H	65	LYS	N-CA-C	-10.53	100.43	113.28
1	C	84	SER	CA-C-O	-10.53	109.77	120.82
1	G	109	LEU	CA-C-N	-10.53	105.12	120.28
1	G	109	LEU	C-N-CA	-10.53	105.12	120.28
2	H	17	LYS	CA-C-N	10.52	135.69	122.43
2	H	17	LYS	C-N-CA	10.52	135.69	122.43
2	B	108	ASN	O-C-N	-10.52	108.33	122.43
1	E	101	LEU	CA-C-O	-10.52	106.27	119.31
2	B	103	PHE	CA-CB-CG	10.52	124.31	113.80
1	G	4	PRO	N-CA-C	-10.52	90.81	112.47
1	G	14	TRP	CA-C-O	10.51	132.06	119.97
2	H	143	HIS	CA-C-O	10.50	132.68	120.92
2	F	69	GLY	CA-C-O	-10.50	107.11	119.50
1	G	21	ALA	CA-C-N	-10.50	100.83	121.41
1	G	21	ALA	C-N-CA	-10.50	100.83	121.41
1	E	124	SER	CA-C-O	-10.49	109.30	120.42
1	G	11	LYS	N-CA-CB	10.49	127.81	110.39
1	G	67	THR	O-C-N	-10.49	107.99	122.46
2	H	40	ARG	NH1-CZ-NH2	10.49	132.94	119.30
2	H	46	GLY	N-CA-C	10.49	124.35	111.45
2	B	57	ASN	O-C-N	-10.48	112.19	121.31
2	F	104	ARG	CB-CA-C	10.48	127.34	110.88
1	G	110	ALA	CA-C-O	-10.48	108.26	120.10
1	C	46	PHE	CB-CG-CD1	-10.48	102.89	120.70
1	C	98	PHE	O-C-N	10.48	133.29	122.08
2	D	20	VAL	CA-CB-CG2	10.48	128.21	110.40
1	A	111	ALA	N-CA-CB	10.47	125.85	110.56
1	E	111	ALA	CA-C-O	10.47	132.84	119.12
2	B	32	LEU	CB-CA-C	10.47	128.17	110.79
1	G	13	ALA	N-CA-C	-10.47	97.90	112.45
1	G	114	PRO	CA-C-O	-10.47	101.55	120.60
1	E	112	HIS	N-CA-CB	-10.46	96.45	110.88
2	H	15	TRP	CZ3-CH2-CZ2	10.46	135.09	121.50
1	A	83	LEU	O-C-N	10.45	135.12	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	141	ARG	CA-CB-CG	-10.45	93.20	114.10
1	G	70	VAL	CA-C-N	-10.45	103.89	120.60
1	G	70	VAL	C-N-CA	-10.45	103.89	120.60
2	B	5	PRO	CB-CA-C	-10.44	95.55	113.20
1	C	53	ALA	N-CA-CB	10.44	126.47	110.28
2	H	125	PRO	CA-CB-CG	-10.44	84.67	104.50
2	H	73	ASP	CA-C-O	-10.43	102.22	118.91
2	D	38	THR	CB-CA-C	10.43	130.71	109.95
2	B	23	VAL	O-C-N	-10.43	111.34	121.87
1	G	66	LEU	CA-C-N	-10.43	102.90	121.14
1	G	66	LEU	C-N-CA	-10.43	102.90	121.14
2	F	63	HIS	CB-CG-ND1	10.42	138.33	122.70
2	B	92	HIS	CA-C-O	10.42	131.59	120.55
1	C	33	PHE	CA-C-O	-10.42	108.33	120.10
1	A	113	LEU	N-CA-CB	-10.41	97.26	110.79
1	A	123	ALA	CA-C-O	10.41	135.40	120.51
1	C	4	PRO	CA-C-N	-10.41	106.49	120.54
1	C	4	PRO	C-N-CA	-10.41	106.49	120.54
1	C	114	PRO	CA-C-N	10.41	140.48	122.79
1	C	114	PRO	C-N-CA	10.41	140.48	122.79
2	H	35	TYR	CB-CG-CD2	-10.40	105.20	120.80
1	C	108	THR	CA-CB-OG1	-10.39	94.01	109.60
1	C	6	ASP	CB-CG-OD1	-10.39	94.50	118.40
1	A	20	HIS	CB-CG-CD2	-10.39	117.69	131.20
2	B	101	GLU	CG-CD-OE1	10.39	142.30	118.40
1	C	122	HIS	CA-C-O	10.39	131.56	120.55
2	H	61	LYS	CA-C-O	-10.38	106.61	119.38
1	C	112	HIS	N-CA-CB	10.38	130.40	110.88
1	G	10	VAL	CA-CB-CG1	-10.38	92.75	110.40
1	C	87	HIS	CB-CG-ND1	-10.38	107.14	122.70
2	D	2	HIS	ND1-CG-CD2	-10.38	95.72	106.10
2	D	48	LEU	N-CA-C	-10.38	98.19	112.30
1	C	58	HIS	O-C-N	-10.38	110.83	122.03
1	A	27	GLU	CG-CD-OE1	10.37	142.25	118.40
1	E	128	PHE	O-C-N	10.37	133.29	122.09
2	D	111	VAL	CA-C-N	10.37	137.67	120.88
2	D	111	VAL	C-N-CA	10.37	137.67	120.88
2	F	7	GLU	O-C-N	10.37	135.02	122.27
2	B	101	GLU	CG-CD-OE2	-10.36	94.56	118.40
1	E	96	VAL	CA-C-O	-10.36	109.48	120.57
1	C	35	SER	O-C-N	-10.36	107.65	122.36
2	H	95	LYS	N-CA-CB	10.36	125.42	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	101	LEU	CA-C-N	10.35	135.18	120.28
1	G	101	LEU	C-N-CA	10.35	135.18	120.28
1	G	140	TYR	N-CA-C	-10.34	98.78	111.40
2	F	145	TYR	CB-CA-C	10.34	127.00	109.53
1	G	92	ARG	CA-CB-CG	10.34	134.78	114.10
1	C	94	ASP	CB-CA-C	10.34	125.85	109.52
1	E	35	SER	CA-CB-OG	-10.34	90.42	111.10
1	A	103	HIS	CG-CD2-NE2	-10.33	96.87	107.20
2	H	6	VAL	CB-CA-C	-10.33	98.92	111.94
2	H	43	GLU	CA-C-O	10.33	133.05	120.55
2	H	103	PHE	O-C-N	-10.33	111.17	122.12
2	B	80	ASN	CA-C-O	10.32	135.27	120.51
1	E	24	TYR	N-CA-CB	10.32	125.29	110.12
2	D	66	LYS	CB-CG-CD	-10.31	87.58	111.30
1	A	24	TYR	CB-CG-CD1	10.31	136.26	120.80
1	A	94	ASP	O-C-N	10.31	130.77	121.18
2	H	40	ARG	NE-CZ-NH1	10.30	131.80	121.50
1	A	127	LYS	CA-C-O	-10.28	109.90	120.90
2	D	99	ASP	N-CA-C	-10.27	87.11	109.81
1	C	89	HIS	CB-CA-C	-10.27	91.27	109.24
1	E	56	LYS	CB-CA-C	10.27	127.83	110.79
2	H	77	HIS	CB-CG-ND1	10.27	138.10	122.70
1	G	70	VAL	O-C-N	10.26	135.90	122.26
2	D	17	LYS	CG-CD-CE	10.25	134.88	111.30
2	F	134	VAL	CA-CB-CG2	10.25	127.83	110.40
1	E	98	PHE	CD1-CG-CD2	10.25	133.98	118.60
2	H	100	PRO	N-CD-CG	-10.25	87.83	103.20
1	G	69	ALA	CB-CA-C	10.25	129.45	110.70
1	A	34	LEU	N-CA-C	-10.25	99.48	112.90
1	E	50	HIS	CA-CB-CG	-10.24	103.56	113.80
2	D	53	ALA	O-C-N	10.24	133.09	122.03
2	F	80	ASN	OD1-CG-ND2	10.24	132.84	122.60
1	C	4	PRO	N-CA-C	-10.23	99.97	114.18
1	C	39	THR	CA-C-N	10.22	135.31	120.38
1	C	39	THR	C-N-CA	10.22	135.31	120.38
1	C	103	HIS	CA-C-N	10.22	141.52	121.58
1	C	103	HIS	C-N-CA	10.22	141.52	121.58
2	H	116	HIS	N-CA-C	-10.22	99.96	111.71
1	A	69	ALA	N-CA-C	-10.22	99.12	111.69
1	A	28	ALA	CB-CA-C	-10.22	90.09	110.42
2	H	124	PRO	CA-N-CD	-10.21	97.70	112.00
2	B	117	HIS	CB-CG-CD2	-10.21	117.93	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	75	ASP	CA-C-N	10.21	136.08	120.97
1	E	75	ASP	C-N-CA	10.21	136.08	120.97
2	H	94	ASP	N-CA-C	10.21	123.69	111.33
1	A	85	ASP	CB-CG-OD2	10.21	141.87	118.40
2	F	101	GLU	CA-C-N	10.20	134.36	120.38
2	F	101	GLU	C-N-CA	10.20	134.36	120.38
2	B	22	GLU	O-C-N	-10.20	110.59	122.32
2	B	144	LYS	O-C-N	-10.20	109.03	122.59
1	C	79	ALA	N-CA-C	10.20	123.46	111.02
2	F	92	HIS	CA-C-O	-10.19	106.67	119.31
1	G	32	MET	CA-CB-CG	-10.19	93.72	114.10
1	G	128	PHE	N-CA-CB	10.19	125.31	109.82
2	F	113	VAL	CA-C-N	10.19	136.10	120.82
2	F	113	VAL	C-N-CA	10.19	136.10	120.82
1	G	30	GLU	N-CA-C	-10.19	100.14	111.14
1	G	106	LEU	CB-CA-C	10.18	127.10	110.81
1	C	105	LEU	CA-C-O	10.18	131.18	120.70
2	D	141	LEU	O-C-N	10.18	134.13	122.22
2	B	123	THR	CA-CB-OG1	-10.17	94.34	109.60
1	E	140	TYR	N-CA-CB	-10.17	95.04	110.20
1	A	54	GLN	CA-CB-CG	-10.17	93.76	114.10
1	G	72	HIS	CA-C-O	-10.17	108.53	120.53
2	F	139	ASN	CA-C-N	10.16	134.26	120.44
2	F	139	ASN	C-N-CA	10.16	134.26	120.44
2	B	65	LYS	N-CA-CB	-10.15	95.20	110.12
1	C	121	VAL	N-CA-C	10.15	120.16	110.42
2	H	80	ASN	CB-CG-ND2	10.15	131.62	116.40
2	F	13	ALA	CB-CA-C	10.14	127.63	110.79
2	F	32	LEU	N-CA-C	-10.14	98.94	111.11
2	D	65	LYS	N-CA-CB	-10.14	94.83	109.94
2	B	78	LEU	O-C-N	10.13	133.70	122.15
1	C	66	LEU	CA-C-N	-10.13	105.69	120.28
1	C	66	LEU	C-N-CA	-10.13	105.69	120.28
2	B	12	THR	CA-C-N	10.13	134.22	120.44
2	B	12	THR	C-N-CA	10.13	134.22	120.44
1	A	123	ALA	CA-C-N	10.13	134.21	120.54
1	A	123	ALA	C-N-CA	10.13	134.21	120.54
2	B	21	ASP	N-CA-CB	-10.12	94.88	110.46
1	E	66	LEU	CA-C-N	10.11	137.87	120.68
1	E	66	LEU	C-N-CA	10.11	137.87	120.68
2	F	145	TYR	CA-C-N	-10.11	103.50	121.70
2	F	145	TYR	C-N-CA	-10.11	103.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	LEU	N-CA-C	10.10	122.29	111.28
2	B	69	GLY	N-CA-C	-10.10	98.35	115.62
2	F	104	ARG	N-CA-CB	-10.10	95.36	110.01
1	A	137	THR	OG1-CB-CG2	10.10	129.50	109.30
2	D	97	HIS	CB-CG-CD2	-10.10	118.07	131.20
1	A	30	GLU	OE1-CD-OE2	-10.09	98.68	122.90
1	C	30	GLU	OE1-CD-OE2	10.09	147.12	122.90
1	E	41	THR	CA-C-O	-10.09	106.08	120.51
2	D	89	SER	CA-C-N	10.09	133.80	120.28
2	D	89	SER	C-N-CA	10.09	133.80	120.28
2	H	77	HIS	CB-CG-CD2	-10.09	118.09	131.20
1	C	106	LEU	N-CA-C	-10.08	89.32	110.80
1	E	106	LEU	CB-CG-CD1	-10.08	80.45	110.70
1	G	30	GLU	CA-C-O	-10.08	110.31	120.70
1	A	121	VAL	CA-CB-CG1	10.08	127.53	110.40
2	H	11	VAL	CA-CB-CG1	10.08	127.53	110.40
2	B	25	GLY	O-C-N	10.08	134.07	122.68
2	H	60	VAL	CA-CB-CG2	10.07	127.52	110.40
2	F	35	TYR	CG-CD2-CE2	10.07	136.30	121.20
1	A	88	ALA	N-CA-C	10.06	123.28	111.71
1	C	22	GLY	O-C-N	-10.05	111.32	122.28
2	B	48	LEU	O-C-N	10.05	135.82	122.15
2	D	94	ASP	CA-C-O	-10.05	109.78	120.63
2	B	8	LYS	N-CA-CB	-10.05	95.35	110.12
1	C	28	ALA	CA-C-O	10.05	134.88	120.51
1	C	45	HIS	CB-CA-C	-10.04	95.52	111.18
2	H	102	ASN	CB-CG-OD1	-10.04	100.72	120.80
2	H	30	ARG	N-CA-CB	10.03	125.67	110.22
2	H	101	GLU	CG-CD-OE2	-10.03	95.32	118.40
2	B	11	VAL	CG1-CB-CG2	-10.03	88.73	110.80
2	F	146	HIS	CB-CG-CD2	10.03	144.24	131.20
2	D	89	SER	N-CA-CB	-10.02	94.80	110.44
1	E	6	ASP	N-CA-C	-10.02	100.20	111.82
1	E	115	ALA	N-CA-C	10.02	128.81	107.67
1	G	58	HIS	CB-CG-CD2	-10.02	118.17	131.20
1	A	48	LEU	CA-C-O	10.02	134.83	120.51
2	F	100	PRO	CA-C-N	10.02	140.67	121.54
2	F	100	PRO	C-N-CA	10.02	140.67	121.54
2	D	134	VAL	CA-C-O	-10.01	110.54	120.95
2	D	22	GLU	CG-CD-OE2	10.01	141.42	118.40
2	D	117	HIS	N-CA-CB	10.01	124.97	110.16
1	A	107	VAL	CA-CB-CG2	10.00	127.41	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	53	ALA	O-C-N	10.00	132.37	122.07
1	E	21	ALA	CA-C-O	-9.99	106.22	120.51
1	C	118	THR	N-CA-CB	-9.99	95.52	110.11
2	B	12	THR	OG1-CB-CG2	-9.99	89.32	109.30
2	F	48	LEU	N-CA-CB	9.98	128.05	111.49
2	H	23	VAL	N-CA-C	-9.98	100.95	113.22
1	E	113	LEU	CB-CA-C	9.97	129.24	111.20
2	D	73	ASP	O-C-N	9.96	132.74	122.08
1	A	67	THR	N-CA-C	-9.96	100.51	111.36
2	H	79	ASP	CA-CB-CG	9.95	122.55	112.60
2	H	25	GLY	O-C-N	-9.95	112.64	122.19
2	D	17	LYS	CB-CG-CD	9.95	134.18	111.30
2	H	23	VAL	CA-C-O	-9.94	108.67	119.20
1	C	50	HIS	CA-CB-CG	-9.93	103.87	113.80
1	C	74	ASP	CB-CA-C	9.93	124.73	109.34
1	G	126	ASP	O-C-N	-9.93	111.45	122.08
1	E	103	HIS	CA-C-N	9.93	134.59	120.79
1	E	103	HIS	C-N-CA	9.93	134.59	120.79
2	H	65	LYS	CA-CB-CG	9.93	133.96	114.10
2	B	11	VAL	CB-CA-C	9.92	127.56	111.29
1	C	19	ALA	N-CA-C	9.92	126.93	112.94
1	C	122	HIS	CA-CB-CG	9.92	123.72	113.80
2	F	35	TYR	CB-CG-CD2	-9.92	105.92	120.80
1	A	128	PHE	O-C-N	9.91	132.28	122.07
2	B	130	TYR	CB-CG-CD1	-9.91	105.94	120.80
1	C	113	LEU	CA-C-N	9.91	130.96	119.47
1	C	113	LEU	C-N-CA	9.91	130.96	119.47
2	D	67	VAL	CA-CB-CG2	9.91	127.24	110.40
2	H	63	HIS	CA-C-N	9.90	130.97	119.98
2	H	63	HIS	C-N-CA	9.90	130.97	119.98
2	D	119	GLY	CA-C-O	-9.90	108.44	121.51
2	F	143	HIS	CE1-NE2-CD2	-9.90	99.10	109.00
2	H	108	ASN	CA-CB-CG	-9.90	102.70	112.60
2	F	127	GLN	CG-CD-NE2	9.90	131.25	116.40
1	G	7	LYS	N-CA-CB	9.90	126.54	109.72
1	C	124	SER	O-C-N	9.89	133.43	122.15
2	F	146	HIS	ND1-CE1-NE2	9.88	118.28	108.40
1	G	111	ALA	N-CA-CB	9.88	125.41	110.79
1	E	23	GLU	CA-C-O	9.88	131.20	120.24
2	F	105	LEU	CA-C-O	-9.88	110.53	120.70
1	G	134	THR	CA-CB-OG1	-9.87	94.79	109.60
2	D	22	GLU	CA-C-O	-9.87	108.05	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	49	SER	N-CA-C	9.87	124.71	112.87
1	E	48	LEU	CB-CA-C	9.87	127.02	111.13
2	F	21	ASP	OD1-CG-OD2	9.87	146.58	122.90
1	A	60	LYS	CA-C-N	9.87	133.86	120.44
1	A	60	LYS	C-N-CA	9.87	133.86	120.44
2	H	116	HIS	CG-CD2-NE2	-9.87	97.33	107.20
1	C	17	VAL	N-CA-CB	9.86	127.50	111.23
2	H	3	LEU	CA-C-O	-9.86	109.65	121.28
2	B	85	PHE	O-C-N	9.85	134.38	122.26
2	F	92	HIS	ND1-CE1-NE2	-9.85	98.55	108.40
1	C	16	LYS	CA-C-N	9.85	139.69	121.97
1	C	16	LYS	C-N-CA	9.85	139.69	121.97
1	G	40	LYS	CA-CB-CG	9.85	133.79	114.10
1	G	101	LEU	O-C-N	-9.84	110.93	122.15
2	D	70	ALA	CA-C-O	-9.83	107.59	119.49
1	E	4	PRO	CA-N-CD	-9.83	98.23	112.00
1	C	128	PHE	N-CA-C	-9.83	99.60	111.69
2	D	109	VAL	N-CA-C	-9.83	100.69	112.98
1	A	109	LEU	N-CA-CB	-9.83	95.05	110.28
1	C	108	THR	CA-C-O	9.82	131.15	120.24
2	F	47	ASP	O-C-N	-9.82	109.51	122.77
2	H	124	PRO	CA-C-O	-9.82	106.32	120.56
2	B	30	ARG	N-CA-CB	-9.82	94.09	110.39
2	D	20	VAL	CB-CA-C	-9.82	95.19	111.29
2	F	102	ASN	O-C-N	-9.82	111.71	122.12
1	C	2	LEU	N-CA-C	-9.81	93.67	109.76
2	D	10	ALA	N-CA-CB	9.81	124.24	110.01
2	H	72	SER	O-C-N	9.81	132.30	122.09
1	C	118	THR	CA-CB-CG2	9.81	127.18	110.50
2	F	10	ALA	N-CA-C	9.81	122.99	111.02
1	A	138	SER	CA-C-N	9.81	140.28	121.54
1	A	138	SER	C-N-CA	9.81	140.28	121.54
2	F	16	GLY	CA-C-O	-9.81	103.50	120.57
2	B	95	LYS	N-CA-C	9.79	126.14	112.04
2	H	7	GLU	CA-C-N	-9.79	105.71	122.56
2	H	7	GLU	C-N-CA	-9.79	105.71	122.56
1	A	35	SER	N-CA-C	9.79	125.22	113.28
2	H	115	ALA	N-CA-CB	9.79	127.03	110.49
2	B	1	VAL	CA-C-O	-9.79	104.17	120.80
1	C	47	ASP	OD1-CG-OD2	-9.78	99.42	122.90
1	E	6	ASP	CB-CA-C	9.78	129.45	110.67
1	E	81	SER	O-C-N	9.78	134.03	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	136	LEU	N-CA-C	-9.78	100.61	112.54
2	H	22	GLU	CA-C-N	-9.78	107.69	121.77
2	H	22	GLU	C-N-CA	-9.78	107.69	121.77
1	C	134	THR	N-CA-CB	9.77	125.34	110.19
2	D	80	ASN	N-CA-C	9.77	122.93	109.54
1	E	30	GLU	CB-CG-CD	9.77	129.21	112.60
1	G	41	THR	CA-C-O	-9.77	106.54	120.51
2	B	114	LEU	N-CA-CB	-9.77	95.71	110.16
2	F	96	LEU	CA-C-O	-9.77	109.40	120.24
2	H	105	LEU	CA-C-N	-9.77	105.47	120.31
2	H	105	LEU	C-N-CA	-9.77	105.47	120.31
1	E	97	ASN	O-C-N	-9.76	110.26	122.27
2	B	111	VAL	N-CA-CB	9.76	128.44	110.77
2	F	114	LEU	O-C-N	9.76	133.34	122.11
1	C	38	THR	OG1-CB-CG2	9.76	128.82	109.30
1	A	40	LYS	N-CA-C	-9.76	100.48	112.38
1	A	48	LEU	CA-C-N	9.75	135.45	121.50
1	A	48	LEU	C-N-CA	9.75	135.45	121.50
2	F	30	ARG	CG-CD-NE	9.75	133.45	112.00
1	E	124	SER	O-C-N	-9.75	111.04	122.15
2	F	80	ASN	CA-CB-CG	-9.75	102.85	112.60
1	A	56	LYS	CB-CG-CD	9.74	133.71	111.30
2	F	96	LEU	N-CA-C	-9.74	99.70	111.69
1	E	4	PRO	O-C-N	9.74	135.71	122.37
1	C	15	GLY	CA-C-N	-9.74	101.90	121.18
1	C	15	GLY	C-N-CA	-9.74	101.90	121.18
2	F	5	PRO	CA-C-O	-9.74	104.19	118.89
1	A	26	ALA	CA-C-N	-9.73	105.52	120.31
1	A	26	ALA	C-N-CA	-9.73	105.52	120.31
2	B	126	VAL	O-C-N	9.73	133.66	122.18
2	H	22	GLU	CB-CG-CD	-9.73	96.06	112.60
1	C	72	HIS	O-C-N	-9.72	109.58	122.22
2	D	56	GLY	O-C-N	-9.72	110.07	122.70
1	C	77	PRO	CA-C-O	-9.71	105.06	119.34
2	H	11	VAL	CA-C-N	-9.71	100.95	121.64
2	H	11	VAL	C-N-CA	-9.71	100.95	121.64
2	B	93	CYS	CA-C-N	-9.70	107.28	120.28
2	B	93	CYS	C-N-CA	-9.70	107.28	120.28
1	E	47	ASP	N-CA-C	-9.70	92.79	108.41
2	F	40	ARG	CA-CB-CG	-9.70	94.70	114.10
2	F	63	HIS	O-C-N	9.70	136.19	122.41
2	D	58	PRO	CB-CA-C	-9.70	95.70	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	62	VAL	CA-CB-CG1	-9.69	93.92	110.40
1	C	138	SER	CA-C-O	-9.69	110.28	120.55
2	F	38	THR	N-CA-CB	9.69	124.50	110.16
2	H	19	ASN	CA-C-O	-9.69	109.19	121.11
2	D	71	PHE	CA-CB-CG	-9.69	104.11	113.80
2	D	94	ASP	O-C-N	9.69	132.39	122.12
2	D	141	LEU	CA-C-O	-9.68	109.16	120.10
1	C	58	HIS	CB-CA-C	9.68	125.95	110.95
1	C	98	PHE	N-CA-CB	9.68	124.53	109.82
2	D	18	VAL	N-CA-C	9.68	123.03	108.23
2	F	62	ALA	N-CA-C	9.67	121.52	110.97
2	B	140	ALA	CA-C-N	-9.67	106.89	122.95
2	B	140	ALA	C-N-CA	-9.67	106.89	122.95
2	D	40	ARG	O-C-N	9.67	135.46	122.59
1	C	62	VAL	CG1-CB-CG2	-9.67	89.52	110.80
2	H	87	THR	CA-CB-OG1	-9.67	95.09	109.60
1	C	105	LEU	O-C-N	-9.67	111.65	122.09
1	E	121	VAL	CA-CB-CG1	-9.66	93.97	110.40
1	G	20	HIS	CA-C-O	-9.66	107.75	119.43
1	G	29	LEU	CA-C-O	9.66	131.06	120.63
2	D	57	ASN	N-CA-CB	-9.65	92.45	109.73
2	F	139	ASN	N-CA-CB	-9.65	95.36	110.22
2	B	75	LEU	CA-C-O	9.64	131.59	119.05
2	H	139	ASN	CA-CB-CG	-9.64	102.96	112.60
1	A	122	HIS	CG-CD2-NE2	9.64	116.84	107.20
2	D	43	GLU	O-C-N	-9.64	106.98	121.63
2	H	17	LYS	CA-CB-CG	-9.64	94.82	114.10
2	B	42	PHE	CA-CB-CG	9.64	123.44	113.80
2	D	13	ALA	N-CA-C	-9.64	99.86	112.68
2	F	55	MET	CB-CG-SD	9.64	141.61	112.70
2	B	52	ASP	CB-CG-OD2	-9.63	96.25	118.40
2	F	92	HIS	O-C-N	9.63	135.75	122.46
2	D	138	ALA	N-CA-C	-9.62	99.57	111.11
2	H	44	SER	CB-CA-C	9.62	125.71	109.55
1	A	119	PRO	CA-C-O	9.61	132.45	119.00
1	A	125	LEU	CA-C-N	-9.61	107.44	120.79
1	A	125	LEU	C-N-CA	-9.61	107.44	120.79
1	G	126	ASP	CB-CG-OD2	-9.61	96.31	118.40
2	D	97	HIS	O-C-N	-9.60	111.82	122.67
2	F	37	TRP	CA-C-N	9.60	133.93	120.29
2	F	37	TRP	C-N-CA	9.60	133.93	120.29
2	H	14	LEU	CB-CA-C	-9.60	95.66	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	106	LEU	CB-CA-C	9.60	129.10	110.67
1	A	29	LEU	O-C-N	9.60	135.70	122.46
1	A	89	HIS	CB-CG-CD2	-9.59	118.73	131.20
1	E	87	HIS	O-C-N	-9.59	109.84	122.59
1	E	1	VAL	N-CA-CB	9.58	127.78	111.50
2	F	114	LEU	CA-CB-CG	-9.57	82.79	116.30
2	D	77	HIS	CG-CD2-NE2	9.57	116.77	107.20
1	G	116	GLU	N-CA-CB	9.57	126.78	110.51
1	C	26	ALA	O-C-N	9.57	135.16	122.33
2	H	129	ALA	CB-CA-C	-9.57	94.59	110.85
1	E	49	SER	CB-CA-C	9.56	126.74	109.62
2	H	76	ALA	CA-C-N	9.56	139.81	121.54
2	H	76	ALA	C-N-CA	9.56	139.81	121.54
1	C	60	LYS	CA-C-O	9.55	130.96	119.97
2	F	98	VAL	CA-C-O	9.55	132.40	120.75
1	G	140	TYR	CB-CG-CD1	-9.55	106.47	120.80
1	E	21	ALA	N-CA-CB	-9.55	94.35	110.49
2	H	31	LEU	CD1-CG-CD2	-9.55	89.79	110.80
1	A	87	HIS	CB-CA-C	9.54	126.10	110.92
1	E	48	LEU	CA-C-N	-9.54	106.34	120.75
1	E	48	LEU	C-N-CA	-9.54	106.34	120.75
2	B	37	TRP	CB-CA-C	9.54	127.18	110.01
2	B	90	GLU	CG-CD-OE2	-9.54	96.47	118.40
1	C	62	VAL	CA-C-N	9.54	132.84	120.44
1	C	62	VAL	C-N-CA	9.54	132.84	120.44
1	G	41	THR	O-C-N	9.54	135.27	122.59
1	A	67	THR	O-C-N	9.53	133.01	122.15
2	B	55	MET	N-CA-CB	-9.53	94.57	110.39
2	B	136	GLY	O-C-N	9.53	133.03	122.54
2	B	1	VAL	CB-CA-C	-9.53	93.30	111.40
2	F	5	PRO	N-CD-CG	-9.53	88.91	103.20
2	F	35	TYR	CA-CB-CG	-9.53	96.75	113.90
1	A	50	HIS	CB-CA-C	-9.52	95.56	109.84
2	H	4	THR	CA-C-N	9.52	131.74	119.84
2	H	4	THR	C-N-CA	9.52	131.74	119.84
2	B	95	LYS	CG-CD-CE	9.52	133.19	111.30
1	G	19	ALA	N-CA-CB	-9.52	96.06	110.33
2	H	54	VAL	CA-CB-CG2	-9.51	94.23	110.40
2	B	13	ALA	CA-C-O	-9.51	110.91	120.70
2	H	145	TYR	N-CA-CB	9.51	124.69	109.95
2	H	34	VAL	CB-CA-C	9.50	124.49	112.04
2	H	116	HIS	O-C-N	9.50	133.34	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	130	ALA	N-CA-CB	9.50	124.92	110.30
1	G	115	ALA	CA-C-N	9.49	142.23	122.58
1	G	115	ALA	C-N-CA	9.49	142.23	122.58
1	G	99	LYS	O-C-N	9.49	135.56	122.46
1	A	3	SER	O-C-N	9.49	137.55	120.56
2	B	51	PRO	O-C-N	9.49	134.46	122.22
1	C	64	ASP	OD1-CG-OD2	9.49	145.68	122.90
2	H	68	LEU	CA-CB-CG	9.49	149.52	116.30
1	E	44	PRO	O-C-N	9.48	133.61	122.23
2	D	51	PRO	N-CA-CB	9.48	113.20	103.25
2	F	141	LEU	CB-CA-C	9.48	129.51	110.17
1	A	129	LEU	N-CA-CB	9.47	125.22	109.78
1	G	45	HIS	CA-C-N	-9.47	106.10	123.05
1	G	45	HIS	C-N-CA	-9.47	106.10	123.05
1	C	41	THR	N-CA-C	-9.47	100.82	111.71
1	G	40	LYS	N-CA-CB	9.47	124.21	109.82
1	C	140	TYR	CG-CD1-CE1	9.46	135.40	121.20
2	H	5	PRO	CB-CA-C	-9.46	95.94	111.56
1	E	7	LYS	N-CA-C	-9.46	100.94	111.07
1	G	54	GLN	CG-CD-OE1	-9.46	101.88	120.80
1	A	98	PHE	CB-CG-CD2	9.46	136.78	120.70
1	G	126	ASP	N-CA-CB	9.46	124.19	109.82
2	D	88	LEU	O-C-N	-9.45	110.10	122.39
1	E	16	LYS	CG-CD-CE	9.45	133.04	111.30
1	G	60	LYS	CA-C-O	9.45	130.08	119.41
1	A	98	PHE	O-C-N	9.44	132.13	122.12
1	G	108	THR	CA-C-N	9.44	136.72	120.58
1	G	108	THR	C-N-CA	9.44	136.72	120.58
1	A	72	HIS	O-C-N	-9.44	109.33	122.26
2	H	35	TYR	O-C-N	9.44	132.17	121.32
2	H	64	GLY	N-CA-C	9.44	124.06	112.73
1	C	35	SER	N-CA-C	9.43	124.92	113.41
2	D	82	LYS	N-CA-CB	9.43	123.98	110.12
1	G	76	MET	CB-CA-C	9.43	128.74	110.17
1	A	19	ALA	CA-C-O	9.42	129.05	118.97
2	B	43	GLU	CG-CD-OE2	9.42	140.06	118.40
2	B	48	LEU	CA-C-N	9.42	136.45	120.72
2	B	48	LEU	C-N-CA	9.42	136.45	120.72
2	F	136	GLY	CA-C-N	9.42	134.20	120.74
2	F	136	GLY	C-N-CA	9.42	134.20	120.74
2	D	57	ASN	CB-CG-ND2	-9.41	102.28	116.40
2	H	102	ASN	CA-C-N	-9.41	107.49	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	102	ASN	C-N-CA	-9.41	107.49	120.38
2	H	80	ASN	CB-CA-C	9.40	127.12	111.51
2	H	127	GLN	CA-CB-CG	-9.40	95.29	114.10
2	F	134	VAL	N-CA-CB	9.40	120.94	110.51
1	E	46	PHE	CB-CG-CD1	-9.40	104.73	120.70
2	F	49	SER	N-CA-C	9.40	124.00	112.54
2	H	100	PRO	CA-C-O	9.40	137.70	120.60
2	D	75	LEU	N-CA-C	-9.39	102.01	113.19
2	F	128	ALA	CA-C-O	-9.39	109.49	120.10
2	F	134	VAL	O-C-N	-9.39	112.55	121.94
2	H	130	TYR	CG-CD2-CE2	9.39	135.29	121.20
1	A	135	VAL	CB-CA-C	9.39	126.68	111.29
1	A	137	THR	N-CA-C	9.38	122.70	111.82
1	C	40	LYS	CG-CD-CE	-9.38	89.72	111.30
2	D	4	THR	OG1-CB-CG2	9.38	128.06	109.30
2	D	14	LEU	CA-C-N	-9.38	107.53	120.38
2	D	14	LEU	C-N-CA	-9.38	107.53	120.38
2	F	98	VAL	CA-CB-CG1	-9.38	94.46	110.40
2	F	145	TYR	CA-CB-CG	9.38	130.78	113.90
1	G	63	ALA	O-C-N	-9.38	108.74	122.43
1	G	86	LEU	CA-C-O	-9.38	107.10	120.51
1	A	35	SER	O-C-N	-9.37	109.10	122.41
1	E	102	SER	N-CA-CB	9.38	124.03	110.16
2	H	125	PRO	CA-C-N	-9.37	108.24	121.55
2	H	125	PRO	C-N-CA	-9.37	108.24	121.55
1	A	101	LEU	CB-CA-C	-9.37	95.40	110.86
1	A	130	ALA	CB-CA-C	-9.37	95.29	110.84
2	B	4	THR	CA-CB-OG1	-9.36	95.55	109.60
2	D	85	PHE	N-CA-C	9.37	125.07	111.87
1	G	60	LYS	CG-CD-CE	9.36	132.83	111.30
2	H	47	ASP	N-CA-C	-9.36	94.93	109.25
2	D	103	PHE	O-C-N	-9.36	112.43	122.07
2	F	30	ARG	CB-CG-CD	9.36	132.82	111.30
2	F	52	ASP	N-CA-C	-9.36	100.64	111.03
2	F	135	ALA	O-C-N	-9.35	112.31	122.03
2	H	128	ALA	CB-CA-C	-9.35	95.22	110.74
2	B	36	PRO	CA-C-N	-9.35	105.46	122.38
2	B	36	PRO	C-N-CA	-9.35	105.46	122.38
1	E	85	ASP	CB-CG-OD2	9.35	139.89	118.40
1	G	70	VAL	CA-CB-CG2	9.35	126.29	110.40
1	A	7	LYS	CA-C-N	-9.34	103.25	121.94
1	A	7	LYS	C-N-CA	-9.34	103.25	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	35	SER	N-CA-C	9.34	124.82	113.23
2	H	119	GLY	O-C-N	9.34	134.84	122.70
1	C	116	GLU	O-C-N	-9.34	112.38	122.09
1	G	92	ARG	NE-CZ-NH1	9.34	130.84	121.50
1	A	31	ARG	O-C-N	9.33	132.01	122.12
1	G	26	ALA	N-CA-CB	9.33	124.67	110.30
1	A	126	ASP	CA-C-N	9.33	133.13	120.54
1	A	126	ASP	C-N-CA	9.33	133.13	120.54
2	B	71	PHE	CA-C-N	9.33	133.71	120.28
2	B	71	PHE	C-N-CA	9.33	133.71	120.28
1	E	122	HIS	O-C-N	9.33	132.16	122.09
1	G	42	TYR	CA-C-N	-9.33	112.11	123.21
1	G	42	TYR	C-N-CA	-9.33	112.11	123.21
2	F	108	ASN	O-C-N	-9.32	109.59	122.46
1	G	77	PRO	CA-C-N	-9.31	107.06	120.29
1	G	77	PRO	C-N-CA	-9.31	107.06	120.29
2	F	112	CYS	CA-C-O	-9.31	111.11	120.70
2	F	61	LYS	CA-C-O	9.31	130.42	120.55
1	C	43	PHE	CB-CA-C	-9.31	99.02	111.21
2	H	50	THR	N-CA-C	9.31	116.51	108.13
2	B	98	VAL	CG1-CB-CG2	-9.31	90.33	110.80
1	G	52	SER	CA-C-N	-9.30	103.68	120.99
1	G	52	SER	C-N-CA	-9.30	103.68	120.99
2	D	102	ASN	N-CA-C	-9.30	101.02	111.71
1	A	118	THR	CA-C-O	9.28	131.08	120.87
2	D	3	LEU	N-CA-CB	9.28	124.88	110.87
1	E	4	PRO	CA-CB-CG	-9.28	86.87	104.50
1	A	129	LEU	CB-CG-CD2	-9.28	82.87	110.70
1	A	42	TYR	CA-C-N	-9.27	112.82	122.28
1	A	42	TYR	C-N-CA	-9.27	112.82	122.28
2	H	5	PRO	CA-N-CD	-9.27	99.03	112.00
2	D	104	ARG	NH1-CZ-NH2	9.26	131.34	119.30
2	H	82	LYS	O-C-N	9.26	132.71	122.15
2	F	70	ALA	CA-C-N	9.26	139.22	121.54
2	F	70	ALA	C-N-CA	9.26	139.22	121.54
1	A	24	TYR	N-CA-C	-9.26	99.58	112.45
1	E	5	ALA	CB-CA-C	-9.26	91.50	110.38
1	C	59	GLY	CA-C-O	-9.25	110.54	120.90
1	G	116	GLU	N-CA-C	-9.25	101.77	113.43
1	E	141	ARG	CD-NE-CZ	9.25	137.35	124.40
2	B	82	LYS	O-C-N	-9.25	111.40	122.22
1	E	43	PHE	CB-CA-C	9.25	124.17	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	98	PHE	CE1-CZ-CE2	-9.24	103.36	120.00
2	F	92	HIS	ND1-CG-CD2	-9.24	96.86	106.10
1	A	112	HIS	CB-CA-C	9.24	124.43	109.27
2	D	92	HIS	N-CA-CB	9.24	124.53	110.30
1	A	74	ASP	CA-CB-CG	-9.24	103.36	112.60
1	E	138	SER	N-CA-C	9.24	121.43	111.36
1	E	14	TRP	N-CA-CB	-9.23	94.23	110.39
1	C	60	LYS	N-CA-C	-9.23	101.12	111.82
2	B	40	ARG	NE-CZ-NH2	-9.22	110.90	119.20
1	E	16	LYS	CA-C-N	9.22	133.51	120.42
1	E	16	LYS	C-N-CA	9.22	133.51	120.42
1	E	9	ASN	O-C-N	9.22	131.89	122.12
2	H	50	THR	CA-C-O	9.22	128.06	120.13
2	D	6	VAL	O-C-N	9.21	134.09	122.57
1	E	65	ALA	N-CA-C	9.21	121.32	111.28
1	E	98	PHE	CE1-CZ-CE2	9.21	136.57	120.00
1	E	92	ARG	NE-CZ-NH2	9.21	127.48	119.20
1	G	52	SER	N-CA-C	9.20	130.40	110.80
2	D	37	TRP	CB-CG-CD2	-9.20	113.92	126.80
2	H	112	CYS	N-CA-CB	9.20	124.13	110.33
1	E	19	ALA	N-CA-CB	9.20	124.40	110.70
2	H	9	SER	N-CA-C	-9.19	101.49	112.89
1	G	139	LYS	CG-CD-CE	-9.19	90.16	111.30
1	A	137	THR	O-C-N	-9.19	110.97	122.27
1	A	44	PRO	CA-C-N	9.19	137.70	122.54
1	A	44	PRO	C-N-CA	9.19	137.70	122.54
1	A	78	ASN	CA-C-O	9.18	130.46	120.82
2	D	37	TRP	CB-CG-CD1	9.18	140.67	126.90
2	D	105	LEU	O-C-N	9.18	134.63	122.33
1	A	90	LYS	CG-CD-CE	9.18	132.41	111.30
1	E	96	VAL	CA-CB-CG2	9.18	126.00	110.40
2	B	41	PHE	N-CA-C	-9.17	101.79	113.16
2	B	124	PRO	N-CA-CB	9.17	111.97	103.08
2	F	104	ARG	CG-CD-NE	9.17	132.17	112.00
2	H	79	ASP	CB-CG-OD2	-9.17	97.31	118.40
2	H	6	VAL	CG1-CB-CG2	-9.17	90.63	110.80
2	B	122	PHE	CG-CD2-CE2	9.16	136.28	120.70
1	C	37	PRO	N-CD-CG	-9.16	89.46	103.20
2	D	101	GLU	CB-CG-CD	9.16	128.17	112.60
1	E	11	LYS	O-C-N	-9.16	112.64	122.07
2	B	40	ARG	O-C-N	-9.16	110.41	122.59
2	D	123	THR	CA-CB-CG2	9.15	126.06	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	74	ASP	O-C-N	-9.15	108.41	122.13
1	A	79	ALA	CA-C-O	9.15	130.69	120.90
2	B	104	ARG	CB-CG-CD	-9.15	90.26	111.30
1	C	50	HIS	CA-C-N	-9.15	112.83	123.08
1	C	50	HIS	C-N-CA	-9.15	112.83	123.08
2	F	28	LEU	N-CA-C	-9.15	100.88	111.03
2	F	84	THR	CA-CB-CG2	9.15	126.05	110.50
1	E	45	HIS	CA-C-O	-9.14	107.55	119.80
2	B	62	ALA	CA-C-O	9.14	131.12	121.07
1	A	122	HIS	CA-C-O	9.14	130.41	120.82
1	C	10	VAL	CB-CA-C	9.14	124.00	111.94
1	E	81	SER	CA-C-N	9.14	134.20	120.31
1	E	81	SER	C-N-CA	9.14	134.20	120.31
2	F	7	GLU	CA-C-N	-9.13	107.32	120.29
2	F	7	GLU	C-N-CA	-9.13	107.32	120.29
1	G	46	PHE	O-C-N	9.13	135.67	122.97
2	D	54	VAL	CA-C-N	9.13	135.33	120.63
2	D	54	VAL	C-N-CA	9.13	135.33	120.63
1	E	67	THR	OG1-CB-CG2	9.13	127.56	109.30
2	D	77	HIS	O-C-N	-9.13	110.41	122.28
2	B	95	LYS	N-CA-CB	-9.12	96.05	110.19
1	A	68	ASN	CB-CG-ND2	-9.12	102.72	116.40
1	G	102	SER	CA-C-O	-9.11	109.80	120.10
2	H	141	LEU	CA-C-O	-9.11	111.25	120.82
2	B	53	ALA	CA-C-O	9.11	130.46	120.63
1	C	49	SER	CA-C-O	-9.11	111.61	121.99
1	E	8	THR	CA-CB-CG2	-9.11	95.02	110.50
1	E	55	VAL	CA-C-O	-9.11	110.36	119.92
1	G	138	SER	N-CA-C	9.10	123.93	113.01
2	D	41	PHE	CA-C-O	-9.10	108.27	119.28
2	D	142	ALA	N-CA-C	9.10	124.51	113.23
2	B	70	ALA	N-CA-C	-9.09	100.94	111.03
1	C	16	LYS	CA-C-O	-9.09	107.24	119.05
2	F	39	GLN	CB-CA-C	9.09	128.09	110.46
2	H	81	LEU	CA-C-O	-9.09	111.26	120.80
1	C	125	LEU	CB-CA-C	9.08	128.49	110.42
2	D	116	HIS	CA-CB-CG	-9.08	104.72	113.80
2	H	91	LEU	CB-CG-CD2	9.08	137.93	110.70
1	C	14	TRP	O-C-N	9.07	134.98	122.46
2	F	50	THR	CA-C-O	-9.07	111.64	120.26
2	H	116	HIS	ND1-CE1-NE2	9.07	117.47	108.40
1	C	43	PHE	CA-C-O	-9.07	110.63	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	54	VAL	CA-CB-CG1	-9.07	94.99	110.40
2	B	138	ALA	CB-CA-C	9.06	128.06	110.67
2	F	15	TRP	N-CA-CB	9.05	124.16	110.22
1	C	118	THR	N-CA-C	-9.05	97.60	110.08
1	G	87	HIS	O-C-N	9.05	131.71	122.12
2	H	103	PHE	CA-C-O	9.05	130.40	120.63
2	B	90	GLU	CB-CA-C	-9.04	95.83	110.84
2	B	62	ALA	CA-C-N	9.04	132.39	120.28
2	B	62	ALA	C-N-CA	9.04	132.39	120.28
1	C	104	CYS	N-CA-CB	9.04	125.59	110.41
2	D	49	SER	CB-CA-C	-9.04	90.42	110.21
2	B	117	HIS	CB-CG-ND1	9.03	136.25	122.70
1	C	60	LYS	CD-CE-NZ	-9.03	83.00	111.90
2	D	44	SER	N-CA-C	-9.03	100.92	112.93
1	C	42	TYR	N-CA-CB	-9.03	96.29	110.46
2	B	71	PHE	O-C-N	-9.02	112.70	122.09
1	E	108	THR	OG1-CB-CG2	9.02	127.34	109.30
1	C	115	ALA	N-CA-CB	-9.02	94.65	110.34
1	A	14	TRP	N-CA-C	-9.01	101.36	111.82
2	D	104	ARG	CG-CD-NE	9.01	131.82	112.00
2	D	103	PHE	CA-CB-CG	-9.00	104.80	113.80
1	A	58	HIS	ND1-CG-CD2	9.00	115.10	106.10
1	C	85	ASP	N-CA-C	9.00	122.06	111.71
2	H	87	THR	N-CA-C	-8.99	91.64	110.80
2	D	32	LEU	CA-C-N	8.99	132.96	122.35
2	D	32	LEU	C-N-CA	8.99	132.96	122.35
2	H	36	PRO	N-CA-CB	-8.99	93.81	103.25
2	H	37	TRP	CA-C-O	8.99	133.07	119.23
1	E	9	ASN	OD1-CG-ND2	-8.98	113.62	122.60
1	C	95	PRO	CA-CB-CG	-8.98	87.44	104.50
2	D	30	ARG	NE-CZ-NH2	-8.97	111.12	119.20
1	G	90	LYS	CG-CD-CE	8.97	131.94	111.30
1	A	106	LEU	CA-C-O	8.97	133.34	120.51
2	D	116	HIS	O-C-N	-8.96	112.62	122.12
1	E	20	HIS	ND1-CG-CD2	8.96	115.06	106.10
1	A	61	LYS	CA-CB-CG	-8.96	96.17	114.10
1	E	104	CYS	CA-CB-SG	-8.96	93.79	114.40
2	F	131	GLN	CG-CD-OE1	8.96	138.72	120.80
1	A	91	LEU	N-CA-C	8.96	126.15	111.37
2	B	35	TYR	CB-CG-CD1	-8.96	107.37	120.80
1	C	7	LYS	N-CA-C	8.95	121.85	111.11
1	C	77	PRO	N-CA-CB	8.95	113.01	103.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	26	GLU	CA-C-N	8.95	135.66	120.71
2	B	26	GLU	C-N-CA	8.95	135.66	120.71
1	G	104	CYS	CB-CA-C	8.95	127.85	110.67
1	C	91	LEU	CA-C-O	8.95	130.40	119.31
1	E	110	ALA	O-C-N	-8.95	110.69	122.59
2	H	73	ASP	OD1-CG-OD2	-8.94	101.44	122.90
1	E	17	VAL	N-CA-C	8.94	119.75	110.72
2	F	33	VAL	N-CA-C	8.94	124.95	112.35
2	B	92	HIS	CB-CG-ND1	-8.93	109.30	122.70
2	D	7	GLU	CA-C-O	8.93	130.38	121.00
2	D	140	ALA	N-CA-C	-8.93	101.20	112.90
2	H	2	HIS	ND1-CG-CD2	-8.93	97.17	106.10
1	C	37	PRO	O-C-N	-8.93	111.36	122.17
2	F	59	LYS	CA-C-O	-8.93	111.08	120.55
1	C	91	LEU	CA-C-N	8.93	138.59	121.54
1	C	91	LEU	C-N-CA	8.93	138.59	121.54
2	F	22	GLU	CB-CA-C	-8.93	95.68	110.85
2	B	73	ASP	N-CA-C	8.92	123.98	113.18
2	D	114	LEU	CA-C-N	-8.92	108.39	120.79
2	D	114	LEU	C-N-CA	-8.92	108.39	120.79
1	A	128	PHE	CA-CB-CG	-8.91	104.89	113.80
1	A	80	LEU	CB-CA-C	8.91	125.78	110.72
1	E	99	LYS	N-CA-CB	8.90	123.20	109.94
1	E	121	VAL	CA-C-O	-8.90	110.58	120.46
2	H	146	HIS	N-CA-C	8.90	135.91	111.00
2	D	10	ALA	CB-CA-C	-8.89	96.93	110.88
2	D	18	VAL	CA-CB-CG2	8.89	125.51	110.40
1	E	1	VAL	CA-C-N	-8.89	109.41	122.65
1	E	1	VAL	C-N-CA	-8.89	109.41	122.65
2	D	15	TRP	CA-C-O	8.88	130.22	120.63
1	E	116	GLU	CA-CB-CG	-8.88	96.35	114.10
1	G	45	HIS	N-CA-C	-8.88	101.71	112.54
1	G	58	HIS	ND1-CE1-NE2	8.88	117.28	108.40
1	E	117	PHE	O-C-N	-8.88	112.52	122.55
2	B	122	PHE	CA-C-N	-8.87	109.16	122.29
2	B	122	PHE	C-N-CA	-8.87	109.16	122.29
2	H	6	VAL	N-CA-C	-8.87	102.18	111.58
2	D	66	LYS	N-CA-CB	8.87	123.88	110.22
2	D	104	ARG	N-CA-CB	-8.87	95.67	110.39
1	E	60	LYS	N-CA-CB	-8.87	95.94	110.40
2	B	128	ALA	CA-C-N	-8.87	104.29	121.58
2	B	128	ALA	C-N-CA	-8.87	104.29	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	38	THR	CB-CA-C	8.86	128.51	109.99
2	F	14	LEU	N-CA-C	-8.86	101.07	112.23
2	F	42	PHE	CA-CB-CG	8.86	122.66	113.80
1	A	13	ALA	CA-C-N	-8.85	106.86	120.31
1	A	13	ALA	C-N-CA	-8.85	106.86	120.31
2	F	92	HIS	CG-ND1-CE1	8.85	124.35	109.30
2	H	84	THR	CA-C-N	8.85	134.65	122.79
2	H	84	THR	C-N-CA	8.85	134.65	122.79
1	G	121	VAL	CB-CA-C	-8.85	100.38	112.24
1	A	34	LEU	CA-C-N	-8.85	105.61	122.06
1	A	34	LEU	C-N-CA	-8.85	105.61	122.06
1	C	74	ASP	CB-CG-OD1	8.84	138.73	118.40
1	G	43	PHE	N-CA-CB	8.84	126.19	110.90
2	H	126	VAL	N-CA-CB	8.84	127.27	111.98
1	A	16	LYS	CA-C-O	8.84	130.18	119.49
2	F	77	HIS	N-CA-CB	-8.84	98.35	111.43
1	G	114	PRO	CA-N-CD	-8.83	99.63	112.00
1	C	74	ASP	CA-CB-CG	8.83	121.43	112.60
1	C	80	LEU	CB-CG-CD2	8.83	137.19	110.70
1	C	99	LYS	CA-C-O	-8.83	109.19	119.61
2	H	53	ALA	N-CA-C	-8.83	101.11	112.23
1	E	109	LEU	CB-CA-C	8.83	126.96	110.63
2	B	38	THR	CA-C-O	8.82	129.96	119.28
1	E	106	LEU	CA-C-O	-8.82	107.90	120.51
2	F	145	TYR	O-C-N	8.82	133.41	123.01
1	C	72	HIS	N-CA-CB	-8.81	96.66	111.20
1	C	118	THR	CA-CB-OG1	-8.81	96.38	109.60
1	E	125	LEU	CA-CB-CG	8.81	147.15	116.30
1	C	115	ALA	CB-CA-C	8.81	123.92	110.08
2	D	96	LEU	CB-CA-C	8.81	128.36	110.38
2	D	126	VAL	CA-CB-CG2	8.81	125.38	110.40
2	F	130	TYR	CG-CD1-CE1	8.81	134.42	121.20
2	H	53	ALA	O-C-N	8.81	134.14	122.33
2	F	80	ASN	CB-CG-OD1	-8.81	103.18	120.80
2	F	81	LEU	N-CA-C	-8.80	101.61	111.82
2	H	129	ALA	O-C-N	8.80	132.19	122.15
1	A	66	LEU	CA-C-O	-8.80	110.47	120.24
2	F	143	HIS	CB-CG-CD2	-8.80	119.76	131.20
2	D	32	LEU	CB-CA-C	8.80	126.91	110.63
1	G	44	PRO	CA-C-N	8.80	135.42	120.72
1	G	44	PRO	C-N-CA	8.80	135.42	120.72
1	C	92	ARG	N-CA-CB	8.80	125.36	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	105	LEU	CA-C-O	8.79	130.06	120.82
2	H	49	SER	N-CA-C	8.79	123.65	113.19
1	A	45	HIS	CA-C-O	-8.79	109.07	119.35
1	A	44	PRO	N-CA-CB	8.79	112.27	103.48
1	C	139	LYS	O-C-N	-8.79	111.12	122.37
2	D	112	CYS	CA-CB-SG	-8.79	94.19	114.40
1	G	79	ALA	O-C-N	8.79	132.48	122.11
1	A	67	THR	CA-C-O	-8.79	111.11	120.42
2	D	143	HIS	N-CA-C	8.79	121.81	111.71
1	G	103	HIS	CB-CG-ND1	8.79	135.88	122.70
2	D	108	ASN	O-C-N	8.78	134.57	122.46
1	E	33	PHE	CA-CB-CG	8.78	122.58	113.80
1	G	67	THR	CB-CA-C	8.78	128.34	109.99
1	G	107	VAL	N-CA-CB	8.78	120.82	110.55
1	C	7	LYS	CA-C-N	8.77	132.75	120.29
1	C	7	LYS	C-N-CA	8.77	132.75	120.29
1	C	59	GLY	N-CA-C	-8.77	101.87	112.49
1	E	68	ASN	N-CA-C	-8.77	100.90	111.69
2	F	89	SER	CB-CA-C	-8.77	96.05	110.79
1	G	20	HIS	CB-CG-CD2	-8.77	119.80	131.20
2	H	8	LYS	CA-CB-CG	8.77	131.63	114.10
2	F	15	TRP	CD2-CE2-CZ2	-8.77	113.64	122.40
2	D	118	PHE	N-CA-CB	-8.76	96.77	110.44
1	E	26	ALA	CA-C-O	-8.76	109.03	119.27
1	G	51	GLY	O-C-N	-8.76	111.32	122.70
1	G	139	LYS	CA-C-O	8.75	131.41	120.65
1	C	110	ALA	N-CA-C	8.75	129.44	110.80
2	H	19	ASN	N-CA-CB	-8.75	94.29	110.56
2	D	94	ASP	CA-C-N	8.75	137.66	122.79
2	D	94	ASP	C-N-CA	8.75	137.66	122.79
2	F	105	LEU	CA-CB-CG	8.74	146.89	116.30
2	F	90	GLU	CG-CD-OE1	-8.74	98.30	118.40
2	B	44	SER	CA-CB-OG	8.74	128.57	111.10
1	C	46	PHE	CB-CG-CD2	8.74	135.55	120.70
2	H	110	LEU	O-C-N	-8.74	111.52	122.27
1	E	3	SER	O-C-N	8.73	131.36	121.32
1	G	30	GLU	N-CA-CB	8.73	122.73	110.07
2	B	31	LEU	CA-C-O	8.72	130.09	119.79
1	A	124	SER	CA-CB-OG	-8.71	93.67	111.10
1	G	32	MET	N-CA-C	8.72	121.65	111.02
2	H	67	VAL	CB-CA-C	8.71	123.11	111.87
2	B	22	GLU	CG-CD-OE2	-8.71	98.37	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	87	HIS	CA-C-N	8.71	131.95	120.28
1	G	87	HIS	C-N-CA	8.71	131.95	120.28
1	A	92	ARG	CA-C-N	-8.71	108.65	121.71
1	A	92	ARG	C-N-CA	-8.71	108.65	121.71
1	C	76	MET	CA-CB-CG	-8.71	96.69	114.10
2	F	32	LEU	CA-C-O	-8.71	111.58	120.90
1	A	117	PHE	N-CA-CB	-8.70	97.46	110.60
2	F	18	VAL	N-CA-C	8.70	121.15	108.53
2	F	57	ASN	CA-CB-CG	-8.70	103.90	112.60
2	H	47	ASP	CB-CG-OD1	8.70	138.41	118.40
1	C	92	ARG	NH1-CZ-NH2	-8.70	107.99	119.30
2	D	59	LYS	CB-CA-C	8.70	125.63	110.85
1	E	48	LEU	CD1-CG-CD2	-8.70	91.67	110.80
2	H	95	LYS	CB-CA-C	-8.69	95.87	109.34
2	D	95	LYS	CB-CG-CD	-8.69	91.31	111.30
2	B	38	THR	N-CA-CB	-8.69	97.15	110.44
2	H	87	THR	O-C-N	8.69	134.14	122.59
1	C	139	LYS	CA-C-N	8.68	132.26	120.54
1	C	139	LYS	C-N-CA	8.68	132.26	120.54
2	B	60	VAL	CA-C-N	-8.67	107.40	121.19
2	B	60	VAL	C-N-CA	-8.67	107.40	121.19
1	C	41	THR	CA-C-N	-8.67	105.94	122.06
1	C	41	THR	C-N-CA	-8.67	105.94	122.06
2	B	53	ALA	CA-C-N	8.66	131.65	120.56
2	B	53	ALA	C-N-CA	8.66	131.65	120.56
1	C	41	THR	CA-CB-CG2	8.66	125.23	110.50
1	G	49	SER	CA-C-N	8.66	138.09	121.54
1	G	49	SER	C-N-CA	8.66	138.09	121.54
1	A	9	ASN	CA-C-N	8.66	134.41	120.55
1	A	9	ASN	C-N-CA	8.66	134.41	120.55
2	B	50	THR	N-CA-C	8.66	132.43	107.84
2	H	57	ASN	O-C-N	8.66	129.23	121.18
2	B	20	VAL	O-C-N	-8.65	110.65	121.90
1	G	82	ALA	N-CA-CB	-8.65	95.86	110.49
2	H	66	LYS	O-C-N	8.65	132.67	122.20
2	F	108	ASN	CA-C-N	8.65	135.17	120.29
2	F	108	ASN	C-N-CA	8.65	135.17	120.29
2	B	2	HIS	CB-CA-C	8.65	123.45	111.51
2	B	82	LYS	N-CA-CB	-8.65	96.90	110.22
2	B	41	PHE	CB-CA-C	8.65	125.57	110.01
2	D	65	LYS	CG-CD-CE	8.64	131.18	111.30
1	E	16	LYS	N-CA-CB	-8.64	95.89	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	45	PHE	CB-CA-C	8.64	127.25	110.57
2	D	127	GLN	OE1-CD-NE2	-8.64	113.96	122.60
2	F	98	VAL	CA-C-N	8.63	140.37	121.63
2	F	98	VAL	C-N-CA	8.63	140.37	121.63
1	G	67	THR	CA-CB-OG1	-8.63	96.65	109.60
1	G	86	LEU	O-C-N	8.63	134.07	122.59
2	D	48	LEU	N-CA-CB	8.63	125.82	111.49
2	B	144	LYS	N-CA-CB	-8.63	95.91	110.49
1	C	42	TYR	O-C-N	8.62	134.66	122.41
2	D	94	ASP	N-CA-C	8.62	121.76	111.33
2	F	50	THR	N-CA-CB	-8.62	102.05	111.10
1	C	104	CYS	CA-CB-SG	8.62	134.22	114.40
1	E	112	HIS	CA-C-O	8.62	128.38	118.90
2	F	37	TRP	N-CA-CB	-8.62	97.26	110.44
2	H	96	LEU	O-C-N	-8.61	111.13	122.59
2	D	30	ARG	NE-CZ-NH1	8.61	130.11	121.50
2	B	92	HIS	CA-C-N	8.60	133.79	120.89
2	B	92	HIS	C-N-CA	8.60	133.79	120.89
2	F	86	ALA	CA-C-O	8.60	129.90	119.49
2	H	109	VAL	O-C-N	8.60	133.70	122.26
2	B	143	HIS	ND1-CG-CD2	-8.60	97.50	106.10
1	C	123	ALA	CA-C-N	8.60	132.50	120.29
1	C	123	ALA	C-N-CA	8.60	132.50	120.29
2	H	129	ALA	N-CA-CB	8.60	122.88	110.16
1	E	126	ASP	CA-C-N	8.60	136.18	121.14
1	E	126	ASP	C-N-CA	8.60	136.18	121.14
1	C	63	ALA	N-CA-C	8.59	120.27	111.07
1	E	123	ALA	CA-C-N	8.59	132.49	120.29
1	E	123	ALA	C-N-CA	8.59	132.49	120.29
2	F	87	THR	N-CA-CB	8.59	122.53	110.07
2	B	39	GLN	N-CA-C	-8.59	100.94	111.33
2	B	22	GLU	CA-CB-CG	-8.59	96.93	114.10
2	B	76	ALA	CA-C-N	-8.59	111.28	122.79
2	B	76	ALA	C-N-CA	-8.59	111.28	122.79
2	H	30	ARG	N-CA-C	8.58	121.58	111.71
2	B	49	SER	O-C-N	-8.58	110.93	122.43
2	F	124	PRO	O-C-N	-8.58	111.34	121.46
1	E	80	LEU	CA-C-N	8.58	134.83	121.19
1	E	80	LEU	C-N-CA	8.58	134.83	121.19
2	B	98	VAL	CA-CB-CG2	-8.57	95.83	110.40
1	C	11	LYS	CD-CE-NZ	8.57	139.33	111.90
2	H	133	VAL	CB-CA-C	8.57	123.25	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	7	GLU	N-CA-CB	-8.56	97.41	109.91
1	E	39	THR	O-C-N	-8.56	108.71	122.41
1	E	107	VAL	CA-C-O	8.56	131.48	120.78
2	B	24	GLY	CA-C-O	8.55	135.45	120.57
2	H	53	ALA	CA-C-N	-8.55	106.57	121.97
2	H	53	ALA	C-N-CA	-8.55	106.57	121.97
2	H	127	GLN	CA-C-O	8.55	132.74	120.51
1	E	53	ALA	CB-CA-C	8.55	128.36	110.32
1	G	56	LYS	N-CA-CB	-8.55	97.03	110.28
2	F	17	LYS	O-C-N	8.55	133.88	122.43
2	D	32	LEU	N-CA-C	-8.54	101.88	111.71
2	H	121	GLU	CB-CG-CD	-8.54	98.09	112.60
2	D	53	ALA	CB-CA-C	-8.53	97.72	110.95
2	F	13	ALA	CA-C-N	-8.53	106.18	120.68
2	F	13	ALA	C-N-CA	-8.53	106.18	120.68
1	A	61	LYS	CA-C-O	8.53	129.48	120.70
2	D	94	ASP	OD1-CG-OD2	8.53	143.37	122.90
2	H	43	GLU	CG-CD-OE1	8.53	138.02	118.40
1	C	59	GLY	CA-C-N	-8.53	107.35	120.31
1	C	59	GLY	C-N-CA	-8.53	107.35	120.31
2	H	40	ARG	CA-CB-CG	8.52	131.14	114.10
2	H	43	GLU	CA-C-N	-8.52	108.72	122.26
2	H	43	GLU	C-N-CA	-8.52	108.72	122.26
2	D	1	VAL	CA-C-O	8.52	135.28	120.80
2	D	3	LEU	N-CA-C	-8.51	97.44	109.69
1	G	86	LEU	CA-C-N	-8.51	108.72	120.38
1	G	86	LEU	C-N-CA	-8.51	108.72	120.38
2	D	133	VAL	CA-C-O	-8.50	111.61	121.05
1	E	65	ALA	O-C-N	8.50	131.13	122.12
1	G	107	VAL	CA-C-O	-8.50	112.16	121.17
1	E	23	GLU	CB-CA-C	8.50	126.25	110.70
1	G	39	THR	N-CA-CB	-8.50	97.12	110.46
1	A	76	MET	O-C-N	-8.49	112.60	120.92
2	D	60	VAL	N-CA-CB	-8.49	98.29	110.52
1	G	74	ASP	CA-C-N	-8.49	108.06	122.92
1	G	74	ASP	C-N-CA	-8.49	108.06	122.92
1	C	27	GLU	CA-CB-CG	8.49	131.08	114.10
2	D	80	ASN	OD1-CG-ND2	-8.48	114.11	122.60
1	C	103	HIS	N-CA-C	8.48	120.61	111.36
2	D	51	PRO	CA-C-N	8.48	131.65	120.28
2	D	51	PRO	C-N-CA	8.48	131.65	120.28
1	E	27	GLU	CA-C-N	8.48	132.58	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	27	GLU	C-N-CA	8.48	132.58	120.79
2	H	128	ALA	CA-C-O	8.48	130.41	120.92
2	D	77	HIS	CA-C-N	8.48	132.33	120.29
2	D	77	HIS	C-N-CA	8.48	132.33	120.29
1	C	26	ALA	N-CA-C	8.47	122.91	112.23
2	F	2	HIS	CB-CG-CD2	-8.47	120.18	131.20
1	C	20	HIS	ND1-CE1-NE2	8.47	116.87	108.40
2	F	44	SER	CA-C-O	-8.47	109.93	119.67
1	G	88	ALA	CB-CA-C	8.47	124.85	110.79
1	A	56	LYS	CB-CA-C	-8.46	96.57	110.79
1	G	73	VAL	CA-C-N	8.46	137.71	121.54
1	G	73	VAL	C-N-CA	8.46	137.71	121.54
2	H	78	LEU	CA-C-O	8.46	131.14	119.80
1	A	72	HIS	N-CA-CB	-8.46	97.45	111.49
1	G	25	GLY	CA-C-O	8.46	130.14	121.00
2	H	110	LEU	N-CA-C	8.46	121.63	111.82
2	D	115	ALA	O-C-N	-8.46	113.03	122.08
2	D	110	LEU	N-CA-C	8.45	123.78	113.38
1	E	89	HIS	CB-CG-ND1	-8.46	110.02	122.70
2	D	2	HIS	N-CA-C	-8.45	95.41	108.76
1	E	55	VAL	CA-CB-CG1	8.45	124.76	110.40
1	A	33	PHE	CD1-CE1-CZ	8.44	135.19	120.00
2	B	34	VAL	N-CA-C	8.44	118.52	110.42
2	H	61	LYS	O-C-N	-8.44	111.12	122.43
1	A	139	LYS	CA-C-N	8.44	134.82	121.66
1	A	139	LYS	C-N-CA	8.44	134.82	121.66
1	G	125	LEU	CB-CG-CD2	-8.44	85.39	110.70
1	C	123	ALA	CA-C-O	-8.43	110.28	119.97
1	E	131	SER	CA-C-N	-8.43	106.48	120.30
1	E	131	SER	C-N-CA	-8.43	106.48	120.30
1	G	34	LEU	CB-CA-C	-8.43	96.52	110.85
2	F	120	LYS	N-CA-C	-8.42	102.05	111.82
1	G	86	LEU	CB-CA-C	-8.42	93.66	110.42
1	A	137	THR	CA-CB-CG2	-8.42	96.19	110.50
2	D	22	GLU	CB-CG-CD	8.41	126.91	112.60
2	B	125	PRO	N-CA-C	-8.41	100.45	114.75
2	H	85	PHE	CB-CA-C	-8.41	98.86	111.72
1	A	93	VAL	O-C-N	8.41	132.64	122.72
1	C	75	ASP	CA-C-O	8.40	129.60	119.43
2	H	7	GLU	N-CA-C	-8.40	100.99	111.75
2	D	111	VAL	CA-CB-CG2	-8.40	96.12	110.40
2	B	66	LYS	CG-CD-CE	8.40	130.61	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	62	ALA	CB-CA-C	-8.39	95.34	110.70
1	C	84	SER	N-CA-CB	8.39	122.18	110.01
2	F	57	ASN	O-C-N	8.39	128.98	121.18
2	H	98	VAL	N-CA-CB	-8.39	99.99	110.31
2	B	45	PHE	CB-CG-CD2	8.39	134.96	120.70
1	E	110	ALA	CA-C-N	8.39	138.72	121.94
1	E	110	ALA	C-N-CA	8.39	138.72	121.94
2	B	84	THR	CB-CA-C	8.38	127.51	109.99
1	E	93	VAL	CA-CB-CG1	-8.38	96.16	110.40
1	A	62	VAL	N-CA-C	-8.37	102.18	110.30
1	A	89	HIS	CE1-NE2-CD2	-8.37	100.63	109.00
1	C	47	ASP	CB-CG-OD1	8.37	137.65	118.40
2	D	60	VAL	O-C-N	-8.37	111.02	121.90
2	F	17	LYS	CB-CA-C	-8.37	92.82	110.31
2	H	123	THR	CA-CB-OG1	8.37	122.15	109.60
1	G	127	LYS	N-CA-CB	8.37	123.36	110.14
2	F	45	PHE	CG-CD1-CE1	8.36	134.91	120.70
1	C	40	LYS	CB-CA-C	8.36	126.68	110.46
1	E	44	PRO	N-CD-CG	-8.36	90.66	103.20
2	D	105	LEU	N-CA-C	-8.35	101.70	112.23
1	G	73	VAL	CA-C-O	-8.35	110.34	120.78
1	A	98	PHE	CZ-CE2-CD2	8.35	135.03	120.00
1	E	8	THR	OG1-CB-CG2	8.35	125.99	109.30
2	H	80	ASN	CB-CG-OD1	-8.35	104.11	120.80
2	F	70	ALA	N-CA-C	-8.34	97.69	111.37
2	H	30	ARG	CB-CA-C	-8.34	95.19	110.63
1	E	77	PRO	CB-CA-C	-8.34	99.20	112.21
1	C	6	ASP	CB-CA-C	-8.33	97.48	110.81
2	F	5	PRO	O-C-N	8.33	134.28	122.37
2	B	41	PHE	N-CA-CB	-8.32	97.70	110.44
2	B	129	ALA	CA-C-N	8.32	137.54	122.06
2	B	129	ALA	C-N-CA	8.32	137.54	122.06
2	B	116	HIS	CG-CD2-NE2	8.32	115.52	107.20
2	H	31	LEU	CA-C-N	8.32	132.53	120.38
2	H	31	LEU	C-N-CA	8.32	132.53	120.38
1	C	35	SER	CA-CB-OG	-8.32	94.47	111.10
1	C	77	PRO	N-CA-C	-8.32	102.67	113.57
2	F	26	GLU	N-CA-C	8.32	121.55	111.40
1	E	122	HIS	ND1-CG-CD2	-8.31	97.79	106.10
1	C	27	GLU	O-C-N	-8.31	111.00	122.46
2	F	77	HIS	CG-CD2-NE2	-8.31	98.89	107.20
2	H	35	TYR	N-CA-CB	-8.30	95.59	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	PRO	O-C-N	-8.30	112.27	122.23
1	A	52	SER	O-C-N	-8.30	112.50	122.96
2	D	49	SER	N-CA-CB	-8.30	95.21	110.32
2	F	73	ASP	N-CA-CB	8.30	124.52	110.49
2	H	110	LEU	CB-CA-C	-8.30	94.73	110.67
1	A	92	ARG	N-CA-CB	-8.30	99.42	111.70
2	B	33	VAL	CA-C-O	-8.30	111.98	120.69
2	H	141	LEU	N-CA-CB	8.30	122.04	110.01
2	H	142	ALA	CA-C-O	8.29	128.60	119.15
1	A	6	ASP	CA-CB-CG	8.29	120.89	112.60
1	C	88	ALA	O-C-N	8.29	131.60	122.15
2	H	11	VAL	CA-C-O	-8.29	109.15	119.43
2	B	38	THR	O-C-N	-8.29	110.94	122.37
2	B	116	HIS	O-C-N	-8.29	111.23	122.33
2	D	127	GLN	CB-CA-C	-8.29	97.87	110.88
2	H	17	LYS	CG-CD-CE	-8.29	92.24	111.30
1	G	62	VAL	CA-C-N	-8.28	105.42	121.58
1	G	62	VAL	C-N-CA	-8.28	105.42	121.58
2	F	32	LEU	CB-CA-C	8.28	124.06	110.81
1	G	84	SER	CB-CA-C	8.28	123.71	110.96
2	D	3	LEU	CD1-CG-CD2	-8.27	92.60	110.80
1	G	129	LEU	CA-CB-CG	-8.27	87.34	116.30
1	C	38	THR	CA-CB-CG2	-8.27	96.44	110.50
1	C	91	LEU	O-C-N	-8.27	111.05	122.46
2	B	82	LYS	CA-CB-CG	8.27	130.63	114.10
2	H	43	GLU	N-CA-CB	8.27	124.73	111.17
2	F	68	LEU	CA-C-O	-8.27	112.06	120.90
2	B	122	PHE	N-CA-CB	-8.26	98.12	110.60
2	F	40	ARG	CD-NE-CZ	8.26	135.97	124.40
2	F	21	ASP	CA-C-N	-8.26	108.56	120.29
2	F	21	ASP	C-N-CA	-8.26	108.56	120.29
1	G	68	ASN	CA-C-N	-8.25	106.47	120.58
1	G	68	ASN	C-N-CA	-8.25	106.47	120.58
1	C	101	LEU	N-CA-C	-8.25	102.36	111.36
2	B	73	ASP	CB-CA-C	-8.25	93.53	109.95
2	D	21	ASP	CB-CG-OD1	-8.25	99.43	118.40
1	C	132	VAL	CA-C-N	-8.25	104.85	121.18
1	C	132	VAL	C-N-CA	-8.25	104.85	121.18
1	A	72	HIS	CB-CG-ND1	-8.24	110.33	122.70
1	C	11	LYS	N-CA-C	-8.24	101.22	111.11
2	D	15	TRP	CA-C-N	8.24	137.56	121.41
2	D	15	TRP	C-N-CA	8.24	137.56	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	GLN	OE1-CD-NE2	-8.24	114.36	122.60
1	E	46	PHE	CD1-CG-CD2	8.24	130.95	118.60
2	H	37	TRP	CA-C-N	8.23	134.65	120.58
2	H	37	TRP	C-N-CA	8.23	134.65	120.58
1	C	45	HIS	N-CA-C	8.23	122.91	111.56
2	D	88	LEU	N-CA-C	-8.23	102.34	112.38
2	F	42	PHE	N-CA-C	8.23	125.56	108.53
1	G	8	THR	CA-CB-CG2	-8.22	96.52	110.50
2	H	82	LYS	N-CA-C	-8.22	102.39	111.36
2	F	111	VAL	N-CA-CB	8.22	126.49	110.95
2	B	43	GLU	OE1-CD-OE2	-8.22	103.18	122.90
2	F	43	GLU	CG-CD-OE1	8.21	137.29	118.40
2	B	146	HIS	CE1-NE2-CD2	-8.21	100.79	109.00
1	C	62	VAL	O-C-N	-8.21	111.01	121.84
2	F	138	ALA	N-CA-C	-8.20	101.93	111.03
2	F	146	HIS	CE1-NE2-CD2	-8.20	100.80	109.00
2	B	45	PHE	O-C-N	-8.20	112.63	122.22
1	C	19	ALA	CB-CA-C	8.20	124.73	110.64
1	C	60	LYS	CA-CB-CG	8.20	130.49	114.10
1	E	68	ASN	CA-C-O	8.20	129.34	120.24
2	D	97	HIS	CB-CG-ND1	8.19	134.99	122.70
2	B	112	CYS	CA-CB-SG	-8.19	95.56	114.40
1	E	32	MET	CB-CA-C	-8.19	97.89	110.92
2	D	144	LYS	CA-C-N	-8.19	105.61	122.07
2	D	144	LYS	C-N-CA	-8.19	105.61	122.07
1	E	82	ALA	CA-C-N	-8.19	106.76	120.68
1	E	82	ALA	C-N-CA	-8.19	106.76	120.68
1	C	10	VAL	O-C-N	-8.19	111.95	121.94
1	C	54	GLN	OE1-CD-NE2	8.18	130.78	122.60
1	E	103	HIS	CA-CB-CG	-8.18	105.62	113.80
1	G	114	PRO	N-CA-CB	8.18	111.84	103.25
1	C	67	THR	CA-C-N	8.18	131.24	120.28
1	C	67	THR	C-N-CA	8.18	131.24	120.28
1	E	107	VAL	O-C-N	8.17	132.79	122.57
2	B	145	TYR	N-CA-CB	-8.17	97.88	110.29
2	D	90	GLU	CG-CD-OE2	-8.17	99.62	118.40
2	F	30	ARG	NE-CZ-NH2	8.17	126.55	119.20
2	B	83	GLY	N-CA-C	8.16	121.97	112.50
1	C	30	GLU	CA-C-N	8.16	134.35	120.72
1	C	30	GLU	C-N-CA	8.16	134.35	120.72
1	A	1	VAL	CA-C-O	-8.16	106.93	120.80
2	F	99	ASP	OD1-CG-OD2	8.16	142.48	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	63	HIS	ND1-CE1-NE2	-8.16	100.24	108.40
1	C	18	GLY	CA-C-N	-8.16	109.81	122.37
1	C	18	GLY	C-N-CA	-8.16	109.81	122.37
1	A	44	PRO	O-C-N	-8.15	111.31	122.24
1	A	76	MET	CB-CA-C	-8.15	96.47	111.64
2	F	144	LYS	O-C-N	8.15	132.70	122.19
1	A	93	VAL	N-CA-CB	8.15	121.42	110.26
1	A	123	ALA	N-CA-CB	-8.15	96.72	110.49
1	C	96	VAL	CA-CB-CG2	-8.15	96.55	110.40
1	G	47	ASP	OD1-CG-OD2	8.15	142.45	122.90
2	H	36	PRO	N-CD-CG	-8.15	90.98	103.20
2	H	38	THR	CB-CA-C	-8.15	95.79	110.70
1	G	22	GLY	O-C-N	-8.14	112.11	122.70
1	C	99	LYS	N-CA-CB	8.14	124.83	110.18
1	G	68	ASN	CB-CG-OD1	8.14	137.08	120.80
2	F	7	GLU	CA-C-O	8.13	129.32	119.97
2	B	22	GLU	CA-C-N	8.13	133.32	120.47
2	B	22	GLU	C-N-CA	8.13	133.32	120.47
1	C	120	ALA	CB-CA-C	8.13	123.48	110.96
1	G	5	ALA	N-CA-CB	-8.13	96.75	110.49
1	G	31	ARG	N-CA-C	-8.13	102.39	111.82
2	H	119	GLY	CA-C-O	-8.13	106.42	120.57
1	C	79	ALA	O-C-N	8.13	130.78	122.08
2	D	63	HIS	CB-CA-C	-8.13	97.03	110.85
1	A	138	SER	CB-CA-C	8.13	124.23	110.74
1	G	130	ALA	CB-CA-C	8.12	126.95	110.38
2	B	31	LEU	O-C-N	8.12	133.21	122.33
2	F	87	THR	O-C-N	8.12	130.85	122.09
2	B	97	HIS	CA-C-N	-8.11	109.58	122.64
2	B	97	HIS	C-N-CA	-8.11	109.58	122.64
2	F	146	HIS	CB-CG-ND1	-8.11	110.53	122.70
2	D	119	GLY	CA-C-N	8.11	132.64	120.31
2	D	119	GLY	C-N-CA	8.11	132.64	120.31
1	A	51	GLY	CA-C-N	8.11	132.92	121.24
1	A	51	GLY	C-N-CA	8.11	132.92	121.24
2	B	20	VAL	N-CA-CB	8.11	122.20	110.52
2	F	78	LEU	O-C-N	8.11	133.37	122.59
1	E	141	ARG	CG-CD-NE	8.11	129.83	112.00
1	A	93	VAL	CA-CB-CG1	8.10	124.16	110.40
1	C	2	LEU	CD1-CG-CD2	8.10	128.61	110.80
1	E	102	SER	N-CA-C	-8.10	102.53	111.36
2	F	63	HIS	CB-CG-CD2	-8.09	120.68	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	50	THR	CA-CB-CG2	-8.09	96.75	110.50
2	D	133	VAL	CA-CB-CG2	8.09	124.15	110.40
2	B	104	ARG	CA-C-O	8.09	129.27	119.97
1	A	40	LYS	CA-CB-CG	8.09	130.27	114.10
2	F	64	GLY	N-CA-C	-8.09	102.42	112.77
2	B	8	LYS	CB-CG-CD	-8.08	92.71	111.30
1	C	22	GLY	CA-C-N	8.08	139.26	121.80
1	C	22	GLY	C-N-CA	8.08	139.26	121.80
1	G	134	THR	N-CA-CB	-8.08	98.24	110.12
2	H	30	ARG	CG-CD-NE	-8.08	94.22	112.00
1	E	141	ARG	NE-CZ-NH1	8.08	129.58	121.50
2	H	21	ASP	N-CA-CB	-8.08	98.29	110.01
2	H	23	VAL	CA-C-N	-8.08	110.16	120.34
2	H	23	VAL	C-N-CA	-8.08	110.16	120.34
1	A	46	PHE	CB-CG-CD2	8.07	134.42	120.70
2	F	1	VAL	O-C-N	-8.07	110.09	123.00
2	F	68	LEU	N-CA-CB	-8.07	97.92	109.94
1	G	99	LYS	CA-C-O	-8.07	108.56	119.05
2	F	137	VAL	CA-CB-CG2	8.06	124.11	110.40
2	H	73	ASP	CB-CG-OD1	8.06	136.95	118.40
2	H	131	GLN	CA-C-O	-8.06	109.31	119.31
1	A	18	GLY	O-C-N	8.06	133.18	122.70
2	D	11	VAL	O-C-N	8.06	132.65	122.57
2	D	75	LEU	CD1-CG-CD2	8.06	128.53	110.80
1	A	112	HIS	CA-CB-CG	8.06	121.86	113.80
2	B	37	TRP	N-CA-CB	-8.06	98.11	110.44
2	B	107	GLY	CA-C-O	8.06	129.16	120.30
1	G	66	LEU	CA-C-O	-8.05	110.71	119.97
2	H	97	HIS	ND1-CG-CD2	8.05	114.15	106.10
1	E	112	HIS	ND1-CG-CD2	-8.04	98.06	106.10
2	F	5	PRO	CB-CA-C	-8.04	99.87	111.62
2	H	50	THR	CA-CB-CG2	8.05	124.18	110.50
2	H	93	CYS	N-CA-CB	-8.04	96.89	110.49
1	A	115	ALA	N-CA-C	8.04	121.55	110.06
2	B	113	VAL	CA-CB-CG1	-8.04	96.74	110.40
2	D	4	THR	CB-CA-C	8.04	120.97	108.84
2	F	25	GLY	CA-C-N	-8.04	107.29	120.71
2	F	25	GLY	C-N-CA	-8.04	107.29	120.71
1	C	108	THR	O-C-N	8.03	132.67	122.23
1	E	47	ASP	CA-C-O	-8.03	111.99	120.58
1	G	70	VAL	N-CA-C	-8.03	102.15	113.07
2	H	10	ALA	CA-C-O	-8.03	112.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	THR	N-CA-C	-8.03	102.53	111.28
2	B	113	VAL	CA-C-O	-8.03	111.89	120.64
2	H	84	THR	N-CA-CB	-8.03	97.62	109.82
2	B	59	LYS	CA-CB-CG	-8.03	98.05	114.10
1	A	36	PHE	CB-CG-CD2	8.02	134.34	120.70
1	A	81	SER	CB-CA-C	8.02	125.47	110.63
1	E	100	LEU	N-CA-CB	-8.02	98.25	110.20
2	F	79	ASP	N-CA-C	-8.02	103.64	113.50
1	A	61	LYS	CB-CG-CD	-8.02	92.86	111.30
2	B	104	ARG	CD-NE-CZ	-8.02	113.18	124.40
2	H	58	PRO	CA-CB-CG	-8.02	89.27	104.50
2	B	30	ARG	N-CA-C	8.01	122.32	112.54
2	F	69	GLY	CA-C-N	-8.01	108.45	121.19
2	F	69	GLY	C-N-CA	-8.01	108.45	121.19
2	D	81	LEU	CA-C-N	-8.01	109.54	120.28
2	D	81	LEU	C-N-CA	-8.01	109.54	120.28
2	B	86	ALA	CA-C-N	8.01	131.34	120.44
2	B	86	ALA	C-N-CA	8.01	131.34	120.44
2	B	117	HIS	CB-CA-C	8.01	126.72	110.38
2	H	55	MET	CB-CA-C	-8.01	93.42	110.32
2	F	111	VAL	O-C-N	-8.01	110.85	121.82
2	B	77	HIS	CB-CA-C	8.01	123.97	111.72
2	H	82	LYS	CG-CD-CE	8.00	129.70	111.30
2	D	68	LEU	CA-C-N	-8.00	105.74	121.41
2	D	68	LEU	C-N-CA	-8.00	105.74	121.41
2	H	106	LEU	N-CA-C	-8.00	102.55	111.82
1	C	129	LEU	CA-C-O	-7.99	109.55	119.38
1	E	141	ARG	NE-CZ-NH2	-7.99	112.00	119.20
1	C	23	GLU	O-C-N	-7.99	111.51	122.30
1	G	58	HIS	ND1-CG-CD2	-7.99	98.11	106.10
2	B	111	VAL	CB-CA-C	-7.99	99.32	112.26
1	E	73	VAL	CA-CB-CG1	7.99	123.98	110.40
1	C	79	ALA	CA-C-N	-7.98	109.40	122.65
1	C	79	ALA	C-N-CA	-7.98	109.40	122.65
2	D	127	GLN	N-CA-CB	7.98	121.59	110.01
1	A	58	HIS	O-C-N	-7.98	112.93	122.11
1	G	61	LYS	CD-CE-NZ	7.98	137.43	111.90
1	E	39	THR	OG1-CB-CG2	7.98	125.25	109.30
1	G	99	LYS	CA-C-N	-7.98	108.12	121.92
1	G	99	LYS	C-N-CA	-7.98	108.12	121.92
2	B	96	LEU	CD1-CG-CD2	7.97	128.34	110.80
2	B	100	PRO	CA-C-N	-7.97	108.19	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	100	PRO	C-N-CA	-7.97	108.19	120.31
1	E	20	HIS	CE1-NE2-CD2	7.97	116.97	109.00
2	F	38	THR	CA-CB-OG1	7.97	121.56	109.60
1	C	16	LYS	CB-CA-C	-7.97	93.92	110.17
1	C	103	HIS	CE1-NE2-CD2	-7.96	101.04	109.00
2	H	60	VAL	O-C-N	-7.96	113.62	121.90
2	D	120	LYS	CA-C-O	-7.96	110.82	119.97
1	E	79	ALA	CA-C-N	-7.96	107.97	122.38
1	E	79	ALA	C-N-CA	-7.96	107.97	122.38
2	B	28	LEU	N-CA-CB	7.96	122.56	110.30
1	C	114	PRO	N-CA-C	7.96	125.35	113.81
1	E	14	TRP	CH2-CZ2-CE2	7.96	127.84	117.50
1	E	97	ASN	CA-C-O	7.95	129.12	119.97
1	E	97	ASN	N-CA-C	7.95	121.05	111.82
1	G	129	LEU	CA-C-N	-7.95	107.16	120.68
1	G	129	LEU	C-N-CA	-7.95	107.16	120.68
2	H	70	ALA	N-CA-C	-7.95	101.71	111.33
1	C	37	PRO	CA-C-O	-7.95	107.08	119.64
2	B	109	VAL	CB-CA-C	-7.94	101.45	111.94
1	E	9	ASN	CB-CG-ND2	7.94	128.32	116.40
2	F	55	MET	CA-C-O	7.94	129.04	119.43
1	A	1	VAL	CA-CB-CG2	7.94	123.90	110.40
2	D	33	VAL	N-CA-C	-7.94	104.98	111.81
1	C	85	ASP	N-CA-CB	7.94	122.44	110.22
1	E	139	LYS	CA-C-N	7.94	134.15	120.58
1	E	139	LYS	C-N-CA	7.94	134.15	120.58
1	A	78	ASN	N-CA-C	7.93	119.56	111.07
2	F	63	HIS	N-CA-CB	7.93	122.92	110.46
2	H	22	GLU	CG-CD-OE2	-7.93	100.15	118.40
2	D	94	ASP	CB-CG-OD2	-7.93	100.15	118.40
2	H	101	GLU	CB-CG-CD	7.93	126.09	112.60
2	B	132	LYS	CA-C-N	-7.93	109.16	120.42
2	B	132	LYS	C-N-CA	-7.93	109.16	120.42
2	B	69	GLY	CA-C-N	-7.92	109.85	120.63
2	B	69	GLY	C-N-CA	-7.92	109.85	120.63
1	E	137	THR	CB-CA-C	7.92	123.86	111.02
2	B	131	GLN	CG-CD-OE1	-7.92	104.96	120.80
2	F	12	THR	CA-CB-OG1	-7.92	97.72	109.60
2	B	143	HIS	O-C-N	7.92	133.12	122.59
1	E	40	LYS	CA-CB-CG	-7.92	98.26	114.10
2	B	5	PRO	N-CD-CG	7.91	115.07	103.20
2	B	105	LEU	N-CA-CB	7.91	121.48	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	9	ASN	N-CA-CB	-7.91	98.54	110.01
2	D	68	LEU	CB-CA-C	7.91	124.49	110.81
2	B	45	PHE	CG-CD2-CE2	7.90	134.14	120.70
2	D	127	GLN	CA-CB-CG	-7.90	98.29	114.10
2	D	95	LYS	CA-C-N	-7.90	107.25	120.68
2	D	95	LYS	C-N-CA	-7.90	107.25	120.68
1	G	73	VAL	CA-CB-CG1	7.90	123.83	110.40
2	D	125	PRO	N-CA-CB	-7.90	95.29	103.19
2	B	131	GLN	CA-C-O	7.90	130.18	120.31
2	D	8	LYS	O-C-N	-7.90	112.09	122.59
1	E	14	TRP	CA-C-N	-7.90	105.93	121.41
1	E	14	TRP	C-N-CA	-7.90	105.93	121.41
2	F	126	VAL	CA-C-N	7.89	130.70	120.44
2	F	126	VAL	C-N-CA	7.89	130.70	120.44
1	A	92	ARG	NH1-CZ-NH2	7.89	129.56	119.30
2	F	39	GLN	CA-C-N	7.89	136.61	121.54
2	F	39	GLN	C-N-CA	7.89	136.61	121.54
1	E	29	LEU	CA-C-N	7.89	131.19	120.54
1	E	29	LEU	C-N-CA	7.89	131.19	120.54
1	A	78	ASN	CA-C-N	7.89	131.19	120.54
1	A	78	ASN	C-N-CA	7.89	131.19	120.54
2	F	142	ALA	O-C-N	-7.89	112.65	122.35
1	E	8	THR	N-CA-CB	7.89	121.45	110.01
2	D	132	LYS	N-CA-C	-7.88	102.57	112.90
1	E	58	HIS	ND1-CG-CD2	7.88	113.98	106.10
2	B	134	VAL	CA-CB-CG2	7.88	123.80	110.40
1	E	12	ALA	CB-CA-C	-7.88	97.55	110.79
1	E	99	LYS	CB-CG-CD	7.88	129.43	111.30
1	E	63	ALA	CA-C-N	7.88	133.87	120.71
1	E	63	ALA	C-N-CA	7.88	133.87	120.71
1	E	72	HIS	O-C-N	-7.88	112.22	121.99
1	A	21	ALA	CB-CA-C	-7.88	94.75	110.42
1	E	16	LYS	CA-CB-CG	-7.87	98.35	114.10
2	H	91	LEU	N-CA-CB	-7.87	98.47	110.20
2	D	23	VAL	CB-CA-C	-7.87	101.51	112.14
2	H	130	TYR	N-CA-CB	7.87	122.42	110.30
1	C	95	PRO	N-CA-CB	7.86	112.11	103.30
1	G	90	LYS	CA-C-O	-7.86	109.27	120.51
1	E	35	SER	N-CA-CB	7.85	122.39	110.30
1	G	72	HIS	CA-CB-CG	7.85	121.65	113.80
2	H	105	LEU	CB-CA-C	-7.85	93.61	109.55
1	E	14	TRP	O-C-N	-7.85	111.63	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	64	GLY	CA-C-N	-7.84	109.95	120.54
2	D	64	GLY	C-N-CA	-7.84	109.95	120.54
2	F	111	VAL	CA-CB-CG2	-7.84	97.06	110.40
2	D	37	TRP	N-CA-C	-7.84	103.44	113.16
2	F	34	VAL	N-CA-CB	7.84	120.60	110.57
1	A	125	LEU	O-C-N	-7.84	113.22	122.15
1	E	91	LEU	CA-C-O	-7.84	112.17	120.55
2	F	117	HIS	CB-CG-CD2	-7.83	121.02	131.20
1	E	103	HIS	ND1-CG-CD2	7.83	113.93	106.10
1	G	12	ALA	N-CA-C	7.82	119.59	111.14
1	G	114	PRO	N-CA-C	-7.82	96.35	112.47
2	F	3	LEU	N-CA-CB	7.82	123.17	110.43
2	F	127	GLN	CA-C-N	-7.81	109.03	120.28
2	F	127	GLN	C-N-CA	-7.81	109.03	120.28
1	E	80	LEU	CA-C-O	-7.81	109.83	119.28
2	H	39	GLN	CG-CD-NE2	7.81	128.12	116.40
1	A	89	HIS	CB-CG-ND1	7.81	134.41	122.70
2	B	41	PHE	CG-CD2-CE2	7.81	133.97	120.70
1	C	86	LEU	O-C-N	-7.81	112.21	122.59
1	A	30	GLU	CB-CG-CD	7.80	125.87	112.60
2	B	117	HIS	CA-C-O	-7.80	110.58	119.79
2	D	44	SER	CA-C-N	7.80	136.62	121.18
2	D	44	SER	C-N-CA	7.80	136.62	121.18
1	E	20	HIS	N-CA-C	-7.80	103.34	113.17
2	D	127	GLN	CG-CD-OE1	7.80	136.40	120.80
2	B	52	ASP	N-CA-C	-7.80	100.81	112.04
2	H	40	ARG	O-C-N	7.80	132.96	122.59
1	C	25	GLY	N-CA-C	-7.79	102.79	112.77
1	G	88	ALA	CA-C-O	-7.79	112.29	120.55
2	D	85	PHE	CA-C-O	-7.79	111.07	120.65
1	E	28	ALA	N-CA-C	-7.79	101.52	111.02
1	A	44	PRO	N-CA-C	7.79	123.96	113.84
1	C	91	LEU	N-CA-C	7.79	122.54	112.89
1	A	128	PHE	N-CA-C	-7.78	102.74	111.07
1	C	119	PRO	CB-CA-C	7.78	123.84	111.31
1	C	4	PRO	N-CA-CB	7.78	110.69	103.46
1	A	132	VAL	CG1-CB-CG2	-7.78	93.69	110.80
1	E	23	GLU	OE1-CD-OE2	-7.78	104.23	122.90
1	E	106	LEU	CB-CG-CD2	7.78	134.03	110.70
2	F	38	THR	CA-C-O	7.78	128.66	120.42
2	D	76	ALA	CA-C-O	-7.77	109.67	119.31
2	H	74	GLY	N-CA-C	-7.77	102.08	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	47	ASP	CB-CG-OD2	-7.77	100.52	118.40
2	H	94	ASP	CA-C-N	7.77	136.62	122.79
2	H	94	ASP	C-N-CA	7.77	136.62	122.79
2	B	89	SER	O-C-N	7.77	130.48	122.09
2	D	62	ALA	CB-CA-C	7.77	122.93	110.96
2	F	117	HIS	CA-CB-CG	-7.76	106.03	113.80
1	A	66	LEU	CB-CA-C	-7.76	96.50	110.70
2	B	53	ALA	O-C-N	-7.76	113.89	122.12
2	B	109	VAL	N-CA-C	-7.76	103.68	110.74
2	D	7	GLU	OE1-CD-OE2	-7.76	104.28	122.90
1	A	43	PHE	CA-C-O	-7.76	113.62	121.07
2	F	22	GLU	N-CA-C	-7.76	102.90	111.36
1	G	98	PHE	N-CA-C	-7.75	101.95	111.33
2	D	67	VAL	O-C-N	7.75	129.82	121.83
2	B	65	LYS	CA-C-N	7.75	136.34	121.54
2	B	65	LYS	C-N-CA	7.75	136.34	121.54
2	H	83	GLY	N-CA-C	-7.75	94.81	113.18
2	B	10	ALA	N-CA-CB	-7.75	98.73	110.12
2	H	1	VAL	CA-CB-CG2	-7.75	97.23	110.40
1	C	69	ALA	CA-C-N	7.75	130.32	120.56
1	C	69	ALA	C-N-CA	7.75	130.32	120.56
2	D	26	GLU	CA-C-O	-7.74	109.29	120.13
2	F	124	PRO	CA-C-O	7.74	131.79	120.56
1	E	33	PHE	N-CA-CB	-7.74	98.74	110.12
1	C	58	HIS	N-CA-C	-7.74	102.44	111.03
2	B	6	VAL	O-C-N	7.74	129.05	122.09
1	A	65	ALA	O-C-N	7.73	133.72	122.43
2	F	11	VAL	N-CA-C	-7.73	101.08	111.44
2	F	65	LYS	CA-CB-CG	7.73	129.56	114.10
1	C	36	PHE	N-CA-CB	-7.73	99.92	110.74
2	D	121	GLU	O-C-N	-7.73	112.76	122.27
2	F	39	GLN	CA-C-O	-7.73	111.55	120.20
1	G	83	LEU	N-CA-C	7.73	121.64	111.75
2	H	39	GLN	CA-CB-CG	7.73	129.56	114.10
1	C	9	ASN	CB-CA-C	-7.73	98.45	110.81
2	H	86	ALA	N-CA-CB	7.73	122.25	110.81
2	F	99	ASP	CB-CG-OD1	-7.72	100.63	118.40
2	H	89	SER	CA-CB-OG	7.72	126.55	111.10
1	A	33	PHE	CA-C-N	-7.72	107.32	121.52
1	A	33	PHE	C-N-CA	-7.72	107.32	121.52
2	B	3	LEU	CB-CG-CD1	7.72	133.86	110.70
1	A	24	TYR	CA-C-N	-7.72	110.42	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	TYR	C-N-CA	-7.72	110.42	120.22
2	B	48	LEU	N-CA-CB	7.72	126.96	111.60
2	B	109	VAL	CA-CB-CG1	-7.72	97.28	110.40
2	D	108	ASN	CB-CA-C	7.71	126.11	109.99
1	G	14	TRP	CB-CG-CD1	7.71	138.47	126.90
1	E	24	TYR	N-CA-C	-7.71	102.88	111.28
1	A	140	TYR	CB-CA-C	7.70	122.38	110.67
2	D	44	SER	CA-CB-OG	-7.70	95.69	111.10
2	H	12	THR	OG1-CB-CG2	-7.70	93.89	109.30
2	H	87	THR	CA-CB-CG2	-7.70	97.41	110.50
1	G	9	ASN	CA-CB-CG	7.70	120.30	112.60
2	H	75	LEU	CB-CA-C	7.70	125.40	110.46
1	A	141	ARG	CB-CG-CD	-7.69	93.61	111.30
1	A	125	LEU	CD1-CG-CD2	-7.69	93.89	110.80
2	B	68	LEU	CA-C-O	-7.69	109.27	119.11
2	F	115	ALA	CA-C-O	-7.69	111.71	120.24
2	H	38	THR	OG1-CB-CG2	-7.69	93.93	109.30
1	E	130	ALA	O-C-N	-7.68	114.16	122.07
1	G	127	LYS	CD-CE-NZ	-7.68	87.31	111.90
2	H	15	TRP	N-CA-C	7.68	127.16	110.80
2	B	15	TRP	CA-C-N	-7.68	110.45	120.13
2	B	15	TRP	C-N-CA	-7.68	110.45	120.13
2	B	41	PHE	CD1-CG-CD2	-7.68	107.08	118.60
2	D	35	TYR	N-CA-CB	-7.68	98.86	110.99
2	H	132	LYS	CA-C-N	-7.67	110.74	120.56
2	H	132	LYS	C-N-CA	-7.67	110.74	120.56
1	C	36	PHE	CB-CG-CD1	-7.67	107.67	120.70
2	H	130	TYR	CA-C-N	-7.67	107.72	121.14
2	H	130	TYR	C-N-CA	-7.67	107.72	121.14
2	F	68	LEU	CD1-CG-CD2	7.67	127.67	110.80
1	G	135	VAL	O-C-N	-7.66	114.05	121.94
2	D	100	PRO	CA-C-O	-7.66	108.88	118.99
2	H	14	LEU	CB-CG-CD1	7.66	133.68	110.70
2	D	137	VAL	O-C-N	7.66	129.72	121.83
1	A	38	THR	OG1-CB-CG2	7.66	124.61	109.30
2	D	135	ALA	CB-CA-C	7.66	123.50	110.79
1	C	6	ASP	CA-C-O	7.66	129.09	120.90
1	C	44	PRO	N-CA-C	-7.65	103.89	113.84
2	H	144	LYS	CA-C-O	-7.65	110.17	119.43
1	E	135	VAL	O-C-N	7.65	129.41	121.91
1	E	104	CYS	CA-C-N	7.65	132.29	120.82
1	E	104	CYS	C-N-CA	7.65	132.29	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	36	PHE	CB-CG-CD1	7.64	133.70	120.70
1	E	4	PRO	CB-CA-C	-7.64	99.50	111.04
1	G	101	LEU	CB-CA-C	7.64	123.84	110.85
1	E	75	ASP	O-C-N	-7.64	111.61	121.92
1	A	53	ALA	O-C-N	7.64	130.91	122.20
2	B	27	ALA	CA-C-O	7.64	128.72	120.55
1	E	134	THR	CA-CB-CG2	7.63	123.48	110.50
2	F	15	TRP	CB-CA-C	-7.63	96.51	110.63
1	E	107	VAL	CA-CB-CG1	7.63	123.37	110.40
1	E	1	VAL	O-C-N	7.63	135.21	123.00
1	C	47	ASP	N-CA-CB	7.62	122.33	110.21
1	E	80	LEU	CA-CB-CG	7.62	142.98	116.30
1	A	20	HIS	CB-CA-C	7.62	125.05	110.27
2	B	110	LEU	CD1-CG-CD2	-7.62	94.03	110.80
1	G	136	LEU	CD1-CG-CD2	7.62	127.57	110.80
2	H	30	ARG	O-C-N	7.62	131.13	122.22
2	H	109	VAL	N-CA-C	-7.62	102.71	113.07
2	D	56	GLY	CA-C-O	7.62	133.82	120.57
1	C	29	LEU	O-C-N	7.61	129.91	122.07
1	E	45	HIS	N-CA-CB	7.61	121.46	110.65
1	G	109	LEU	CB-CG-CD1	-7.61	87.87	110.70
2	H	41	PHE	CA-C-N	-7.61	112.70	123.20
2	H	41	PHE	C-N-CA	-7.61	112.70	123.20
2	B	144	LYS	CA-C-O	-7.61	109.63	120.51
1	A	12	ALA	CA-C-O	-7.61	110.81	119.79
1	G	61	LYS	CA-C-N	-7.61	110.39	121.65
1	G	61	LYS	C-N-CA	-7.61	110.39	121.65
2	B	59	LYS	CG-CD-CE	7.61	128.79	111.30
2	B	133	VAL	CA-C-O	-7.61	112.79	120.85
1	E	77	PRO	CA-C-N	-7.61	107.58	120.58
1	E	77	PRO	C-N-CA	-7.61	107.58	120.58
1	G	21	ALA	CB-CA-C	-7.61	98.22	110.84
2	B	78	LEU	CB-CA-C	7.60	123.78	110.85
2	H	46	GLY	O-C-N	-7.60	118.14	123.08
2	F	14	LEU	N-CA-CB	-7.60	98.60	110.30
2	H	143	HIS	CA-CB-CG	-7.60	106.20	113.80
1	A	84	SER	O-C-N	-7.59	113.49	122.15
1	E	29	LEU	CA-C-O	7.59	129.02	120.90
2	B	65	LYS	O-C-N	-7.59	114.07	122.12
2	B	86	ALA	CA-C-O	7.59	128.47	120.42
1	E	46	PHE	CA-C-N	7.59	132.52	122.42
1	E	46	PHE	C-N-CA	7.59	132.52	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	11	VAL	CA-CB-CG2	-7.59	97.49	110.40
1	C	97	ASN	CB-CG-OD1	7.59	135.98	120.80
2	B	30	ARG	CA-C-O	-7.59	110.05	119.38
2	D	41	PHE	N-CA-C	7.59	122.57	113.16
1	G	50	HIS	ND1-CE1-NE2	7.58	115.98	108.40
2	B	75	LEU	N-CA-CB	7.58	123.65	110.39
2	H	7	GLU	CB-CG-CD	7.58	125.48	112.60
2	F	99	ASP	O-C-N	7.57	128.02	121.20
2	D	28	LEU	N-CA-C	-7.57	102.02	111.11
2	B	68	LEU	CA-C-N	-7.57	102.02	122.46
2	B	68	LEU	C-N-CA	-7.57	102.02	122.46
1	E	17	VAL	CA-CB-CG2	-7.57	97.53	110.40
1	C	74	ASP	OD1-CG-OD2	-7.56	104.75	122.90
2	D	133	VAL	CA-C-N	-7.56	110.10	120.46
2	D	133	VAL	C-N-CA	-7.56	110.10	120.46
1	E	69	ALA	CB-CA-C	7.56	125.79	109.99
1	G	135	VAL	CA-CB-CG2	-7.56	97.55	110.40
2	H	46	GLY	CA-C-N	7.56	132.68	121.72
2	H	46	GLY	C-N-CA	7.56	132.68	121.72
1	A	76	MET	N-CA-CB	-7.56	98.22	110.39
2	B	84	THR	CA-CB-OG1	-7.55	98.27	109.60
2	H	5	PRO	O-C-N	7.55	132.83	122.64
2	H	93	CYS	CA-C-O	7.55	131.30	120.51
2	B	98	VAL	CA-C-N	7.54	131.76	121.20
2	B	98	VAL	C-N-CA	7.54	131.76	121.20
2	F	38	THR	CA-CB-CG2	-7.54	97.67	110.50
2	B	60	VAL	CA-CB-CG1	-7.54	97.58	110.40
2	D	39	GLN	CA-C-N	7.54	135.94	121.54
2	D	39	GLN	C-N-CA	7.54	135.94	121.54
1	G	112	HIS	ND1-CG-CD2	7.54	113.64	106.10
2	H	19	ASN	OD1-CG-ND2	7.54	130.14	122.60
1	G	10	VAL	O-C-N	-7.54	114.06	121.90
2	B	35	TYR	CA-C-N	7.54	129.26	119.84
2	B	35	TYR	C-N-CA	7.54	129.26	119.84
2	F	61	LYS	CG-CD-CE	7.53	128.63	111.30
2	D	44	SER	O-C-N	-7.53	111.79	122.03
2	F	50	THR	CA-C-N	7.53	127.56	119.28
2	F	50	THR	C-N-CA	7.53	127.56	119.28
2	F	131	GLN	N-CA-C	-7.53	103.89	113.23
2	D	122	PHE	CA-CB-CG	7.52	121.32	113.80
1	E	112	HIS	O-C-N	-7.52	113.55	122.27
1	G	10	VAL	CG1-CB-CG2	7.52	127.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	19	ALA	O-C-N	-7.51	113.10	122.19
1	E	94	ASP	N-CA-CB	-7.51	99.55	110.14
2	F	39	GLN	CB-CG-CD	-7.51	99.83	112.60
2	B	143	HIS	CB-CA-C	-7.51	95.47	110.42
2	F	85	PHE	O-C-N	-7.51	113.10	122.19
2	F	92	HIS	CB-CG-CD2	7.51	140.96	131.20
1	C	109	LEU	N-CA-C	-7.50	94.82	110.80
2	D	101	GLU	CG-CD-OE1	-7.50	101.14	118.40
1	G	128	PHE	CB-CA-C	-7.50	98.99	110.92
1	E	58	HIS	CB-CG-ND1	-7.50	111.45	122.70
2	D	102	ASN	CA-C-O	-7.50	111.63	120.10
2	F	98	VAL	N-CA-CB	7.50	120.53	111.31
1	C	78	ASN	CA-C-N	-7.50	110.37	120.79
1	C	78	ASN	C-N-CA	-7.50	110.37	120.79
1	C	140	TYR	N-CA-CB	7.49	121.10	109.94
1	G	43	PHE	CB-CG-CD1	-7.48	107.98	120.70
1	E	76	MET	CA-CB-CG	7.48	129.06	114.10
2	F	42	PHE	CB-CA-C	-7.48	99.85	111.74
2	H	34	VAL	N-CA-CB	-7.47	99.76	110.52
1	A	9	ASN	N-CA-C	7.47	121.64	112.23
2	F	45	PHE	N-CA-CB	-7.47	95.13	110.67
1	G	127	LYS	CA-CB-CG	7.47	129.04	114.10
2	D	129	ALA	O-C-N	-7.47	113.13	122.17
2	H	14	LEU	CD1-CG-CD2	-7.47	94.36	110.80
1	A	141	ARG	CB-CA-C	7.47	124.29	110.10
1	E	97	ASN	CB-CG-OD1	7.47	135.73	120.80
2	D	10	ALA	N-CA-C	-7.46	103.08	111.07
2	F	71	PHE	O-C-N	-7.46	112.66	122.59
2	D	12	THR	O-C-N	-7.46	112.16	122.46
1	A	23	GLU	CG-CD-OE2	-7.46	101.24	118.40
2	B	2	HIS	CE1-NE2-CD2	7.46	116.46	109.00
2	F	66	LYS	CB-CG-CD	7.46	128.46	111.30
1	G	64	ASP	N-CA-CB	7.46	120.80	109.91
1	E	31	ARG	N-CA-C	-7.46	102.84	110.97
2	H	72	SER	CA-C-O	-7.46	112.92	120.90
1	E	27	GLU	CB-CG-CD	7.46	125.28	112.60
1	C	72	HIS	CB-CA-C	7.45	123.10	111.02
1	E	117	PHE	CB-CA-C	7.45	123.38	112.05
2	D	56	GLY	CA-C-N	7.44	130.77	120.65
2	D	56	GLY	C-N-CA	7.44	130.77	120.65
1	C	46	PHE	CB-CA-C	7.44	121.98	109.48
2	D	135	ALA	N-CA-CB	-7.44	99.18	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	129	ALA	CA-C-N	-7.44	109.57	120.28
2	D	129	ALA	C-N-CA	-7.44	109.57	120.28
2	F	15	TRP	CE3-CZ3-CH2	-7.44	111.43	121.10
1	A	31	ARG	NH1-CZ-NH2	-7.43	109.64	119.30
1	C	80	LEU	N-CA-C	-7.43	104.61	112.93
2	F	7	GLU	CB-CG-CD	-7.43	99.97	112.60
1	E	3	SER	N-CA-CB	-7.43	97.15	110.37
1	C	11	LYS	CA-C-O	-7.42	112.96	120.90
2	H	89	SER	CA-C-N	-7.42	109.59	120.28
2	H	89	SER	C-N-CA	-7.42	109.59	120.28
1	E	24	TYR	CZ-CE2-CD2	-7.42	106.25	119.60
2	F	98	VAL	O-C-N	-7.42	113.57	122.77
2	F	130	TYR	CD1-CG-CD2	-7.42	106.98	118.10
2	F	130	TYR	N-CA-CB	7.42	122.93	110.32
1	G	58	HIS	CG-CD2-NE2	7.42	114.61	107.20
2	B	108	ASN	OD1-CG-ND2	-7.41	115.19	122.60
2	D	38	THR	CA-C-N	-7.41	109.56	120.38
2	D	38	THR	C-N-CA	-7.41	109.56	120.38
1	C	56	LYS	CA-C-N	-7.41	101.39	122.06
1	C	56	LYS	C-N-CA	-7.41	101.39	122.06
2	H	7	GLU	CA-C-O	-7.41	111.90	120.20
1	G	78	ASN	N-CA-C	7.41	119.43	111.36
1	A	52	SER	CA-CB-OG	-7.40	96.30	111.10
2	D	136	GLY	CA-C-O	7.40	128.01	120.09
1	A	55	VAL	N-CA-C	7.39	122.78	112.50
2	D	98	VAL	CA-C-N	7.39	139.84	121.80
2	D	98	VAL	C-N-CA	7.39	139.84	121.80
2	F	127	GLN	OE1-CD-NE2	-7.39	115.21	122.60
2	D	1	VAL	CA-CB-CG2	7.39	122.97	110.40
1	G	42	TYR	CB-CG-CD1	7.39	131.89	120.80
2	B	59	LYS	O-C-N	7.39	129.95	122.12
1	C	84	SER	CA-CB-OG	-7.39	96.32	111.10
2	H	18	VAL	N-CA-C	7.39	119.25	107.73
2	H	1	VAL	CA-CB-CG1	7.38	122.95	110.40
2	H	138	ALA	CB-CA-C	7.38	122.62	110.81
1	C	124	SER	CA-C-O	-7.38	112.59	120.42
1	C	38	THR	CB-CA-C	7.38	124.84	110.67
1	C	115	ALA	N-CA-C	7.38	122.74	112.93
2	D	102	ASN	CA-CB-CG	7.38	119.98	112.60
2	B	72	SER	N-CA-C	-7.37	103.23	111.71
1	G	71	ALA	CA-C-O	7.37	128.41	119.49
1	E	14	TRP	CG-CD2-CE3	7.37	141.27	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	116	HIS	O-C-N	-7.37	114.31	122.12
2	F	54	VAL	CA-C-O	-7.37	112.51	120.47
2	D	92	HIS	CA-C-N	-7.37	107.47	121.54
2	D	92	HIS	C-N-CA	-7.37	107.47	121.54
1	E	78	ASN	CA-C-O	7.37	128.42	120.24
1	E	24	TYR	CB-CG-CD1	7.37	131.85	120.80
1	C	89	HIS	N-CA-C	7.36	122.39	113.41
1	E	108	THR	CA-CB-OG1	-7.36	98.56	109.60
2	F	13	ALA	CA-C-O	-7.36	112.75	120.55
1	G	19	ALA	N-CA-C	7.36	122.54	112.90
2	B	133	VAL	N-CA-C	7.36	118.15	110.72
2	H	81	LEU	N-CA-C	-7.36	101.75	111.24
2	H	102	ASN	N-CA-C	-7.36	102.86	111.03
1	E	17	VAL	CA-C-O	7.36	128.65	120.85
1	G	124	SER	CA-CB-OG	-7.36	96.39	111.10
2	H	66	LYS	CG-CD-CE	-7.36	94.38	111.30
2	D	50	THR	N-CA-CB	7.35	120.99	110.77
1	E	10	VAL	N-CA-C	7.35	119.02	111.00
1	G	58	HIS	N-CA-CB	7.35	122.59	110.39
1	G	74	ASP	N-CA-CB	7.35	122.92	110.49
2	H	103	PHE	N-CA-CB	-7.35	99.03	110.06
2	D	104	ARG	CB-CG-CD	-7.35	94.40	111.30
1	A	47	ASP	O-C-N	7.35	131.79	123.05
1	G	140	TYR	CB-CA-C	7.35	123.13	110.79
2	D	15	TRP	CB-CA-C	-7.35	98.19	110.68
2	F	99	ASP	CA-CB-CG	-7.34	105.26	112.60
1	E	42	TYR	N-CA-C	-7.34	104.32	113.20
2	H	98	VAL	CA-C-N	-7.34	108.66	121.35
2	H	98	VAL	C-N-CA	-7.34	108.66	121.35
2	B	41	PHE	CG-CD1-CE1	7.34	133.17	120.70
1	A	69	ALA	CA-C-O	-7.33	112.10	120.24
2	F	75	LEU	CB-CG-CD1	-7.33	88.70	110.70
2	H	125	PRO	N-CD-CG	-7.33	92.20	103.20
2	D	111	VAL	CB-CA-C	7.33	122.06	112.24
1	E	33	PHE	CA-C-N	7.33	133.13	120.68
1	E	33	PHE	C-N-CA	7.33	133.13	120.68
2	D	12	THR	N-CA-C	-7.32	104.22	113.01
2	F	20	VAL	CA-C-O	7.32	128.93	119.85
1	G	78	ASN	CA-CB-CG	7.32	119.92	112.60
2	H	49	SER	CA-C-O	7.32	130.62	118.91
2	B	70	ALA	CA-C-N	7.32	130.42	120.54
2	B	70	ALA	C-N-CA	7.32	130.42	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	116	HIS	CE1-NE2-CD2	-7.32	101.68	109.00
2	F	86	ALA	CA-C-N	-7.32	110.49	120.44
2	F	86	ALA	C-N-CA	-7.32	110.49	120.44
2	D	73	ASP	N-CA-CB	-7.32	98.70	109.82
1	E	48	LEU	N-CA-C	-7.32	102.60	112.26
1	E	42	TYR	CA-C-O	-7.31	109.54	119.12
1	G	132	VAL	CA-CB-CG2	7.31	122.83	110.40
1	C	88	ALA	CA-C-N	-7.31	109.01	122.09
1	C	88	ALA	C-N-CA	-7.31	109.01	122.09
2	D	88	LEU	CB-CA-C	7.31	125.74	110.32
2	B	106	LEU	CA-C-N	-7.31	110.94	120.22
2	B	106	LEU	C-N-CA	-7.31	110.94	120.22
2	D	65	LYS	N-CA-C	-7.31	102.34	111.11
1	E	79	ALA	O-C-N	7.30	129.59	122.07
2	B	130	TYR	O-C-N	7.30	132.78	122.41
2	F	66	LYS	N-CA-CB	-7.30	99.43	110.01
2	D	87	THR	N-CA-CB	7.30	120.56	109.98
2	F	1	VAL	CA-C-N	7.29	135.47	121.54
2	F	1	VAL	C-N-CA	7.29	135.47	121.54
2	F	132	LYS	CA-C-N	-7.29	109.52	120.82
2	F	132	LYS	C-N-CA	-7.29	109.52	120.82
1	C	136	LEU	N-CA-CB	-7.29	99.41	110.12
1	A	106	LEU	N-CA-CB	-7.28	98.18	110.49
2	B	32	LEU	CD1-CG-CD2	-7.28	94.78	110.80
2	B	104	ARG	N-CA-CB	-7.28	98.99	110.28
1	A	30	GLU	N-CA-C	-7.28	103.34	111.28
1	C	95	PRO	CA-C-O	7.28	131.14	119.64
2	D	1	VAL	CA-C-N	7.28	135.61	121.63
2	D	1	VAL	C-N-CA	7.28	135.61	121.63
2	F	95	LYS	CB-CA-C	7.28	123.34	111.26
2	B	4	THR	N-CA-C	7.28	119.85	110.39
2	D	67	VAL	CA-C-N	-7.28	110.57	122.65
2	D	67	VAL	C-N-CA	-7.28	110.57	122.65
1	C	2	LEU	CA-C-O	-7.27	112.72	120.80
1	G	112	HIS	O-C-N	7.27	132.26	122.59
2	F	101	GLU	OE1-CD-OE2	-7.27	105.45	122.90
2	B	116	HIS	CA-C-N	-7.27	108.32	120.68
2	B	116	HIS	C-N-CA	-7.27	108.32	120.68
2	F	118	PHE	CA-C-N	-7.27	107.16	121.41
2	F	118	PHE	C-N-CA	-7.27	107.16	121.41
2	F	35	TYR	CD1-CE1-CZ	7.27	132.68	119.60
2	F	115	ALA	N-CA-C	-7.27	102.75	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	97	HIS	CB-CG-CD2	-7.27	121.75	131.20
2	H	120	LYS	N-CA-C	7.27	121.84	113.19
1	G	109	LEU	CD1-CG-CD2	-7.26	94.82	110.80
1	C	54	GLN	CB-CA-C	-7.26	99.48	110.88
2	B	122	PHE	CA-CB-CG	-7.26	106.54	113.80
2	D	120	LYS	CB-CA-C	7.26	124.60	110.67
1	C	24	TYR	O-C-N	7.25	130.71	122.22
2	B	72	SER	CA-C-N	7.25	135.72	121.58
2	B	72	SER	C-N-CA	7.25	135.72	121.58
1	E	39	THR	CA-CB-OG1	-7.25	98.72	109.60
2	F	3	LEU	CB-CA-C	-7.25	97.78	109.75
1	G	41	THR	N-CA-CB	-7.25	98.23	110.49
2	H	87	THR	OG1-CB-CG2	7.25	123.80	109.30
1	C	130	ALA	O-C-N	-7.25	112.61	122.33
1	G	69	ALA	CA-C-O	-7.25	112.19	120.24
1	A	98	PHE	CB-CG-CD1	-7.25	108.38	120.70
1	C	60	LYS	CA-C-N	-7.25	110.00	120.29
1	C	60	LYS	C-N-CA	-7.25	110.00	120.29
1	E	50	HIS	CA-C-N	7.25	134.60	121.85
1	E	50	HIS	C-N-CA	7.25	134.60	121.85
1	G	64	ASP	CA-C-N	-7.25	107.70	121.54
1	G	64	ASP	C-N-CA	-7.25	107.70	121.54
1	G	30	GLU	CB-CA-C	7.25	122.35	110.90
2	D	22	GLU	CB-CA-C	7.24	124.23	109.67
2	D	37	TRP	CA-C-O	-7.24	110.52	119.28
2	B	39	GLN	CA-C-N	7.24	135.37	121.54
2	B	39	GLN	C-N-CA	7.24	135.37	121.54
1	G	121	VAL	CA-CB-CG1	7.24	122.71	110.40
2	F	105	LEU	N-CA-C	-7.24	103.32	111.14
2	H	40	ARG	CA-C-N	-7.24	109.74	122.26
2	H	40	ARG	C-N-CA	-7.24	109.74	122.26
2	B	34	VAL	CG1-CB-CG2	7.23	126.71	110.80
1	E	11	LYS	N-CA-C	7.23	118.81	111.07
2	H	75	LEU	N-CA-CB	7.23	121.56	110.14
2	F	12	THR	OG1-CB-CG2	7.23	123.76	109.30
2	F	61	LYS	CB-CG-CD	-7.23	94.68	111.30
1	A	88	ALA	CA-C-N	7.23	136.19	122.60
1	A	88	ALA	C-N-CA	7.23	136.19	122.60
1	E	28	ALA	CA-C-O	7.23	129.02	121.07
2	B	135	ALA	N-CA-C	-7.22	103.01	111.03
1	G	103	HIS	CB-CA-C	-7.22	96.47	110.11
1	E	2	LEU	CB-CG-CD2	-7.22	89.05	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	59	LYS	CA-CB-CG	7.21	128.53	114.10
1	E	99	LYS	O-C-N	7.21	129.59	122.09
2	F	23	VAL	CB-CA-C	7.21	123.94	112.26
2	B	13	ALA	N-CA-CB	7.21	120.52	110.07
2	H	1	VAL	CA-C-N	-7.21	111.25	121.99
2	H	1	VAL	C-N-CA	-7.21	111.25	121.99
1	A	122	HIS	CG-ND1-CE1	7.21	121.55	109.30
2	D	63	HIS	CA-C-O	7.21	128.06	120.42
1	E	98	PHE	N-CA-C	-7.21	103.50	111.36
1	G	17	VAL	CA-CB-CG2	7.20	122.64	110.40
2	F	52	ASP	CA-C-N	7.19	129.79	120.44
2	F	52	ASP	C-N-CA	7.19	129.79	120.44
2	D	113	VAL	CA-C-N	7.19	129.92	120.28
2	D	113	VAL	C-N-CA	7.19	129.92	120.28
1	G	102	SER	CB-CA-C	7.19	123.94	110.63
1	C	59	GLY	O-C-N	7.18	129.09	122.19
1	E	42	TYR	OH-CZ-CE2	7.18	141.45	119.90
2	H	29	GLY	CA-C-N	7.18	130.62	120.28
2	H	29	GLY	C-N-CA	7.18	130.62	120.28
2	D	31	LEU	N-CA-CB	7.18	120.39	109.98
2	D	124	PRO	CB-CA-C	7.17	119.67	110.92
2	B	110	LEU	CB-CG-CD2	7.16	132.19	110.70
2	B	120	LYS	CA-C-N	-7.16	108.50	120.68
2	B	120	LYS	C-N-CA	-7.16	108.50	120.68
1	G	117	PHE	CA-C-O	7.16	130.75	120.51
1	C	112	HIS	CA-CB-CG	-7.16	106.64	113.80
2	F	36	PRO	O-C-N	-7.16	112.97	122.64
2	F	40	ARG	CA-C-N	-7.16	111.20	122.65
2	F	40	ARG	C-N-CA	-7.16	111.20	122.65
1	A	40	LYS	CB-CA-C	7.15	125.42	110.32
1	A	24	TYR	CB-CA-C	-7.15	96.59	110.11
1	A	76	MET	CA-C-O	7.15	124.92	117.98
2	F	17	LYS	CA-C-O	-7.15	110.59	119.38
1	E	111	ALA	N-CA-CB	-7.15	98.84	110.42
1	G	91	LEU	O-C-N	-7.15	113.09	122.59
1	A	113	LEU	CA-CB-CG	-7.14	91.29	116.30
1	A	131	SER	CA-CB-OG	-7.14	96.81	111.10
1	A	37	PRO	O-C-N	-7.13	113.01	122.64
1	E	6	ASP	CA-C-N	-7.13	111.16	120.44
1	E	6	ASP	C-N-CA	-7.13	111.16	120.44
1	G	127	LYS	CA-C-N	7.13	130.71	120.79
1	G	127	LYS	C-N-CA	7.13	130.71	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	137	THR	N-CA-C	-7.13	104.58	113.28
1	A	29	LEU	CA-C-O	-7.13	110.47	119.31
2	B	63	HIS	CA-C-O	7.13	128.10	120.55
2	H	15	TRP	CE3-CZ3-CH2	-7.13	111.83	121.10
1	A	98	PHE	N-CA-C	-7.12	103.52	111.28
2	B	120	LYS	O-C-N	7.12	133.81	122.41
1	E	102	SER	CA-C-N	7.12	130.41	120.29
1	E	102	SER	C-N-CA	7.12	130.41	120.29
2	F	100	PRO	CB-CA-C	7.12	125.03	112.64
2	B	121	GLU	CG-CD-OE1	-7.12	102.02	118.40
1	G	110	ALA	O-C-N	7.12	130.55	122.22
2	F	108	ASN	CB-CG-OD1	7.12	135.04	120.80
2	F	129	ALA	N-CA-CB	-7.12	99.63	110.16
1	G	24	TYR	O-C-N	7.12	130.26	122.15
1	G	122	HIS	CB-CA-C	7.12	122.05	110.88
2	B	28	LEU	CB-CA-C	7.11	124.88	110.38
1	E	106	LEU	O-C-N	-7.11	113.13	122.59
1	G	114	PRO	N-CD-CG	-7.11	92.54	103.20
2	B	44	SER	N-CA-C	-7.11	104.08	112.89
2	D	78	LEU	CA-C-N	7.11	131.11	120.31
2	D	78	LEU	C-N-CA	7.11	131.11	120.31
2	D	102	ASN	CB-CG-OD1	7.11	135.01	120.80
2	H	26	GLU	CA-C-N	7.11	135.11	121.54
2	H	26	GLU	C-N-CA	7.11	135.11	121.54
2	B	87	THR	O-C-N	-7.10	114.42	122.09
1	E	9	ASN	CA-C-O	-7.10	112.96	120.63
1	C	30	GLU	CG-CD-OE1	-7.10	102.07	118.40
1	C	64	ASP	CA-C-O	7.10	128.08	119.49
2	D	133	VAL	N-CA-CB	7.10	119.65	110.57
2	F	133	VAL	O-C-N	7.10	132.68	122.04
2	D	49	SER	CA-CB-OG	-7.09	96.91	111.10
2	D	50	THR	CA-CB-OG1	7.09	120.24	109.60
2	F	21	ASP	O-C-N	7.09	132.02	122.59
2	F	74	GLY	N-CA-C	-7.09	104.59	115.66
2	F	131	GLN	N-CA-CB	7.09	121.50	110.44
2	F	143	HIS	CB-CG-ND1	7.09	133.34	122.70
1	C	134	THR	CA-C-N	-7.09	109.20	121.97
1	C	134	THR	C-N-CA	-7.09	109.20	121.97
2	D	53	ALA	N-CA-C	-7.09	103.16	111.03
1	A	20	HIS	CA-C-N	7.09	135.08	121.54
1	A	20	HIS	C-N-CA	7.09	135.08	121.54
2	F	43	GLU	CA-CB-CG	7.09	128.28	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	LEU	CB-CA-C	7.09	121.39	109.84
1	A	21	ALA	CA-C-N	-7.09	107.52	121.41
1	A	21	ALA	C-N-CA	-7.09	107.52	121.41
2	B	98	VAL	N-CA-C	-7.09	97.98	108.97
2	D	19	ASN	CA-CB-CG	7.09	119.69	112.60
2	F	117	HIS	CG-CD2-NE2	-7.09	100.11	107.20
2	H	131	GLN	CG-CD-OE1	7.09	134.97	120.80
2	H	146	HIS	CG-ND1-CE1	7.08	121.34	109.30
1	G	20	HIS	CG-ND1-CE1	-7.08	97.26	109.30
1	E	83	LEU	CB-CG-CD2	-7.08	89.45	110.70
1	G	81	SER	CA-C-N	7.08	135.06	121.54
1	G	81	SER	C-N-CA	7.08	135.06	121.54
1	G	117	PHE	N-CA-C	7.08	125.88	110.80
2	H	86	ALA	CB-CA-C	7.08	121.76	109.15
2	B	67	VAL	CB-CA-C	-7.08	102.91	111.97
1	E	26	ALA	CB-CA-C	7.08	123.92	109.55
2	D	102	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	C	16	LYS	O-C-N	7.07	132.22	122.46
2	D	146	HIS	CE1-NE2-CD2	-7.07	101.93	109.00
1	A	30	GLU	CG-CD-OE1	7.07	134.66	118.40
1	E	98	PHE	CG-CD2-CE2	-7.07	108.68	120.70
2	B	130	TYR	CG-CD1-CE1	-7.07	110.60	121.20
1	E	8	THR	CA-CB-OG1	-7.07	99.00	109.60
2	F	84	THR	N-CA-CB	7.07	120.59	110.13
2	H	17	LYS	N-CA-C	7.07	121.92	113.16
1	G	121	VAL	O-C-N	7.06	131.16	121.84
1	A	76	MET	CG-SD-CE	-7.06	85.36	100.90
1	E	14	TRP	CB-CA-C	7.06	124.58	110.17
2	F	42	PHE	O-C-N	7.06	137.98	121.74
2	H	33	VAL	CA-CB-CG2	-7.06	98.40	110.40
2	H	67	VAL	CA-CB-CG2	7.06	122.40	110.40
1	C	24	TYR	CA-C-O	-7.06	112.12	120.10
1	C	90	LYS	CB-CA-C	7.06	124.47	110.42
1	C	104	CYS	O-C-N	7.06	132.73	122.43
2	B	14	LEU	N-CA-CB	7.05	120.54	109.82
1	A	76	MET	N-CA-C	7.05	123.30	113.57
2	B	97	HIS	CB-CG-CD2	-7.05	122.04	131.20
1	A	64	ASP	N-CA-C	7.04	119.04	111.36
2	B	141	LEU	CB-CA-C	7.04	120.93	111.14
2	B	66	LYS	N-CA-CB	7.04	122.39	110.49
1	G	49	SER	CB-CA-C	7.04	121.98	110.22
1	E	47	ASP	CA-C-N	-7.04	112.09	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	47	ASP	C-N-CA	-7.04	112.09	122.86
1	G	84	SER	N-CA-CB	7.04	120.19	109.91
1	E	83	LEU	O-C-N	-7.04	112.90	122.33
1	G	104	CYS	CA-C-N	7.04	129.94	120.65
1	G	104	CYS	C-N-CA	7.04	129.94	120.65
2	D	71	PHE	CB-CG-CD2	7.03	132.66	120.70
2	F	31	LEU	N-CA-C	-7.03	103.04	111.69
2	H	54	VAL	CA-C-N	7.03	131.85	120.60
2	H	54	VAL	C-N-CA	7.03	131.85	120.60
1	E	6	ASP	CA-C-O	7.03	128.06	119.97
1	G	42	TYR	CB-CG-CD2	-7.03	110.25	120.80
2	B	110	LEU	N-CA-C	-7.03	103.63	111.71
1	G	4	PRO	N-CA-CB	7.03	110.63	103.25
2	H	107	GLY	CA-C-O	-7.03	111.20	119.50
2	B	7	GLU	CA-CB-CG	-7.03	100.04	114.10
1	A	46	PHE	CB-CG-CD1	-7.03	108.75	120.70
2	F	14	LEU	CD1-CG-CD2	7.03	126.26	110.80
1	G	27	GLU	N-CA-CB	7.03	121.12	110.30
1	C	60	LYS	CB-CA-C	7.03	124.16	110.67
2	F	82	LYS	CG-CD-CE	-7.03	95.14	111.30
1	A	68	ASN	CA-C-O	7.02	128.04	119.97
2	B	127	GLN	CG-CD-NE2	7.02	126.93	116.40
2	B	110	LEU	CB-CG-CD1	-7.02	89.65	110.70
1	A	15	GLY	CA-C-N	7.01	131.82	120.60
1	A	15	GLY	C-N-CA	7.01	131.82	120.60
2	H	45	PHE	O-C-N	-7.01	113.03	122.43
2	B	81	LEU	CA-C-N	-7.01	110.18	120.28
2	B	81	LEU	C-N-CA	-7.01	110.18	120.28
2	D	53	ALA	CA-C-O	7.01	128.12	120.90
1	C	8	THR	CA-CB-OG1	-7.01	99.09	109.60
1	E	74	ASP	N-CA-C	-7.01	104.86	113.41
1	G	43	PHE	CA-CB-CG	-7.01	106.79	113.80
2	D	86	ALA	CA-C-N	7.00	130.16	120.63
2	D	86	ALA	C-N-CA	7.00	130.16	120.63
2	F	54	VAL	CA-CB-CG2	7.00	122.31	110.40
1	G	23	GLU	OE1-CD-OE2	-7.00	106.09	122.90
1	A	27	GLU	CG-CD-OE2	-7.00	102.30	118.40
2	B	35	TYR	CG-CD2-CE2	7.00	131.70	121.20
1	E	70	VAL	CA-CB-CG2	7.00	122.30	110.40
2	F	19	ASN	N-CA-C	-7.00	97.14	108.41
1	C	132	VAL	CA-C-O	-7.00	113.80	121.29
2	H	65	LYS	N-CA-CB	7.00	121.45	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	52	ASP	CA-C-N	-6.99	110.80	120.38
2	B	52	ASP	C-N-CA	-6.99	110.80	120.38
2	D	37	TRP	CA-CB-CG	-6.99	100.31	113.60
1	G	20	HIS	CA-C-N	6.99	132.31	121.19
1	G	20	HIS	C-N-CA	6.99	132.31	121.19
2	H	100	PRO	O-C-N	-6.99	113.20	122.64
2	B	66	LYS	CD-CE-NZ	-6.99	89.53	111.90
1	E	106	LEU	N-CA-C	-6.99	95.92	110.80
1	C	68	ASN	N-CA-C	6.99	118.89	111.28
1	C	20	HIS	O-C-N	6.98	131.07	122.34
1	E	21	ALA	CB-CA-C	6.98	124.32	110.42
2	H	27	ALA	CA-C-N	-6.98	110.38	120.29
2	H	27	ALA	C-N-CA	-6.98	110.38	120.29
2	H	58	PRO	CA-C-N	6.98	134.37	121.52
2	H	58	PRO	C-N-CA	6.98	134.37	121.52
1	C	61	LYS	N-CA-CB	6.98	120.49	110.16
1	G	117	PHE	CB-CA-C	-6.98	96.53	110.42
2	H	87	THR	CB-CA-C	-6.98	96.54	110.42
2	H	4	THR	O-C-N	-6.98	112.70	121.70
1	E	47	ASP	N-CA-CB	6.97	121.30	110.21
1	E	139	LYS	N-CA-CB	-6.97	101.08	111.25
1	A	134	THR	CA-CB-CG2	6.97	122.34	110.50
1	C	131	SER	N-CA-C	-6.97	103.12	111.69
2	F	5	PRO	CA-N-CD	6.97	121.75	112.00
1	C	129	LEU	N-CA-C	-6.96	104.04	112.54
2	D	59	LYS	CA-C-N	6.96	130.70	120.74
2	D	59	LYS	C-N-CA	6.96	130.70	120.74
1	E	67	THR	CA-CB-CG2	-6.96	98.66	110.50
1	G	103	HIS	ND1-CE1-NE2	-6.96	101.44	108.40
2	H	84	THR	CA-CB-CG2	6.96	122.33	110.50
1	C	58	HIS	ND1-CE1-NE2	6.96	115.36	108.40
1	E	125	LEU	CA-C-N	6.96	129.48	120.44
1	E	125	LEU	C-N-CA	6.96	129.48	120.44
1	C	125	LEU	N-CA-CB	-6.95	98.74	110.49
2	D	142	ALA	N-CA-CB	-6.95	99.59	110.44
2	D	106	LEU	O-C-N	-6.95	112.06	122.28
1	G	36	PHE	CB-CG-CD2	-6.95	108.88	120.70
1	G	104	CYS	O-C-N	6.95	130.82	122.27
2	H	142	ALA	N-CA-CB	-6.95	100.17	110.53
1	E	66	LEU	CA-C-O	-6.95	113.47	120.90
1	E	78	ASN	CA-CB-CG	-6.95	105.65	112.60
2	H	42	PHE	CA-C-N	-6.95	112.23	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	42	PHE	C-N-CA	-6.95	112.23	122.86
1	A	112	HIS	CA-C-O	6.95	126.68	118.69
1	C	121	VAL	CA-CB-CG1	-6.95	98.59	110.40
2	H	71	PHE	CA-C-O	-6.95	113.71	121.00
2	H	38	THR	CA-C-N	6.94	134.80	121.54
2	H	38	THR	C-N-CA	6.94	134.80	121.54
2	B	66	LYS	N-CA-C	-6.94	96.01	110.80
1	E	36	PHE	CG-CD1-CE1	6.94	132.50	120.70
1	A	103	HIS	O-C-N	6.94	129.22	122.07
2	F	43	GLU	CA-C-N	6.94	135.14	122.79
2	F	43	GLU	C-N-CA	6.94	135.14	122.79
2	F	109	VAL	CA-CB-CG2	6.94	122.19	110.40
2	H	88	LEU	CA-C-N	6.94	134.79	121.54
2	H	88	LEU	C-N-CA	6.94	134.79	121.54
1	E	73	VAL	CG1-CB-CG2	-6.94	95.54	110.80
2	B	130	TYR	CA-C-N	6.93	136.77	121.80
2	B	130	TYR	C-N-CA	6.93	136.77	121.80
2	F	22	GLU	O-C-N	6.93	130.05	122.15
1	E	56	LYS	CA-CB-CG	6.93	127.96	114.10
1	C	102	SER	CA-C-O	-6.93	113.15	120.63
1	G	23	GLU	CG-CD-OE2	-6.92	102.47	118.40
2	F	114	LEU	CD1-CG-CD2	6.92	126.03	110.80
2	H	134	VAL	N-CA-C	6.92	121.73	112.04
1	A	43	PHE	CD1-CG-CD2	-6.91	108.23	118.60
1	C	116	GLU	N-CA-C	-6.91	102.81	111.11
2	D	79	ASP	CB-CG-OD1	-6.91	102.50	118.40
2	F	75	LEU	CB-CA-C	6.91	121.33	109.24
1	G	54	GLN	CB-CG-CD	-6.91	100.86	112.60
1	A	8	THR	CB-CA-C	-6.91	96.99	110.11
2	D	95	LYS	N-CA-C	6.91	122.11	112.93
1	A	91	LEU	CA-C-O	6.90	128.65	120.92
2	B	101	GLU	CA-C-O	-6.90	112.04	119.97
2	B	124	PRO	CA-C-N	6.90	127.85	120.47
2	B	124	PRO	C-N-CA	6.90	127.85	120.47
1	C	64	ASP	CB-CA-C	6.90	124.87	110.32
1	C	8	THR	N-CA-CB	6.89	120.36	110.16
1	G	35	SER	N-CA-CB	-6.89	99.69	110.44
1	C	138	SER	CA-C-N	6.89	134.09	122.65
1	C	138	SER	C-N-CA	6.89	134.09	122.65
2	B	145	TYR	CB-CA-C	6.89	122.14	109.46
2	H	141	LEU	O-C-N	6.89	129.17	122.07
1	C	24	TYR	CA-C-N	6.89	127.58	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	24	TYR	C-N-CA	6.89	127.58	120.00
1	A	3	SER	CA-C-O	-6.88	109.34	121.67
1	E	121	VAL	CA-CB-CG2	6.88	122.10	110.40
2	F	124	PRO	CB-CA-C	6.88	119.32	110.92
1	C	32	MET	CA-C-O	6.88	130.35	120.51
2	B	74	GLY	CA-C-O	-6.88	108.60	120.57
2	B	77	HIS	ND1-CE1-NE2	6.88	115.28	108.40
2	B	117	HIS	CA-CB-CG	6.88	120.68	113.80
2	D	7	GLU	CG-CD-OE1	6.88	134.22	118.40
1	G	61	LYS	N-CA-CB	-6.88	99.98	110.16
2	H	18	VAL	CA-CB-CG1	-6.88	98.71	110.40
1	C	65	ALA	N-CA-CB	-6.88	98.87	110.49
1	C	95	PRO	N-CD-CG	-6.88	92.89	103.20
2	H	40	ARG	CA-C-O	-6.88	110.68	120.51
2	H	72	SER	CA-CB-OG	-6.88	97.35	111.10
2	B	122	PHE	CZ-CE2-CD2	-6.88	107.62	120.00
2	F	104	ARG	NE-CZ-NH2	-6.88	113.01	119.20
1	A	25	GLY	N-CA-C	-6.87	104.16	113.37
2	D	26	GLU	CG-CD-OE1	6.87	134.21	118.40
1	E	139	LYS	CG-CD-CE	-6.87	95.49	111.30
2	H	140	ALA	CA-C-O	-6.87	113.61	120.82
1	E	72	HIS	N-CA-CB	-6.87	102.03	111.65
1	C	52	SER	CA-C-N	-6.87	109.87	120.31
1	C	52	SER	C-N-CA	-6.87	109.87	120.31
1	E	119	PRO	CA-CB-CG	-6.87	91.45	104.50
2	F	103	PHE	CA-CB-CG	-6.87	106.93	113.80
1	A	16	LYS	CB-CG-CD	6.87	127.09	111.30
1	A	72	HIS	CE1-NE2-CD2	6.87	115.86	109.00
2	D	106	LEU	N-CA-CB	-6.86	100.03	110.26
2	D	123	THR	N-CA-C	6.86	119.55	110.08
2	F	40	ARG	CG-CD-NE	-6.86	96.90	112.00
2	D	120	LYS	N-CA-CB	-6.86	99.65	110.28
2	F	51	PRO	N-CA-C	6.86	122.91	113.65
1	E	24	TYR	CB-CA-C	-6.86	99.41	110.79
1	G	85	ASP	OD1-CG-OD2	-6.86	106.44	122.90
1	A	24	TYR	CA-CB-CG	-6.86	101.56	113.90
1	E	118	THR	CA-CB-OG1	-6.86	99.32	109.60
1	E	129	LEU	N-CA-CB	-6.86	100.04	110.12
2	F	35	TYR	CA-C-N	-6.86	111.27	119.84
2	F	35	TYR	C-N-CA	-6.86	111.27	119.84
1	G	140	TYR	CG-CD2-CE2	-6.85	110.92	121.20
2	B	42	PHE	N-CA-CB	-6.85	101.37	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	PRO	CA-CB-CG	-6.85	91.49	104.50
1	A	102	SER	CA-C-O	6.85	127.80	119.38
1	E	54	GLN	CG-CD-NE2	-6.85	106.13	116.40
2	F	6	VAL	CA-C-N	-6.85	109.91	120.31
2	F	6	VAL	C-N-CA	-6.85	109.91	120.31
1	A	95	PRO	CA-N-CD	-6.84	102.42	112.00
1	E	116	GLU	OE1-CD-OE2	-6.84	106.49	122.90
2	D	111	VAL	CA-C-O	6.83	128.02	120.71
1	E	114	PRO	CA-C-N	6.83	134.88	122.92
1	E	114	PRO	C-N-CA	6.83	134.88	122.92
1	A	102	SER	N-CA-C	-6.83	104.21	112.54
1	G	106	LEU	CB-CG-CD1	6.83	131.20	110.70
1	A	94	ASP	N-CA-CB	6.83	122.48	109.44
1	E	36	PHE	CA-C-N	-6.83	111.31	119.84
1	E	36	PHE	C-N-CA	-6.83	111.31	119.84
1	A	43	PHE	O-C-N	6.83	127.06	121.05
2	H	123	THR	OG1-CB-CG2	-6.83	95.65	109.30
1	C	7	LYS	CG-CD-CE	6.82	126.99	111.30
1	G	14	TRP	CD2-CE2-CZ2	6.82	129.22	122.40
1	C	137	THR	CA-CB-OG1	-6.82	99.37	109.60
2	B	67	VAL	CA-C-N	-6.82	108.28	121.58
2	B	67	VAL	C-N-CA	-6.82	108.28	121.58
2	B	77	HIS	N-CA-C	-6.82	99.43	109.11
2	H	74	GLY	CA-C-O	6.82	128.76	119.28
2	H	85	PHE	CB-CG-CD1	-6.82	109.11	120.70
1	A	31	ARG	N-CA-C	6.82	119.58	111.33
1	A	37	PRO	CA-N-CD	6.82	121.54	112.00
1	G	44	PRO	CB-CA-C	-6.82	102.33	112.55
1	A	23	GLU	CG-CD-OE1	6.81	134.07	118.40
1	A	112	HIS	CB-CG-CD2	6.81	140.06	131.20
1	G	85	ASP	CA-C-O	-6.81	113.67	120.82
2	F	35	TYR	O-C-N	-6.81	113.49	121.32
1	E	1	VAL	CA-CB-CG2	6.80	121.97	110.40
1	E	111	ALA	N-CA-C	6.80	121.43	113.20
1	E	10	VAL	N-CA-CB	6.80	121.92	110.56
2	B	59	LYS	N-CA-CB	6.80	120.11	110.12
1	C	139	LYS	CA-C-O	6.80	127.95	119.59
2	H	37	TRP	CE2-CD2-CE3	6.79	125.59	118.80
2	H	39	GLN	CG-CD-OE1	6.79	134.39	120.80
2	B	71	PHE	N-CA-C	6.78	119.25	111.11
2	D	59	LYS	CB-CG-CD	6.78	126.90	111.30
1	G	129	LEU	N-CA-CB	-6.78	98.79	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	33	VAL	CA-CB-CG1	-6.78	98.87	110.40
1	C	139	LYS	CB-CA-C	6.78	122.54	110.81
2	D	80	ASN	CA-C-O	-6.78	110.55	121.94
2	H	26	GLU	CB-CA-C	-6.78	100.23	110.88
1	G	96	VAL	CA-CB-CG1	6.78	121.92	110.40
1	C	28	ALA	O-C-N	-6.78	113.58	122.59
1	E	122	HIS	CG-CD2-NE2	6.77	113.97	107.20
2	B	90	GLU	N-CA-C	-6.77	100.27	111.37
1	E	91	LEU	O-C-N	6.77	130.36	122.17
2	D	54	VAL	CA-CB-CG2	6.76	121.90	110.40
2	F	94	ASP	OD1-CG-OD2	-6.76	106.67	122.90
1	G	113	LEU	CB-CA-C	6.76	122.31	111.15
2	H	68	LEU	N-CA-CB	-6.76	98.01	110.32
2	D	101	GLU	CG-CD-OE2	-6.76	102.85	118.40
2	F	5	PRO	N-CA-CB	-6.76	97.10	103.52
1	G	43	PHE	CA-C-O	-6.76	112.49	120.87
2	H	36	PRO	CA-C-N	6.76	135.83	122.31
2	H	36	PRO	C-N-CA	6.76	135.83	122.31
2	D	69	GLY	O-C-N	6.76	131.49	122.70
2	D	73	ASP	OD1-CG-OD2	6.76	139.12	122.90
2	F	12	THR	CA-CB-CG2	6.76	121.99	110.50
1	C	88	ALA	CB-CA-C	6.76	122.34	110.85
2	F	22	GLU	CG-CD-OE1	6.76	133.94	118.40
1	G	81	SER	O-C-N	6.76	131.58	122.59
1	A	42	TYR	CD1-CE1-CZ	-6.75	107.44	119.60
1	G	67	THR	N-CA-CB	-6.75	99.39	110.40
1	C	128	PHE	CE1-CZ-CE2	6.75	132.15	120.00
1	A	129	LEU	O-C-N	-6.75	114.35	122.11
1	A	68	ASN	CA-CB-CG	-6.75	105.85	112.60
2	H	75	LEU	CD1-CG-CD2	-6.75	95.96	110.80
1	E	64	ASP	N-CA-CB	6.75	120.11	110.13
2	H	113	VAL	CA-CB-CG1	6.75	121.87	110.40
2	B	16	GLY	O-C-N	-6.74	115.25	122.19
2	F	140	ALA	N-CA-C	-6.74	103.86	111.14
1	C	88	ALA	CA-C-O	-6.74	113.27	120.42
2	D	71	PHE	CB-CA-C	6.74	121.40	110.95
1	G	10	VAL	N-CA-CB	6.74	119.20	110.57
2	D	5	PRO	N-CD-CG	6.74	113.31	103.20
2	D	93	CYS	CA-CB-SG	6.74	129.90	114.40
1	E	53	ALA	N-CA-C	-6.74	104.16	112.38
1	E	85	ASP	N-CA-CB	6.74	120.17	110.06
1	G	132	VAL	CG1-CB-CG2	-6.74	95.98	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	25	GLY	N-CA-C	-6.74	106.01	114.16
2	H	50	THR	CB-CA-C	6.74	119.26	110.03
1	E	82	ALA	N-CA-C	-6.73	104.01	111.82
1	E	15	GLY	N-CA-C	-6.73	97.23	113.18
2	H	92	HIS	N-CA-CB	6.73	120.01	110.12
1	E	101	LEU	CD1-CG-CD2	6.73	125.60	110.80
1	A	54	GLN	N-CA-CB	6.72	119.73	109.91
2	F	128	ALA	CB-CA-C	6.72	123.07	110.63
2	H	67	VAL	N-CA-CB	-6.72	103.05	110.65
1	G	100	LEU	CB-CG-CD1	-6.72	90.53	110.70
2	H	26	GLU	CA-C-O	6.72	127.88	120.82
2	D	77	HIS	ND1-CE1-NE2	-6.72	101.68	108.40
1	C	16	LYS	N-CA-C	6.71	121.07	113.01
1	G	46	PHE	CB-CG-CD1	-6.71	109.28	120.70
1	A	49	SER	O-C-N	6.71	130.89	123.04
1	E	61	LYS	CB-CA-C	6.71	124.07	110.38
1	E	33	PHE	CG-CD1-CE1	6.71	132.10	120.70
2	F	127	GLN	N-CA-CB	-6.71	100.29	110.01
1	A	2	LEU	O-C-N	6.71	130.88	123.04
2	H	144	LYS	CA-C-N	-6.71	111.91	121.50
2	H	144	LYS	C-N-CA	-6.71	111.91	121.50
1	G	112	HIS	CG-ND1-CE1	-6.70	97.90	109.30
2	H	124	PRO	N-CA-C	-6.70	102.52	110.70
2	F	65	LYS	CA-C-O	-6.70	111.00	119.31
2	D	26	GLU	CG-CD-OE2	-6.70	102.99	118.40
2	F	28	LEU	CA-C-N	-6.70	112.51	119.94
2	F	28	LEU	C-N-CA	-6.70	112.51	119.94
2	H	134	VAL	O-C-N	-6.70	113.28	122.05
2	F	29	GLY	O-C-N	-6.70	115.75	122.18
1	G	1	VAL	CG1-CB-CG2	6.70	125.53	110.80
1	C	61	LYS	CA-C-N	-6.69	109.84	120.55
1	C	61	LYS	C-N-CA	-6.69	109.84	120.55
1	A	42	TYR	CZ-CE2-CD2	6.69	131.65	119.60
2	D	44	SER	CA-C-O	6.69	129.10	120.07
1	A	39	THR	N-CA-CB	6.69	119.95	110.12
2	B	3	LEU	N-CA-C	-6.69	99.77	110.14
1	C	100	LEU	CB-CA-C	6.69	122.75	110.11
1	G	123	ALA	CA-C-O	-6.68	113.33	120.42
2	D	20	VAL	CG1-CB-CG2	-6.68	96.10	110.80
2	F	104	ARG	N-CA-C	-6.68	103.92	111.07
1	A	86	LEU	CA-C-N	-6.68	111.50	120.79
1	A	86	LEU	C-N-CA	-6.68	111.50	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	102	ASN	N-CA-CB	6.68	120.08	110.06
2	H	98	VAL	CA-CB-CG2	6.68	121.75	110.40
2	D	75	LEU	O-C-N	-6.67	111.73	122.41
1	C	90	LYS	CA-C-N	6.67	132.82	121.14
1	C	90	LYS	C-N-CA	6.67	132.82	121.14
1	E	62	VAL	CA-C-N	6.67	129.52	120.38
1	E	62	VAL	C-N-CA	6.67	129.52	120.38
1	G	107	VAL	CG1-CB-CG2	-6.67	96.12	110.80
2	D	139	ASN	CA-CB-CG	6.67	119.27	112.60
2	D	62	ALA	CA-C-N	6.67	129.75	120.29
2	D	62	ALA	C-N-CA	6.67	129.75	120.29
1	G	107	VAL	O-C-N	-6.67	115.38	121.91
1	E	44	PRO	CA-CB-CG	-6.66	91.84	104.50
1	G	138	SER	CA-CB-OG	-6.66	97.77	111.10
1	A	72	HIS	CB-CG-CD2	6.66	139.86	131.20
1	C	31	ARG	O-C-N	6.66	131.35	122.43
1	C	31	ARG	N-CA-C	-6.66	104.41	112.54
1	G	98	PHE	CA-CB-CG	6.66	120.46	113.80
2	H	48	LEU	CB-CA-C	-6.66	98.29	109.75
2	D	43	GLU	CB-CG-CD	-6.66	101.28	112.60
1	A	80	LEU	O-C-N	6.66	130.17	122.25
2	H	35	TYR	CG-CD1-CE1	-6.65	111.22	121.20
2	D	37	TRP	CZ3-CH2-CZ2	-6.65	112.86	121.50
2	B	56	GLY	CA-C-N	-6.65	109.85	121.35
2	B	56	GLY	C-N-CA	-6.65	109.85	121.35
1	E	43	PHE	CB-CG-CD1	6.65	132.00	120.70
1	A	69	ALA	O-C-N	6.64	130.87	122.23
2	B	22	GLU	N-CA-CB	-6.64	99.78	110.14
2	D	101	GLU	CA-C-O	-6.64	111.21	119.38
1	E	46	PHE	CA-CB-CG	-6.64	107.16	113.80
1	E	68	ASN	CA-CB-CG	6.64	119.24	112.60
2	F	105	LEU	CA-C-N	6.64	129.84	120.28
2	F	105	LEU	C-N-CA	6.64	129.84	120.28
2	B	64	GLY	N-CA-C	-6.64	104.80	112.50
2	D	127	GLN	O-C-N	6.64	128.91	122.07
2	F	21	ASP	CA-CB-CG	-6.64	105.96	112.60
2	F	121	GLU	CB-CG-CD	6.63	123.88	112.60
2	D	31	LEU	CB-CA-C	-6.63	100.67	110.95
2	D	118	PHE	CD1-CG-CD2	-6.63	108.65	118.60
2	F	107	GLY	CA-C-O	-6.63	109.03	120.57
1	E	81	SER	CA-CB-OG	-6.63	97.84	111.10
1	E	101	LEU	N-CA-CB	6.63	121.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	38	THR	N-CA-C	-6.63	104.67	112.89
1	G	138	SER	CA-C-O	-6.63	110.44	119.05
2	D	95	LYS	CD-CE-NZ	6.62	133.10	111.90
2	D	143	HIS	O-C-N	-6.62	114.47	122.22
1	C	49	SER	CA-C-N	-6.62	111.70	121.24
1	C	49	SER	C-N-CA	-6.62	111.70	121.24
1	C	68	ASN	CB-CA-C	-6.62	99.79	110.79
1	C	42	TYR	CA-CB-CG	-6.62	101.98	113.90
2	D	42	PHE	N-CA-C	6.62	121.74	109.56
2	D	51	PRO	N-CD-CG	-6.62	93.27	103.20
1	G	6	ASP	CA-C-N	6.62	131.72	121.19
1	G	6	ASP	C-N-CA	6.62	131.72	121.19
1	A	58	HIS	CB-CG-ND1	6.62	132.63	122.70
1	C	70	VAL	N-CA-CB	6.62	118.29	110.55
1	E	138	SER	N-CA-CB	6.62	119.95	110.16
1	G	139	LYS	CD-CE-NZ	-6.62	90.73	111.90
2	H	65	LYS	O-C-N	6.62	131.81	122.41
2	B	121	GLU	CG-CD-OE2	-6.61	103.19	118.40
1	E	103	HIS	O-C-N	6.61	129.69	122.15
1	E	116	GLU	CB-CA-C	-6.61	98.43	109.27
2	H	76	ALA	CB-CA-C	-6.61	100.78	110.96
1	A	74	ASP	CB-CG-OD1	-6.61	103.20	118.40
1	A	9	ASN	CB-CG-OD1	6.61	134.01	120.80
1	A	33	PHE	CG-CD1-CE1	-6.61	109.47	120.70
2	B	54	VAL	N-CA-CB	6.61	119.03	110.57
2	F	108	ASN	CA-CB-CG	6.61	119.21	112.60
1	A	42	TYR	CG-CD2-CE2	-6.60	111.30	121.20
2	H	130	TYR	CZ-CE2-CD2	-6.60	107.72	119.60
1	A	48	LEU	N-CA-CB	-6.60	99.34	110.49
2	H	127	GLN	CB-CG-CD	6.60	123.81	112.60
1	G	123	ALA	N-CA-CB	6.59	119.92	110.16
1	A	105	LEU	CA-CB-CG	6.59	139.37	116.30
2	D	38	THR	CA-CB-CG2	6.59	121.71	110.50
2	B	6	VAL	CA-CB-CG1	6.59	121.60	110.40
1	E	11	LYS	N-CA-CB	6.59	119.56	110.01
2	F	37	TRP	CB-CA-C	6.59	121.87	110.01
2	D	124	PRO	N-CD-CG	6.59	113.08	103.20
2	B	91	LEU	N-CA-CB	-6.59	100.12	110.46
2	D	1	VAL	N-CA-CB	6.59	122.70	111.50
1	E	88	ALA	N-CA-CB	6.59	121.62	110.49
2	H	55	MET	N-CA-C	6.59	120.42	112.38
1	E	73	VAL	CA-C-N	-6.58	110.31	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	73	VAL	C-N-CA	-6.58	110.31	122.09
2	D	34	VAL	CA-CB-CG1	6.58	121.59	110.40
2	D	121	GLU	CA-C-N	-6.58	108.97	121.54
2	D	121	GLU	C-N-CA	-6.58	108.97	121.54
2	H	31	LEU	CB-CG-CD1	-6.58	90.97	110.70
1	C	68	ASN	O-C-N	-6.58	115.15	122.12
1	G	30	GLU	CG-CD-OE1	6.58	133.53	118.40
1	A	89	HIS	CB-CA-C	-6.58	99.26	110.24
1	E	67	THR	N-CA-C	-6.58	103.94	112.23
1	E	40	LYS	CA-C-O	6.57	127.53	119.97
2	H	125	PRO	CA-N-CD	-6.57	102.80	112.00
1	A	36	PHE	CA-CB-CG	6.57	120.37	113.80
2	B	109	VAL	N-CA-CB	6.57	118.52	110.64
2	D	68	LEU	CA-C-O	6.57	127.67	119.59
1	C	98	PHE	CA-C-O	-6.56	113.85	121.07
1	A	64	ASP	O-C-N	6.56	129.63	122.15
2	D	123	THR	CB-CA-C	-6.56	98.71	109.27
2	D	60	VAL	CA-C-O	6.56	128.76	120.96
2	D	31	LEU	N-CA-C	6.55	118.31	111.03
2	F	132	LYS	CB-CA-C	6.55	121.25	110.90
1	A	17	VAL	CG1-CB-CG2	6.55	125.21	110.80
2	B	137	VAL	N-CA-C	-6.55	104.26	110.42
2	H	86	ALA	O-C-N	6.55	130.11	122.25
2	H	133	VAL	N-CA-CB	6.55	118.95	110.57
2	H	23	VAL	O-C-N	6.54	128.74	122.20
2	H	71	PHE	CB-CA-C	6.54	121.03	110.96
2	H	121	GLU	CG-CD-OE1	6.54	133.45	118.40
2	D	42	PHE	CA-C-N	-6.54	112.09	122.95
2	D	42	PHE	C-N-CA	-6.54	112.09	122.95
1	C	60	LYS	O-C-N	6.54	130.31	122.27
1	A	29	LEU	CB-CA-C	6.53	123.64	109.99
1	A	129	LEU	CB-CG-CD1	6.53	130.30	110.70
1	E	61	LYS	CA-C-O	-6.53	112.08	119.79
1	A	6	ASP	CB-CG-OD2	-6.53	103.38	118.40
2	B	99	ASP	CA-CB-CG	6.53	119.13	112.60
2	H	12	THR	CB-CA-C	6.53	122.45	110.11
2	H	22	GLU	CA-CB-CG	-6.53	101.04	114.10
1	C	97	ASN	CB-CG-ND2	-6.53	106.61	116.40
1	E	14	TRP	CD2-CE3-CZ3	6.52	127.08	118.60
1	A	36	PHE	CZ-CE2-CD2	-6.52	108.26	120.00
1	A	125	LEU	N-CA-C	6.52	118.47	111.36
1	C	85	ASP	O-C-N	-6.52	114.59	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	48	LEU	N-CA-CB	6.52	121.86	111.17
2	D	111	VAL	O-C-N	-6.52	113.24	121.84
1	G	10	VAL	CA-C-O	-6.52	113.82	121.05
1	G	31	ARG	NE-CZ-NH1	-6.52	114.98	121.50
2	B	28	LEU	CA-C-N	-6.51	112.71	119.94
2	B	28	LEU	C-N-CA	-6.51	112.71	119.94
1	C	19	ALA	CA-C-N	6.51	133.29	122.54
1	C	19	ALA	C-N-CA	6.51	133.29	122.54
1	E	17	VAL	CG1-CB-CG2	6.51	125.13	110.80
2	F	88	LEU	N-CA-CB	6.51	121.20	110.39
1	A	30	GLU	O-C-N	6.51	129.02	122.12
1	A	90	LYS	N-CA-CB	6.51	120.41	110.39
1	E	5	ALA	N-CA-C	-6.51	104.03	112.23
1	G	1	VAL	CA-C-N	6.51	132.35	122.65
1	G	1	VAL	C-N-CA	6.51	132.35	122.65
2	B	26	GLU	CA-CB-CG	-6.50	101.10	114.10
1	G	103	HIS	ND1-CG-CD2	-6.50	99.60	106.10
2	H	14	LEU	N-CA-CB	6.50	119.70	109.82
2	F	14	LEU	CA-C-N	-6.49	110.93	120.28
2	F	14	LEU	C-N-CA	-6.49	110.93	120.28
2	F	19	ASN	OD1-CG-ND2	6.49	129.09	122.60
1	C	80	LEU	CD1-CG-CD2	-6.49	96.52	110.80
2	F	60	VAL	N-CA-CB	-6.49	100.84	110.58
1	G	84	SER	CA-C-N	6.49	128.88	120.44
1	G	84	SER	C-N-CA	6.49	128.88	120.44
1	A	139	LYS	CA-CB-CG	-6.49	101.12	114.10
2	D	28	LEU	CA-C-O	6.49	127.84	120.90
2	D	72	SER	CA-CB-OG	6.49	124.08	111.10
1	A	94	ASP	CB-CA-C	-6.49	99.12	109.82
2	B	22	GLU	CG-CD-OE1	6.49	133.32	118.40
2	B	67	VAL	CA-CB-CG2	6.49	121.42	110.40
2	D	138	ALA	O-C-N	-6.49	115.34	122.09
2	H	93	CYS	CB-CA-C	6.49	123.33	110.42
2	B	12	THR	O-C-N	-6.48	115.35	122.09
1	G	119	PRO	CB-CA-C	-6.48	100.86	111.56
1	A	85	ASP	CB-CA-C	6.48	123.85	110.31
1	A	92	ARG	NE-CZ-NH2	6.48	125.03	119.20
2	F	23	VAL	CA-CB-CG2	6.48	121.41	110.40
1	A	54	GLN	CG-CD-OE1	6.48	133.75	120.80
1	A	53	ALA	N-CA-C	-6.47	103.46	111.75
1	A	44	PRO	CB-CA-C	-6.47	102.66	111.85
1	C	100	LEU	CD1-CG-CD2	6.47	125.04	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	114	LEU	CA-C-N	-6.47	111.80	120.79
2	B	114	LEU	C-N-CA	-6.47	111.80	120.79
1	G	28	ALA	N-CA-C	-6.47	97.02	110.80
1	E	12	ALA	N-CA-C	-6.47	103.51	111.40
2	F	37	TRP	CB-CG-CD1	-6.46	117.20	126.90
2	B	3	LEU	CD1-CG-CD2	-6.46	96.58	110.80
2	D	23	VAL	O-C-N	6.46	128.14	121.87
2	B	60	VAL	N-CA-CB	6.46	119.82	110.52
2	D	112	CYS	N-CA-C	-6.46	102.91	111.24
2	F	79	ASP	CB-CG-OD2	-6.46	103.55	118.40
1	G	4	PRO	CA-CB-CG	-6.46	92.23	104.50
2	H	94	ASP	CB-CG-OD2	-6.46	103.55	118.40
1	E	12	ALA	CA-C-O	-6.46	113.64	120.55
2	F	4	THR	N-CA-CB	-6.46	101.33	110.04
1	E	93	VAL	CG1-CB-CG2	6.45	125.00	110.80
1	E	139	LYS	N-CA-C	6.45	121.75	111.81
1	G	43	PHE	N-CA-C	6.45	121.51	110.02
1	A	33	PHE	CB-CA-C	-6.45	98.70	110.63
1	G	88	ALA	O-C-N	-6.45	115.28	122.12
1	G	121	VAL	N-CA-C	6.45	118.03	111.00
2	H	2	HIS	N-CA-C	6.45	118.66	108.67
2	D	88	LEU	N-CA-CB	-6.44	99.36	110.32
1	A	94	ASP	CA-C-N	6.44	127.89	119.84
1	A	94	ASP	C-N-CA	6.44	127.89	119.84
1	C	75	ASP	CB-CG-OD2	6.44	133.21	118.40
1	C	113	LEU	CB-CG-CD1	6.44	130.02	110.70
1	C	52	SER	CA-CB-OG	6.44	123.97	111.10
2	H	124	PRO	CB-CA-C	6.43	118.77	110.92
1	E	116	GLU	CA-C-N	-6.43	113.34	122.41
1	E	116	GLU	C-N-CA	-6.43	113.34	122.41
2	D	98	VAL	O-C-N	6.43	129.93	123.18
2	H	24	GLY	CA-C-N	6.43	126.95	119.94
2	H	24	GLY	C-N-CA	6.43	126.95	119.94
2	B	10	ALA	CA-C-N	-6.43	110.40	121.97
2	B	10	ALA	C-N-CA	-6.43	110.40	121.97
1	G	27	GLU	CG-CD-OE2	-6.43	103.62	118.40
2	D	145	TYR	CB-CA-C	6.42	121.07	109.83
1	E	101	LEU	CB-CA-C	-6.42	96.56	109.99
2	B	91	LEU	CB-CA-C	-6.42	97.39	109.72
2	B	126	VAL	CA-C-O	-6.42	112.23	119.42
1	E	125	LEU	CB-CG-CD1	6.42	129.94	110.70
1	E	37	PRO	CA-C-O	6.41	132.27	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	117	HIS	O-C-N	6.41	129.46	122.15
1	E	5	ALA	CA-C-O	-6.41	112.22	119.79
2	B	108	ASN	CB-CG-OD1	6.41	133.62	120.80
2	B	130	TYR	CD1-CG-CD2	6.41	127.71	118.10
2	H	77	HIS	CA-CB-CG	-6.41	107.39	113.80
2	F	114	LEU	CA-C-O	6.41	128.09	120.92
2	F	110	LEU	O-C-N	6.40	128.91	122.12
2	H	111	VAL	N-CA-C	-6.40	104.09	110.62
2	D	82	LYS	N-CA-C	-6.40	104.31	111.28
1	A	87	HIS	CA-C-N	6.39	129.49	120.28
1	A	87	HIS	C-N-CA	6.39	129.49	120.28
1	G	6	ASP	CA-C-O	6.39	127.72	121.00
1	C	117	PHE	CA-C-N	-6.39	110.96	120.68
1	C	117	PHE	C-N-CA	-6.39	110.96	120.68
1	G	31	ARG	CB-CA-C	6.39	122.94	110.67
2	B	137	VAL	CA-CB-CG2	6.39	121.26	110.40
2	B	9	SER	CA-C-N	6.39	128.84	120.28
2	B	9	SER	C-N-CA	6.39	128.84	120.28
2	B	41	PHE	CA-C-N	-6.39	111.06	123.13
2	B	41	PHE	C-N-CA	-6.39	111.06	123.13
1	C	33	PHE	CB-CA-C	-6.39	98.81	110.63
1	E	125	LEU	CD1-CG-CD2	-6.39	96.75	110.80
2	B	78	LEU	N-CA-CB	-6.38	100.71	110.16
2	D	26	GLU	CA-C-N	-6.38	112.14	120.44
2	D	26	GLU	C-N-CA	-6.38	112.14	120.44
2	D	117	HIS	N-CA-C	6.38	118.32	111.36
1	E	87	HIS	CE1-NE2-CD2	6.38	115.39	109.00
1	A	91	LEU	CA-CB-CG	-6.38	93.97	116.30
1	G	27	GLU	CA-C-N	6.38	133.73	121.54
1	G	27	GLU	C-N-CA	6.38	133.73	121.54
1	A	33	PHE	N-CA-CB	6.38	120.04	110.22
1	A	107	VAL	CG1-CB-CG2	-6.38	96.77	110.80
1	C	138	SER	N-CA-C	6.38	118.23	111.28
2	F	1	VAL	CA-CB-CG1	6.37	121.23	110.40
1	C	56	LYS	CA-CB-CG	-6.37	101.36	114.10
2	F	20	VAL	CA-CB-CG1	6.37	121.23	110.40
1	C	5	ALA	CA-C-N	6.37	129.14	120.54
1	C	5	ALA	C-N-CA	6.37	129.14	120.54
1	C	16	LYS	N-CA-CB	-6.37	99.25	110.39
1	C	98	PHE	CA-C-N	6.36	130.87	120.63
1	C	98	PHE	C-N-CA	6.36	130.87	120.63
2	B	74	GLY	O-C-N	6.36	130.97	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	22	GLU	OE1-CD-OE2	-6.36	107.63	122.90
2	H	1	VAL	N-CA-C	-6.36	93.19	111.00
2	H	134	VAL	CA-C-N	6.36	129.98	120.31
2	H	134	VAL	C-N-CA	6.36	129.98	120.31
2	B	12	THR	N-CA-C	-6.36	103.48	111.11
2	B	33	VAL	CA-C-N	-6.36	112.55	120.56
2	B	33	VAL	C-N-CA	-6.36	112.55	120.56
1	C	136	LEU	N-CA-C	-6.36	104.35	111.28
2	B	48	LEU	CA-C-O	-6.36	112.90	119.51
1	E	45	HIS	O-C-N	-6.36	113.54	122.06
2	B	45	PHE	N-CA-C	6.36	119.02	111.71
2	B	145	TYR	CG-CD1-CE1	6.35	130.73	121.20
1	C	121	VAL	CA-C-N	6.35	128.79	120.28
1	C	121	VAL	C-N-CA	6.35	128.79	120.28
1	A	68	ASN	OD1-CG-ND2	6.35	128.95	122.60
2	B	6	VAL	N-CA-CB	-6.35	102.82	112.15
2	F	8	LYS	CD-CE-NZ	6.35	132.22	111.90
1	A	37	PRO	CA-C-N	6.35	128.79	120.28
1	A	37	PRO	C-N-CA	6.35	128.79	120.28
2	D	73	ASP	CA-C-N	-6.35	109.49	120.79
2	D	73	ASP	C-N-CA	-6.35	109.49	120.79
2	D	9	SER	CA-CB-OG	-6.34	98.41	111.10
1	A	135	VAL	CA-CB-CG1	6.34	121.18	110.40
2	H	65	LYS	CA-C-N	-6.34	111.11	121.19
2	H	65	LYS	C-N-CA	-6.34	111.11	121.19
1	A	39	THR	CA-C-N	-6.34	110.45	120.60
1	A	39	THR	C-N-CA	-6.34	110.45	120.60
1	A	105	LEU	CA-C-O	-6.34	113.76	120.55
1	C	108	THR	N-CA-C	-6.34	103.89	111.69
2	B	120	LYS	CB-CA-C	-6.34	97.97	110.27
1	E	129	LEU	N-CA-C	6.34	118.19	111.28
2	F	42	PHE	N-CA-CB	6.34	121.34	111.64
1	G	60	LYS	CB-CA-C	-6.34	98.14	109.24
1	A	88	ALA	CB-CA-C	-6.34	98.90	110.63
2	F	5	PRO	CA-CB-CG	-6.34	92.46	104.50
2	F	15	TRP	N-CA-C	-6.34	104.42	111.71
1	G	7	LYS	CB-CA-C	-6.34	100.32	110.84
2	D	62	ALA	CA-C-O	-6.33	114.35	121.00
1	A	99	LYS	O-C-N	-6.33	114.81	122.22
1	C	32	MET	N-CA-CB	6.33	121.19	110.49
1	G	17	VAL	N-CA-CB	6.33	122.11	110.40
1	G	34	LEU	N-CA-C	6.33	118.26	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	95	LYS	O-C-N	6.33	130.84	122.30
1	C	1	VAL	CA-CB-CG1	6.33	121.15	110.40
2	D	78	LEU	CA-C-O	6.33	127.12	120.42
1	A	84	SER	N-CA-CB	-6.32	100.80	110.16
1	A	120	ALA	N-CA-C	-6.32	105.06	112.89
2	H	31	LEU	CB-CA-C	6.32	120.88	110.90
1	A	10	VAL	CA-CB-CG1	6.31	121.13	110.40
2	B	37	TRP	CE2-CD2-CE3	6.31	125.11	118.80
2	D	9	SER	CA-C-O	-6.31	112.30	120.00
1	G	44	PRO	N-CA-C	-6.31	104.94	113.40
2	D	117	HIS	CG-CD2-NE2	-6.31	100.89	107.20
1	G	71	ALA	CB-CA-C	6.31	123.63	110.32
2	H	21	ASP	CA-C-O	6.31	127.44	120.82
2	F	35	TYR	CZ-CE2-CD2	-6.31	108.25	119.60
1	C	136	LEU	CA-C-N	-6.30	110.33	122.06
1	C	136	LEU	C-N-CA	-6.30	110.33	122.06
2	D	36	PRO	N-CA-C	6.30	125.46	112.47
1	E	43	PHE	CG-CD2-CE2	6.30	131.42	120.70
1	A	6	ASP	CB-CA-C	6.30	120.89	110.81
1	C	139	LYS	N-CA-C	6.30	119.99	112.93
2	B	85	PHE	CA-C-O	-6.30	112.52	119.95
2	H	66	LYS	CA-CB-CG	-6.30	101.50	114.10
1	E	115	ALA	CA-C-N	6.30	131.62	121.98
1	E	115	ALA	C-N-CA	6.30	131.62	121.98
1	C	49	SER	CA-CB-OG	-6.30	98.51	111.10
1	C	96	VAL	CG1-CB-CG2	6.30	124.65	110.80
2	B	118	PHE	CB-CG-CD1	-6.29	110.00	120.70
1	A	23	GLU	N-CA-CB	6.29	118.96	110.59
1	A	63	ALA	O-C-N	6.29	131.62	122.43
1	G	33	PHE	N-CA-C	-6.29	103.34	111.02
1	G	43	PHE	CB-CG-CD2	6.29	131.39	120.70
1	E	92	ARG	O-C-N	6.29	130.95	122.59
1	E	98	PHE	CD1-CE1-CZ	-6.29	108.69	120.00
1	E	120	ALA	CA-C-O	6.28	127.15	119.11
1	G	20	HIS	CE1-NE2-CD2	6.28	115.28	109.00
1	C	128	PHE	N-CA-CB	6.28	119.55	110.20
2	D	144	LYS	N-CA-C	6.28	119.62	112.97
2	F	117	HIS	N-CA-CB	-6.28	100.97	110.07
1	G	141	ARG	CB-CA-C	6.28	122.03	110.10
2	B	103	PHE	CA-C-O	-6.28	113.85	120.63
2	D	50	THR	CA-CB-CG2	6.27	121.17	110.50
2	D	123	THR	CA-C-N	-6.27	113.92	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	123	THR	C-N-CA	-6.27	113.92	120.38
2	F	15	TRP	CE2-CD2-CE3	6.27	125.07	118.80
2	B	47	ASP	O-C-N	-6.27	114.67	123.01
2	F	11	VAL	CA-C-O	6.27	127.02	120.25
1	E	137	THR	CA-CB-CG2	6.27	121.16	110.50
1	G	75	ASP	OD1-CG-OD2	6.27	137.94	122.90
2	F	130	TYR	CB-CG-CD2	6.26	130.19	120.80
2	B	99	ASP	N-CA-C	-6.26	100.16	109.42
1	G	49	SER	CA-C-O	6.26	127.44	120.43
1	C	77	PRO	CA-N-CD	-6.25	103.24	112.00
1	E	92	ARG	CA-CB-CG	6.25	126.61	114.10
1	A	13	ALA	CB-CA-C	-6.25	100.22	110.85
2	D	109	VAL	O-C-N	6.25	129.86	122.17
1	E	68	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	A	43	PHE	CG-CD1-CE1	6.25	131.33	120.70
2	H	59	LYS	CG-CD-CE	6.25	125.68	111.30
2	H	85	PHE	CG-CD1-CE1	6.25	131.33	120.70
2	H	132	LYS	CA-CB-CG	-6.25	101.60	114.10
1	G	89	HIS	N-CA-CB	-6.25	102.59	110.90
1	C	123	ALA	CB-CA-C	-6.24	98.68	110.67
1	E	98	PHE	CA-C-N	6.24	128.97	120.54
1	E	98	PHE	C-N-CA	6.24	128.97	120.54
2	F	36	PRO	CA-CB-CG	6.24	116.36	104.50
2	F	77	HIS	CB-CG-ND1	6.24	132.06	122.70
2	D	54	VAL	N-CA-CB	6.24	121.52	111.23
1	E	47	ASP	OD1-CG-OD2	6.24	137.87	122.90
2	F	88	LEU	CA-CB-CG	6.24	138.13	116.30
1	A	28	ALA	N-CA-CB	6.23	121.03	110.49
1	G	10	VAL	CA-CB-CG2	6.23	121.00	110.40
1	A	91	LEU	N-CA-CB	-6.23	99.62	109.78
1	G	82	ALA	CA-C-O	-6.23	111.60	120.51
2	F	134	VAL	N-CA-C	-6.23	103.82	110.36
2	H	130	TYR	CD1-CE1-CZ	6.23	130.82	119.60
2	H	92	HIS	CA-CB-CG	-6.23	107.57	113.80
1	A	104	CYS	CB-CA-C	-6.22	97.19	110.32
2	D	42	PHE	CD1-CE1-CZ	-6.22	108.80	120.00
1	G	7	LYS	CA-CB-CG	6.22	126.54	114.10
1	A	33	PHE	CE1-CZ-CE2	-6.22	108.80	120.00
1	E	18	GLY	CA-C-N	-6.22	112.72	122.73
1	E	18	GLY	C-N-CA	-6.22	112.72	122.73
1	E	18	GLY	CA-C-O	6.22	131.39	120.57
2	B	118	PHE	CB-CG-CD2	6.22	131.27	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	97	ASN	N-CA-CB	-6.22	100.27	110.40
2	F	144	LYS	CB-CA-C	-6.22	101.42	111.06
2	D	22	GLU	OE1-CD-OE2	-6.21	107.99	122.90
2	D	77	HIS	CA-C-O	6.21	132.38	121.94
2	D	102	ASN	CA-C-N	-6.21	112.36	120.44
2	D	102	ASN	C-N-CA	-6.21	112.36	120.44
1	A	85	ASP	O-C-N	-6.21	114.11	122.43
1	E	11	LYS	CA-CB-CG	-6.21	101.69	114.10
2	B	61	LYS	CB-CA-C	6.20	121.14	110.84
2	D	77	HIS	CE1-NE2-CD2	-6.20	102.80	109.00
1	E	39	THR	CB-CA-C	-6.20	98.23	110.27
2	F	47	ASP	OD1-CG-OD2	-6.20	108.01	122.90
1	A	10	VAL	N-CA-CB	-6.20	100.20	110.56
2	H	6	VAL	CA-CB-CG2	6.20	120.94	110.40
2	B	38	THR	CA-CB-OG1	-6.20	100.30	109.60
1	A	6	ASP	N-CA-CB	6.20	119.17	109.94
2	F	129	ALA	CA-C-N	6.20	130.51	120.60
2	F	129	ALA	C-N-CA	6.20	130.51	120.60
1	G	91	LEU	N-CA-C	6.20	124.00	110.80
1	C	127	LYS	CB-CG-CD	6.19	125.54	111.30
2	F	80	ASN	CA-C-O	-6.19	111.66	120.51
1	G	64	ASP	CA-C-O	6.19	127.50	121.00
2	H	63	HIS	CB-CG-ND1	-6.19	113.42	122.70
1	C	33	PHE	N-CA-CB	6.19	119.75	110.22
1	E	72	HIS	N-CA-C	6.19	118.34	110.61
2	H	118	PHE	CB-CG-CD1	6.19	131.22	120.70
2	B	119	GLY	CA-C-O	-6.19	112.92	121.46
1	C	87	HIS	ND1-CG-CD2	-6.18	99.92	106.10
2	D	2	HIS	CG-CD2-NE2	6.18	113.39	107.20
2	F	35	TYR	CB-CA-C	-6.18	97.98	110.17
1	G	114	PRO	CB-CA-C	-6.18	101.36	111.56
1	G	46	PHE	CA-C-N	-6.18	113.80	123.13
1	G	46	PHE	C-N-CA	-6.18	113.80	123.13
2	F	45	PHE	CB-CG-CD1	6.18	131.20	120.70
2	F	115	ALA	N-CA-CB	6.18	119.41	110.20
1	E	59	GLY	CA-C-N	-6.18	110.33	121.14
1	E	59	GLY	C-N-CA	-6.18	110.33	121.14
1	E	62	VAL	CB-CA-C	6.18	120.11	112.02
2	H	133	VAL	N-CA-C	-6.18	104.72	110.53
1	G	25	GLY	CA-C-N	6.17	131.18	120.68
1	G	25	GLY	C-N-CA	6.17	131.18	120.68
2	B	108	ASN	N-CA-C	6.17	120.06	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	61	LYS	CB-CG-CD	6.17	125.48	111.30
2	F	35	TYR	CA-C-O	6.17	128.61	120.16
2	H	109	VAL	CA-CB-CG1	-6.16	99.92	110.40
1	E	14	TRP	CE2-CD2-CE3	-6.16	112.64	118.80
2	H	128	ALA	N-CA-C	6.16	121.53	111.37
2	F	10	ALA	CA-C-O	-6.16	114.30	121.07
1	A	131	SER	N-CA-C	-6.16	104.48	111.07
1	A	78	ASN	CB-CA-C	6.15	120.54	110.88
1	A	85	ASP	CA-C-N	6.15	135.09	121.80
1	A	85	ASP	C-N-CA	6.15	135.09	121.80
1	A	9	ASN	CB-CG-ND2	-6.15	107.18	116.40
2	F	97	HIS	CE1-NE2-CD2	-6.15	102.85	109.00
1	G	42	TYR	N-CA-CB	6.15	120.74	110.41
1	E	89	HIS	ND1-CG-CD2	-6.15	99.95	106.10
2	F	75	LEU	O-C-N	6.15	131.09	122.36
2	F	136	GLY	CA-C-O	-6.14	109.88	120.57
1	C	32	MET	CA-CB-CG	-6.14	101.82	114.10
2	H	107	GLY	O-C-N	6.14	129.62	122.68
2	D	137	VAL	CA-CB-CG1	-6.14	99.97	110.40
2	H	69	GLY	CA-C-O	6.13	131.25	120.57
2	D	106	LEU	CA-C-N	6.13	126.90	120.03
2	D	106	LEU	C-N-CA	6.13	126.90	120.03
1	A	103	HIS	CA-C-O	6.13	127.25	120.82
2	F	42	PHE	CD1-CE1-CZ	-6.13	108.97	120.00
1	G	7	LYS	O-C-N	-6.13	114.78	122.20
2	H	54	VAL	CB-CA-C	6.13	121.34	111.29
1	G	50	HIS	N-CA-C	-6.13	97.75	110.80
2	F	21	ASP	N-CA-CB	6.12	120.84	110.49
1	G	27	GLU	CA-CB-CG	6.12	126.35	114.10
1	G	136	LEU	CA-CB-CG	-6.12	94.87	116.30
2	H	73	ASP	CB-CA-C	6.12	122.15	110.27
1	E	114	PRO	O-C-N	-6.12	114.38	122.64
2	B	42	PHE	CG-CD2-CE2	-6.12	110.30	120.70
1	E	47	ASP	CB-CG-OD2	-6.12	104.33	118.40
1	E	78	ASN	N-CA-CB	-6.12	101.09	110.20
1	G	78	ASN	CA-C-O	-6.12	113.94	120.42
2	H	15	TRP	O-C-N	-6.12	114.46	122.59
1	E	83	LEU	N-CA-CB	-6.11	100.89	110.30
1	A	85	ASP	CB-CG-OD1	-6.11	104.36	118.40
1	E	24	TYR	CB-CG-CD2	-6.11	111.64	120.80
2	F	34	VAL	N-CA-C	6.11	116.27	110.53
1	C	81	SER	N-CA-C	6.10	123.80	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	121	VAL	CA-CB-CG2	-6.10	100.02	110.40
2	H	28	LEU	CB-CA-C	6.10	121.23	110.85
1	G	17	VAL	O-C-N	6.10	133.51	121.91
1	G	56	LYS	CG-CD-CE	6.10	125.33	111.30
2	H	67	VAL	CA-C-N	-6.10	109.64	120.99
2	H	67	VAL	C-N-CA	-6.10	109.64	120.99
2	D	45	PHE	CB-CG-CD2	6.10	131.06	120.70
1	E	126	ASP	OD1-CG-OD2	-6.10	108.27	122.90
1	E	81	SER	N-CA-C	6.09	121.36	111.37
1	E	131	SER	O-C-N	-6.09	115.75	122.09
1	E	132	VAL	CA-CB-CG1	-6.09	100.04	110.40
1	G	31	ARG	N-CA-CB	-6.09	100.84	110.28
2	H	15	TRP	CE2-CD2-CE3	-6.09	112.71	118.80
2	H	118	PHE	CA-C-O	6.09	126.42	119.18
2	B	99	ASP	CA-C-N	6.08	125.78	119.82
2	B	99	ASP	C-N-CA	6.08	125.78	119.82
1	C	117	PHE	N-CA-C	6.08	123.75	110.80
2	D	38	THR	CA-CB-OG1	-6.08	100.49	109.60
2	D	97	HIS	CA-C-O	6.08	128.63	121.40
1	A	50	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	E	91	LEU	CB-CA-C	6.07	120.99	110.79
1	G	103	HIS	CG-CD2-NE2	-6.07	101.13	107.20
2	D	11	VAL	CA-C-O	6.07	128.36	120.78
2	F	37	TRP	CD1-NE1-CE2	-6.07	97.98	108.90
2	H	129	ALA	N-CA-C	-6.07	104.75	111.36
1	A	41	THR	CB-CA-C	6.07	122.23	110.46
1	A	70	VAL	N-CA-CB	6.07	118.79	110.54
1	C	45	HIS	O-C-N	6.06	130.32	122.19
1	A	61	LYS	CD-CE-NZ	-6.06	92.51	111.90
1	C	24	TYR	CD1-CG-CD2	-6.06	109.01	118.10
2	H	104	ARG	CG-CD-NE	6.06	125.33	112.00
2	B	29	GLY	N-CA-C	-6.06	105.47	112.50
1	C	86	LEU	CA-C-O	-6.05	111.85	120.51
1	G	47	ASP	O-C-N	6.05	132.16	122.96
2	B	142	ALA	CA-C-N	6.05	133.10	121.54
2	B	142	ALA	C-N-CA	6.05	133.10	121.54
1	E	86	LEU	O-C-N	-6.05	113.38	122.28
1	G	140	TYR	CA-C-O	-6.05	114.07	120.55
1	C	85	ASP	CB-CA-C	-6.05	99.43	110.63
2	D	2	HIS	CG-ND1-CE1	6.05	119.59	109.30
1	E	129	LEU	CA-C-N	6.05	128.31	120.44
1	E	129	LEU	C-N-CA	6.05	128.31	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	92	HIS	CA-CB-CG	6.05	119.85	113.80
1	E	91	LEU	N-CA-C	-6.05	104.02	111.40
1	G	32	MET	O-C-N	-6.05	115.61	122.08
1	C	69	ALA	N-CA-C	-6.04	104.32	111.03
1	A	77	PRO	N-CD-CG	-6.04	94.14	103.20
2	F	38	THR	OG1-CB-CG2	-6.04	97.21	109.30
2	F	107	GLY	O-C-N	6.04	130.56	122.70
1	C	135	VAL	CA-CB-CG2	-6.04	100.13	110.40
2	D	87	THR	CA-CB-OG1	-6.04	100.54	109.60
1	G	106	LEU	CA-C-O	6.04	127.36	120.90
1	A	38	THR	CB-CA-C	-6.04	100.77	110.79
2	D	114	LEU	CA-CB-CG	-6.04	95.17	116.30
1	E	14	TRP	CB-CG-CD2	6.04	135.25	126.80
2	F	1	VAL	CA-C-O	6.04	131.06	120.80
1	E	128	PHE	CZ-CE2-CD2	-6.03	109.14	120.00
1	A	107	VAL	O-C-N	6.03	127.97	121.94
1	G	97	ASN	O-C-N	-6.03	114.14	122.46
1	C	45	HIS	CA-C-O	6.03	127.64	120.53
1	E	117	PHE	CZ-CE2-CD2	6.03	130.85	120.00
1	G	109	LEU	CB-CA-C	-6.03	99.67	110.70
2	F	15	TRP	CH2-CZ2-CE2	6.02	125.33	117.50
1	G	87	HIS	N-CA-CB	6.02	119.09	110.06
2	H	93	CYS	CA-CB-SG	-6.02	100.56	114.40
1	G	76	MET	N-CA-CB	-6.02	99.66	110.37
1	E	35	SER	N-CA-C	-6.01	104.66	112.23
2	D	141	LEU	CB-CG-CD1	-6.01	92.67	110.70
1	E	16	LYS	O-C-N	6.01	130.58	122.59
2	D	134	VAL	O-C-N	-6.01	116.04	121.87
1	E	118	THR	OG1-CB-CG2	6.01	121.31	109.30
2	H	35	TYR	CD1-CG-CD2	6.01	127.11	118.10
1	C	125	LEU	CA-C-O	-6.00	111.92	120.51
1	C	68	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	60	LYS	O-C-N	-6.00	115.89	122.07
1	E	135	VAL	CA-C-N	6.00	130.74	120.72
1	E	135	VAL	C-N-CA	6.00	130.74	120.72
2	D	31	LEU	CA-CB-CG	6.00	137.30	116.30
1	G	14	TRP	CG-CD2-CE3	6.00	139.90	133.90
1	A	20	HIS	CA-C-O	6.00	128.51	118.91
1	A	131	SER	N-CA-CB	6.00	118.71	110.01
2	D	139	ASN	CB-CG-OD1	-6.00	108.80	120.80
1	G	45	HIS	CB-CA-C	6.00	122.85	110.31
1	G	110	ALA	N-CA-CB	6.00	119.46	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	78	LEU	N-CA-CB	-6.00	101.28	110.16
2	D	84	THR	CA-C-O	6.00	126.87	120.10
1	G	9	ASN	CB-CG-ND2	6.00	125.39	116.40
1	C	34	LEU	CB-CG-CD2	-5.99	92.72	110.70
2	H	33	VAL	O-C-N	-5.99	110.52	121.91
2	D	59	LYS	N-CA-C	-5.99	104.83	111.36
1	A	2	LEU	CA-C-O	5.99	127.52	120.69
1	E	54	GLN	CA-C-O	5.99	127.66	121.07
2	F	52	ASP	CA-CB-CG	-5.99	106.61	112.60
2	F	92	HIS	N-CA-CB	-5.99	100.64	110.40
1	E	6	ASP	N-CA-CB	5.99	119.56	110.28
1	C	27	GLU	CG-CD-OE2	5.99	132.17	118.40
1	A	6	ASP	OD1-CG-OD2	5.99	137.26	122.90
1	A	41	THR	OG1-CB-CG2	5.99	121.27	109.30
2	B	64	GLY	O-C-N	-5.99	116.43	122.18
2	D	16	GLY	O-C-N	5.99	130.48	122.70
1	C	107	VAL	N-CA-CB	5.98	118.68	110.54
2	F	18	VAL	CA-C-N	5.98	130.38	122.42
2	F	18	VAL	C-N-CA	5.98	130.38	122.42
2	F	51	PRO	CA-C-O	-5.98	110.45	119.55
1	G	20	HIS	ND1-CE1-NE2	5.98	114.38	108.40
2	H	90	GLU	N-CA-CB	5.98	119.44	110.22
2	F	6	VAL	CG1-CB-CG2	5.98	123.96	110.80
2	H	117	HIS	CE1-NE2-CD2	5.98	114.98	109.00
1	C	140	TYR	CZ-CE2-CD2	5.98	130.37	119.60
2	H	49	SER	O-C-N	-5.98	112.84	122.41
1	G	50	HIS	CE1-NE2-CD2	-5.98	103.02	109.00
2	H	117	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	A	8	THR	CA-C-O	5.98	126.95	119.12
1	C	62	VAL	N-CA-CB	-5.98	100.58	110.56
2	F	132	LYS	CG-CD-CE	5.97	125.04	111.30
2	H	98	VAL	CA-CB-CG1	-5.97	100.25	110.40
2	D	42	PHE	CB-CA-C	-5.97	99.64	112.12
1	G	123	ALA	CA-C-N	-5.97	111.81	120.29
1	G	123	ALA	C-N-CA	-5.97	111.81	120.29
1	A	7	LYS	CB-CG-CD	5.96	125.02	111.30
1	A	43	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	122	HIS	O-C-N	-5.96	115.93	122.07
2	B	67	VAL	N-CA-C	-5.96	104.70	110.42
2	F	41	PHE	CA-C-N	-5.96	113.56	123.04
2	F	41	PHE	C-N-CA	-5.96	113.56	123.04
2	F	90	GLU	CG-CD-OE2	-5.96	104.69	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	36	PHE	N-CA-CB	-5.96	103.04	110.79
2	H	41	PHE	N-CA-CB	-5.96	101.65	110.53
2	B	131	GLN	CB-CA-C	-5.96	99.66	110.56
1	G	46	PHE	N-CA-CB	5.96	119.58	110.70
2	B	49	SER	CB-CA-C	5.96	122.76	110.31
1	E	83	LEU	CA-C-O	5.96	126.82	119.79
1	E	128	PHE	CB-CG-CD2	-5.96	110.57	120.70
1	A	58	HIS	N-CA-C	5.95	121.19	111.37
2	D	37	TRP	CG-CD2-CE3	5.95	139.85	133.90
1	G	74	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	110	ALA	N-CA-CB	-5.95	101.38	110.01
1	E	102	SER	CA-CB-OG	5.95	123.00	111.10
1	G	56	LYS	CB-CA-C	5.95	122.09	110.67
2	H	15	TRP	CG-CD2-CE3	5.95	139.85	133.90
1	A	131	SER	CA-C-N	5.95	128.05	120.56
1	A	131	SER	C-N-CA	5.95	128.05	120.56
1	C	6	ASP	OD1-CG-OD2	5.95	137.17	122.90
1	E	94	ASP	OD1-CG-OD2	5.94	137.16	122.90
2	B	12	THR	CA-CB-CG2	5.94	120.60	110.50
1	C	62	VAL	CA-C-O	5.94	127.07	120.71
2	F	75	LEU	CA-C-O	5.94	126.12	119.41
2	H	35	TYR	CG-CD2-CE2	-5.94	112.29	121.20
1	G	120	ALA	CA-C-O	-5.94	114.22	120.63
1	A	90	LYS	CB-CA-C	-5.94	101.37	112.00
1	E	24	TYR	CA-C-N	-5.94	113.38	120.03
1	E	24	TYR	C-N-CA	-5.94	113.38	120.03
1	E	73	VAL	O-C-N	-5.94	115.15	122.57
2	B	116	HIS	ND1-CG-CD2	-5.94	100.16	106.10
2	F	103	PHE	N-CA-C	-5.94	104.89	111.36
2	F	117	HIS	ND1-CG-CD2	5.93	112.03	106.10
1	C	71	ALA	N-CA-CB	-5.93	100.01	110.39
1	G	36	PHE	CB-CA-C	5.93	119.99	111.27
1	G	127	LYS	CB-CA-C	-5.93	98.95	110.46
1	E	87	HIS	CA-C-O	-5.93	112.03	120.51
1	A	87	HIS	N-CA-CB	-5.93	100.81	109.82
1	G	72	HIS	CG-CD2-NE2	-5.93	101.27	107.20
1	A	110	ALA	N-CA-C	-5.92	104.73	111.07
2	H	128	ALA	O-C-N	5.92	128.92	122.11
1	C	85	ASP	CA-CB-CG	5.92	118.52	112.60
2	D	59	LYS	CA-C-O	-5.92	114.14	120.42
2	D	35	TYR	CA-C-N	5.92	127.24	119.84
2	D	35	TYR	C-N-CA	5.92	127.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	81	LEU	O-C-N	-5.92	114.53	122.23
1	E	85	ASP	OD1-CG-OD2	-5.92	108.69	122.90
1	C	76	MET	CA-C-N	5.92	125.46	119.19
1	C	76	MET	C-N-CA	5.92	125.46	119.19
2	F	86	ALA	N-CA-CB	-5.92	100.26	110.32
1	G	118	THR	CA-CB-OG1	5.92	118.47	109.60
2	D	36	PRO	N-CD-CG	5.92	112.07	103.20
1	E	70	VAL	CG1-CB-CG2	-5.92	97.79	110.80
1	G	10	VAL	N-CA-C	-5.92	104.97	110.53
1	A	27	GLU	CB-CG-CD	-5.91	102.55	112.60
1	A	116	GLU	CG-CD-OE1	5.91	132.00	118.40
2	F	138	ALA	CA-C-N	-5.91	111.77	120.28
2	F	138	ALA	C-N-CA	-5.91	111.77	120.28
2	H	86	ALA	CA-C-O	-5.91	111.67	119.06
2	B	106	LEU	N-CA-CB	-5.91	100.05	110.39
1	E	72	HIS	CB-CG-CD2	-5.91	123.52	131.20
2	F	84	THR	OG1-CB-CG2	-5.91	97.48	109.30
1	G	112	HIS	CA-C-O	-5.91	112.06	120.51
2	H	106	LEU	CA-C-O	-5.91	113.18	119.97
2	D	3	LEU	CA-C-O	-5.91	114.45	121.60
2	B	34	VAL	O-C-N	-5.91	116.12	121.91
2	H	1	VAL	O-C-N	5.90	132.45	123.00
2	D	94	ASP	N-CA-CB	5.90	118.92	110.06
2	H	96	LEU	CB-CA-C	5.90	122.17	110.42
1	A	20	HIS	CB-CG-ND1	5.90	131.55	122.70
1	E	50	HIS	N-CA-CB	-5.90	100.31	109.34
1	E	112	HIS	CB-CA-C	5.90	119.29	109.38
2	B	45	PHE	CD1-CE1-CZ	5.90	130.62	120.00
1	E	84	SER	CB-CA-C	5.90	121.49	110.70
1	G	105	LEU	N-CA-C	5.90	117.40	110.97
1	A	29	LEU	N-CA-CB	-5.89	100.80	110.40
1	A	41	THR	N-CA-CB	-5.89	100.83	110.14
1	A	122	HIS	ND1-CG-CD2	-5.89	100.21	106.10
1	G	28	ALA	CA-C-O	5.89	128.93	120.51
1	G	36	PHE	N-CA-C	5.89	118.76	108.75
1	G	107	VAL	CB-CA-C	5.89	119.51	111.97
1	G	133	SER	CB-CA-C	5.89	121.53	110.63
2	H	146	HIS	CB-CA-C	-5.89	98.91	110.10
2	D	88	LEU	CB-CG-CD2	5.89	128.37	110.70
1	C	70	VAL	CA-C-N	-5.89	109.53	121.18
1	C	70	VAL	C-N-CA	-5.89	109.53	121.18
1	E	33	PHE	CB-CA-C	5.89	120.56	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	51	GLY	O-C-N	-5.88	115.63	122.22
2	H	136	GLY	N-CA-C	-5.88	99.23	113.18
1	E	125	LEU	CA-C-O	5.88	126.62	119.38
2	H	70	ALA	N-CA-CB	5.88	118.89	110.06
2	D	80	ASN	CB-CA-C	-5.88	98.14	111.83
2	D	95	LYS	N-CA-CB	-5.88	100.11	110.34
2	D	10	ALA	CA-C-O	-5.88	114.65	120.82
1	E	9	ASN	N-CA-C	5.88	118.44	111.33
2	D	79	ASP	O-C-N	-5.87	115.05	122.27
1	C	55	VAL	CA-CB-CG2	5.87	120.38	110.40
1	A	112	HIS	N-CA-C	-5.87	105.88	114.39
2	H	84	THR	OG1-CB-CG2	5.87	121.04	109.30
2	B	28	LEU	CB-CG-CD2	5.87	128.31	110.70
2	D	79	ASP	CB-CG-OD2	5.87	131.90	118.40
2	F	40	ARG	N-CA-CB	-5.87	100.58	110.49
1	G	29	LEU	CB-CG-CD2	5.87	128.30	110.70
1	C	46	PHE	CE1-CZ-CE2	5.86	130.56	120.00
2	B	54	VAL	CA-CB-CG1	5.86	120.36	110.40
1	A	55	VAL	CB-CA-C	-5.86	95.64	111.34
1	A	75	ASP	CB-CG-OD1	5.86	131.87	118.40
1	A	40	LYS	CB-CG-CD	-5.86	97.83	111.30
1	A	38	THR	N-CA-CB	-5.85	101.52	110.12
1	C	105	LEU	CB-CA-C	5.85	120.15	110.90
2	D	139	ASN	CB-CG-ND2	5.85	125.18	116.40
1	E	94	ASP	CB-CA-C	5.85	117.86	109.26
2	B	143	HIS	CG-ND1-CE1	5.85	119.24	109.30
2	H	52	ASP	CA-C-N	-5.85	110.74	120.68
2	H	52	ASP	C-N-CA	-5.85	110.74	120.68
2	D	45	PHE	CA-C-N	-5.85	112.68	122.62
2	D	45	PHE	C-N-CA	-5.85	112.68	122.62
1	E	66	LEU	CB-CG-CD1	5.84	128.23	110.70
2	B	140	ALA	N-CA-C	-5.84	104.99	111.36
1	C	125	LEU	CB-CG-CD2	5.84	128.22	110.70
1	E	37	PRO	CA-C-N	-5.84	112.65	120.54
1	E	37	PRO	C-N-CA	-5.84	112.65	120.54
1	E	85	ASP	CA-CB-CG	-5.84	106.76	112.60
1	A	100	LEU	CB-CA-C	5.84	120.48	110.79
1	A	103	HIS	CB-CG-CD2	5.84	138.79	131.20
1	E	72	HIS	CB-CG-ND1	5.84	131.46	122.70
2	D	23	VAL	CA-CB-CG2	-5.84	100.48	110.40
2	B	30	ARG	O-C-N	5.83	130.25	122.43
2	B	87	THR	CA-C-O	5.83	126.71	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	56	LYS	CB-CG-CD	-5.83	97.89	111.30
1	E	135	VAL	N-CA-CB	-5.83	103.73	110.55
1	G	3	SER	N-CA-C	-5.83	96.92	109.81
1	A	135	VAL	N-CA-CB	-5.83	101.61	111.23
2	F	26	GLU	CA-C-O	5.83	126.79	120.55
2	B	46	GLY	CA-C-N	5.83	129.65	121.02
2	B	46	GLY	C-N-CA	5.83	129.65	121.02
1	A	8	THR	N-CA-C	5.83	120.25	113.20
1	C	116	GLU	CB-CG-CD	-5.83	102.70	112.60
2	F	116	HIS	CG-CD2-NE2	-5.83	101.37	107.20
1	G	112	HIS	CB-CA-C	-5.83	98.83	110.42
1	C	38	THR	N-CA-C	-5.82	105.07	111.82
2	F	37	TRP	CA-C-O	5.82	126.32	119.28
1	G	132	VAL	N-CA-C	-5.82	104.84	110.72
2	D	80	ASN	CB-CG-ND2	5.82	125.12	116.40
1	G	124	SER	N-CA-C	-5.82	105.02	111.36
1	G	78	ASN	CB-CG-OD1	5.81	132.42	120.80
1	C	114	PRO	CA-C-O	5.81	128.82	119.64
2	D	55	MET	N-CA-C	5.81	119.89	112.34
1	E	100	LEU	CA-C-O	-5.81	113.79	120.24
2	F	122	PHE	O-C-N	-5.81	114.71	122.38
2	F	125	PRO	CA-C-O	5.81	128.92	119.86
2	H	113	VAL	CA-CB-CG2	-5.81	100.53	110.40
2	H	122	PHE	CZ-CE2-CD2	-5.80	109.55	120.00
2	F	106	LEU	N-CA-CB	5.80	119.16	110.22
2	F	76	ALA	O-C-N	5.80	128.36	122.09
1	C	101	LEU	CA-C-N	-5.80	112.43	120.38
1	C	101	LEU	C-N-CA	-5.80	112.43	120.38
2	D	103	PHE	CA-C-N	5.80	130.41	120.72
2	D	103	PHE	C-N-CA	5.80	130.41	120.72
2	B	57	ASN	N-CA-CB	5.80	121.45	109.45
2	D	14	LEU	CB-CG-CD1	-5.80	93.31	110.70
1	G	130	ALA	CA-C-O	5.80	126.63	119.79
1	A	47	ASP	CA-CB-CG	5.80	118.40	112.60
1	C	20	HIS	N-CA-C	-5.79	105.87	113.17
1	E	106	LEU	CD1-CG-CD2	-5.79	98.06	110.80
2	B	131	GLN	N-CA-C	-5.79	103.70	112.04
1	E	62	VAL	O-C-N	-5.79	115.88	121.90
2	F	44	SER	CA-CB-OG	5.79	122.68	111.10
2	H	61	LYS	N-CA-CB	-5.79	100.78	110.39
1	G	61	LYS	O-C-N	5.79	128.75	122.15
2	B	28	LEU	CA-C-O	5.79	126.62	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	127	GLN	CA-C-O	-5.79	114.74	120.82
2	F	94	ASP	CA-C-N	5.79	131.08	122.17
2	F	94	ASP	C-N-CA	5.79	131.08	122.17
1	A	52	SER	CB-CA-C	-5.79	101.58	110.26
2	H	26	GLU	CA-CB-CG	5.79	125.67	114.10
1	A	83	LEU	CA-C-N	-5.78	112.08	120.29
1	A	83	LEU	C-N-CA	-5.78	112.08	120.29
2	B	13	ALA	CB-CA-C	-5.78	101.76	110.90
1	E	11	LYS	CG-CD-CE	-5.78	98.00	111.30
2	H	8	LYS	N-CA-C	5.78	119.96	113.02
1	C	7	LYS	CA-C-O	5.78	127.08	120.90
1	E	20	HIS	CB-CA-C	5.78	119.74	110.09
2	F	94	ASP	CB-CG-OD2	5.78	131.69	118.40
2	H	45	PHE	CA-C-O	5.78	126.49	119.38
1	C	61	LYS	CG-CD-CE	-5.77	98.03	111.30
2	D	28	LEU	CA-C-N	5.77	132.72	121.41
2	D	28	LEU	C-N-CA	5.77	132.72	121.41
2	F	65	LYS	N-CA-C	-5.77	105.73	112.89
2	F	90	GLU	CB-CG-CD	-5.77	102.79	112.60
1	G	128	PHE	CA-C-O	-5.77	114.72	121.07
2	F	146	HIS	CA-C-O	-5.77	103.70	121.00
1	G	66	LEU	N-CA-C	5.77	118.51	111.82
1	A	4	PRO	CB-CG-CD	-5.77	87.65	106.10
2	H	32	LEU	O-C-N	-5.77	115.63	122.20
1	C	2	LEU	N-CA-CB	5.76	120.03	110.52
1	E	60	LYS	CA-C-N	-5.76	110.89	120.68
1	E	60	LYS	C-N-CA	-5.76	110.89	120.68
2	H	18	VAL	N-CA-CB	5.76	118.39	111.31
2	H	139	ASN	CA-C-N	5.76	127.93	120.44
2	H	139	ASN	C-N-CA	5.76	127.93	120.44
2	D	51	PRO	CA-CB-CG	-5.75	93.56	104.50
1	A	63	ALA	CB-CA-C	5.75	121.40	109.95
1	E	20	HIS	CB-CG-CD2	5.75	138.68	131.20
1	A	63	ALA	N-CA-C	5.75	120.14	113.18
2	H	131	GLN	CG-CD-NE2	5.75	125.03	116.40
1	C	79	ALA	CA-C-O	5.75	127.39	121.07
2	H	114	LEU	N-CA-C	-5.75	105.53	112.54
1	G	114	PRO	CB-CG-CD	-5.75	87.71	106.10
1	C	38	THR	CA-C-O	5.75	126.58	119.97
1	E	53	ALA	CA-C-O	-5.75	112.54	119.49
1	C	48	LEU	CA-C-O	-5.74	114.05	121.17
1	G	57	GLY	N-CA-C	5.74	121.06	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	131	GLN	O-C-N	-5.74	114.54	122.46
1	C	37	PRO	CA-CB-CG	-5.74	93.59	104.50
1	G	136	LEU	O-C-N	5.74	130.12	122.43
2	H	59	LYS	CA-C-O	5.74	126.32	119.60
1	A	45	HIS	O-C-N	5.74	129.51	122.34
1	E	67	THR	O-C-N	-5.74	114.64	122.33
2	H	138	ALA	O-C-N	-5.74	116.12	122.09
1	G	103	HIS	O-C-N	5.74	130.71	122.28
1	A	32	MET	N-CA-C	-5.74	104.72	110.97
1	A	71	ALA	CB-CA-C	-5.74	98.32	110.31
2	B	29	GLY	CA-C-N	5.74	130.30	120.72
2	B	29	GLY	C-N-CA	5.74	130.30	120.72
1	C	95	PRO	CB-CA-C	-5.74	102.68	112.26
2	D	6	VAL	CA-C-O	-5.73	113.61	120.78
1	E	129	LEU	CB-CG-CD1	5.73	127.90	110.70
1	C	114	PRO	CB-CA-C	-5.73	102.69	112.26
1	A	133	SER	CA-C-N	5.73	132.48	121.54
1	A	133	SER	C-N-CA	5.73	132.48	121.54
2	B	12	THR	CB-CA-C	5.73	119.97	110.81
2	B	40	ARG	CA-C-O	5.73	128.70	120.51
1	C	11	LYS	CB-CG-CD	-5.73	98.13	111.30
1	C	92	ARG	CG-CD-NE	-5.73	99.40	112.00
1	E	95	PRO	CA-C-O	-5.73	110.24	118.89
1	G	92	ARG	CB-CA-C	5.73	121.82	110.42
1	A	110	ALA	O-C-N	-5.72	116.17	122.07
2	D	94	ASP	CB-CA-C	-5.72	100.95	110.68
1	E	87	HIS	ND1-CE1-NE2	-5.72	102.68	108.40
1	E	87	HIS	N-CA-CB	5.72	120.16	110.49
1	A	37	PRO	CB-CA-C	-5.72	102.12	111.56
1	C	110	ALA	CA-C-O	-5.72	112.33	120.51
1	A	57	GLY	O-C-N	5.71	130.13	122.70
2	B	52	ASP	CA-CB-CG	5.71	118.31	112.60
2	D	130	TYR	CG-CD2-CE2	5.71	129.77	121.20
1	E	88	ALA	CB-CA-C	-5.71	99.05	110.42
2	H	22	GLU	CB-CA-C	5.71	121.64	110.67
1	G	45	HIS	N-CA-CB	5.71	119.87	110.39
1	C	104	CYS	CA-C-O	-5.71	111.80	119.11
2	F	18	VAL	N-CA-CB	-5.71	100.65	111.21
1	C	84	SER	CB-CA-C	-5.71	101.92	110.88
2	H	31	LEU	N-CA-CB	-5.70	101.80	110.07
1	A	36	PHE	CE1-CZ-CE2	5.70	130.26	120.00
1	C	90	LYS	O-C-N	-5.70	115.01	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	29	LEU	N-CA-C	5.70	117.95	111.11
1	A	17	VAL	CB-CA-C	-5.70	94.47	111.05
2	D	125	PRO	CB-CG-CD	-5.70	87.87	106.10
1	E	39	THR	CA-C-O	5.70	128.03	118.91
2	F	18	VAL	CA-C-O	5.70	127.22	120.72
2	H	139	ASN	N-CA-CB	5.70	118.59	110.16
1	G	50	HIS	CB-CA-C	-5.70	99.08	110.42
2	D	130	TYR	CB-CG-CD2	5.69	129.34	120.80
1	C	73	VAL	N-CA-CB	-5.69	101.85	111.23
2	D	132	LYS	CA-CB-CG	5.69	125.47	114.10
2	D	16	GLY	CA-C-O	-5.68	110.68	120.57
2	D	37	TRP	CE2-CD2-CE3	-5.68	113.11	118.80
2	B	90	GLU	CB-CG-CD	5.68	122.26	112.60
2	B	126	VAL	N-CA-CB	5.68	123.81	111.76
1	E	24	TYR	OH-CZ-CE2	-5.68	102.86	119.90
2	F	81	LEU	CA-CB-CG	5.68	136.18	116.30
1	G	14	TRP	CH2-CZ2-CE2	-5.68	110.12	117.50
1	A	128	PHE	CA-C-O	5.68	126.78	120.82
1	E	39	THR	CA-CB-CG2	-5.68	100.85	110.50
1	G	141	ARG	N-CA-C	-5.68	95.11	111.00
1	A	107	VAL	CA-C-N	-5.67	111.21	121.14
1	A	107	VAL	C-N-CA	-5.67	111.21	121.14
2	F	3	LEU	O-C-N	5.67	129.68	123.27
2	H	52	ASP	CA-CB-CG	-5.67	106.92	112.60
2	B	47	ASP	CA-C-N	5.67	131.64	121.15
2	B	47	ASP	C-N-CA	5.67	131.64	121.15
2	F	126	VAL	CB-CA-C	5.67	120.05	112.22
1	A	8	THR	OG1-CB-CG2	5.67	120.64	109.30
1	C	1	VAL	O-C-N	5.67	132.07	123.00
1	E	132	VAL	CA-C-N	5.67	128.44	120.28
1	E	132	VAL	C-N-CA	5.67	128.44	120.28
1	G	38	THR	CA-C-O	-5.67	112.28	119.31
1	C	66	LEU	N-CA-CB	5.67	119.80	110.39
2	D	61	LYS	O-C-N	5.67	129.24	122.27
1	A	8	THR	CA-C-N	5.66	130.31	120.68
1	A	8	THR	C-N-CA	5.66	130.31	120.68
1	C	42	TYR	CE1-CZ-OH	5.66	136.89	119.90
2	D	72	SER	N-CA-C	-5.66	98.74	110.80
2	D	74	GLY	O-C-N	-5.66	116.29	122.68
1	G	9	ASN	CB-CG-OD1	-5.66	109.49	120.80
1	A	26	ALA	N-CA-CB	-5.66	101.85	110.33
2	D	81	LEU	CD1-CG-CD2	5.65	123.23	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	116	GLU	CG-CD-OE2	-5.65	105.41	118.40
2	H	121	GLU	CA-C-O	5.65	125.88	119.27
2	F	140	ALA	CB-CA-C	5.64	119.82	110.90
1	G	46	PHE	CG-CD2-CE2	-5.64	111.11	120.70
2	B	139	ASN	N-CA-C	-5.64	104.50	111.33
2	H	113	VAL	CG1-CB-CG2	-5.64	98.39	110.80
1	E	94	ASP	O-C-N	5.64	129.31	121.64
2	F	117	HIS	CE1-NE2-CD2	5.64	114.64	109.00
2	H	48	LEU	N-CA-CB	5.64	119.07	110.95
2	B	6	VAL	CA-C-N	5.64	129.54	121.71
2	B	6	VAL	C-N-CA	5.64	129.54	121.71
1	G	1	VAL	N-CA-CB	-5.64	101.92	111.50
2	H	60	VAL	N-CA-CB	5.63	117.78	110.57
1	C	14	TRP	CB-CG-CD2	-5.63	118.92	126.80
1	C	117	PHE	O-C-N	-5.62	115.11	122.59
1	C	117	PHE	CA-CB-CG	-5.62	108.17	113.80
1	E	66	LEU	O-C-N	5.62	127.94	122.09
1	A	35	SER	N-CA-CB	-5.62	101.63	110.46
1	E	11	LYS	CB-CG-CD	5.62	124.23	111.30
1	G	122	HIS	CE1-NE2-CD2	5.62	114.62	109.00
1	A	130	ALA	CA-C-O	-5.62	114.44	121.02
2	B	133	VAL	CA-CB-CG2	5.62	119.96	110.40
1	A	133	SER	O-C-N	-5.62	114.71	122.46
1	C	90	LYS	CA-CB-CG	-5.62	102.86	114.10
1	C	140	TYR	CD1-CG-CD2	-5.62	109.67	118.10
1	E	20	HIS	O-C-N	5.62	129.36	122.34
1	E	14	TRP	CB-CG-CD1	-5.62	118.47	126.90
2	F	18	VAL	CA-CB-CG1	5.62	119.95	110.40
1	G	30	GLU	CG-CD-OE2	-5.62	105.48	118.40
2	B	19	ASN	CA-C-N	5.62	128.77	120.74
2	B	19	ASN	C-N-CA	5.62	128.77	120.74
2	B	126	VAL	CA-C-N	5.62	129.98	120.88
2	B	126	VAL	C-N-CA	5.62	129.98	120.88
1	C	42	TYR	CB-CG-CD1	-5.62	112.38	120.80
2	H	38	THR	CA-CB-CG2	-5.61	100.96	110.50
1	A	58	HIS	CB-CA-C	5.61	120.06	110.74
2	D	96	LEU	CA-C-O	-5.61	113.17	119.79
1	G	4	PRO	CA-C-N	-5.61	110.83	121.54
1	G	4	PRO	C-N-CA	-5.61	110.83	121.54
2	D	33	VAL	CA-C-N	-5.61	112.13	120.82
2	D	33	VAL	C-N-CA	-5.61	112.13	120.82
1	E	10	VAL	CA-CB-CG2	-5.61	100.87	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	87	THR	OG1-CB-CG2	5.60	120.50	109.30
1	G	29	LEU	O-C-N	-5.60	116.18	122.12
1	E	110	ALA	N-CA-C	-5.60	98.87	110.80
1	G	137	THR	CA-CB-CG2	5.60	120.02	110.50
1	C	122	HIS	CB-CG-ND1	-5.60	114.30	122.70
1	E	47	ASP	CB-CA-C	-5.60	101.57	110.81
2	H	36	PRO	CB-CG-CD	-5.60	88.18	106.10
1	A	40	LYS	O-C-N	-5.60	115.11	122.39
1	A	61	LYS	CG-CD-CE	-5.60	98.43	111.30
1	G	74	ASP	CA-C-O	5.60	128.51	120.51
2	B	67	VAL	CA-CB-CG1	5.60	119.91	110.40
1	E	27	GLU	CA-C-O	5.59	126.40	119.97
2	F	83	GLY	CA-C-O	-5.59	110.36	119.31
1	G	27	GLU	CG-CD-OE1	5.59	131.26	118.40
1	G	78	ASN	N-CA-CB	-5.59	101.88	110.16
2	H	8	LYS	CA-C-O	-5.59	112.66	119.43
2	D	48	LEU	CA-C-O	5.59	126.27	119.78
1	A	68	ASN	O-C-N	-5.59	115.40	122.27
2	F	70	ALA	N-CA-CB	5.58	119.21	109.72
2	H	108	ASN	O-C-N	5.58	130.34	122.41
1	G	20	HIS	CG-CD2-NE2	-5.58	101.62	107.20
1	G	40	LYS	CB-CG-CD	5.58	124.14	111.30
2	H	45	PHE	CG-CD2-CE2	5.58	130.19	120.70
2	B	116	HIS	N-CA-CB	5.58	118.89	110.30
1	C	115	ALA	O-C-N	-5.58	114.44	122.03
1	E	21	ALA	N-CA-C	5.58	122.69	110.80
1	G	8	THR	CA-C-O	-5.58	114.51	120.42
1	G	125	LEU	N-CA-C	-5.58	105.35	111.82
2	B	93	CYS	CA-C-O	-5.58	115.04	120.89
1	C	112	HIS	CA-C-N	-5.57	116.83	122.74
1	C	112	HIS	C-N-CA	-5.57	116.83	122.74
1	G	37	PRO	N-CD-CG	-5.57	94.84	103.20
1	E	133	SER	O-C-N	5.57	128.74	122.22
1	C	65	ALA	CB-CA-C	5.57	121.50	110.42
2	B	85	PHE	N-CA-C	5.57	119.38	112.59
2	D	132	LYS	CA-C-O	5.56	126.11	119.60
2	D	51	PRO	CA-N-CD	-5.56	104.21	112.00
2	B	142	ALA	N-CA-C	5.56	121.85	114.12
1	C	135	VAL	CB-CA-C	5.56	120.41	111.29
1	A	23	GLU	N-CA-C	-5.56	107.04	113.88
1	G	12	ALA	N-CA-CB	-5.56	102.01	110.07
2	B	18	VAL	O-C-N	-5.55	115.63	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	47	ASP	CB-CG-OD2	-5.55	105.63	118.40
1	A	120	ALA	CA-C-O	5.55	126.19	119.31
1	G	77	PRO	O-C-N	5.55	130.13	122.64
2	D	43	GLU	CA-C-O	5.55	129.75	120.65
2	F	64	GLY	O-C-N	-5.55	116.81	122.19
2	H	99	ASP	N-CA-CB	5.55	120.93	109.45
2	B	104	ARG	CG-CD-NE	5.55	124.20	112.00
2	D	40	ARG	N-CA-CB	-5.55	101.12	110.49
2	D	41	PHE	CA-C-N	-5.55	114.52	122.67
2	D	41	PHE	C-N-CA	-5.55	114.52	122.67
1	G	81	SER	CB-CA-C	-5.54	99.39	110.42
2	B	130	TYR	CD1-CE1-CZ	5.54	129.57	119.60
2	F	2	HIS	CA-C-N	5.54	130.37	122.72
2	F	2	HIS	C-N-CA	5.54	130.37	122.72
1	G	93	VAL	CA-CB-CG2	-5.54	100.98	110.40
2	F	35	TYR	CG-CD1-CE1	-5.54	112.89	121.20
2	D	6	VAL	CG1-CB-CG2	-5.54	98.62	110.80
1	A	5	ALA	O-C-N	-5.54	114.91	122.33
2	D	32	LEU	O-C-N	-5.54	115.74	122.22
1	G	96	VAL	N-CA-CB	5.54	118.07	110.54
2	H	85	PHE	CD1-CG-CD2	-5.54	110.30	118.60
2	D	130	TYR	CB-CA-C	-5.53	100.39	110.63
1	E	138	SER	CB-CA-C	-5.53	101.44	110.85
1	A	132	VAL	CA-CB-CG2	-5.53	101.00	110.40
2	B	104	ARG	N-CA-C	5.53	118.24	111.82
1	E	134	THR	CB-CA-C	-5.53	101.45	110.85
2	F	106	LEU	CB-CA-C	-5.53	100.40	110.63
1	G	125	LEU	CD1-CG-CD2	5.53	122.97	110.80
2	B	60	VAL	O-C-N	5.53	129.09	121.90
2	H	120	LYS	CA-CB-CG	5.53	125.15	114.10
2	H	125	PRO	O-C-N	5.52	129.94	122.37
1	G	47	ASP	N-CA-C	-5.52	96.59	107.69
2	B	26	GLU	CB-CG-CD	5.52	121.98	112.60
1	A	60	LYS	CA-CB-CG	5.51	125.13	114.10
1	G	77	PRO	N-CA-CB	5.51	109.04	103.25
2	B	45	PHE	CD1-CG-CD2	-5.51	110.33	118.60
2	B	98	VAL	CA-C-O	-5.51	114.48	121.48
2	F	104	ARG	NH1-CZ-NH2	-5.51	112.14	119.30
1	A	11	LYS	CA-C-N	-5.51	111.32	120.68
1	A	11	LYS	C-N-CA	-5.51	111.32	120.68
1	C	86	LEU	CB-CG-CD1	-5.51	94.18	110.70
2	B	36	PRO	CA-N-CD	-5.51	104.29	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	113	VAL	N-CA-CB	-5.51	101.89	110.54
1	C	128	PHE	CD1-CE1-CZ	-5.51	110.09	120.00
1	E	113	LEU	CA-CB-CG	-5.51	97.02	116.30
1	C	136	LEU	CB-CA-C	5.50	119.93	110.79
2	D	42	PHE	CD1-CG-CD2	5.50	126.86	118.60
1	E	43	PHE	N-CA-C	-5.50	101.10	109.30
2	H	88	LEU	CB-CG-CD1	5.50	127.21	110.70
2	H	27	ALA	CB-CA-C	-5.50	99.47	110.42
2	D	63	HIS	ND1-CG-CD2	5.50	111.60	106.10
1	G	42	TYR	CA-CB-CG	-5.50	104.00	113.90
2	D	116	HIS	CA-C-O	5.50	126.57	120.63
2	F	99	ASP	CA-C-N	5.50	125.59	119.32
2	F	99	ASP	C-N-CA	5.50	125.59	119.32
1	C	49	SER	O-C-N	-5.49	115.95	122.65
1	G	131	SER	CA-C-N	5.49	128.22	120.42
1	G	131	SER	C-N-CA	5.49	128.22	120.42
2	H	43	GLU	CG-CD-OE2	-5.49	105.78	118.40
2	H	94	ASP	OD1-CG-OD2	5.49	136.07	122.90
2	H	111	VAL	CA-CB-CG2	5.49	119.73	110.40
2	D	117	HIS	CA-C-N	-5.49	112.00	121.66
2	D	117	HIS	C-N-CA	-5.49	112.00	121.66
1	E	129	LEU	CA-CB-CG	-5.48	97.11	116.30
2	B	17	LYS	CB-CA-C	5.48	120.00	110.79
2	F	52	ASP	OD1-CG-OD2	5.48	136.06	122.90
1	A	62	VAL	O-C-N	5.48	127.58	121.94
1	A	46	PHE	CA-CB-CG	-5.48	108.32	113.80
2	B	39	GLN	OE1-CD-NE2	5.48	128.08	122.60
2	D	131	GLN	O-C-N	-5.48	115.91	122.15
1	A	141	ARG	CD-NE-CZ	-5.48	116.73	124.40
2	D	131	GLN	CA-CB-CG	-5.48	103.15	114.10
1	A	139	LYS	O-C-N	5.47	129.87	122.59
1	G	55	VAL	CA-CB-CG1	-5.47	101.10	110.40
1	A	72	HIS	N-CA-C	5.47	119.74	112.30
1	A	106	LEU	N-CA-C	-5.47	99.15	110.80
2	B	141	LEU	CB-CG-CD1	5.47	127.11	110.70
1	C	88	ALA	N-CA-CB	-5.47	102.07	110.16
1	C	26	ALA	CA-C-N	5.46	132.00	121.18
1	C	26	ALA	C-N-CA	5.46	132.00	121.18
1	G	54	GLN	CG-CD-NE2	-5.46	108.20	116.40
2	H	32	LEU	N-CA-C	5.46	118.75	111.75
2	H	79	ASP	O-C-N	-5.46	115.03	122.19
2	H	72	SER	CB-CA-C	-5.46	102.07	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	55	MET	CA-C-O	5.46	126.10	119.38
2	H	13	ALA	N-CA-C	5.46	117.09	111.03
2	H	116	HIS	CA-C-O	-5.46	113.93	120.10
2	D	35	TYR	CB-CG-CD2	-5.46	112.62	120.80
2	D	91	LEU	CB-CA-C	-5.45	102.32	110.88
2	D	95	LYS	CA-CB-CG	-5.45	103.19	114.10
2	D	47	ASP	CA-C-N	-5.45	113.03	122.14
2	D	47	ASP	C-N-CA	-5.45	113.03	122.14
2	H	135	ALA	CB-CA-C	5.45	121.14	110.67
1	A	109	LEU	CB-CA-C	5.45	121.14	110.67
1	E	62	VAL	CA-C-O	5.45	127.10	121.05
1	E	51	GLY	O-C-N	5.45	128.82	122.45
1	A	58	HIS	CG-ND1-CE1	-5.45	100.04	109.30
2	B	71	PHE	CB-CG-CD2	-5.45	111.44	120.70
2	D	124	PRO	CA-C-O	5.44	128.45	120.56
2	F	26	GLU	CB-CG-CD	-5.44	103.34	112.60
1	A	47	ASP	CB-CA-C	5.44	119.49	110.78
1	A	119	PRO	O-C-N	-5.44	114.90	122.30
2	B	65	LYS	CA-CB-CG	-5.44	103.22	114.10
1	E	119	PRO	CB-CG-CD	-5.44	88.68	106.10
2	B	121	GLU	O-C-N	5.44	129.62	122.33
2	H	136	GLY	CA-C-O	-5.44	111.11	120.57
1	C	33	PHE	CB-CG-CD1	-5.44	111.46	120.70
1	C	95	PRO	CA-N-CD	-5.43	104.39	112.00
2	D	59	LYS	CG-CD-CE	-5.43	98.80	111.30
1	G	92	ARG	NH1-CZ-NH2	-5.43	112.23	119.30
2	F	60	VAL	CA-C-N	5.43	127.56	120.28
2	F	60	VAL	C-N-CA	5.43	127.56	120.28
1	C	118	THR	O-C-N	5.43	127.50	121.53
1	E	121	VAL	N-CA-CB	5.43	120.44	110.40
2	H	5	PRO	CA-C-O	-5.43	110.72	120.60
1	E	61	LYS	N-CA-CB	5.42	118.65	110.30
2	F	26	GLU	CA-CB-CG	-5.42	103.25	114.10
2	F	79	ASP	OD1-CG-OD2	5.42	135.92	122.90
1	C	3	SER	CA-C-N	5.42	125.12	119.64
1	C	3	SER	C-N-CA	5.42	125.12	119.64
1	A	40	LYS	CA-C-N	-5.42	112.47	120.38
1	A	40	LYS	C-N-CA	-5.42	112.47	120.38
2	B	48	LEU	CB-CA-C	-5.42	98.65	110.41
2	D	19	ASN	CB-CG-ND2	-5.42	108.27	116.40
1	E	31	ARG	N-CA-CB	-5.42	102.00	109.91
2	F	61	LYS	CA-C-N	5.42	127.80	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	61	LYS	C-N-CA	5.42	127.80	120.65
1	G	29	LEU	CA-C-N	-5.42	113.07	120.44
1	G	29	LEU	C-N-CA	-5.42	113.07	120.44
1	A	4	PRO	CA-CB-CG	-5.41	94.22	104.50
1	A	21	ALA	CA-C-O	5.41	128.25	120.51
1	C	105	LEU	CB-CG-CD2	5.41	126.94	110.70
1	A	33	PHE	O-C-N	5.41	128.55	122.22
1	E	57	GLY	CA-C-O	-5.41	114.84	120.90
2	F	97	HIS	CA-C-O	5.41	128.36	122.03
2	F	139	ASN	CB-CG-OD1	5.41	131.62	120.80
2	B	65	LYS	N-CA-C	5.41	117.17	111.28
2	D	60	VAL	N-CA-C	-5.41	105.58	110.82
2	F	72	SER	CB-CA-C	-5.41	99.66	110.42
2	H	65	LYS	CD-CE-NZ	5.41	129.20	111.90
2	D	103	PHE	CD1-CE1-CZ	-5.40	110.28	120.00
1	G	80	LEU	CB-CA-C	5.40	121.17	110.42
2	F	19	ASN	CB-CG-OD1	-5.40	110.00	120.80
1	A	11	LYS	CG-CD-CE	5.40	123.71	111.30
2	D	51	PRO	CB-CA-C	5.40	120.47	111.56
1	G	50	HIS	N-CA-CB	5.40	119.61	110.49
2	H	58	PRO	CB-CA-C	5.40	119.19	111.04
2	H	107	GLY	CA-C-N	-5.40	112.02	122.06
2	H	107	GLY	C-N-CA	-5.40	112.02	122.06
1	E	64	ASP	N-CA-C	-5.39	104.82	111.40
1	G	60	LYS	CA-CB-CG	5.39	124.89	114.10
2	B	105	LEU	CA-C-N	-5.39	110.50	121.18
2	B	105	LEU	C-N-CA	-5.39	110.50	121.18
1	C	68	ASN	CA-CB-CG	5.39	117.99	112.60
1	E	44	PRO	CB-CG-CD	-5.39	88.84	106.10
2	B	97	HIS	CB-CG-ND1	5.39	130.78	122.70
2	F	42	PHE	CG-CD1-CE1	5.39	129.86	120.70
2	F	128	ALA	O-C-N	5.39	128.53	122.22
1	A	117	PHE	CB-CA-C	5.39	120.67	112.00
1	A	77	PRO	CB-CA-C	-5.39	104.10	113.20
2	D	26	GLU	CB-CA-C	-5.39	101.25	110.24
1	C	21	ALA	CB-CA-C	5.38	121.14	110.42
1	A	125	LEU	CB-CG-CD2	5.38	126.84	110.70
1	C	50	HIS	CG-CD2-NE2	-5.38	101.82	107.20
1	C	103	HIS	CA-CB-CG	5.38	119.18	113.80
1	G	80	LEU	N-CA-C	-5.38	99.34	110.80
2	B	4	THR	CB-CA-C	-5.38	100.38	108.61
2	F	48	LEU	O-C-N	-5.38	114.89	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	117	HIS	ND1-CG-CD2	5.38	111.48	106.10
1	A	63	ALA	N-CA-CB	-5.38	101.38	110.41
2	B	97	HIS	CB-CA-C	5.38	121.12	110.42
1	E	68	ASN	CB-CG-OD1	-5.38	110.05	120.80
1	E	108	THR	N-CA-C	-5.38	104.31	111.24
1	C	140	TYR	CA-C-O	5.37	126.65	120.90
2	H	123	THR	CA-C-O	5.37	124.70	120.19
2	H	140	ALA	O-C-N	5.37	127.60	122.07
1	C	2	LEU	CA-C-N	5.37	134.90	121.80
1	C	2	LEU	C-N-CA	5.37	134.90	121.80
1	C	139	LYS	CD-CE-NZ	-5.36	94.73	111.90
2	F	43	GLU	N-CA-CB	-5.36	103.50	111.43
1	G	93	VAL	O-C-N	5.36	128.81	123.18
1	A	124	SER	CA-C-O	5.36	126.63	120.90
1	E	94	ASP	CB-CG-OD1	-5.36	106.08	118.40
2	D	66	LYS	O-C-N	5.36	128.49	122.22
1	E	92	ARG	NH1-CZ-NH2	-5.36	112.34	119.30
2	B	44	SER	O-C-N	5.35	129.85	122.46
2	F	102	ASN	CB-CG-OD1	5.35	131.51	120.80
1	G	24	TYR	CG-CD1-CE1	-5.35	113.17	121.20
1	C	134	THR	N-CA-C	-5.35	104.33	112.04
2	F	74	GLY	CA-C-O	5.35	128.48	119.59
2	B	45	PHE	CB-CA-C	5.35	120.53	110.63
1	E	139	LYS	CD-CE-NZ	-5.35	94.78	111.90
2	H	27	ALA	N-CA-CB	-5.35	101.45	110.49
2	H	114	LEU	CA-CB-CG	5.35	135.03	116.30
1	A	50	HIS	CB-CG-ND1	5.35	130.72	122.70
1	G	116	GLU	CG-CD-OE1	5.35	130.70	118.40
2	F	102	ASN	CA-C-O	-5.34	114.86	120.63
1	G	20	HIS	ND1-CG-CD2	5.34	111.44	106.10
1	G	71	ALA	CA-C-N	-5.34	112.77	122.50
1	G	71	ALA	C-N-CA	-5.34	112.77	122.50
1	C	82	ALA	O-C-N	-5.34	115.97	122.22
2	D	134	VAL	N-CA-CB	5.34	117.81	110.54
1	A	128	PHE	CB-CA-C	-5.34	102.50	110.88
1	C	30	GLU	CB-CA-C	5.34	119.33	110.90
2	F	43	GLU	CG-CD-OE2	-5.34	106.12	118.40
2	F	93	CYS	CA-C-N	5.34	130.92	120.99
2	F	93	CYS	C-N-CA	5.34	130.92	120.99
1	G	55	VAL	CG1-CB-CG2	5.34	122.54	110.80
1	A	47	ASP	CA-C-N	-5.33	111.35	121.54
1	A	47	ASP	C-N-CA	-5.33	111.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	142	ALA	N-CA-C	5.33	120.65	113.72
1	E	23	GLU	CB-CG-CD	-5.33	103.53	112.60
2	D	131	GLN	OE1-CD-NE2	5.33	127.93	122.60
1	E	36	PHE	CD1-CE1-CZ	-5.33	110.42	120.00
2	H	37	TRP	CE2-CD2-CG	-5.33	100.81	107.20
1	A	27	GLU	O-C-N	-5.32	115.72	122.27
1	E	100	LEU	O-C-N	-5.32	115.31	122.23
2	H	68	LEU	N-CA-C	-5.32	106.48	112.87
2	H	117	HIS	CB-CA-C	-5.32	99.83	110.42
1	A	41	THR	O-C-N	-5.32	116.13	122.20
1	A	92	ARG	CB-CA-C	5.32	119.45	111.89
1	C	97	ASN	CA-C-O	5.32	125.91	119.31
1	G	22	GLY	N-CA-C	-5.32	100.57	113.18
1	G	24	TYR	CB-CA-C	5.32	119.89	110.85
1	G	122	HIS	CB-CG-ND1	-5.32	114.72	122.70
1	A	93	VAL	CA-CB-CG2	-5.31	101.37	110.40
2	F	40	ARG	CB-CG-CD	-5.31	99.08	111.30
1	E	41	THR	OG1-CB-CG2	-5.31	98.68	109.30
1	A	32	MET	N-CA-CB	5.31	117.66	109.91
2	B	73	ASP	OD1-CG-OD2	5.31	135.64	122.90
1	E	32	MET	CA-C-N	5.31	127.39	120.28
1	E	32	MET	C-N-CA	5.31	127.39	120.28
2	F	10	ALA	CB-CA-C	-5.31	102.48	110.92
1	G	118	THR	CB-CA-C	5.31	117.62	109.50
2	D	50	THR	CA-C-O	-5.31	114.61	119.76
2	D	85	PHE	CB-CG-CD1	5.30	129.72	120.70
1	E	108	THR	N-CA-CB	5.30	117.87	110.07
2	H	122	PHE	CD1-CG-CD2	5.30	126.56	118.60
2	B	21	ASP	N-CA-C	-5.30	106.84	113.15
1	A	75	ASP	O-C-N	-5.30	115.42	121.99
2	B	84	THR	OG1-CB-CG2	5.30	119.90	109.30
1	G	4	PRO	CA-N-CD	-5.30	104.58	112.00
2	H	85	PHE	CA-C-N	5.30	131.80	122.42
2	H	85	PHE	C-N-CA	5.30	131.80	122.42
2	D	143	HIS	CA-CB-CG	-5.30	108.50	113.80
1	G	41	THR	CA-CB-CG2	-5.30	101.49	110.50
1	C	95	PRO	N-CA-C	5.30	121.49	113.81
2	F	27	ALA	CA-C-O	-5.30	115.24	121.07
1	G	80	LEU	CA-C-N	5.30	131.66	121.54
1	G	80	LEU	C-N-CA	5.30	131.66	121.54
2	H	54	VAL	CG1-CB-CG2	5.30	122.45	110.80
2	F	67	VAL	CA-CB-CG1	5.29	119.40	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	51	GLY	N-CA-C	-5.29	100.63	113.18
1	C	95	PRO	O-C-N	5.29	128.57	122.17
1	C	98	PHE	N-CA-C	-5.29	104.56	111.02
1	C	130	ALA	CA-C-O	-5.29	113.54	119.79
2	F	10	ALA	N-CA-CB	5.29	117.87	109.82
2	H	72	SER	N-CA-C	-5.29	104.76	111.11
2	B	90	GLU	OE1-CD-OE2	5.29	135.60	122.90
2	B	116	HIS	N-CA-C	-5.29	105.56	112.23
2	D	83	GLY	N-CA-C	-5.29	100.64	113.18
2	D	78	LEU	CA-CB-CG	5.29	134.82	116.30
1	C	128	PHE	CZ-CE2-CD2	-5.29	110.48	120.00
1	A	82	ALA	CB-CA-C	5.29	119.18	110.88
1	A	43	PHE	CG-CD2-CE2	5.28	129.68	120.70
2	B	22	GLU	CA-C-O	5.28	126.95	120.56
1	E	114	PRO	N-CA-CB	-5.28	97.71	103.25
2	B	47	ASP	N-CA-C	5.28	117.83	109.96
2	B	142	ALA	CB-CA-C	-5.28	100.51	109.38
2	F	130	TYR	CD1-CE1-CZ	-5.28	110.10	119.60
1	A	46	PHE	O-C-N	-5.28	117.07	123.03
1	E	91	LEU	N-CA-CB	5.28	117.94	110.13
2	H	132	LYS	CA-C-O	5.28	126.44	120.00
2	B	102	ASN	OD1-CG-ND2	5.28	127.88	122.60
2	D	71	PHE	CB-CG-CD1	-5.28	111.73	120.70
2	D	128	ALA	N-CA-C	5.28	117.11	111.36
2	F	21	ASP	CB-CG-OD2	-5.28	106.26	118.40
2	H	144	LYS	CB-CA-C	5.28	119.76	110.37
1	G	20	HIS	N-CA-C	-5.27	106.69	113.02
2	F	17	LYS	CA-CB-CG	-5.27	103.56	114.10
2	D	132	LYS	CB-CG-CD	5.27	123.42	111.30
2	F	121	GLU	O-C-N	-5.27	116.61	122.09
1	E	58	HIS	ND1-CE1-NE2	5.27	113.67	108.40
2	H	39	GLN	N-CA-C	-5.27	99.58	110.80
2	F	30	ARG	CD-NE-CZ	-5.26	117.03	124.40
1	G	140	TYR	CZ-CE2-CD2	5.26	129.08	119.60
2	H	77	HIS	CA-C-N	-5.26	114.08	122.66
2	H	77	HIS	C-N-CA	-5.26	114.08	122.66
2	D	144	LYS	CB-CA-C	5.26	119.22	111.17
2	D	69	GLY	N-CA-C	-5.26	100.71	113.18
1	G	105	LEU	CA-C-N	5.26	127.64	120.54
1	G	105	LEU	C-N-CA	5.26	127.64	120.54
1	A	14	TRP	NE1-CE2-CD2	-5.26	100.56	107.40
1	C	91	LEU	N-CA-CB	-5.26	101.83	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	80	LEU	CA-CB-CG	5.26	134.71	116.30
2	H	115	ALA	CB-CA-C	-5.26	99.95	110.42
1	G	62	VAL	CA-CB-CG2	5.26	119.34	110.40
1	A	36	PHE	N-CA-C	5.25	116.33	108.76
2	D	144	LYS	CA-C-O	5.25	126.84	119.80
2	F	58	PRO	CA-C-O	5.25	130.16	120.60
1	A	127	LYS	CB-CA-C	-5.25	102.41	110.81
2	H	77	HIS	CG-CD2-NE2	5.25	112.45	107.20
2	D	2	HIS	CB-CA-C	5.25	119.76	110.16
1	E	38	THR	CA-CB-OG1	5.25	117.47	109.60
2	H	52	ASP	CA-C-O	-5.25	113.60	119.79
2	F	49	SER	CB-CA-C	-5.24	99.35	110.31
1	G	83	LEU	CA-C-O	5.24	126.07	120.20
1	C	17	VAL	N-CA-C	-5.24	98.44	109.34
1	C	32	MET	CG-SD-CE	-5.24	89.37	100.90
1	C	109	LEU	N-CA-CB	5.24	119.35	110.49
1	E	60	LYS	CB-CG-CD	5.24	123.35	111.30
1	E	77	PRO	O-C-N	5.24	128.98	122.22
2	D	47	ASP	CB-CG-OD2	-5.24	106.35	118.40
2	D	122	PHE	N-CA-CB	5.24	119.34	110.49
2	B	108	ASN	N-CA-CB	-5.24	101.70	110.39
2	F	89	SER	N-CA-CB	5.24	117.88	110.13
1	A	92	ARG	N-CA-C	5.23	118.61	111.39
2	B	135	ALA	O-C-N	-5.23	116.38	122.03
2	B	38	THR	N-CA-C	-5.23	106.67	113.16
2	D	104	ARG	CA-C-N	5.23	129.57	120.68
2	D	104	ARG	C-N-CA	5.23	129.57	120.68
2	F	100	PRO	CB-CG-CD	-5.23	89.36	106.10
1	G	33	PHE	CB-CA-C	5.23	119.23	110.92
1	C	49	SER	N-CA-CB	-5.23	103.22	110.38
2	D	28	LEU	CB-CG-CD2	-5.23	95.02	110.70
1	E	103	HIS	CB-CA-C	-5.23	101.96	110.85
1	G	4	PRO	CA-C-O	-5.23	111.08	120.60
2	H	61	LYS	N-CA-C	5.23	118.92	112.54
2	F	89	SER	CA-C-O	5.23	126.14	120.55
1	C	56	LYS	CD-CE-NZ	5.22	128.62	111.90
1	C	129	LEU	CD1-CG-CD2	5.22	122.30	110.80
2	F	37	TRP	N-CA-C	-5.22	106.68	113.16
2	F	55	MET	N-CA-CB	-5.22	102.89	110.47
1	C	24	TYR	CB-CG-CD2	-5.22	112.97	120.80
1	C	125	LEU	CB-CG-CD1	-5.22	95.04	110.70
2	B	82	LYS	N-CA-C	-5.22	105.71	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	112	HIS	CA-CB-CG	5.22	119.02	113.80
2	D	92	HIS	CG-ND1-CE1	-5.22	100.43	109.30
2	B	105	LEU	CD1-CG-CD2	-5.21	99.33	110.80
2	D	22	GLU	N-CA-CB	5.21	118.15	110.33
2	H	130	TYR	CG-CD1-CE1	-5.21	113.38	121.20
1	A	72	HIS	CB-CA-C	-5.21	102.30	110.85
2	H	146	HIS	CE1-NE2-CD2	5.21	114.21	109.00
2	B	16	GLY	CA-C-N	-5.21	112.01	120.71
2	B	16	GLY	C-N-CA	-5.21	112.01	120.71
1	G	3	SER	CA-C-O	-5.21	113.02	120.16
1	G	99	LYS	N-CA-C	5.21	119.26	113.01
2	H	75	LEU	CB-CG-CD1	5.21	126.32	110.70
1	E	22	GLY	CA-C-N	-5.21	111.68	120.58
1	E	22	GLY	C-N-CA	-5.21	111.68	120.58
1	E	133	SER	CA-C-N	5.21	127.68	120.29
1	E	133	SER	C-N-CA	5.21	127.68	120.29
1	C	71	ALA	O-C-N	-5.20	115.28	122.46
2	D	19	ASN	N-CA-C	-5.20	99.31	108.20
1	G	90	LYS	N-CA-C	-5.20	99.72	110.80
2	F	50	THR	N-CA-C	-5.20	103.54	108.22
1	G	139	LYS	CA-CB-CG	5.20	124.50	114.10
2	F	25	GLY	CA-C-O	-5.20	112.25	119.01
1	C	5	ALA	N-CA-CB	5.20	117.68	109.94
2	D	92	HIS	CE1-NE2-CD2	-5.20	103.81	109.00
2	D	141	LEU	CA-C-N	5.20	130.80	121.66
2	D	141	LEU	C-N-CA	5.20	130.80	121.66
1	A	131	SER	CA-C-O	5.19	126.27	120.82
2	D	35	TYR	CB-CA-C	5.19	119.24	111.14
2	F	111	VAL	CA-CB-CG1	5.19	119.23	110.40
1	C	97	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	G	8	THR	CA-CB-OG1	-5.19	101.81	109.60
2	H	3	LEU	CB-CG-CD2	-5.19	95.13	110.70
1	C	87	HIS	CB-CA-C	-5.19	99.47	110.31
1	E	65	ALA	CB-CA-C	5.19	119.40	110.79
2	D	13	ALA	CA-C-N	-5.18	110.92	121.18
2	D	13	ALA	C-N-CA	-5.18	110.92	121.18
2	H	49	SER	CB-CA-C	-5.18	100.22	110.27
2	D	39	GLN	O-C-N	-5.18	116.29	122.20
1	A	43	PHE	CD1-CE1-CZ	-5.18	110.68	120.00
1	A	122	HIS	N-CA-C	-5.18	105.53	111.07
1	E	25	GLY	N-CA-C	5.18	119.15	112.83
1	A	60	LYS	CB-CG-CD	5.18	123.20	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	100	PRO	CA-C-N	5.18	129.37	120.72
2	D	100	PRO	C-N-CA	5.18	129.37	120.72
1	E	67	THR	CA-C-O	5.18	125.90	119.79
2	F	139	ASN	N-CA-C	5.18	117.66	111.71
1	G	123	ALA	CB-CA-C	5.17	119.65	110.85
1	E	6	ASP	CB-CG-OD1	5.17	130.30	118.40
1	A	116	GLU	CA-C-O	5.17	125.53	119.06
1	A	119	PRO	CA-C-N	5.17	130.19	121.14
1	A	119	PRO	C-N-CA	5.17	130.19	121.14
1	E	125	LEU	N-CA-C	-5.17	106.23	112.54
1	C	136	LEU	CA-C-O	-5.17	115.07	120.55
1	A	65	ALA	N-CA-CB	5.17	119.09	110.41
2	D	35	TYR	CG-CD1-CE1	-5.17	113.45	121.20
2	D	36	PRO	CB-CA-C	5.17	120.09	111.56
2	F	14	LEU	CA-C-O	-5.17	113.69	119.79
2	F	120	LYS	CB-CG-CD	5.17	123.18	111.30
1	G	9	ASN	CB-CA-C	5.17	118.99	110.88
1	G	62	VAL	N-CA-CB	5.17	118.58	110.31
1	G	119	PRO	CA-N-CD	5.16	119.23	112.00
2	B	15	TRP	N-CA-C	5.16	118.68	112.38
1	G	103	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	G	119	PRO	N-CA-C	-5.16	101.84	112.47
2	H	55	MET	N-CA-CB	5.16	119.09	110.32
2	F	120	LYS	CB-CA-C	5.16	120.58	110.67
2	H	122	PHE	CE1-CZ-CE2	5.16	129.29	120.00
2	D	40	ARG	CA-CB-CG	5.16	124.41	114.10
1	G	115	ALA	N-CA-C	5.16	117.00	108.49
1	A	119	PRO	CA-N-CD	5.15	119.21	112.00
1	E	118	THR	CA-C-N	-5.15	113.45	119.32
1	E	118	THR	C-N-CA	-5.15	113.45	119.32
2	B	1	VAL	N-CA-CB	5.15	120.26	111.50
1	E	96	VAL	CA-C-N	5.15	128.14	120.31
1	E	96	VAL	C-N-CA	5.15	128.14	120.31
2	F	118	PHE	CB-CG-CD2	5.15	129.46	120.70
2	H	19	ASN	CB-CG-ND2	-5.15	108.67	116.40
2	B	41	PHE	O-C-N	-5.15	115.26	122.37
2	D	15	TRP	O-C-N	-5.15	116.66	122.12
2	D	96	LEU	N-CA-CB	-5.15	102.37	110.30
2	F	63	HIS	ND1-CG-CD2	-5.15	100.95	106.10
2	H	31	LEU	O-C-N	-5.15	116.53	122.09
2	H	35	TYR	CB-CA-C	5.15	120.31	110.17
2	H	57	ASN	N-CA-CB	5.15	119.27	109.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	127	GLN	CB-CA-C	-5.15	102.37	110.86
2	F	31	LEU	CB-CA-C	-5.14	101.29	110.70
1	A	74	ASP	CB-CA-C	-5.14	99.33	109.67
2	D	73	ASP	CB-CG-OD2	-5.14	106.57	118.40
1	E	72	HIS	CB-CA-C	5.14	120.19	111.35
2	F	54	VAL	CA-C-N	-5.14	113.71	122.56
2	F	54	VAL	C-N-CA	-5.14	113.71	122.56
1	E	59	GLY	N-CA-C	-5.14	106.42	112.64
1	A	126	ASP	O-C-N	-5.14	116.58	122.08
2	B	23	VAL	CA-CB-CG2	-5.14	101.67	110.40
2	D	47	ASP	CB-CG-OD1	5.14	130.21	118.40
1	A	1	VAL	O-C-N	5.13	131.22	123.00
2	F	41	PHE	CB-CA-C	5.13	119.24	110.56
2	H	68	LEU	CA-C-O	5.13	125.57	119.10
2	D	21	ASP	N-CA-C	5.13	117.27	111.11
1	C	65	ALA	N-CA-C	-5.13	99.87	110.80
1	E	9	ASN	CB-CA-C	-5.13	101.96	110.68
2	F	37	TRP	O-C-N	-5.13	115.29	122.37
1	C	14	TRP	CA-CB-CG	-5.13	103.86	113.60
2	F	6	VAL	CA-C-O	5.13	126.15	120.46
2	F	73	ASP	CA-CB-CG	-5.13	107.47	112.60
1	G	136	LEU	N-CA-CB	5.13	118.90	110.39
1	C	12	ALA	CB-CA-C	-5.12	102.14	110.85
1	C	4	PRO	CA-N-CD	-5.12	104.83	112.00
2	B	8	LYS	CB-CA-C	-5.12	102.29	110.79
1	C	78	ASN	CA-C-O	5.12	125.66	119.31
1	E	33	PHE	CD1-CE1-CZ	-5.12	110.79	120.00
2	H	27	ALA	CA-C-O	5.12	127.83	120.51
2	H	66	LYS	N-CA-CB	5.12	118.42	109.72
1	A	88	ALA	O-C-N	-5.12	116.23	122.22
2	B	107	GLY	O-C-N	5.12	127.86	122.28
1	A	38	THR	CA-CB-CG2	-5.11	101.81	110.50
2	B	100	PRO	CB-CA-C	-5.11	104.16	111.62
2	H	122	PHE	CB-CG-CD2	-5.11	112.01	120.70
2	F	72	SER	CA-CB-OG	-5.11	100.89	111.10
1	G	89	HIS	ND1-CE1-NE2	5.11	113.51	108.40
1	G	135	VAL	CA-CB-CG1	5.11	119.08	110.40
1	G	26	ALA	CB-CA-C	-5.10	99.97	110.38
1	A	57	GLY	CA-C-N	-5.10	113.17	120.82
1	A	57	GLY	C-N-CA	-5.10	113.17	120.82
1	C	103	HIS	CG-ND1-CE1	-5.10	100.63	109.30
2	D	36	PRO	CA-CB-CG	5.10	114.19	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	78	LEU	CA-C-N	5.10	130.74	121.92
2	F	78	LEU	C-N-CA	5.10	130.74	121.92
2	H	91	LEU	CD1-CG-CD2	-5.10	99.58	110.80
2	H	111	VAL	CG1-CB-CG2	-5.10	99.58	110.80
1	E	98	PHE	CB-CG-CD1	-5.10	112.04	120.70
1	G	64	ASP	CB-CG-OD1	5.10	130.12	118.40
2	B	130	TYR	OH-CZ-CE2	5.09	135.18	119.90
2	F	141	LEU	CA-C-N	5.09	130.36	122.26
2	F	141	LEU	C-N-CA	5.09	130.36	122.26
2	B	69	GLY	O-C-N	5.09	129.87	122.18
2	D	57	ASN	CA-C-O	-5.09	114.96	119.75
1	C	104	CYS	N-CA-C	-5.09	107.02	113.18
2	F	42	PHE	CA-C-O	-5.09	112.36	122.23
2	F	120	LYS	CA-CB-CG	5.09	124.28	114.10
1	A	93	VAL	CA-C-O	-5.09	115.06	121.11
2	D	17	LYS	N-CA-CB	-5.09	101.89	110.49
1	C	30	GLU	O-C-N	-5.08	116.60	122.09
1	C	66	LEU	CB-CG-CD1	-5.08	95.45	110.70
2	F	100	PRO	N-CD-CG	-5.08	95.57	103.20
1	A	59	GLY	CA-C-N	5.08	127.05	120.44
1	A	59	GLY	C-N-CA	5.08	127.05	120.44
2	D	68	LEU	N-CA-CB	-5.08	103.55	110.56
1	E	40	LYS	N-CA-CB	-5.08	102.40	110.28
2	H	37	TRP	O-C-N	-5.08	114.24	122.42
1	A	112	HIS	N-CA-CB	-5.08	104.27	110.98
1	A	135	VAL	CA-C-N	5.08	127.80	120.38
1	A	135	VAL	C-N-CA	5.08	127.80	120.38
2	D	64	GLY	N-CA-C	-5.08	106.61	112.50
2	D	40	ARG	NE-CZ-NH1	5.08	126.58	121.50
2	F	20	VAL	O-C-N	5.08	128.70	122.05
2	F	54	VAL	N-CA-C	5.08	117.44	111.09
1	G	133	SER	N-CA-CB	5.08	118.04	110.22
1	A	35	SER	CA-C-O	5.08	125.22	119.18
1	C	89	HIS	N-CA-CB	5.08	117.88	110.47
2	F	133	VAL	CA-C-N	-5.07	114.05	120.60
2	F	133	VAL	C-N-CA	-5.07	114.05	120.60
2	B	14	LEU	CA-CB-CG	5.07	134.05	116.30
2	H	82	LYS	CD-CE-NZ	5.07	128.13	111.90
2	B	49	SER	N-CA-C	5.07	118.73	112.54
1	C	113	LEU	CA-C-O	5.07	127.10	121.22
2	D	115	ALA	CA-C-N	5.07	127.32	120.38
2	D	115	ALA	C-N-CA	5.07	127.32	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	28	LEU	O-C-N	5.07	127.50	122.03
2	F	116	HIS	CB-CA-C	5.07	119.20	110.79
1	C	9	ASN	N-CA-C	-5.07	105.03	111.11
2	H	45	PHE	CZ-CE2-CD2	-5.07	110.88	120.00
2	F	79	ASP	CA-C-N	-5.06	111.87	121.54
2	F	79	ASP	C-N-CA	-5.06	111.87	121.54
2	B	116	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
1	E	73	VAL	N-CA-C	-5.06	98.81	109.34
2	F	15	TRP	CB-CG-CD2	5.06	133.89	126.80
2	F	32	LEU	N-CA-CB	5.06	117.48	109.94
1	E	104	CYS	N-CA-CB	5.06	117.51	109.82
2	H	56	GLY	CA-C-N	-5.06	112.97	121.17
2	H	56	GLY	C-N-CA	-5.06	112.97	121.17
1	C	84	SER	CA-C-N	-5.06	113.00	120.28
1	C	84	SER	C-N-CA	-5.06	113.00	120.28
1	G	66	LEU	N-CA-CB	5.05	118.11	110.28
1	C	130	ALA	CA-C-N	5.05	129.22	120.58
1	C	130	ALA	C-N-CA	5.05	129.22	120.58
2	D	146	HIS	CB-CA-C	-5.05	100.50	110.10
2	F	80	ASN	CB-CG-ND2	5.05	123.98	116.40
1	G	49	SER	CA-CB-OG	-5.05	101.00	111.10
2	H	95	LYS	CA-CB-CG	5.05	124.20	114.10
2	D	45	PHE	CB-CG-CD1	-5.05	112.12	120.70
2	F	62	ALA	CA-C-O	-5.05	115.70	121.00
2	F	47	ASP	N-CA-C	5.04	116.41	109.15
2	H	52	ASP	O-C-N	5.04	129.09	122.33
1	E	56	LYS	CD-CE-NZ	-5.04	95.77	111.90
1	A	10	VAL	CA-CB-CG2	-5.04	101.83	110.40
2	H	116	HIS	CG-ND1-CE1	-5.04	100.74	109.30
2	D	46	GLY	CA-C-N	5.04	129.02	121.72
2	D	46	GLY	C-N-CA	5.04	129.02	121.72
2	D	71	PHE	CG-CD1-CE1	5.04	129.26	120.70
2	D	143	HIS	N-CA-CB	-5.04	102.47	110.22
2	F	15	TRP	NE1-CE2-CZ2	5.04	137.66	130.10
2	F	143	HIS	CA-C-O	-5.04	113.31	120.51
2	B	110	LEU	CB-CA-C	-5.03	101.32	110.63
1	G	117	PHE	O-C-N	-5.03	115.90	122.59
1	C	86	LEU	CA-C-N	5.03	129.12	120.72
1	C	86	LEU	C-N-CA	5.03	129.12	120.72
2	F	10	ALA	CA-C-N	5.03	128.94	120.29
2	F	10	ALA	C-N-CA	5.03	128.94	120.29
2	H	101	GLU	CB-CA-C	-5.03	101.32	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	30	ARG	N-CA-CB	-5.03	102.04	110.39
1	C	109	LEU	O-C-N	5.03	129.28	122.59
2	D	42	PHE	O-C-N	5.03	130.88	121.63
2	H	22	GLU	OE1-CD-OE2	5.03	134.97	122.90
2	F	45	PHE	CD1-CE1-CZ	-5.03	110.95	120.00
1	C	15	GLY	O-C-N	-5.02	116.17	122.70
1	C	118	THR	CA-C-O	-5.02	115.23	120.70
2	B	15	TRP	CB-CG-CD2	-5.02	119.78	126.80
2	B	121	GLU	CB-CA-C	-5.02	100.14	110.38
1	C	60	LYS	CG-CD-CE	-5.02	99.76	111.30
1	G	100	LEU	N-CA-C	5.02	119.67	113.50
2	H	37	TRP	CD2-CE2-CZ2	-5.02	117.38	122.40
2	D	89	SER	CA-CB-OG	-5.01	101.07	111.10
1	E	15	GLY	CA-C-N	-5.01	111.96	121.54
1	E	15	GLY	C-N-CA	-5.01	111.96	121.54
2	H	63	HIS	CB-CA-C	-5.01	102.95	110.92
2	B	9	SER	N-CA-C	-5.01	105.51	110.97
1	E	112	HIS	CA-C-N	-5.01	116.11	122.98
1	E	112	HIS	C-N-CA	-5.01	116.11	122.98
1	E	25	GLY	CA-C-N	-5.01	112.84	121.66
1	E	25	GLY	C-N-CA	-5.01	112.84	121.66
2	F	18	VAL	CB-CA-C	-5.01	103.20	110.81
1	A	85	ASP	CA-C-O	-5.01	113.22	119.38
1	C	135	VAL	CA-CB-CG1	5.01	118.91	110.40
1	E	139	LYS	CA-C-O	5.01	127.38	121.17
2	F	2	HIS	CB-CG-ND1	5.01	130.21	122.70
2	B	50	THR	CA-C-N	5.00	124.78	119.28
2	B	50	THR	C-N-CA	5.00	124.78	119.28
2	B	143	HIS	ND1-CE1-NE2	-5.00	103.40	108.40
2	H	82	LYS	CA-C-O	5.00	125.72	120.42
2	F	77	HIS	CB-CG-CD2	-5.00	124.70	131.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	20	HIS	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	141	ARG	Sidechain
2	F	23	VAL	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1060	340	0
1	C	1069	0	1048	410	3
1	E	1069	0	1058	341	0
1	G	1069	0	1056	418	0
2	B	1121	0	1111	385	0
2	D	1121	0	1103	481	3
2	F	1121	0	1101	360	3
2	H	1121	0	1103	445	0
3	A	43	0	30	23	0
3	B	43	0	30	14	0
3	C	43	0	30	15	0
3	D	43	0	30	25	0
3	E	43	0	30	24	0
3	F	43	0	30	16	1
3	G	43	0	30	21	0
3	H	43	0	30	7	0
All	All	9104	0	8880	3081	5

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 171.

All (3081) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:CA	1:A:76:MET:CB	1.76	1.64
2:D:104:ARG:CB	2:D:104:ARG:CG	1.74	1.64
2:F:29:GLY:HA3	2:F:55:MET:SD	1.32	1.64
2:H:14:LEU:CD2	2:H:14:LEU:CG	1.76	1.63
1:G:32:MET:CA	1:G:32:MET:CB	1.75	1.62
2:B:3:LEU:CD2	2:B:3:LEU:CG	1.77	1.62
1:G:107:VAL:HG13	2:H:112:CYS:SG	1.36	1.62
2:H:137:VAL:CB	2:H:137:VAL:CG2	1.77	1.62
1:A:61:LYS:CG	1:A:61:LYS:CB	1.78	1.61
2:B:30:ARG:CB	2:B:30:ARG:CG	1.75	1.61
1:E:43:PHE:CZ	3:E:142:HEM:HBC2	1.28	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:LEU:CG	1:G:101:LEU:CD1	1.78	1.61
2:D:14:LEU:CG	2:D:14:LEU:CD1	1.76	1.61
2:D:49:SER:CA	2:D:49:SER:CB	1.77	1.61
2:B:18:VAL:CG1	2:B:18:VAL:CB	1.78	1.60
1:G:61:LYS:CG	1:G:61:LYS:CD	1.76	1.60
1:G:47:ASP:CA	1:G:47:ASP:C	1.74	1.60
2:B:98:VAL:CB	2:B:98:VAL:CG2	1.78	1.60
1:G:112:HIS:CA	1:G:112:HIS:CB	1.79	1.60
1:C:38:THR:CB	1:C:38:THR:CA	1.75	1.60
2:D:141:LEU:CD1	2:D:141:LEU:CG	1.77	1.59
2:H:123:THR:CB	2:H:123:THR:CG2	1.75	1.59
2:B:17:LYS:CG	2:B:17:LYS:CD	1.75	1.59
1:C:64:ASP:CA	1:C:64:ASP:CB	1.76	1.58
2:F:90:GLU:CG	2:F:90:GLU:CD	1.75	1.58
1:C:40:LYS:CD	1:C:40:LYS:CG	1.81	1.58
1:C:132:VAL:CG1	1:C:132:VAL:CB	1.80	1.58
1:E:106:LEU:CG	1:E:106:LEU:CD1	1.77	1.58
2:H:127:GLN:CG	2:H:127:GLN:CB	1.80	1.58
2:B:8:LYS:CB	2:B:8:LYS:CG	1.75	1.58
2:F:8:LYS:CB	2:F:8:LYS:CG	1.80	1.58
2:F:39:GLN:CG	2:F:39:GLN:CD	1.76	1.58
2:F:40:ARG:CG	2:F:40:ARG:CD	1.79	1.57
2:F:110:LEU:CB	2:F:110:LEU:CA	1.81	1.57
1:E:11:LYS:CA	1:E:11:LYS:CB	1.75	1.57
2:F:82:LYS:CD	2:F:82:LYS:CE	1.81	1.57
1:C:118:THR:N	1:C:118:THR:CA	1.68	1.56
1:C:91:LEU:CD2	1:C:91:LEU:CG	1.77	1.56
2:H:22:GLU:CB	2:H:22:GLU:CG	1.78	1.56
1:A:41:THR:N	1:A:41:THR:CA	1.67	1.56
1:G:109:LEU:CD1	1:G:109:LEU:CG	1.80	1.56
1:C:78:ASN:N	1:C:78:ASN:CA	1.69	1.56
1:E:20:HIS:N	1:E:20:HIS:CA	1.67	1.55
2:D:142:ALA:CA	2:D:142:ALA:CB	1.75	1.55
1:G:66:LEU:CD1	1:G:132:VAL:HG11	1.35	1.55
1:A:61:LYS:CD	1:A:61:LYS:CE	1.79	1.54
1:A:121:VAL:N	1:A:121:VAL:CA	1.68	1.54
1:G:117:PHE:CB	1:G:117:PHE:CA	1.78	1.54
2:H:91:LEU:CD1	2:H:91:LEU:CG	1.76	1.54
2:F:48:LEU:CB	2:F:48:LEU:CG	1.74	1.54
3:A:142:HEM:CAD	3:A:142:HEM:CBD	1.80	1.54
2:H:103:PHE:N	2:H:103:PHE:CA	1.67	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:HIS:CA	2:D:77:HIS:CB	1.79	1.53
2:F:40:ARG:CD	2:F:40:ARG:NE	1.67	1.53
2:F:95:LYS:NZ	2:F:95:LYS:CE	1.68	1.53
2:B:38:THR:N	2:B:38:THR:CA	1.68	1.52
1:C:16:LYS:CG	1:C:16:LYS:CD	1.82	1.52
1:C:141:ARG:NE	1:C:141:ARG:CD	1.72	1.52
2:H:30:ARG:NE	2:H:30:ARG:CD	1.73	1.52
2:H:99:ASP:N	2:H:99:ASP:CA	1.72	1.51
2:H:61:LYS:NZ	2:H:61:LYS:CE	1.72	1.51
1:G:60:LYS:NZ	1:G:60:LYS:CE	1.68	1.51
1:C:13:ALA:N	1:C:13:ALA:CA	1.68	1.51
2:D:65:LYS:CE	2:D:65:LYS:NZ	1.72	1.51
2:H:68:LEU:N	2:H:68:LEU:CA	1.68	1.51
1:A:37:PRO:CB	1:A:37:PRO:CA	1.77	1.50
1:E:69:ALA:N	1:E:69:ALA:CA	1.68	1.50
1:E:99:LYS:NZ	1:E:99:LYS:CE	1.71	1.50
2:F:17:LYS:NZ	2:F:17:LYS:CE	1.70	1.50
2:D:125:PRO:CA	2:D:125:PRO:CB	1.74	1.49
1:A:61:LYS:CE	1:A:61:LYS:NZ	1.71	1.49
1:G:67:THR:N	1:G:67:THR:CA	1.72	1.48
2:H:21:ASP:CG	2:H:65:LYS:HG3	1.38	1.48
2:D:14:LEU:HD21	2:D:126:VAL:CG1	1.45	1.47
1:A:77:PRO:CB	1:A:77:PRO:CG	1.75	1.45
1:A:60:LYS:NZ	1:A:60:LYS:CE	1.79	1.45
2:D:4:THR:OG1	2:D:4:THR:CB	1.65	1.45
1:G:30:GLU:HG3	1:G:50:HIS:NE2	1.23	1.45
1:E:137:THR:OG1	1:E:137:THR:CB	1.66	1.44
2:H:4:THR:CB	2:H:7:GLU:HB2	1.45	1.43
2:H:84:THR:OG1	2:H:84:THR:CB	1.64	1.43
1:G:118:THR:CG2	1:G:120:ALA:HB3	1.47	1.43
2:D:80:ASN:ND2	2:D:83:GLY:CA	1.82	1.43
1:C:3:SER:CB	1:C:3:SER:OG	1.66	1.42
1:E:35:SER:OG	1:E:35:SER:CB	1.66	1.42
2:D:14:LEU:CD2	2:D:126:VAL:HG11	1.48	1.42
2:H:100:PRO:CG	2:H:100:PRO:CD	1.76	1.41
2:B:95:LYS:NZ	2:B:95:LYS:CE	1.79	1.41
2:B:12:THR:OG1	2:B:12:THR:CB	1.68	1.41
2:B:38:THR:OG1	2:B:38:THR:CB	1.67	1.41
1:G:81:SER:OG	1:G:81:SER:CB	1.67	1.41
1:E:43:PHE:CZ	3:E:142:HEM:CBC	2.03	1.40
1:G:87:HIS:CA	1:G:91:LEU:HD12	1.50	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:THR:O	2:B:38:THR:C	1.65	1.38
2:D:3:LEU:CD2	2:D:132:LYS:HB3	1.53	1.38
1:C:64:ASP:CA	1:C:64:ASP:OD1	1.68	1.37
2:H:4:THR:HB	2:H:7:GLU:CB	1.52	1.37
1:C:118:THR:HG22	1:C:121:VAL:N	1.37	1.36
1:A:87:HIS:CG	1:A:136:LEU:HD11	1.60	1.36
2:F:4:THR:HB	2:F:7:GLU:CG	1.52	1.36
2:F:2:HIS:ND1	2:F:132:LYS:NZ	1.73	1.34
1:C:39:THR:OG1	1:C:39:THR:CB	1.73	1.34
2:D:107:GLY:CA	2:D:134:VAL:HG21	1.58	1.34
2:D:32:LEU:HD21	2:D:42:PHE:CE1	1.61	1.33
1:G:66:LEU:HD11	1:G:132:VAL:CG2	1.59	1.32
3:B:147:HEM:HBC2	3:B:147:HEM:CMC	1.43	1.32
1:G:14:TRP:NE1	1:G:67:THR:OG1	1.56	1.32
2:B:45:PHE:CE1	2:B:60:VAL:HG23	1.63	1.32
1:G:95:PRO:HA	1:G:98:PHE:CD2	1.64	1.32
2:H:117:HIS:HD2	2:H:118:PHE:CD1	1.45	1.32
2:F:39:GLN:HB3	2:F:39:GLN:NE2	1.44	1.31
2:B:7:GLU:O	2:B:11:VAL:HG23	1.22	1.31
2:H:26:GLU:O	2:H:30:ARG:HG3	1.20	1.30
2:D:80:ASN:ND2	2:D:83:GLY:HA3	0.99	1.30
2:F:39:GLN:HE21	2:F:39:GLN:CB	1.43	1.29
1:G:87:HIS:HA	1:G:91:LEU:CD1	1.61	1.29
2:F:1:VAL:CG1	2:F:132:LYS:HE2	1.62	1.28
2:F:29:GLY:HA3	2:F:55:MET:CE	1.62	1.28
2:H:20:VAL:CG1	2:H:65:LYS:HB2	1.63	1.28
2:B:50:THR:O	2:B:54:VAL:HG23	1.30	1.27
2:D:15:TRP:CD1	2:D:130:TYR:HH	1.52	1.27
2:H:117:HIS:HD2	2:H:118:PHE:CE1	1.50	1.27
2:F:28:LEU:O	2:F:32:LEU:HB2	1.34	1.26
1:A:118:THR:OG1	1:A:121:VAL:HG21	1.26	1.26
1:E:106:LEU:CD1	1:E:106:LEU:CB	2.14	1.26
1:G:30:GLU:CD	1:G:50:HIS:CD2	2.14	1.26
2:D:77:HIS:CB	2:D:77:HIS:N	1.99	1.26
1:G:79:ALA:O	1:G:82:ALA:HB3	1.30	1.25
1:G:107:VAL:CG1	2:H:112:CYS:SG	2.23	1.25
2:H:20:VAL:O	2:H:24:GLY:N	1.66	1.25
1:C:66:LEU:HD21	1:C:129:LEU:CD2	1.65	1.25
2:F:29:GLY:CA	2:F:55:MET:SD	2.23	1.24
2:F:29:GLY:N	2:F:55:MET:HE1	1.48	1.24
2:D:101:GLU:HA	2:D:104:ARG:NH1	1.50	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:GLU:CA	2:D:104:ARG:HH11	1.50	1.23
2:F:25:GLY:O	2:F:55:MET:HE3	1.11	1.23
2:H:3:LEU:CD2	2:H:8:LYS:HE2	1.69	1.23
2:F:80:ASN:HD21	2:F:83:GLY:N	1.38	1.22
1:A:29:LEU:CD2	1:A:101:LEU:HD12	1.67	1.22
3:D:147:HEM:HBB2	3:D:147:HEM:CMB	1.56	1.20
2:H:117:HIS:CD2	2:H:118:PHE:CD1	2.29	1.20
1:E:6:ASP:HB3	1:E:124:SER:OG	1.37	1.20
1:G:4:PRO:HG2	1:G:5:ALA:N	1.54	1.20
2:B:98:VAL:CG2	2:B:98:VAL:N	2.03	1.20
1:A:139:LYS:O	1:A:141:ARG:HG3	1.38	1.19
1:C:6:ASP:OD2	1:C:127:LYS:HE2	1.39	1.19
1:C:141:ARG:NE	1:C:141:ARG:CG	2.05	1.19
2:H:31:LEU:CD2	2:H:106:LEU:HB2	1.72	1.19
1:C:107:VAL:O	1:C:110:ALA:HB3	1.40	1.18
2:F:1:VAL:HG12	2:F:132:LYS:CE	1.72	1.18
1:G:114:PRO:HG2	1:G:115:ALA:H	1.06	1.18
2:H:80:ASN:CG	2:H:83:GLY:HA3	1.69	1.18
2:D:3:LEU:HD22	2:D:132:LYS:HB3	1.19	1.18
2:H:137:VAL:O	2:H:141:LEU:HD23	1.02	1.18
3:B:147:HEM:CMC	3:B:147:HEM:CBC	2.20	1.18
2:D:104:ARG:N	2:D:104:ARG:HG2	1.59	1.18
1:G:30:GLU:CG	1:G:50:HIS:NE2	2.06	1.18
1:E:1:VAL:HG12	1:E:2:LEU:N	1.57	1.17
1:G:84:SER:CA	1:G:136:LEU:HD23	1.75	1.17
2:D:101:GLU:CA	2:D:104:ARG:HD2	1.74	1.17
2:D:107:GLY:HA3	2:D:134:VAL:CG2	1.73	1.17
1:E:102:SER:HB3	1:E:129:LEU:CD2	1.72	1.17
3:B:147:HEM:HBC2	3:B:147:HEM:HMC3	1.21	1.17
2:F:20:VAL:O	2:F:68:LEU:CD1	1.93	1.17
1:G:66:LEU:CD1	1:G:132:VAL:CG1	2.22	1.17
1:A:53:ALA:HA	1:A:56:LYS:HD3	1.24	1.16
3:A:142:HEM:CAD	3:A:142:HEM:O2D	1.92	1.16
2:B:51:PRO:O	2:B:55:MET:HG2	1.02	1.16
2:D:91:LEU:HD12	2:D:95:LYS:HB2	1.21	1.16
2:D:104:ARG:HG2	2:D:104:ARG:H	1.04	1.16
2:H:51:PRO:O	2:H:55:MET:HG2	1.44	1.16
1:C:66:LEU:HD23	1:C:128:PHE:CZ	1.81	1.16
2:F:29:GLY:CA	2:F:55:MET:HE1	1.76	1.16
1:A:127:LYS:HD2	1:C:141:ARG:HD3	1.22	1.16
1:C:40:LYS:CD	1:C:40:LYS:CB	2.23	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:LEU:HD11	1:G:132:VAL:CG1	1.74	1.15
1:A:98:PHE:HD1	1:A:133:SER:OG	1.28	1.15
1:E:66:LEU:HD11	3:E:142:HEM:CMB	1.76	1.14
1:C:118:THR:HG23	1:C:120:ALA:HB3	1.26	1.14
1:G:80:LEU:CB	1:G:135:VAL:HG11	1.78	1.14
2:B:68:LEU:N	2:B:68:LEU:HD23	1.62	1.14
2:H:3:LEU:HD21	2:H:8:LYS:HE2	1.24	1.14
1:C:62:VAL:O	1:C:65:ALA:HB3	1.46	1.13
2:D:81:LEU:CD1	2:D:137:VAL:HG23	1.78	1.13
2:H:137:VAL:O	2:H:141:LEU:CD2	1.97	1.13
3:D:147:HEM:HMC2	3:D:147:HEM:HBC2	1.13	1.13
1:A:29:LEU:HD21	1:A:101:LEU:CD1	1.76	1.13
2:F:25:GLY:O	2:F:55:MET:CE	1.97	1.13
1:E:106:LEU:HD12	1:E:106:LEU:HA	1.31	1.13
2:H:117:HIS:CD2	2:H:118:PHE:CE1	2.36	1.13
2:D:82:LYS:HA	2:D:140:ALA:HB1	1.22	1.13
2:D:104:ARG:CG	2:D:104:ARG:H	1.61	1.12
1:E:66:LEU:HD11	3:E:142:HEM:HMB2	1.16	1.12
3:E:142:HEM:CMB	3:E:142:HEM:HBB2	1.58	1.12
2:B:7:GLU:O	2:B:11:VAL:CG2	1.96	1.12
1:G:109:LEU:HD12	1:G:109:LEU:HA	1.28	1.12
1:G:112:HIS:ND1	1:G:112:HIS:HA	1.63	1.12
2:H:20:VAL:HG12	2:H:65:LYS:HB2	1.22	1.12
2:D:10:ALA:O	2:D:14:LEU:HG	1.49	1.12
1:E:76:MET:SD	1:E:135:VAL:HG21	1.88	1.12
1:A:3:SER:CB	1:A:4:PRO:HD2	1.65	1.11
2:B:28:LEU:CD1	2:B:32:LEU:HD22	1.78	1.11
2:H:123:THR:HG22	2:H:124:PRO:HD2	1.18	1.11
2:F:20:VAL:O	2:F:68:LEU:HD13	1.47	1.11
2:B:101:GLU:OE1	2:B:104:ARG:NE	1.82	1.11
2:B:129:ALA:HA	2:B:132:LYS:HG3	1.31	1.11
1:G:112:HIS:CA	1:G:112:HIS:CG	2.32	1.11
2:B:28:LEU:HD11	2:B:32:LEU:HD22	1.32	1.11
2:B:129:ALA:O	2:B:133:VAL:HG23	1.51	1.11
1:E:44:PRO:HG2	1:E:45:HIS:H	1.15	1.11
1:G:84:SER:HA	1:G:136:LEU:HD23	1.29	1.11
1:C:118:THR:CG2	1:C:121:VAL:H	1.62	1.10
2:F:29:GLY:CA	2:F:55:MET:CE	2.28	1.10
1:G:14:TRP:HA	1:G:14:TRP:CE3	1.52	1.10
2:F:68:LEU:O	2:F:71:PHE:HB3	1.49	1.10
1:G:79:ALA:O	1:G:82:ALA:CB	1.97	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:CE	1:C:141:ARG:O	2.00	1.10
2:B:4:THR:HG23	2:B:5:PRO:CD	1.80	1.10
2:H:84:THR:OG1	2:H:84:THR:N	1.83	1.10
2:B:19:ASN:O	2:B:23:VAL:HG13	1.50	1.10
2:D:21:ASP:OD1	2:D:21:ASP:N	1.63	1.10
2:F:14:LEU:O	2:F:17:LYS:HB2	1.49	1.10
1:G:49:SER:O	1:G:52:SER:N	1.84	1.10
1:G:87:HIS:CD2	1:G:91:LEU:HD13	1.86	1.10
2:B:51:PRO:O	2:B:55:MET:CG	1.97	1.09
1:C:106:LEU:O	1:C:110:ALA:N	1.84	1.09
1:E:86:LEU:HD11	1:E:90:LYS:HD2	1.28	1.09
2:B:45:PHE:HE1	2:B:60:VAL:CG2	1.64	1.09
1:G:104:CYS:O	1:G:108:THR:OG1	1.69	1.09
1:C:116:GLU:OE1	1:C:116:GLU:HA	1.48	1.09
2:D:113:VAL:HG12	2:D:114:LEU:HD23	1.10	1.09
1:E:106:LEU:O	1:E:110:ALA:HB2	1.53	1.09
2:F:2:HIS:O	2:F:132:LYS:NZ	1.85	1.09
1:G:66:LEU:CD1	1:G:132:VAL:HG21	1.81	1.09
2:D:131:GLN:HA	2:D:131:GLN:NE2	1.65	1.08
2:F:37:TRP:NE1	1:G:94:ASP:OD1	1.86	1.08
1:C:27:GLU:HG2	1:C:108:THR:HG23	1.17	1.08
1:E:10:VAL:HG13	1:E:125:LEU:HD23	1.33	1.08
1:E:99:LYS:HB3	1:E:100:LEU:HD23	1.09	1.08
1:G:87:HIS:CG	1:G:91:LEU:HD13	1.87	1.08
1:G:112:HIS:CA	1:G:112:HIS:ND1	2.15	1.08
1:A:100:LEU:O	1:A:103:HIS:HB3	1.54	1.08
2:B:96:LEU:HD22	2:B:98:VAL:HG21	1.33	1.08
1:E:86:LEU:CD1	1:E:90:LYS:HD2	1.84	1.08
2:F:4:THR:HB	2:F:7:GLU:HG3	1.12	1.07
1:G:121:VAL:O	1:G:125:LEU:N	1.87	1.07
1:G:118:THR:HG23	1:G:120:ALA:HB3	1.17	1.07
1:C:31:ARG:HG2	2:D:127:GLN:OE1	1.54	1.07
2:D:104:ARG:CG	2:D:104:ARG:CA	2.31	1.07
1:G:118:THR:CG2	1:G:120:ALA:CB	2.32	1.07
1:C:64:ASP:OD1	1:C:64:ASP:HA	1.27	1.06
2:D:45:PHE:HD2	2:D:45:PHE:N	1.37	1.06
2:F:26:GLU:O	2:F:30:ARG:HB2	1.53	1.06
1:G:95:PRO:CA	1:G:98:PHE:HD2	1.67	1.06
2:H:24:GLY:HA2	2:H:68:LEU:HD13	1.12	1.06
1:C:16:LYS:CG	1:C:16:LYS:CE	2.32	1.06
1:C:93:VAL:HG11	3:C:142:HEM:CAC	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:ARG:CG	2:D:104:ARG:N	2.14	1.06
1:G:60:LYS:O	1:G:64:ASP:HB2	1.55	1.06
1:A:3:SER:HB2	1:A:4:PRO:HD2	1.07	1.06
1:A:127:LYS:HE3	1:C:141:ARG:O	1.54	1.06
2:B:67:VAL:C	2:B:68:LEU:HD23	1.79	1.06
2:D:91:LEU:HD12	2:D:95:LYS:CB	1.83	1.06
1:G:109:LEU:CD1	1:G:109:LEU:CB	2.33	1.06
2:B:17:LYS:HE2	2:B:17:LYS:HB2	1.34	1.06
1:G:109:LEU:CD1	1:G:109:LEU:CD2	2.33	1.06
1:G:112:HIS:HB3	1:G:113:LEU:HD13	1.34	1.06
2:H:21:ASP:OD1	2:H:65:LYS:HG3	1.53	1.06
3:B:147:HEM:CBC	3:B:147:HEM:HMC1	1.81	1.05
1:C:40:LYS:CG	1:C:40:LYS:CE	2.33	1.05
1:C:84:SER:CB	1:C:139:LYS:HD2	1.85	1.05
1:E:101:LEU:O	1:E:101:LEU:HD22	1.55	1.05
1:G:83:LEU:HD11	3:G:142:HEM:HMA1	1.35	1.05
1:C:16:LYS:CD	1:C:16:LYS:CB	2.35	1.05
2:B:98:VAL:CG2	2:B:98:VAL:CG1	2.33	1.05
2:D:26:GLU:OE1	2:D:30:ARG:NH1	1.89	1.05
1:A:98:PHE:CD1	1:A:133:SER:OG	2.02	1.05
1:C:12:ALA:C	1:C:13:ALA:CA	2.30	1.05
2:D:110:LEU:HD23	2:D:110:LEU:C	1.81	1.05
1:E:109:LEU:O	1:E:113:LEU:HD12	1.57	1.05
2:H:20:VAL:HG12	2:H:65:LYS:CB	1.85	1.05
1:A:41:THR:N	1:A:41:THR:HG23	1.70	1.04
3:D:147:HEM:CMB	3:D:147:HEM:CBB	2.33	1.04
2:D:107:GLY:O	2:D:111:VAL:CG2	2.05	1.04
1:E:66:LEU:CD1	3:E:142:HEM:HMB2	1.85	1.04
3:A:142:HEM:CAD	3:A:142:HEM:CGD	2.35	1.04
1:E:14:TRP:HA	1:E:17:VAL:CG2	1.87	1.04
1:E:67:THR:HG22	1:E:68:ASN:N	1.72	1.04
1:E:112:HIS:C	1:E:113:LEU:HG	1.74	1.04
1:G:114:PRO:HG2	1:G:115:ALA:N	1.71	1.04
2:B:96:LEU:HD22	2:B:98:VAL:CG2	1.88	1.04
2:B:106:LEU:HA	2:B:109:VAL:HG23	1.33	1.04
2:H:80:ASN:ND2	2:H:83:GLY:HA3	1.71	1.04
1:C:7:LYS:HE2	1:C:74:ASP:OD2	1.58	1.03
2:D:91:LEU:HG	2:D:91:LEU:O	1.58	1.03
2:D:131:GLN:CA	2:D:131:GLN:HE21	1.53	1.03
1:E:102:SER:HB3	1:E:129:LEU:HD22	1.06	1.03
1:E:126:ASP:OD2	1:G:141:ARG:NH2	1.90	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:LEU:HD13	1:G:132:VAL:HG11	1.35	1.03
1:A:127:LYS:O	1:A:130:ALA:HB3	1.59	1.03
2:B:1:VAL:C	2:B:2:HIS:ND1	2.16	1.03
1:C:66:LEU:CD2	1:C:129:LEU:CD2	2.37	1.03
2:D:101:GLU:O	2:D:104:ARG:CG	2.06	1.03
1:E:1:VAL:HG12	1:E:2:LEU:H	0.87	1.03
1:E:66:LEU:CD1	3:E:142:HEM:CMB	2.37	1.03
1:A:139:LYS:N	1:A:139:LYS:HD2	1.69	1.03
1:C:77:PRO:C	1:C:78:ASN:CA	2.30	1.03
1:C:107:VAL:HG13	2:D:112:CYS:SG	1.98	1.03
1:E:62:VAL:O	1:E:66:LEU:HD13	1.59	1.03
2:H:130:TYR:O	2:H:134:VAL:HG23	1.58	1.03
1:E:96:VAL:HG21	2:H:101:GLU:CD	1.84	1.02
1:A:58:HIS:O	1:A:62:VAL:N	1.93	1.02
1:A:110:ALA:HB1	2:B:115:ALA:HB3	1.40	1.02
1:G:14:TRP:CE3	1:G:14:TRP:CA	2.42	1.02
1:A:121:VAL:N	1:A:121:VAL:HG23	1.74	1.02
2:H:14:LEU:CD2	2:H:14:LEU:CB	2.37	1.02
2:H:31:LEU:HD22	2:H:106:LEU:HB2	1.03	1.02
1:A:76:MET:CA	1:A:76:MET:CG	2.37	1.02
3:A:142:HEM:O2D	3:A:142:HEM:HAD2	1.56	1.02
2:B:3:LEU:HD22	2:B:7:GLU:HB3	1.38	1.02
1:E:101:LEU:O	1:E:105:LEU:HD12	1.57	1.02
2:F:4:THR:CB	2:F:7:GLU:HG3	1.88	1.02
2:D:14:LEU:CD1	2:D:14:LEU:CB	2.36	1.02
2:D:131:GLN:NE2	2:D:131:GLN:CA	2.10	1.02
2:F:2:HIS:CG	2:F:132:LYS:HZ1	1.78	1.02
2:F:39:GLN:CG	2:F:39:GLN:NE2	2.22	1.02
1:G:83:LEU:HD11	3:G:142:HEM:CMA	1.90	1.02
2:D:82:LYS:HA	2:D:140:ALA:CB	1.90	1.01
1:A:66:LEU:O	1:A:70:VAL:HG23	1.60	1.01
2:B:4:THR:HG23	2:B:5:PRO:HD2	1.39	1.01
2:D:141:LEU:CD1	2:D:141:LEU:CB	2.37	1.01
1:G:87:HIS:CG	1:G:91:LEU:CD1	2.43	1.01
1:C:16:LYS:HD3	1:C:116:GLU:HG3	1.41	1.01
1:C:27:GLU:HG2	1:C:108:THR:CG2	1.89	1.01
1:E:132:VAL:O	1:E:136:LEU:HD12	1.60	1.01
3:E:142:HEM:HBB2	3:E:142:HEM:HMB2	1.01	1.01
2:F:130:TYR:O	2:F:134:VAL:HG23	1.60	1.01
2:H:21:ASP:CG	2:H:65:LYS:CG	2.34	1.01
1:C:141:ARG:CD	1:C:141:ARG:CZ	2.37	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ALA:HB3	2:D:77:HIS:CG	1.94	1.01
2:D:113:VAL:HG12	2:D:114:LEU:CD2	1.91	1.00
1:E:33:PHE:CD2	1:E:48:LEU:HD23	1.95	1.00
1:E:43:PHE:HZ	3:E:142:HEM:CBC	1.57	1.00
2:B:59:LYS:CE	2:B:59:LYS:HA	1.72	1.00
1:C:7:LYS:NZ	1:C:74:ASP:OD1	1.92	1.00
2:D:104:ARG:CB	2:D:104:ARG:CD	2.39	1.00
2:D:107:GLY:HA3	2:D:134:VAL:HG21	1.03	1.00
2:B:3:LEU:CD2	2:B:7:GLU:HB3	1.90	1.00
2:H:81:LEU:O	2:H:85:PHE:CE1	2.13	1.00
2:D:3:LEU:CD1	2:D:133:VAL:HG23	1.92	1.00
2:F:141:LEU:HD11	3:F:147:HEM:CAB	1.92	1.00
1:C:64:ASP:CA	1:C:64:ASP:CG	2.34	1.00
3:D:147:HEM:HBB2	3:D:147:HEM:HMB3	1.42	1.00
3:C:142:HEM:HMC2	3:C:142:HEM:HBC2	1.42	0.99
2:H:125:PRO:HG2	2:H:126:VAL:N	1.75	0.99
2:B:15:TRP:CE3	2:B:18:VAL:HG21	1.95	0.99
2:F:80:ASN:ND2	2:F:83:GLY:H	1.59	0.99
2:F:7:GLU:O	2:F:11:VAL:HG12	1.63	0.99
1:A:2:LEU:N	1:A:2:LEU:HD23	1.77	0.99
1:E:31:ARG:NH1	2:F:122:PHE:O	1.96	0.99
1:G:66:LEU:HD11	1:G:132:VAL:HG21	1.01	0.99
2:B:50:THR:O	2:B:54:VAL:CG2	2.09	0.99
2:B:98:VAL:O	2:B:145:TYR:OH	1.79	0.99
1:C:107:VAL:HA	1:C:110:ALA:HB2	1.45	0.99
1:G:32:MET:CB	1:G:32:MET:C	2.35	0.99
1:A:17:VAL:O	1:A:17:VAL:HG12	1.61	0.99
2:B:8:LYS:CB	2:B:8:LYS:CD	2.40	0.99
2:F:48:LEU:CB	2:F:48:LEU:CD2	2.41	0.99
1:A:3:SER:CB	1:A:4:PRO:CD	2.41	0.99
2:H:93:CYS:HB2	2:H:145:TYR:CE1	1.98	0.99
1:A:118:THR:OG1	1:A:121:VAL:CG2	2.10	0.98
2:H:102:ASN:C	2:H:103:PHE:CA	2.35	0.98
1:C:40:LYS:CD	1:C:40:LYS:HB3	1.91	0.98
2:D:54:VAL:O	2:D:57:ASN:HB2	1.64	0.98
1:E:107:VAL:C	1:E:110:ALA:HB3	1.87	0.98
1:G:117:PHE:CA	1:G:117:PHE:CG	2.46	0.98
2:H:35:TYR:O	2:H:38:THR:HG23	1.63	0.98
2:H:36:PRO:HG2	2:H:37:TRP:CE3	1.96	0.98
1:G:113:LEU:O	1:G:117:PHE:HB2	1.63	0.98
2:D:101:GLU:HA	2:D:104:ARG:HD2	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:ALA:O	2:D:131:GLN:HB2	1.62	0.98
1:E:99:LYS:HB3	1:E:100:LEU:CD2	1.93	0.98
1:E:102:SER:CB	1:E:129:LEU:HD22	1.94	0.98
1:C:118:THR:HG22	1:C:121:VAL:H	0.94	0.98
1:C:107:VAL:O	1:C:110:ALA:CB	2.12	0.98
1:E:1:VAL:CG1	1:E:2:LEU:H	1.74	0.98
1:A:77:PRO:O	1:A:81:SER:HB2	1.64	0.98
1:A:83:LEU:HD11	3:A:142:HEM:HMA1	1.46	0.98
1:C:78:ASN:N	1:C:78:ASN:CB	2.27	0.98
3:D:147:HEM:CBB	3:D:147:HEM:HMB1	1.93	0.98
2:F:43:GLU:OE2	1:G:92:ARG:NH1	1.96	0.98
1:G:84:SER:N	1:G:136:LEU:CD2	2.26	0.98
2:H:123:THR:CG2	2:H:124:PRO:HD2	1.92	0.98
1:E:141:ARG:HB3	2:H:36:PRO:HG3	1.42	0.98
1:G:118:THR:HG23	1:G:120:ALA:CB	1.91	0.98
1:A:61:LYS:CB	1:A:61:LYS:CD	2.41	0.97
2:D:45:PHE:N	2:D:45:PHE:CD2	2.08	0.97
2:D:49:SER:CB	2:D:49:SER:C	2.36	0.97
1:G:48:LEU:N	1:G:48:LEU:HD23	1.77	0.97
1:E:19:ALA:C	1:E:20:HIS:CA	2.37	0.97
1:G:20:HIS:HB3	1:G:23:GLU:HB2	1.44	0.97
1:A:33:PHE:CD1	1:A:40:LYS:HG2	2.00	0.97
1:A:52:SER:O	1:A:55:VAL:HG22	1.65	0.97
2:D:24:GLY:HA3	2:D:68:LEU:CD2	1.95	0.97
1:G:3:SER:HB2	1:G:4:PRO:HD2	1.47	0.97
2:D:80:ASN:HD21	2:D:83:GLY:CA	1.64	0.97
1:A:87:HIS:CB	1:A:136:LEU:HD11	1.95	0.97
2:D:81:LEU:HD13	2:D:137:VAL:HG23	1.45	0.97
1:G:80:LEU:HB2	1:G:135:VAL:HG11	1.45	0.97
2:H:21:ASP:HA	2:H:65:LYS:HB3	1.44	0.97
2:B:3:LEU:CD2	2:B:3:LEU:CD1	2.43	0.96
2:H:82:LYS:O	2:H:83:GLY:C	2.06	0.96
2:B:96:LEU:CD2	2:B:98:VAL:HG21	1.94	0.96
2:B:98:VAL:H	2:B:98:VAL:HG23	1.25	0.96
1:C:118:THR:CG2	1:C:120:ALA:HB3	1.94	0.96
1:G:80:LEU:HD11	1:G:132:VAL:HG13	1.47	0.96
2:H:32:LEU:HA	2:H:38:THR:OG1	1.64	0.96
1:A:45:HIS:N	1:A:45:HIS:ND1	2.13	0.96
2:F:141:LEU:HD11	3:F:147:HEM:HAB	1.46	0.96
1:A:139:LYS:N	1:A:139:LYS:CD	2.23	0.96
2:B:98:VAL:CG2	2:B:98:VAL:CA	2.42	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:LEU:O	2:H:85:PHE:HE1	1.48	0.96
2:B:28:LEU:HD11	2:B:32:LEU:CD2	1.95	0.96
1:G:84:SER:OG	1:G:136:LEU:HA	1.64	0.96
2:H:26:GLU:O	2:H:30:ARG:CG	2.13	0.96
1:E:104:CYS:O	1:E:108:THR:OG1	1.83	0.96
1:G:118:THR:HG21	1:G:120:ALA:HB3	1.48	0.96
2:B:146:HIS:CD2	2:B:146:HIS:N	2.32	0.95
1:E:128:PHE:O	1:E:131:SER:HB2	1.66	0.95
1:A:118:THR:HG1	1:A:121:VAL:HG21	1.27	0.95
2:B:92:HIS:HA	2:B:96:LEU:CD1	1.95	0.95
2:D:11:VAL:HG12	2:D:12:THR:N	1.79	0.95
2:D:24:GLY:HA3	2:D:68:LEU:HD21	1.46	0.95
2:D:80:ASN:HD22	2:D:83:GLY:HA3	1.23	0.95
2:F:33:VAL:HG21	2:F:51:PRO:HB3	1.45	0.95
2:B:38:THR:OG1	2:B:38:THR:CG2	2.13	0.95
2:D:44:SER:OG	2:D:45:PHE:HE2	1.50	0.95
2:F:72:SER:O	2:F:75:LEU:HB2	1.66	0.95
1:G:105:LEU:O	1:G:109:LEU:HB2	1.67	0.95
2:B:73:ASP:O	2:B:77:HIS:CE1	2.20	0.95
1:A:61:LYS:CG	1:A:61:LYS:CA	2.44	0.95
2:B:98:VAL:N	2:B:98:VAL:HG23	1.75	0.95
1:A:6:ASP:O	1:A:10:VAL:HG23	1.65	0.95
1:A:53:ALA:CA	1:A:56:LYS:HD3	1.95	0.95
3:D:147:HEM:HMC2	3:D:147:HEM:CBC	1.97	0.95
1:G:121:VAL:HA	1:G:124:SER:OG	1.67	0.95
2:H:91:LEU:CD1	2:H:91:LEU:CD2	2.45	0.94
1:A:41:THR:HG23	1:A:41:THR:H	1.25	0.94
1:C:118:THR:HB	1:C:121:VAL:HB	1.45	0.94
2:D:47:ASP:OD2	2:D:49:SER:HB3	1.68	0.94
1:G:32:MET:CA	1:G:32:MET:CG	2.45	0.94
2:B:101:GLU:OE1	2:B:104:ARG:NH1	2.00	0.94
2:D:81:LEU:HD11	2:D:137:VAL:HG23	1.46	0.94
2:D:146:HIS:CD2	2:D:146:HIS:N	2.29	0.94
1:E:123:ALA:O	1:E:126:ASP:HB3	1.66	0.94
1:A:100:LEU:N	1:A:100:LEU:HD23	1.80	0.94
1:A:112:HIS:O	1:A:113:LEU:HD23	1.67	0.94
1:C:66:LEU:HD23	1:C:128:PHE:HZ	1.26	0.94
1:G:107:VAL:HG13	2:H:112:CYS:HG	1.15	0.94
3:A:142:HEM:CBD	3:A:142:HEM:C3D	2.51	0.94
1:C:123:ALA:O	1:C:127:LYS:HG3	1.68	0.94
1:C:84:SER:OG	1:C:139:LYS:HD2	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:TYR:CD1	1:G:93:VAL:HG13	2.03	0.94
1:C:13:ALA:N	1:C:13:ALA:CB	2.31	0.94
2:F:33:VAL:CG2	2:F:51:PRO:HB3	1.97	0.94
2:F:80:ASN:ND2	2:F:80:ASN:O	2.00	0.94
2:F:91:LEU:HD21	2:F:96:LEU:CD1	1.98	0.94
2:H:3:LEU:HD23	2:H:4:THR:N	1.83	0.93
1:G:49:SER:O	1:G:52:SER:OG	1.86	0.93
2:H:78:LEU:HD23	2:H:133:VAL:CG2	1.97	0.93
2:F:94:ASP:OD1	2:F:146:HIS:NE2	2.01	0.93
1:A:86:LEU:HD13	1:A:90:LYS:NZ	1.82	0.93
2:B:114:LEU:O	2:B:118:PHE:HB2	1.68	0.93
1:C:40:LYS:HB3	1:C:40:LYS:HD2	1.50	0.93
2:D:77:HIS:O	2:D:81:LEU:HD23	1.68	0.93
2:F:29:GLY:H	2:F:55:MET:HE1	1.18	0.93
1:G:46:PHE:HE2	3:G:142:HEM:O1D	1.50	0.93
1:G:118:THR:HB	1:G:121:VAL:CG2	1.97	0.93
2:H:24:GLY:HA2	2:H:68:LEU:CD1	1.97	0.93
1:A:4:PRO:HG2	1:A:5:ALA:H	1.34	0.93
1:G:14:TRP:HA	1:G:14:TRP:HE3	1.23	0.93
2:H:82:LYS:O	2:H:83:GLY:O	1.87	0.93
1:G:118:THR:CB	1:G:121:VAL:HG23	1.98	0.93
2:D:3:LEU:CD2	2:D:132:LYS:CB	2.46	0.93
2:F:39:GLN:NE2	2:F:39:GLN:CB	2.14	0.93
2:H:14:LEU:CD2	2:H:14:LEU:CD1	2.46	0.93
3:E:142:HEM:HMB2	3:E:142:HEM:CBB	1.97	0.93
1:G:29:LEU:HD21	1:G:58:HIS:NE2	1.83	0.93
2:B:92:HIS:O	2:B:96:LEU:HB3	1.67	0.93
2:B:103:PHE:CZ	2:B:141:LEU:HD12	2.03	0.93
2:F:4:THR:HB	2:F:7:GLU:CD	1.93	0.93
2:F:93:CYS:O	2:F:97:HIS:HA	1.69	0.92
1:G:66:LEU:O	1:G:69:ALA:HB3	1.69	0.92
3:D:147:HEM:HBC2	3:D:147:HEM:CMC	1.89	0.92
2:F:43:GLU:CD	1:G:92:ARG:HH12	1.77	0.92
1:A:112:HIS:O	1:A:113:LEU:CD2	2.17	0.92
2:D:32:LEU:CD2	2:D:42:PHE:CE1	2.51	0.92
1:C:66:LEU:CD2	1:C:129:LEU:HD23	1.99	0.92
1:G:83:LEU:O	1:G:87:HIS:N	2.03	0.92
1:A:41:THR:N	1:A:41:THR:CG2	2.31	0.92
1:C:68:ASN:O	1:C:72:HIS:HD2	1.53	0.92
1:E:44:PRO:HG2	1:E:45:HIS:N	1.80	0.92
1:A:118:THR:HB	1:A:121:VAL:HG23	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:SER:CB	2:D:49:SER:N	2.33	0.92
2:H:39:GLN:O	2:H:42:PHE:N	2.02	0.92
2:D:24:GLY:CA	2:D:68:LEU:HD21	2.00	0.92
2:F:1:VAL:CG1	2:F:132:LYS:CE	2.38	0.92
1:A:121:VAL:N	1:A:121:VAL:CG2	2.31	0.92
1:E:96:VAL:CG2	2:H:101:GLU:HG2	2.00	0.92
2:B:30:ARG:O	2:B:34:VAL:HG23	1.68	0.92
1:A:98:PHE:HB3	1:A:133:SER:HB3	1.49	0.91
2:B:51:PRO:HA	2:B:54:VAL:HB	1.48	0.91
2:D:81:LEU:HD13	2:D:137:VAL:CG2	1.99	0.91
3:D:147:HEM:HBB2	3:D:147:HEM:HMB1	1.47	0.91
2:B:21:ASP:OD2	2:B:21:ASP:N	2.01	0.91
2:F:82:LYS:CE	2:F:82:LYS:CG	2.48	0.91
2:B:3:LEU:CD2	2:B:3:LEU:CB	2.49	0.91
2:F:74:GLY:O	2:F:78:LEU:HD13	1.70	0.91
2:H:31:LEU:HD22	2:H:106:LEU:CB	1.98	0.91
1:C:31:ARG:O	1:C:35:SER:OG	1.87	0.91
2:D:11:VAL:HG21	2:D:133:VAL:HG21	1.52	0.91
2:H:33:VAL:HG22	2:H:54:VAL:HG11	1.51	0.91
1:A:47:ASP:OD1	1:A:49:SER:HB3	1.71	0.91
2:F:20:VAL:C	2:F:68:LEU:HD13	1.96	0.91
2:F:141:LEU:CD1	3:F:147:HEM:HAB	2.01	0.91
2:H:3:LEU:HD22	2:H:8:LYS:HE2	1.52	0.91
2:B:101:GLU:CD	2:B:104:ARG:HE	1.79	0.91
1:C:84:SER:HB3	1:C:139:LYS:HD2	1.53	0.91
1:C:91:LEU:CD2	1:C:91:LEU:CB	2.49	0.91
2:F:99:ASP:O	2:F:102:ASN:HB2	1.69	0.91
2:H:114:LEU:HD23	2:H:118:PHE:CE1	2.05	0.91
2:B:18:VAL:CG1	2:B:20:VAL:HG23	2.00	0.91
1:E:14:TRP:HA	1:E:17:VAL:HG21	1.52	0.91
1:G:14:TRP:CD1	1:G:67:THR:OG1	2.23	0.91
1:E:109:LEU:O	1:E:113:LEU:CD1	2.19	0.91
2:F:1:VAL:HG11	2:F:132:LYS:CD	1.99	0.91
2:F:91:LEU:HD21	2:F:96:LEU:HD11	1.53	0.91
2:H:127:GLN:CG	2:H:127:GLN:CA	2.49	0.91
2:D:68:LEU:HD13	2:D:68:LEU:N	1.86	0.90
1:E:6:ASP:CB	1:E:124:SER:OG	2.20	0.90
1:E:88:ALA:HA	1:E:140:TYR:CE2	2.05	0.90
1:E:92:ARG:HB3	2:H:37:TRP:HB2	1.50	0.90
2:F:24:GLY:HA3	2:F:68:LEU:HD12	1.51	0.90
1:A:31:ARG:NH1	2:B:122:PHE:O	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:O	1:C:72:HIS:HB2	1.71	0.90
1:G:4:PRO:HG2	1:G:5:ALA:H	1.24	0.90
1:G:118:THR:O	1:G:119:PRO:C	2.07	0.90
2:H:103:PHE:N	2:H:103:PHE:CB	2.34	0.90
1:C:47:ASP:O	1:C:52:SER:OG	1.89	0.90
2:F:49:SER:O	2:F:50:THR:HG23	1.70	0.90
2:H:30:ARG:NE	2:H:30:ARG:CG	2.34	0.90
1:C:119:PRO:HA	1:C:122:HIS:HB3	1.53	0.90
2:B:51:PRO:O	2:B:55:MET:N	2.04	0.90
1:G:109:LEU:HD12	1:G:109:LEU:CA	2.00	0.90
2:H:20:VAL:HG11	2:H:65:LYS:HB2	1.51	0.90
2:D:10:ALA:HB1	2:D:126:VAL:HG13	1.53	0.90
1:G:112:HIS:CB	1:G:113:LEU:HD13	2.02	0.90
2:H:20:VAL:HG13	2:H:68:LEU:HD22	1.54	0.90
1:C:107:VAL:CG1	2:D:112:CYS:SG	2.59	0.90
2:H:34:VAL:C	2:H:36:PRO:HD2	1.96	0.90
1:A:59:GLY:O	1:A:63:ALA:N	2.05	0.90
1:C:38:THR:CA	1:C:38:THR:CG2	2.49	0.90
1:C:118:THR:N	1:C:118:THR:CB	2.35	0.90
2:F:15:TRP:O	2:F:18:VAL:HG23	1.72	0.89
2:D:113:VAL:CG1	2:D:114:LEU:HD23	2.02	0.89
1:G:118:THR:CG2	1:G:121:VAL:HG23	2.02	0.89
2:H:123:THR:HB	2:H:125:PRO:HD2	1.54	0.89
2:B:93:CYS:HB2	2:B:145:TYR:CZ	2.07	0.89
2:B:106:LEU:HA	2:B:109:VAL:CG2	2.01	0.89
1:C:104:CYS:HA	1:C:107:VAL:CG2	2.02	0.89
2:D:114:LEU:HD23	2:D:114:LEU:N	1.87	0.89
2:H:57:ASN:HB3	2:H:60:VAL:HB	1.54	0.89
2:H:114:LEU:HD23	2:H:118:PHE:CD1	2.06	0.89
2:F:1:VAL:HG11	2:F:132:LYS:HD2	1.54	0.89
2:H:22:GLU:CB	2:H:22:GLU:CD	2.45	0.89
2:D:101:GLU:CB	2:D:104:ARG:HD2	2.03	0.89
1:G:87:HIS:CE1	1:G:91:LEU:HD13	2.08	0.89
3:H:147:HEM:CMC	3:H:147:HEM:HBC2	2.01	0.89
1:A:47:ASP:OD1	1:A:49:SER:CB	2.20	0.89
1:A:117:PHE:CD2	1:A:117:PHE:O	2.26	0.89
1:A:134:THR:O	1:A:137:THR:N	2.04	0.89
1:C:117:PHE:C	1:C:118:THR:CA	2.45	0.89
1:G:20:HIS:O	1:G:23:GLU:N	2.05	0.89
2:H:20:VAL:HB	2:H:21:ASP:OD1	1.71	0.89
2:H:86:ALA:HB1	2:H:144:LYS:CE	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:CB	1:A:76:MET:C	2.45	0.89
1:G:66:LEU:C	1:G:67:THR:CA	2.45	0.89
1:G:76:MET:HE2	1:G:131:SER:HB2	1.54	0.89
2:D:146:HIS:HD2	2:D:146:HIS:H	1.10	0.88
2:H:38:THR:O	2:H:41:PHE:CD1	2.26	0.88
2:B:59:LYS:HA	2:B:59:LYS:NZ	1.87	0.88
2:B:65:LYS:O	2:B:69:GLY:N	2.05	0.88
2:D:32:LEU:HD21	2:D:42:PHE:HE1	1.36	0.88
2:D:107:GLY:O	2:D:111:VAL:HG23	1.73	0.88
2:B:58:PRO:HA	2:B:61:LYS:HB2	1.54	0.88
1:C:116:GLU:OE1	1:C:116:GLU:CA	2.19	0.88
1:E:43:PHE:CE2	3:E:142:HEM:HBC2	2.08	0.88
1:E:106:LEU:CD1	1:E:106:LEU:HA	2.01	0.88
1:G:4:PRO:CG	1:G:5:ALA:N	2.37	0.88
2:H:86:ALA:HB1	2:H:144:LYS:HE3	1.55	0.88
2:H:28:LEU:HD21	2:H:63:HIS:CD2	2.09	0.88
2:H:68:LEU:N	2:H:68:LEU:CB	2.36	0.88
2:H:93:CYS:HB2	2:H:145:TYR:CD1	2.08	0.88
1:C:64:ASP:OD1	1:C:64:ASP:N	2.07	0.88
2:D:51:PRO:CA	2:D:54:VAL:HG23	2.03	0.88
2:D:142:ALA:CB	2:D:142:ALA:N	2.37	0.87
2:F:135:ALA:O	2:F:138:ALA:HB3	1.74	0.87
1:G:101:LEU:CD1	1:G:101:LEU:CB	2.52	0.87
1:G:29:LEU:HD21	1:G:58:HIS:CD2	2.08	0.87
2:H:38:THR:O	2:H:41:PHE:HD1	1.55	0.87
1:E:38:THR:HG23	1:E:39:THR:N	1.88	0.87
2:D:14:LEU:HD21	2:D:126:VAL:HG13	1.56	0.87
2:D:44:SER:C	2:D:45:PHE:HD2	1.82	0.87
1:E:129:LEU:HD23	1:E:129:LEU:O	1.75	0.87
2:F:39:GLN:HB3	2:F:39:GLN:HE21	0.71	0.87
1:G:109:LEU:CD1	1:G:109:LEU:CA	2.53	0.87
1:G:118:THR:HB	1:G:121:VAL:HG23	1.56	0.87
2:H:98:VAL:C	2:H:99:ASP:CA	2.46	0.87
1:A:110:ALA:HB1	2:B:115:ALA:CB	2.04	0.87
3:E:142:HEM:CMB	3:E:142:HEM:CBB	2.51	0.87
1:C:7:LYS:CE	1:C:74:ASP:OD1	2.23	0.86
1:C:118:THR:O	1:C:122:HIS:N	2.08	0.86
1:E:99:LYS:CB	1:E:100:LEU:HD23	2.02	0.86
2:H:20:VAL:HG13	2:H:68:LEU:CD2	2.05	0.86
1:A:87:HIS:CB	1:A:136:LEU:CD1	2.54	0.86
1:C:45:HIS:ND1	1:C:45:HIS:N	2.16	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:LYS:CG	1:G:61:LYS:CE	2.54	0.86
1:A:76:MET:CB	1:A:76:MET:N	2.37	0.86
1:C:132:VAL:CG1	1:C:132:VAL:CA	2.52	0.86
1:C:24:TYR:CD2	1:C:24:TYR:N	2.38	0.86
2:D:80:ASN:CG	2:D:83:GLY:HA3	2.01	0.86
2:D:110:LEU:O	2:D:110:LEU:CG	2.24	0.86
1:G:84:SER:N	1:G:136:LEU:HD23	1.89	0.86
1:C:24:TYR:N	1:C:24:TYR:HD2	1.72	0.86
2:F:31:LEU:HD13	2:F:109:VAL:CG2	2.04	0.86
1:A:1:VAL:C	1:A:2:LEU:HD23	2.00	0.86
1:E:106:LEU:CD1	1:E:106:LEU:CD2	2.54	0.86
1:A:20:HIS:H	1:A:20:HIS:CD2	1.93	0.86
1:A:51:GLY:O	1:A:56:LYS:CE	2.23	0.86
1:A:61:LYS:CG	1:A:61:LYS:CE	2.53	0.86
2:B:141:LEU:HD21	3:B:147:HEM:HBB2	1.56	0.86
1:C:88:ALA:C	1:C:89:HIS:ND1	2.34	0.86
1:C:130:ALA:HA	1:C:133:SER:OG	1.74	0.86
1:E:2:LEU:HA	1:E:127:LYS:NZ	1.91	0.86
1:G:103:HIS:O	1:G:107:VAL:CG2	2.24	0.86
2:H:98:VAL:HG13	2:H:102:ASN:OD1	1.74	0.86
3:H:147:HEM:CBC	3:H:147:HEM:HMC1	2.05	0.86
2:F:14:LEU:O	2:F:17:LYS:CB	2.21	0.86
1:G:31:ARG:NH1	2:H:122:PHE:O	2.09	0.86
1:G:87:HIS:ND1	1:G:91:LEU:CD1	2.38	0.86
2:H:9:SER:O	2:H:13:ALA:HB3	1.75	0.86
1:C:141:ARG:NE	1:C:141:ARG:HG2	1.89	0.86
2:D:51:PRO:O	2:D:55:MET:HB2	1.74	0.86
2:H:82:LYS:H	2:H:82:LYS:HD3	1.39	0.85
2:F:4:THR:CB	2:F:7:GLU:CG	2.47	0.85
1:A:87:HIS:CG	1:A:136:LEU:CD1	2.54	0.85
1:C:110:ALA:HB1	2:D:115:ALA:HB1	1.58	0.85
2:D:11:VAL:HG21	2:D:133:VAL:CG2	2.06	0.85
1:A:40:LYS:C	1:A:41:THR:CA	2.49	0.85
1:C:16:LYS:CG	1:C:16:LYS:HE2	2.06	0.85
1:C:68:ASN:O	1:C:72:HIS:CD2	2.29	0.85
2:D:14:LEU:CD1	2:D:14:LEU:CD2	2.55	0.85
2:D:64:GLY:O	2:D:68:LEU:HD22	1.76	0.85
1:G:112:HIS:CB	1:G:112:HIS:C	2.49	0.85
1:G:117:PHE:CB	1:G:117:PHE:C	2.49	0.85
1:A:118:THR:HB	1:A:121:VAL:CG2	2.06	0.85
1:C:16:LYS:CD	1:C:16:LYS:HB2	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:LEU:HD13	2:F:109:VAL:HG21	1.56	0.85
1:G:32:MET:SD	1:G:101:LEU:HB2	2.17	0.85
1:A:118:THR:HG22	1:A:119:PRO:HD2	1.55	0.85
2:D:76:ALA:HB3	2:D:77:HIS:ND1	1.91	0.85
1:A:100:LEU:N	1:A:100:LEU:CD2	2.39	0.85
1:C:118:THR:CB	1:C:121:VAL:HB	2.07	0.85
2:D:15:TRP:CD1	2:D:130:TYR:OH	2.28	0.85
1:A:4:PRO:HG2	1:A:5:ALA:N	1.91	0.85
1:C:118:THR:HG23	1:C:120:ALA:CB	2.07	0.85
1:G:103:HIS:O	1:G:107:VAL:HG22	1.77	0.85
1:C:3:SER:O	1:C:6:ASP:HB2	1.77	0.85
2:F:98:VAL:O	2:F:145:TYR:OH	1.94	0.85
1:C:16:LYS:HZ2	1:C:116:GLU:HG3	1.41	0.84
2:F:63:HIS:HE1	3:F:147:HEM:ND	1.75	0.84
1:G:27:GLU:O	1:G:31:ARG:HB2	1.76	0.84
1:A:20:HIS:CD2	1:A:20:HIS:N	2.40	0.84
1:A:51:GLY:O	1:A:56:LYS:HE2	1.76	0.84
2:D:33:VAL:HG22	2:D:54:VAL:HG21	1.58	0.84
2:D:107:GLY:CA	2:D:134:VAL:CG2	2.42	0.84
1:G:30:GLU:HG3	1:G:50:HIS:CD2	2.12	0.84
1:E:6:ASP:HA	1:E:124:SER:OG	1.75	0.84
2:H:78:LEU:HB3	2:H:81:LEU:HD21	1.57	0.84
2:D:101:GLU:HA	2:D:104:ARG:HH11	0.71	0.84
1:C:58:HIS:O	1:C:62:VAL:N	2.11	0.84
2:H:82:LYS:H	2:H:82:LYS:CD	1.90	0.84
2:B:59:LYS:O	2:B:62:ALA:HB3	1.77	0.84
1:E:52:SER:HB2	1:E:54:GLN:H	1.43	0.84
2:F:127:GLN:O	2:F:131:GLN:N	2.11	0.84
1:G:93:VAL:HG11	3:G:142:HEM:CAC	2.08	0.84
1:A:87:HIS:O	1:A:91:LEU:HB2	1.77	0.84
2:F:50:THR:O	2:F:53:ALA:HB3	1.77	0.84
1:C:17:VAL:CG1	1:C:21:ALA:HA	2.07	0.84
1:A:127:LYS:HE2	1:C:141:ARG:O	1.78	0.83
1:E:15:GLY:O	1:E:16:LYS:C	2.14	0.83
2:F:90:GLU:CD	2:F:90:GLU:CB	2.50	0.83
2:B:42:PHE:O	2:B:45:PHE:HB2	1.79	0.83
1:C:7:LYS:CE	1:C:74:ASP:OD2	2.26	0.83
2:B:17:LYS:HE2	2:B:17:LYS:CB	2.08	0.83
2:F:58:PRO:O	2:F:62:ALA:HB3	1.77	0.83
2:F:80:ASN:HD21	2:F:83:GLY:H	0.90	0.83
2:H:21:ASP:OD1	2:H:21:ASP:N	2.06	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:109:VAL:HG13	2:H:109:VAL:O	1.77	0.83
1:C:118:THR:N	1:C:118:THR:C	2.35	0.83
1:C:132:VAL:CG1	1:C:132:VAL:CG2	2.56	0.83
1:E:13:ALA:O	1:E:16:LYS:HB2	1.78	0.83
1:C:78:ASN:N	1:C:78:ASN:CG	2.36	0.83
2:B:110:LEU:HD12	2:B:110:LEU:O	1.79	0.83
2:F:90:GLU:CG	2:F:90:GLU:OE1	2.26	0.83
1:A:36:PHE:CE1	1:A:100:LEU:HD13	2.14	0.83
1:C:93:VAL:HG11	3:C:142:HEM:HAC	1.61	0.83
2:H:137:VAL:C	2:H:141:LEU:HD23	2.02	0.83
2:B:92:HIS:HA	2:B:96:LEU:HD12	1.58	0.83
2:D:14:LEU:C	2:D:14:LEU:HD12	2.04	0.83
2:F:49:SER:C	2:F:50:THR:HG23	2.03	0.83
2:H:86:ALA:HB1	2:H:144:LYS:NZ	1.94	0.83
2:D:63:HIS:O	2:D:67:VAL:N	2.11	0.83
2:H:68:LEU:O	2:H:72:SER:OG	1.96	0.83
2:B:38:THR:N	2:B:38:THR:CB	2.40	0.82
1:G:87:HIS:CE1	1:G:91:LEU:CD1	2.61	0.82
1:A:88:ALA:HB2	1:A:139:LYS:CB	2.09	0.82
1:E:122:HIS:CE1	2:F:30:ARG:HD3	2.14	0.82
2:H:22:GLU:CG	2:H:22:GLU:CA	2.56	0.82
2:B:17:LYS:CG	2:B:17:LYS:CE	2.57	0.82
2:H:67:VAL:C	2:H:68:LEU:CA	2.53	0.82
2:B:107:GLY:HA3	2:B:134:VAL:HG22	1.61	0.82
1:E:11:LYS:CA	1:E:11:LYS:CG	2.57	0.82
2:H:4:THR:HG22	2:H:7:GLU:H	1.44	0.82
2:D:44:SER:OG	2:D:45:PHE:CE2	2.26	0.82
1:E:122:HIS:ND1	2:F:30:ARG:NE	2.28	0.82
2:F:11:VAL:HG23	2:F:130:TYR:CE1	2.13	0.82
1:G:109:LEU:CD1	1:G:109:LEU:HA	2.06	0.82
1:G:112:HIS:O	1:G:113:LEU:HD12	1.80	0.82
1:C:37:PRO:O	1:C:40:LYS:HB2	1.80	0.82
2:D:91:LEU:O	2:D:91:LEU:CG	2.27	0.82
2:F:8:LYS:CB	2:F:8:LYS:CD	2.57	0.82
1:E:66:LEU:CD1	3:E:142:HEM:HMB1	2.10	0.82
2:H:146:HIS:H	2:H:146:HIS:CD2	1.95	0.82
2:B:4:THR:CG2	2:B:5:PRO:HD2	2.09	0.82
2:H:9:SER:O	2:H:13:ALA:CB	2.28	0.82
1:C:27:GLU:CG	1:C:108:THR:HG23	2.06	0.82
2:D:47:ASP:OD2	2:D:49:SER:CB	2.27	0.82
2:F:80:ASN:ND2	2:F:83:GLY:N	2.21	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:CA	1:A:76:MET:HG2	2.08	0.82
2:D:44:SER:HB3	2:D:45:PHE:CD2	2.14	0.82
2:F:4:THR:HG22	2:F:6:VAL:H	1.44	0.82
1:G:29:LEU:HB2	1:G:101:LEU:HD11	1.62	0.82
2:H:93:CYS:CB	2:H:145:TYR:CE1	2.62	0.82
2:D:51:PRO:C	2:D:54:VAL:HG23	2.05	0.81
1:E:27:GLU:O	1:E:31:ARG:HB2	1.80	0.81
1:G:88:ALA:HB2	1:G:140:TYR:CD2	2.15	0.81
1:A:38:THR:O	1:A:41:THR:HG23	1.79	0.81
2:B:28:LEU:HD12	2:B:32:LEU:HD22	1.60	0.81
2:B:107:GLY:CA	2:B:134:VAL:HG21	2.10	0.81
2:B:107:GLY:HA2	2:B:134:VAL:HG21	1.61	0.81
2:D:68:LEU:HD22	2:D:68:LEU:H	1.44	0.81
2:D:75:LEU:HD13	2:D:75:LEU:N	1.95	0.81
1:A:38:THR:O	1:A:41:THR:CG2	2.28	0.81
1:A:87:HIS:ND1	1:A:136:LEU:HD11	1.95	0.81
2:B:59:LYS:CE	2:B:59:LYS:CA	2.57	0.81
2:B:146:HIS:N	2:B:146:HIS:HD2	1.75	0.81
2:D:65:LYS:NZ	2:D:65:LYS:CD	2.43	0.81
2:D:72:SER:HA	2:D:75:LEU:HD22	1.62	0.81
1:E:88:ALA:HB2	1:E:140:TYR:CD2	2.15	0.81
1:G:75:ASP:C	1:G:77:PRO:HD2	2.05	0.81
1:A:65:ALA:HB1	1:A:80:LEU:CD2	2.10	0.81
1:C:27:GLU:CG	1:C:108:THR:CG2	2.57	0.81
1:C:47:ASP:O	1:C:52:SER:CB	2.28	0.81
1:G:66:LEU:HD21	1:G:132:VAL:HG21	1.61	0.81
1:G:80:LEU:CG	1:G:135:VAL:HG11	2.10	0.81
2:H:21:ASP:OD1	2:H:65:LYS:CG	2.27	0.81
2:H:26:GLU:OE1	2:H:30:ARG:NH1	2.13	0.81
2:H:31:LEU:HD23	2:H:106:LEU:CD2	2.11	0.81
2:H:117:HIS:CD2	2:H:118:PHE:CZ	2.68	0.81
2:B:14:LEU:HD11	2:B:114:LEU:HD13	1.60	0.81
2:B:72:SER:HA	2:B:75:LEU:CD1	2.10	0.81
2:D:48:LEU:HD21	2:D:60:VAL:HG21	1.62	0.81
2:D:87:THR:CG2	2:D:88:LEU:N	2.44	0.81
1:E:43:PHE:HZ	3:E:142:HEM:HBC2	1.00	0.81
1:G:87:HIS:N	1:G:91:LEU:HD12	1.94	0.81
1:A:6:ASP:O	1:A:10:VAL:CG2	2.29	0.81
1:C:16:LYS:CD	1:C:116:GLU:HG3	2.10	0.81
2:D:24:GLY:CA	2:D:68:LEU:CD2	2.57	0.81
2:D:81:LEU:HA	2:D:84:THR:HG22	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:LEU:CD1	2:D:141:LEU:CD2	2.57	0.81
1:A:98:PHE:HE1	3:A:142:HEM:CAB	1.92	0.81
2:B:96:LEU:O	2:B:97:HIS:HB2	1.80	0.81
1:C:7:LYS:HE2	1:C:74:ASP:OD1	1.81	0.81
1:C:66:LEU:HD21	1:C:129:LEU:HD21	1.61	0.81
1:C:113:LEU:HD22	1:C:116:GLU:CB	2.10	0.81
2:D:26:GLU:CD	2:D:30:ARG:HH11	1.86	0.81
2:H:84:THR:OG1	2:H:84:THR:CA	2.28	0.81
1:C:10:VAL:HG23	1:C:125:LEU:HD23	1.63	0.81
1:C:31:ARG:NH1	2:D:127:GLN:OE1	2.14	0.81
2:D:72:SER:CA	2:D:75:LEU:HD22	2.11	0.81
1:G:6:ASP:OD1	1:G:127:LYS:CE	2.29	0.81
1:G:110:ALA:HB3	2:H:115:ALA:HB3	1.61	0.81
2:H:66:LYS:HB3	2:H:67:VAL:HG23	1.63	0.81
1:C:16:LYS:CG	1:C:16:LYS:O	2.27	0.81
1:E:35:SER:OG	1:E:35:SER:CA	2.29	0.81
1:E:93:VAL:HG11	3:E:142:HEM:HAC	1.63	0.81
1:E:106:LEU:CD1	1:E:106:LEU:HB2	2.10	0.81
1:A:37:PRO:CB	1:A:37:PRO:C	2.53	0.80
2:H:26:GLU:CD	2:H:30:ARG:HH11	1.87	0.80
2:H:46:GLY:O	2:H:48:LEU:HD23	1.81	0.80
1:A:127:LYS:CD	1:C:141:ARG:HD3	2.09	0.80
1:C:16:LYS:O	1:C:16:LYS:HG3	1.80	0.80
2:D:87:THR:HG23	2:D:88:LEU:N	1.97	0.80
1:E:27:GLU:CD	1:E:112:HIS:HE2	1.90	0.80
3:H:147:HEM:CMC	3:H:147:HEM:CBC	2.55	0.80
1:C:43:PHE:HD2	1:C:46:PHE:CG	1.99	0.80
1:E:120:ALA:O	1:E:123:ALA:HB3	1.82	0.80
2:F:1:VAL:CG1	2:F:132:LYS:CD	2.57	0.80
2:H:135:ALA:O	2:H:138:ALA:HB3	1.81	0.80
2:B:92:HIS:CA	2:B:96:LEU:HD13	2.12	0.80
2:H:80:ASN:O	2:H:84:THR:OG1	1.98	0.80
2:H:117:HIS:CD2	2:H:118:PHE:CG	2.69	0.80
1:A:30:GLU:OE1	1:A:50:HIS:ND1	2.15	0.80
1:A:98:PHE:CE1	3:A:142:HEM:HAB	2.17	0.80
2:B:21:ASP:HB3	2:B:65:LYS:HB2	1.64	0.80
2:B:35:TYR:HB3	2:B:37:TRP:CZ2	2.17	0.80
2:D:110:LEU:O	2:D:110:LEU:CD2	2.29	0.80
2:D:146:HIS:N	2:D:146:HIS:HD2	1.69	0.80
2:F:63:HIS:HE1	3:F:147:HEM:C1D	2.00	0.80
2:F:114:LEU:C	2:F:114:LEU:HD23	2.04	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:HIS:HA	2:B:96:LEU:HD13	1.63	0.80
2:D:121:GLU:O	2:D:123:THR:N	2.15	0.80
1:G:17:VAL:HG13	1:G:24:TYR:CD1	2.16	0.80
1:A:10:VAL:HG13	1:A:125:LEU:HD23	1.64	0.80
2:B:4:THR:CG2	2:B:5:PRO:CD	2.59	0.80
2:B:88:LEU:H	2:B:88:LEU:HD12	1.45	0.80
1:A:88:ALA:HB2	1:A:139:LYS:HB2	1.62	0.80
1:E:52:SER:HB2	1:E:54:GLN:HB3	1.64	0.80
3:G:142:HEM:HBB2	3:G:142:HEM:HMB1	1.63	0.80
2:D:71:PHE:O	2:D:75:LEU:HD13	1.82	0.80
1:G:62:VAL:O	1:G:65:ALA:HB3	1.82	0.80
1:E:32:MET:HG2	1:E:39:THR:HG21	1.63	0.80
2:F:63:HIS:HE1	3:F:147:HEM:C4D	1.99	0.80
2:H:91:LEU:CD1	2:H:91:LEU:CB	2.58	0.79
2:H:98:VAL:O	2:H:98:VAL:HG12	1.81	0.79
1:C:55:VAL:O	1:C:55:VAL:HG13	1.82	0.79
2:D:14:LEU:HD11	2:D:130:TYR:HE2	1.47	0.79
2:D:127:GLN:O	2:D:131:GLN:HG2	1.82	0.79
2:F:1:VAL:CB	2:F:132:LYS:HG3	2.13	0.79
1:G:83:LEU:C	1:G:136:LEU:CD2	2.55	0.79
1:A:139:LYS:C	1:A:141:ARG:HG3	2.08	0.79
2:B:111:VAL:CG1	2:B:111:VAL:O	2.28	0.79
1:G:29:LEU:HD13	1:G:33:PHE:CE2	2.17	0.79
1:C:119:PRO:O	1:C:120:ALA:C	2.17	0.79
2:D:14:LEU:O	2:D:15:TRP:C	2.23	0.79
2:D:42:PHE:O	2:D:45:PHE:HB2	1.80	0.79
1:E:4:PRO:HA	1:E:7:LYS:HD2	1.63	0.79
2:F:2:HIS:CE1	2:F:132:LYS:HZ1	1.97	0.79
2:F:22:GLU:HG2	2:F:23:VAL:N	1.80	0.79
2:B:131:GLN:O	2:B:135:ALA:CB	2.31	0.79
2:D:77:HIS:CB	2:D:77:HIS:H	1.96	0.79
1:G:17:VAL:O	1:G:19:ALA:N	2.16	0.79
1:G:30:GLU:CG	1:G:50:HIS:HE2	1.82	0.79
2:H:30:ARG:CD	2:H:30:ARG:CZ	2.61	0.79
2:B:107:GLY:CA	2:B:134:VAL:CG2	2.60	0.79
1:E:129:LEU:HD23	1:E:129:LEU:C	2.05	0.79
2:B:92:HIS:O	2:B:97:HIS:N	2.16	0.79
1:E:141:ARG:CG	2:H:37:TRP:HZ3	1.95	0.79
1:G:20:HIS:HB3	1:G:23:GLU:CB	2.12	0.79
2:H:92:HIS:CD2	2:H:103:PHE:CZ	2.71	0.79
2:D:14:LEU:HD21	2:D:126:VAL:HG11	0.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:73:ASP:O	2:H:76:ALA:CB	2.30	0.79
1:G:67:THR:N	1:G:67:THR:CB	2.46	0.79
2:H:4:THR:CG2	2:H:7:GLU:HB2	2.13	0.79
2:H:117:HIS:HD2	2:H:118:PHE:CZ	2.00	0.79
1:A:80:LEU:O	1:A:84:SER:N	2.16	0.79
1:G:47:ASP:C	1:G:48:LEU:HD23	2.08	0.79
1:C:141:ARG:NE	1:C:141:ARG:HG3	1.98	0.78
1:G:76:MET:CE	1:G:131:SER:HB2	2.13	0.78
1:A:98:PHE:HB3	1:A:133:SER:CB	2.13	0.78
1:C:7:LYS:HE2	1:C:74:ASP:CG	2.08	0.78
2:D:80:ASN:HD21	2:D:83:GLY:HA2	1.47	0.78
2:D:128:ALA:C	2:D:131:GLN:HB2	2.08	0.78
1:E:68:ASN:C	1:E:69:ALA:CA	2.54	0.78
1:G:109:LEU:CD1	1:G:109:LEU:HD22	2.12	0.78
2:D:73:ASP:O	2:D:76:ALA:CB	2.31	0.78
2:D:101:GLU:O	2:D:104:ARG:HG2	1.83	0.78
2:D:107:GLY:HA2	2:D:134:VAL:HG21	1.63	0.78
2:F:20:VAL:O	2:F:68:LEU:HD12	1.81	0.78
2:B:4:THR:CG2	2:B:5:PRO:N	2.45	0.78
2:D:113:VAL:O	2:D:116:HIS:HB3	1.83	0.78
1:E:68:ASN:OD1	1:E:72:HIS:NE2	2.16	0.78
1:G:30:GLU:CD	1:G:50:HIS:NE2	2.36	0.78
2:D:11:VAL:CG1	2:D:12:THR:N	2.45	0.78
1:A:110:ALA:O	2:B:116:HIS:HA	1.84	0.78
1:A:118:THR:CB	1:A:121:VAL:CG2	2.62	0.78
2:D:110:LEU:C	2:D:110:LEU:CD2	2.48	0.78
2:H:34:VAL:O	2:H:36:PRO:HD2	1.83	0.78
1:C:55:VAL:O	1:C:55:VAL:CG1	2.24	0.78
1:E:121:VAL:O	1:E:121:VAL:CG1	2.32	0.78
1:E:141:ARG:HG2	2:H:37:TRP:HZ3	1.47	0.78
2:F:49:SER:O	2:F:50:THR:CG2	2.31	0.78
1:E:107:VAL:O	1:E:110:ALA:HB3	1.84	0.78
2:H:80:ASN:OD1	2:H:83:GLY:HA3	1.84	0.78
2:H:92:HIS:CD2	2:H:98:VAL:HG21	2.19	0.78
1:A:120:ALA:C	1:A:121:VAL:CA	2.55	0.78
1:G:80:LEU:CB	1:G:135:VAL:CG1	2.59	0.78
1:A:61:LYS:CG	1:A:61:LYS:HA	2.14	0.77
2:B:18:VAL:CG1	2:B:18:VAL:CG2	2.60	0.77
2:D:58:PRO:O	2:D:62:ALA:CB	2.32	0.77
1:C:16:LYS:HD3	1:C:116:GLU:CG	2.14	0.77
1:C:39:THR:OG1	1:C:39:THR:CA	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:THR:HG22	1:G:121:VAL:HG23	1.64	0.77
2:H:92:HIS:O	2:H:96:LEU:HB2	1.85	0.77
2:H:21:ASP:CA	2:H:65:LYS:HB3	2.14	0.77
2:H:24:GLY:CA	2:H:68:LEU:HD13	2.06	0.77
1:G:84:SER:CA	1:G:136:LEU:CD2	2.59	0.77
2:B:60:VAL:O	2:B:61:LYS:C	2.23	0.77
1:G:47:ASP:C	1:G:47:ASP:CG	2.53	0.77
2:H:6:VAL:O	2:H:7:GLU:C	2.23	0.77
2:B:68:LEU:N	2:B:68:LEU:CD2	2.46	0.77
1:E:52:SER:CB	1:E:54:GLN:HB3	2.14	0.77
1:A:111:ALA:HB1	2:B:119:GLY:HA2	1.65	0.77
1:C:40:LYS:CG	1:C:40:LYS:HE2	2.15	0.77
2:H:137:VAL:CG2	2:H:137:VAL:CG1	2.61	0.77
1:G:3:SER:HB2	1:G:4:PRO:CD	2.15	0.77
2:H:39:GLN:O	2:H:41:PHE:N	2.18	0.77
2:B:57:ASN:O	2:B:61:LYS:N	2.16	0.77
2:F:14:LEU:HD21	2:F:118:PHE:CD2	2.19	0.77
2:H:23:VAL:HG23	2:H:68:LEU:HD21	1.66	0.77
2:B:92:HIS:CG	2:B:96:LEU:CD1	2.68	0.76
1:E:16:LYS:HE2	1:E:116:GLU:OE2	1.84	0.76
2:D:141:LEU:CD1	2:D:141:LEU:HB3	2.13	0.76
2:F:54:VAL:O	2:F:54:VAL:HG12	1.84	0.76
1:G:112:HIS:HB3	1:G:113:LEU:CD1	2.13	0.76
2:H:20:VAL:CG1	2:H:65:LYS:CB	2.51	0.76
1:A:86:LEU:HD13	1:A:90:LYS:HZ1	1.47	0.76
2:B:15:TRP:CH2	2:B:71:PHE:CE2	2.74	0.76
2:D:112:CYS:O	2:D:115:ALA:HB3	1.85	0.76
1:E:88:ALA:HA	1:E:140:TYR:CD2	2.20	0.76
1:E:96:VAL:HG23	2:H:101:GLU:HG2	1.67	0.76
2:H:123:THR:CG2	2:H:123:THR:OG1	2.33	0.76
2:B:92:HIS:CG	2:B:96:LEU:HD13	2.19	0.76
2:D:91:LEU:CD1	2:D:95:LYS:CB	2.62	0.76
2:D:125:PRO:CB	2:D:125:PRO:C	2.56	0.76
1:E:69:ALA:N	1:E:69:ALA:CB	2.48	0.76
2:H:84:THR:H	2:H:84:THR:HG1	1.33	0.76
2:B:8:LYS:HD3	2:B:8:LYS:HB3	1.67	0.76
2:B:73:ASP:O	2:B:77:HIS:HE1	1.68	0.76
2:D:67:VAL:C	2:D:68:LEU:HD13	2.11	0.76
1:E:13:ALA:O	1:E:17:VAL:HG23	1.86	0.76
2:F:1:VAL:HG12	2:F:132:LYS:HE2	0.83	0.76
2:H:35:TYR:O	2:H:38:THR:CG2	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:VAL:CG1	2:B:18:VAL:C	2.59	0.76
1:C:110:ALA:CB	2:D:115:ALA:HB1	2.15	0.76
2:D:44:SER:CB	2:D:45:PHE:CD2	2.69	0.76
2:H:93:CYS:CB	2:H:145:TYR:CD1	2.69	0.76
1:G:28:ALA:HA	1:G:108:THR:HG21	1.68	0.76
1:G:121:VAL:CA	1:G:124:SER:OG	2.34	0.76
2:F:6:VAL:O	2:F:9:SER:HB3	1.84	0.76
2:F:8:LYS:CG	2:F:8:LYS:CA	2.62	0.76
2:F:90:GLU:CG	2:F:90:GLU:OE2	2.34	0.76
1:G:4:PRO:O	1:G:5:ALA:C	2.27	0.76
1:G:114:PRO:CG	1:G:115:ALA:N	2.46	0.76
2:B:14:LEU:CD1	2:B:114:LEU:HD13	2.15	0.76
1:E:114:PRO:O	2:F:116:HIS:NE2	2.18	0.76
2:H:137:VAL:CG2	2:H:137:VAL:CA	2.63	0.76
2:B:37:TRP:C	2:B:38:THR:CA	2.57	0.75
2:F:91:LEU:CD2	2:F:96:LEU:CD1	2.63	0.75
1:G:6:ASP:OD1	1:G:127:LYS:HE3	1.84	0.75
2:B:101:GLU:OE1	2:B:104:ARG:CZ	2.34	0.75
1:C:119:PRO:HB3	2:D:30:ARG:HG3	1.67	0.75
2:D:15:TRP:O	2:D:18:VAL:HG23	1.85	0.75
1:E:106:LEU:CD1	1:E:106:LEU:CA	2.64	0.75
2:F:124:PRO:N	2:F:125:PRO:CD	2.49	0.75
2:H:4:THR:HB	2:H:7:GLU:HB2	0.78	0.75
1:A:134:THR:C	1:A:137:THR:H	1.94	0.75
2:B:52:ASP:O	2:B:53:ALA:C	2.28	0.75
1:E:141:ARG:HG2	2:H:37:TRP:CZ3	2.21	0.75
1:G:66:LEU:HD12	1:G:132:VAL:HG11	1.63	0.75
2:H:31:LEU:HD23	2:H:106:LEU:HD23	1.67	0.75
2:D:113:VAL:HG12	2:D:114:LEU:N	2.00	0.75
2:F:40:ARG:CD	2:F:40:ARG:CB	2.63	0.75
2:H:87:THR:O	2:H:88:LEU:C	2.29	0.75
1:A:127:LYS:HD2	1:C:141:ARG:CD	2.12	0.75
1:C:31:ARG:HG2	2:D:127:GLN:CD	2.12	0.75
1:C:64:ASP:CB	1:C:64:ASP:N	2.48	0.75
1:G:66:LEU:HD11	1:G:132:VAL:HG11	1.16	0.75
1:A:87:HIS:HB3	1:A:136:LEU:CD1	2.17	0.75
2:D:51:PRO:HA	2:D:54:VAL:HG23	1.65	0.75
2:F:81:LEU:HD22	2:F:85:PHE:HE1	1.51	0.75
2:H:32:LEU:HD12	2:H:38:THR:OG1	1.87	0.75
2:B:4:THR:HG22	2:B:6:VAL:H	1.49	0.75
2:B:15:TRP:HE1	2:B:72:SER:HB3	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:LYS:CD	2:B:17:LYS:CB	2.65	0.75
2:B:51:PRO:CA	2:B:54:VAL:HB	2.16	0.75
1:C:17:VAL:HG11	1:C:21:ALA:HA	1.69	0.75
1:G:130:ALA:O	1:G:134:THR:N	2.20	0.75
2:H:85:PHE:CD1	2:H:85:PHE:N	2.53	0.75
1:A:65:ALA:HB1	1:A:80:LEU:HD21	1.67	0.75
2:B:131:GLN:O	2:B:135:ALA:HB3	1.87	0.75
1:C:77:PRO:O	1:C:78:ASN:CA	2.34	0.75
1:E:39:THR:O	1:E:43:PHE:CE1	2.39	0.75
1:E:45:HIS:N	1:E:45:HIS:ND1	2.22	0.75
1:G:47:ASP:C	1:G:47:ASP:N	2.44	0.75
1:G:84:SER:N	1:G:136:LEU:HD21	2.02	0.75
2:H:11:VAL:HG23	2:H:12:THR:N	2.01	0.75
2:D:3:LEU:HD23	2:D:132:LYS:HB3	1.68	0.75
1:G:66:LEU:HD11	1:G:132:VAL:CB	2.17	0.75
2:H:109:VAL:O	2:H:109:VAL:CG1	2.34	0.75
1:C:13:ALA:N	1:C:13:ALA:C	2.44	0.74
2:D:90:GLU:O	2:D:94:ASP:N	2.19	0.74
2:F:101:GLU:O	2:F:104:ARG:HB2	1.86	0.74
2:B:59:LYS:HE3	2:B:62:ALA:CB	2.16	0.74
1:C:7:LYS:CE	1:C:74:ASP:CG	2.58	0.74
2:D:146:HIS:CD2	2:D:146:HIS:H	1.93	0.74
2:F:2:HIS:CE1	2:F:132:LYS:NZ	2.54	0.74
2:F:45:PHE:O	2:F:57:ASN:ND2	2.20	0.74
2:F:80:ASN:O	2:F:84:THR:OG1	2.05	0.74
1:G:43:PHE:N	1:G:43:PHE:CD1	2.55	0.74
1:G:60:LYS:NZ	1:G:60:LYS:CD	2.50	0.74
2:H:93:CYS:HB2	2:H:145:TYR:CZ	2.22	0.74
2:B:18:VAL:HG11	2:B:20:VAL:HG23	1.69	0.74
1:C:36:PHE:HZ	1:C:103:HIS:CE1	2.04	0.74
1:C:113:LEU:HB3	1:C:116:GLU:HB2	1.67	0.74
2:D:26:GLU:O	2:D:30:ARG:N	2.20	0.74
1:G:30:GLU:HG3	1:G:50:HIS:HE2	0.87	0.74
2:B:92:HIS:CB	2:B:96:LEU:HD13	2.17	0.74
1:C:6:ASP:OD2	1:C:127:LYS:CE	2.29	0.74
1:E:107:VAL:C	1:E:110:ALA:CB	2.60	0.74
1:E:96:VAL:CG2	2:H:101:GLU:CG	2.65	0.74
2:H:21:ASP:CB	2:H:65:LYS:HG3	2.18	0.74
1:A:98:PHE:HE1	3:A:142:HEM:HAB	1.51	0.74
2:D:101:GLU:CB	2:D:104:ARG:HH11	2.01	0.74
1:G:30:GLU:CG	1:G:50:HIS:CD2	2.58	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:SER:HG	1:G:136:LEU:HA	1.52	0.74
1:G:118:THR:HB	1:G:121:VAL:HG21	1.69	0.74
2:B:88:LEU:HD21	2:H:6:VAL:HG13	1.67	0.74
2:D:58:PRO:O	2:D:62:ALA:HB2	1.85	0.74
1:G:42:TYR:CE1	1:G:93:VAL:HG13	2.23	0.74
2:B:107:GLY:HA3	2:B:134:VAL:CG2	2.17	0.74
2:D:44:SER:CB	2:D:45:PHE:CE2	2.70	0.74
2:D:28:LEU:O	2:D:28:LEU:HD12	1.88	0.74
1:C:66:LEU:HD21	1:C:129:LEU:HD22	1.64	0.74
2:D:77:HIS:N	2:D:77:HIS:HB2	1.99	0.74
1:E:14:TRP:HA	1:E:17:VAL:CB	2.17	0.74
1:E:88:ALA:HB2	1:E:140:TYR:HD2	1.53	0.74
1:A:138:SER:C	1:A:139:LYS:HD2	2.13	0.73
1:E:106:LEU:HD12	1:E:106:LEU:CA	2.15	0.73
1:G:80:LEU:HB3	1:G:135:VAL:HG11	1.66	0.73
2:D:3:LEU:HD22	2:D:132:LYS:CB	2.11	0.73
2:D:124:PRO:N	2:D:125:PRO:HD2	2.03	0.73
1:G:36:PHE:N	1:G:37:PRO:HD3	2.01	0.73
1:C:107:VAL:CA	1:C:110:ALA:HB2	2.17	0.73
2:D:101:GLU:O	2:D:104:ARG:HD2	1.88	0.73
1:E:43:PHE:CE1	3:E:142:HEM:CBC	2.69	0.73
1:G:118:THR:HG22	1:G:121:VAL:N	2.04	0.73
2:H:4:THR:CG2	2:H:7:GLU:H	2.01	0.73
1:G:87:HIS:NE2	1:G:91:LEU:HD13	2.03	0.73
2:B:146:HIS:HD2	2:B:146:HIS:H	1.34	0.73
2:F:14:LEU:HA	2:F:17:LYS:HG3	1.69	0.73
1:C:70:VAL:HA	1:C:73:VAL:HG23	1.70	0.73
1:C:84:SER:OG	1:C:139:LYS:CD	2.37	0.73
1:A:80:LEU:O	1:A:84:SER:HB2	1.89	0.73
1:A:93:VAL:HG21	3:A:142:HEM:CAC	2.19	0.73
1:E:14:TRP:HA	1:E:17:VAL:HB	1.69	0.73
2:H:61:LYS:NZ	2:H:61:LYS:CD	2.51	0.73
2:H:89:SER:HB3	2:H:144:LYS:HB2	1.69	0.73
3:H:147:HEM:HBC2	3:H:147:HEM:HMC3	1.69	0.73
1:A:29:LEU:HD21	1:A:101:LEU:HD12	0.82	0.73
1:C:36:PHE:N	1:C:37:PRO:CD	2.50	0.73
2:D:99:ASP:OD2	2:D:100:PRO:HD2	1.88	0.73
1:E:121:VAL:O	1:E:121:VAL:HG13	1.89	0.73
1:G:76:MET:N	1:G:77:PRO:CD	2.51	0.73
1:C:37:PRO:O	1:C:40:LYS:CB	2.37	0.72
2:H:26:GLU:OE1	2:H:30:ARG:HD2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:PRO:O	2:H:55:MET:CG	2.32	0.72
1:A:116:GLU:O	1:A:121:VAL:HG11	1.89	0.72
2:B:93:CYS:HB2	2:B:145:TYR:CE2	2.23	0.72
1:C:109:LEU:O	1:C:113:LEU:HD12	1.89	0.72
2:F:80:ASN:ND2	2:F:80:ASN:C	2.47	0.72
2:F:94:ASP:CG	2:F:146:HIS:HE2	1.97	0.72
2:H:3:LEU:HD23	2:H:4:THR:H	1.53	0.72
2:B:3:LEU:CD2	2:B:3:LEU:HB3	2.20	0.72
2:B:45:PHE:HE1	2:B:60:VAL:HG23	0.71	0.72
1:E:14:TRP:CA	1:E:17:VAL:CG2	2.66	0.72
1:E:10:VAL:O	1:E:10:VAL:HG12	1.87	0.72
1:G:80:LEU:HG	1:G:135:VAL:HG11	1.71	0.72
2:D:11:VAL:HG12	2:D:12:THR:H	1.53	0.72
2:D:94:ASP:OD1	2:D:146:HIS:CE1	2.43	0.72
1:E:82:ALA:HA	1:E:85:ASP:HB2	1.71	0.72
1:G:31:ARG:HG3	1:G:31:ARG:HH21	1.55	0.72
2:B:18:VAL:CG1	2:B:18:VAL:CA	2.66	0.72
1:C:16:LYS:HZ2	1:C:113:LEU:HD23	1.53	0.72
1:E:39:THR:O	1:E:43:PHE:CD1	2.42	0.72
1:E:117:PHE:CD2	1:E:117:PHE:O	2.42	0.72
1:E:125:LEU:O	1:E:129:LEU:HB2	1.89	0.72
1:G:46:PHE:C	1:G:48:LEU:HD21	2.15	0.72
1:E:32:MET:HG3	1:E:32:MET:O	1.89	0.72
2:F:48:LEU:CB	2:F:48:LEU:CD1	2.67	0.72
2:H:49:SER:O	2:H:50:THR:HG23	1.89	0.72
2:B:105:LEU:O	2:B:109:VAL:HG23	1.90	0.72
2:D:44:SER:HG	2:D:45:PHE:HE2	0.74	0.72
1:E:76:MET:N	1:E:77:PRO:HD2	2.04	0.72
1:E:141:ARG:CB	2:H:36:PRO:HG3	2.18	0.72
1:E:128:PHE:O	1:E:132:VAL:N	2.22	0.72
2:D:15:TRP:CE3	2:D:18:VAL:HB	2.24	0.72
2:D:85:PHE:HB3	2:D:88:LEU:HB3	1.72	0.72
2:F:67:VAL:HG22	3:F:147:HEM:NB	2.05	0.72
2:F:124:PRO:CD	2:F:125:PRO:HD3	2.19	0.72
1:G:61:LYS:CD	1:G:61:LYS:CB	2.65	0.72
2:B:59:LYS:O	2:B:59:LYS:HE3	1.88	0.71
2:D:21:ASP:HA	2:D:65:LYS:HG2	1.72	0.71
2:D:37:TRP:O	2:D:40:ARG:HB2	1.90	0.71
2:H:7:GLU:O	2:H:10:ALA:HB3	1.90	0.71
1:A:61:LYS:CD	1:A:61:LYS:NZ	2.53	0.71
1:C:31:ARG:CG	2:D:127:GLN:OE1	2.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:LEU:CD1	2:D:137:VAL:CG2	2.60	0.71
1:E:33:PHE:CD2	1:E:48:LEU:CD2	2.72	0.71
1:G:14:TRP:O	1:G:15:GLY:C	2.34	0.71
2:H:138:ALA:O	2:H:141:LEU:HB2	1.90	0.71
1:A:8:THR:CG2	1:A:8:THR:O	2.38	0.71
1:C:73:VAL:HA	1:C:76:MET:HG3	1.73	0.71
2:F:99:ASP:O	2:F:102:ASN:CB	2.38	0.71
2:F:110:LEU:HD12	2:F:110:LEU:O	1.89	0.71
2:B:4:THR:HG23	2:B:5:PRO:N	2.04	0.71
2:F:114:LEU:HD23	2:F:114:LEU:O	1.91	0.71
1:G:80:LEU:HB3	1:G:135:VAL:CG1	2.20	0.71
2:H:34:VAL:C	2:H:36:PRO:CD	2.64	0.71
2:H:139:ASN:HD22	2:H:139:ASN:N	1.79	0.71
2:B:4:THR:O	2:B:8:LYS:HB2	1.91	0.71
2:B:98:VAL:N	2:B:98:VAL:HG22	2.03	0.71
2:D:63:HIS:CE1	3:D:147:HEM:C4D	2.78	0.71
2:F:28:LEU:O	2:F:32:LEU:CB	2.27	0.71
2:H:20:VAL:O	2:H:24:GLY:CA	2.38	0.71
2:H:68:LEU:N	2:H:68:LEU:HB2	2.05	0.71
2:H:102:ASN:HB3	3:H:147:HEM:HMC1	1.71	0.71
2:B:3:LEU:CD1	2:B:133:VAL:HG22	2.20	0.71
1:E:28:ALA:O	1:E:29:LEU:C	2.32	0.71
2:H:78:LEU:HB3	2:H:81:LEU:CD2	2.19	0.71
1:A:6:ASP:OD1	1:A:124:SER:HA	1.89	0.71
1:A:83:LEU:HD11	3:A:142:HEM:CMA	2.19	0.71
2:F:69:GLY:O	2:F:70:ALA:C	2.31	0.71
1:G:97:ASN:O	1:G:98:PHE:C	2.33	0.71
2:H:33:VAL:CG2	2:H:54:VAL:HG11	2.19	0.71
1:A:125:LEU:O	1:A:126:ASP:C	2.34	0.71
2:B:12:THR:OG1	2:B:12:THR:CG2	2.38	0.71
1:C:99:LYS:HE2	1:C:100:LEU:CD2	2.20	0.71
2:D:20:VAL:O	2:D:20:VAL:CG1	2.37	0.71
2:H:36:PRO:HG2	2:H:37:TRP:CZ3	2.25	0.71
2:B:98:VAL:CG2	2:B:98:VAL:HG13	2.18	0.71
2:D:41:PHE:CZ	2:D:98:VAL:HG13	2.26	0.71
1:A:92:ARG:HG2	2:D:37:TRP:HA	1.73	0.70
2:B:138:ALA:O	2:B:139:ASN:C	2.30	0.70
2:D:73:ASP:O	2:D:76:ALA:HB3	1.91	0.70
2:D:110:LEU:O	2:D:110:LEU:HG	1.88	0.70
1:E:20:HIS:N	1:E:20:HIS:C	2.49	0.70
1:E:20:HIS:N	1:E:20:HIS:CB	2.51	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:142:HEM:HBB2	3:G:142:HEM:CMB	2.19	0.70
2:B:3:LEU:HD11	2:B:133:VAL:HG22	1.73	0.70
1:C:57:GLY:O	1:C:61:LYS:HB2	1.91	0.70
2:D:101:GLU:CD	2:D:104:ARG:HD3	2.15	0.70
1:E:78:ASN:O	1:E:81:SER:HB2	1.91	0.70
1:G:60:LYS:O	1:G:64:ASP:CB	2.35	0.70
2:B:45:PHE:CE1	2:B:60:VAL:CG2	2.52	0.70
2:D:14:LEU:HD22	2:D:126:VAL:HG11	1.69	0.70
1:E:62:VAL:O	1:E:66:LEU:CD1	2.38	0.70
1:E:66:LEU:HD12	3:E:142:HEM:CMB	2.20	0.70
2:F:20:VAL:CG2	2:F:21:ASP:N	2.54	0.70
2:B:8:LYS:CB	2:B:8:LYS:HD3	2.20	0.70
2:B:96:LEU:CG	2:B:98:VAL:HG21	2.20	0.70
3:C:142:HEM:HBC2	3:C:142:HEM:CMC	2.17	0.70
2:H:54:VAL:HG12	2:H:55:MET:SD	2.32	0.70
2:D:17:LYS:H	2:D:17:LYS:HD3	1.56	0.70
2:H:81:LEU:C	2:H:85:PHE:HE1	1.97	0.70
2:B:62:ALA:O	2:B:65:LYS:HG2	1.91	0.70
2:B:111:VAL:HG13	2:B:122:PHE:CZ	2.26	0.70
2:D:101:GLU:C	2:D:104:ARG:HD2	2.15	0.70
1:E:10:VAL:O	1:E:10:VAL:CG1	2.38	0.70
2:D:124:PRO:O	2:D:127:GLN:HB3	1.91	0.70
1:E:4:PRO:HG2	1:E:5:ALA:N	2.05	0.70
1:E:88:ALA:CB	1:E:140:TYR:CD2	2.75	0.70
1:G:79:ALA:O	1:G:80:LEU:C	2.35	0.70
1:C:10:VAL:HG23	1:C:125:LEU:CD2	2.22	0.70
1:C:25:GLY:O	1:C:28:ALA:HB3	1.91	0.70
1:C:104:CYS:HA	1:C:107:VAL:HG22	1.72	0.70
2:D:123:THR:HB	2:D:125:PRO:HD2	1.72	0.70
1:G:51:GLY:O	1:G:52:SER:C	2.30	0.70
1:G:87:HIS:HA	1:G:91:LEU:HD12	0.76	0.70
1:G:111:ALA:HB1	2:H:119:GLY:C	2.16	0.70
1:A:113:LEU:O	1:A:117:PHE:HB3	1.92	0.69
2:B:15:TRP:HA	2:B:18:VAL:HB	1.72	0.69
2:D:94:ASP:OD1	2:D:146:HIS:NE2	2.25	0.69
2:H:73:ASP:O	2:H:76:ALA:HB2	1.92	0.69
2:H:92:HIS:CD2	2:H:103:PHE:HZ	2.10	0.69
2:B:106:LEU:CA	2:B:109:VAL:HG23	2.18	0.69
1:G:110:ALA:HB3	2:H:115:ALA:CB	2.21	0.69
1:C:38:THR:CG2	1:C:38:THR:N	2.55	0.69
1:G:118:THR:HG22	1:G:120:ALA:C	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:VAL:HG21	2:B:51:PRO:HB3	1.74	0.69
2:B:38:THR:N	2:B:38:THR:C	2.50	0.69
1:C:113:LEU:HD22	1:C:116:GLU:HB3	1.73	0.69
2:F:2:HIS:ND1	2:F:132:LYS:CE	2.53	0.69
2:B:93:CYS:HB2	2:B:145:TYR:CE1	2.28	0.69
1:C:118:THR:N	1:C:118:THR:HB	2.05	0.69
2:F:25:GLY:C	2:F:55:MET:HE3	2.14	0.69
2:F:70:ALA:O	2:F:73:ASP:CG	2.35	0.69
1:C:60:LYS:O	1:C:64:ASP:HB2	1.92	0.69
2:D:42:PHE:N	2:D:42:PHE:CD1	2.58	0.69
1:A:127:LYS:HE3	1:C:141:ARG:HB2	1.75	0.69
1:E:29:LEU:CD2	1:E:101:LEU:HG	2.22	0.69
1:E:97:ASN:OD1	2:H:99:ASP:OD1	2.10	0.69
1:G:2:LEU:HA	1:G:6:ASP:OD2	1.93	0.69
1:A:65:ALA:O	1:A:80:LEU:HD21	1.93	0.69
1:A:77:PRO:O	1:A:81:SER:CB	2.40	0.69
2:B:92:HIS:CD2	2:B:103:PHE:HE1	2.11	0.69
2:B:107:GLY:HA2	2:B:134:VAL:CG2	2.20	0.69
1:C:110:ALA:HB1	2:D:115:ALA:CB	2.21	0.69
2:D:3:LEU:HD11	2:D:133:VAL:HG23	1.72	0.69
1:G:48:LEU:N	1:G:48:LEU:CD2	2.46	0.69
1:A:14:TRP:NE1	1:A:67:THR:OG1	2.25	0.69
1:C:118:THR:CG2	1:C:121:VAL:N	2.28	0.69
2:D:101:GLU:OE1	2:D:104:ARG:CZ	2.41	0.69
2:H:93:CYS:HA	2:H:145:TYR:CE1	2.28	0.69
2:B:99:ASP:OD2	2:B:100:PRO:HD2	1.93	0.69
1:C:106:LEU:N	1:C:109:LEU:HB2	2.08	0.69
2:F:63:HIS:CE1	3:F:147:HEM:C4D	2.80	0.69
1:A:83:LEU:HD23	1:A:136:LEU:CD2	2.23	0.68
2:B:4:THR:HG22	2:B:6:VAL:N	2.07	0.68
2:D:73:ASP:OD1	2:D:73:ASP:N	2.24	0.68
2:D:92:HIS:HA	2:D:96:LEU:HB2	1.74	0.68
2:H:93:CYS:SG	2:H:145:TYR:CD1	2.86	0.68
1:E:86:LEU:HD12	1:E:90:LYS:HD2	1.74	0.68
2:F:4:THR:CG2	2:F:6:VAL:HG12	2.23	0.68
2:H:37:TRP:O	2:H:40:ARG:HB2	1.93	0.68
1:A:27:GLU:O	1:A:28:ALA:C	2.37	0.68
2:B:50:THR:OG1	2:B:53:ALA:HB2	1.93	0.68
1:C:89:HIS:ND1	1:C:89:HIS:N	2.24	0.68
1:E:30:GLU:OE2	1:E:50:HIS:ND1	2.27	0.68
1:G:1:VAL:HG13	1:G:2:LEU:N	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ASN:O	2:B:23:VAL:CG1	2.37	0.68
2:B:58:PRO:O	2:B:62:ALA:HB2	1.93	0.68
1:G:76:MET:HE2	1:G:131:SER:CB	2.23	0.68
2:B:1:VAL:O	2:B:2:HIS:ND1	2.24	0.68
1:G:75:ASP:C	1:G:77:PRO:CD	2.67	0.68
2:H:2:HIS:O	2:H:132:LYS:HD3	1.94	0.68
2:H:92:HIS:HA	2:H:96:LEU:HB2	1.76	0.68
1:A:98:PHE:CE1	3:A:142:HEM:CAB	2.75	0.68
2:F:100:PRO:HD3	2:F:145:TYR:CE1	2.27	0.68
1:C:31:ARG:CG	1:C:31:ARG:HH11	2.05	0.68
1:A:47:ASP:OD1	1:A:49:SER:HB2	1.91	0.68
2:B:87:THR:O	2:B:91:LEU:N	2.27	0.68
2:D:51:PRO:O	2:D:54:VAL:HG23	1.93	0.68
1:G:49:SER:C	1:G:52:SER:HG	2.02	0.68
1:G:80:LEU:O	1:G:81:SER:C	2.36	0.68
2:B:59:LYS:HA	2:B:59:LYS:HZ2	1.58	0.68
1:C:78:ASN:CG	1:C:78:ASN:H	2.02	0.68
2:D:69:GLY:O	2:D:72:SER:HB2	1.93	0.68
1:E:96:VAL:HG21	2:H:101:GLU:CG	2.22	0.68
2:F:1:VAL:HB	2:F:132:LYS:HG3	1.74	0.68
2:H:88:LEU:O	2:H:91:LEU:HB3	1.94	0.68
1:A:41:THR:N	1:A:41:THR:CB	2.56	0.68
1:A:111:ALA:CB	2:B:119:GLY:HA2	2.23	0.68
2:B:15:TRP:CH2	2:B:71:PHE:HE2	2.11	0.68
1:C:13:ALA:N	1:C:14:TRP:N	2.41	0.68
2:F:26:GLU:O	2:F:55:MET:HE2	1.94	0.68
2:H:84:THR:HB	2:H:85:PHE:CE1	2.28	0.68
1:A:9:ASN:ND2	1:A:124:SER:OG	2.26	0.67
1:C:66:LEU:HD21	1:C:129:LEU:HD23	1.59	0.67
2:F:49:SER:C	2:F:50:THR:CG2	2.65	0.67
2:F:74:GLY:C	2:F:75:LEU:HD22	2.19	0.67
2:F:100:PRO:O	2:F:101:GLU:C	2.37	0.67
1:G:31:ARG:CG	2:H:127:GLN:OE1	2.43	0.67
1:A:3:SER:OG	1:A:4:PRO:CD	2.42	0.67
1:C:91:LEU:CD2	1:C:91:LEU:CD1	2.67	0.67
2:D:77:HIS:H	2:D:77:HIS:HB2	1.54	0.67
2:D:97:HIS:C	2:D:98:VAL:CG2	2.59	0.67
2:D:101:GLU:HA	2:D:104:ARG:CZ	2.23	0.67
1:E:36:PHE:O	1:E:37:PRO:C	2.34	0.67
1:G:47:ASP:CA	1:G:48:LEU:N	2.56	0.67
1:A:38:THR:OG1	1:A:39:THR:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:TRP:CZ3	2:B:18:VAL:HG21	2.29	0.67
2:D:101:GLU:O	2:D:104:ARG:CD	2.41	0.67
2:H:20:VAL:CG1	2:H:68:LEU:HD22	2.25	0.67
2:B:28:LEU:CD1	2:B:32:LEU:CD2	2.60	0.67
1:C:102:SER:HA	1:C:129:LEU:HD11	1.74	0.67
1:G:21:ALA:O	1:G:22:GLY:C	2.36	0.67
2:D:3:LEU:HD21	2:D:132:LYS:C	2.19	0.67
2:D:3:LEU:HD12	2:D:133:VAL:HG23	1.73	0.67
1:E:122:HIS:HE1	2:F:30:ARG:HD3	1.60	0.67
1:G:27:GLU:OE1	1:G:31:ARG:NE	2.28	0.67
1:G:80:LEU:HB2	1:G:135:VAL:CG1	2.22	0.67
2:B:4:THR:CG2	2:B:6:VAL:H	2.07	0.67
1:E:36:PHE:C	1:E:38:THR:N	2.50	0.67
2:F:71:PHE:O	2:F:72:SER:C	2.38	0.67
1:G:30:GLU:OE2	1:G:50:HIS:CE1	2.47	0.67
2:H:20:VAL:HG13	2:H:68:LEU:HB3	1.75	0.67
2:H:93:CYS:CA	2:H:145:TYR:CE1	2.77	0.67
1:G:94:ASP:C	1:G:96:VAL:H	2.03	0.67
2:D:77:HIS:N	2:D:77:HIS:CG	2.62	0.67
1:G:11:LYS:HG3	1:G:70:VAL:HG23	1.77	0.67
1:G:30:GLU:OE1	1:G:50:HIS:CD2	2.47	0.67
2:H:92:HIS:C	2:H:96:LEU:HB2	2.19	0.67
1:A:134:THR:O	1:A:135:VAL:C	2.34	0.67
2:H:20:VAL:O	2:H:68:LEU:HD22	1.93	0.67
2:B:15:TRP:C	2:B:17:LYS:N	2.52	0.66
2:F:58:PRO:O	2:F:59:LYS:C	2.32	0.66
1:G:6:ASP:OD1	1:G:127:LYS:HE2	1.95	0.66
1:G:6:ASP:CG	1:G:127:LYS:HE3	2.20	0.66
1:G:30:GLU:CD	1:G:50:HIS:CG	2.72	0.66
2:H:47:ASP:HB3	2:H:49:SER:OG	1.95	0.66
1:C:66:LEU:HD23	1:C:128:PHE:CE2	2.30	0.66
1:C:129:LEU:O	1:C:133:SER:N	2.27	0.66
2:D:58:PRO:HA	2:D:61:LYS:HG2	1.75	0.66
2:F:41:PHE:CD1	3:F:147:HEM:HBC1	2.29	0.66
2:H:87:THR:O	2:H:88:LEU:O	2.14	0.66
1:A:39:THR:O	1:A:40:LYS:C	2.33	0.66
2:B:111:VAL:O	2:B:111:VAL:HG13	1.95	0.66
2:D:39:GLN:O	2:D:41:PHE:N	2.28	0.66
1:E:20:HIS:N	1:E:21:ALA:N	2.43	0.66
1:E:29:LEU:HD21	1:E:101:LEU:CD1	2.24	0.66
1:E:44:PRO:CG	1:E:45:HIS:N	2.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:LEU:O	1:E:109:LEU:HB2	1.94	0.66
2:F:4:THR:HG22	2:F:6:VAL:HG12	1.75	0.66
1:A:118:THR:CB	1:A:121:VAL:HG21	2.25	0.66
2:D:78:LEU:HD11	2:D:133:VAL:HG22	1.77	0.66
1:E:33:PHE:CE2	1:E:48:LEU:CD2	2.77	0.66
2:F:4:THR:HB	2:F:7:GLU:OE2	1.94	0.66
2:F:63:HIS:CE1	3:F:147:HEM:C1D	2.84	0.66
1:G:31:ARG:HG2	2:H:127:GLN:OE1	1.95	0.66
1:G:47:ASP:O	1:G:52:SER:HB3	1.95	0.66
1:G:66:LEU:CD2	1:G:132:VAL:HG21	2.25	0.66
1:E:22:GLY:O	1:E:26:ALA:N	2.27	0.66
1:E:66:LEU:HD12	3:E:142:HEM:HMB1	1.74	0.66
1:E:88:ALA:CA	1:E:140:TYR:CD2	2.78	0.66
2:H:78:LEU:CD2	2:H:133:VAL:CG2	2.72	0.66
1:A:20:HIS:H	1:A:20:HIS:HD2	1.39	0.66
1:A:121:VAL:N	1:A:121:VAL:CB	2.56	0.66
2:B:41:PHE:CG	3:B:147:HEM:HAC	2.30	0.66
2:D:33:VAL:HG12	2:D:34:VAL:CG2	2.25	0.66
2:F:73:ASP:OD1	2:F:73:ASP:N	2.24	0.66
2:F:124:PRO:HD2	2:F:125:PRO:HD3	1.75	0.66
1:G:6:ASP:O	1:G:10:VAL:HG23	1.96	0.66
2:B:96:LEU:HD22	2:B:98:VAL:HG22	1.75	0.66
2:D:3:LEU:HD21	2:D:132:LYS:HB3	1.66	0.66
2:D:14:LEU:CD2	2:D:126:VAL:CG1	2.33	0.66
2:D:51:PRO:HA	2:D:54:VAL:CG2	2.25	0.66
2:H:33:VAL:CG1	2:H:51:PRO:HB3	2.25	0.66
1:A:127:LYS:O	1:A:130:ALA:CB	2.41	0.66
1:E:15:GLY:O	1:E:17:VAL:N	2.29	0.66
2:F:77:HIS:HB2	2:F:84:THR:HG21	1.78	0.66
2:H:22:GLU:CB	2:H:22:GLU:OE2	2.44	0.66
2:B:23:VAL:HG23	2:B:24:GLY:N	2.10	0.66
2:H:78:LEU:HD23	2:H:133:VAL:HG23	1.78	0.66
1:A:31:ARG:O	1:A:35:SER:N	2.25	0.65
1:A:126:ASP:OD2	1:C:141:ARG:NH1	2.30	0.65
1:C:7:LYS:HE3	1:C:73:VAL:HG12	1.77	0.65
2:D:14:LEU:HD11	2:D:130:TYR:CE2	2.31	0.65
2:D:49:SER:HG	2:D:53:ALA:HB2	1.60	0.65
2:D:72:SER:HB3	2:D:73:ASP:OD1	1.96	0.65
1:E:78:ASN:O	1:E:81:SER:CB	2.43	0.65
2:F:43:GLU:CD	1:G:92:ARG:NH1	2.46	0.65
1:G:80:LEU:O	1:G:82:ALA:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:GLN:O	2:H:40:ARG:C	2.38	0.65
2:H:42:PHE:N	2:H:42:PHE:CD1	2.62	0.65
1:E:141:ARG:HD2	1:E:141:ARG:O	1.95	0.65
2:F:40:ARG:CG	2:F:40:ARG:NE	2.59	0.65
2:B:30:ARG:CB	2:B:30:ARG:CD	2.71	0.65
1:C:43:PHE:CD2	1:C:46:PHE:CG	2.82	0.65
2:D:49:SER:OG	2:D:53:ALA:HB2	1.96	0.65
1:G:33:PHE:CZ	1:G:43:PHE:CE1	2.84	0.65
2:H:8:LYS:HG2	2:H:78:LEU:HD11	1.77	0.65
2:B:96:LEU:O	2:B:97:HIS:CB	2.40	0.65
1:C:68:ASN:OD1	1:C:72:HIS:CD2	2.49	0.65
2:D:42:PHE:HB3	2:D:45:PHE:CG	2.31	0.65
2:D:80:ASN:ND2	2:D:83:GLY:HA2	1.98	0.65
1:G:106:LEU:O	1:G:110:ALA:N	2.30	0.65
1:C:83:LEU:HD21	3:C:142:HEM:CMA	2.26	0.65
1:C:99:LYS:HG2	1:C:100:LEU:HD23	1.77	0.65
1:C:119:PRO:O	1:C:120:ALA:O	2.14	0.65
1:G:4:PRO:CG	1:G:5:ALA:H	2.03	0.65
2:D:71:PHE:O	2:D:75:LEU:CD1	2.45	0.65
1:E:105:LEU:O	1:E:109:LEU:N	2.26	0.65
2:F:63:HIS:CE1	3:F:147:HEM:ND	2.63	0.65
2:D:110:LEU:HD23	2:D:110:LEU:O	1.91	0.65
2:D:131:GLN:HE21	2:D:131:GLN:C	2.04	0.65
2:F:3:LEU:HB3	2:F:8:LYS:HB2	1.78	0.65
2:B:41:PHE:CE2	2:B:98:VAL:HG12	2.31	0.65
2:B:59:LYS:CE	2:B:62:ALA:CB	2.75	0.65
1:C:136:LEU:N	1:C:136:LEU:HD23	2.11	0.65
2:F:19:ASN:O	2:F:23:VAL:N	2.26	0.65
2:H:17:LYS:HB3	2:H:118:PHE:CE2	2.32	0.65
1:A:92:ARG:CB	2:D:37:TRP:HB2	2.27	0.65
1:A:137:THR:O	1:A:140:TYR:HB2	1.96	0.65
1:E:14:TRP:CA	1:E:17:VAL:HG21	2.26	0.65
2:B:3:LEU:HD23	2:B:7:GLU:HB3	1.74	0.65
1:C:38:THR:N	1:C:38:THR:HG22	2.12	0.65
2:D:87:THR:CG2	2:D:88:LEU:H	2.10	0.65
2:D:91:LEU:CD1	2:D:95:LYS:HB3	2.27	0.65
1:E:93:VAL:HG11	3:E:142:HEM:CAC	2.27	0.64
1:E:127:LYS:HG2	1:G:141:ARG:HD3	1.79	0.64
1:G:11:LYS:O	1:G:15:GLY:CA	2.45	0.64
1:G:77:PRO:O	1:G:81:SER:HB2	1.97	0.64
2:H:99:ASP:C	2:H:101:GLU:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:THR:CB	2:B:5:PRO:HD2	2.24	0.64
2:B:72:SER:O	2:B:75:LEU:HD12	1.97	0.64
1:E:127:LYS:HG2	1:G:141:ARG:CD	2.27	0.64
2:D:26:GLU:OE1	2:D:30:ARG:CZ	2.45	0.64
2:D:67:VAL:HG12	3:D:147:HEM:C4A	2.31	0.64
1:E:75:ASP:OD2	1:E:78:ASN:OD1	2.15	0.64
1:C:66:LEU:CD2	1:C:129:LEU:HD21	2.20	0.64
1:E:101:LEU:O	1:E:101:LEU:CD2	2.40	0.64
2:H:31:LEU:CD2	2:H:106:LEU:CD2	2.75	0.64
1:C:128:PHE:CE2	1:C:129:LEU:HD23	2.32	0.64
2:D:41:PHE:CE2	2:D:98:VAL:HG13	2.32	0.64
2:D:85:PHE:CD2	2:D:88:LEU:HD13	2.32	0.64
1:G:106:LEU:O	1:G:109:LEU:HB3	1.98	0.64
2:D:101:GLU:HA	2:D:104:ARG:CD	2.26	0.64
2:F:95:LYS:NZ	2:F:95:LYS:CD	2.57	0.64
1:A:92:ARG:HB3	2:D:37:TRP:HB2	1.80	0.64
1:C:43:PHE:HD2	1:C:46:PHE:CD2	2.15	0.64
1:E:141:ARG:HG2	2:H:36:PRO:HG3	1.79	0.64
1:A:16:LYS:HG3	1:A:116:GLU:OE2	1.97	0.64
2:B:113:VAL:HG12	2:B:114:LEU:N	2.07	0.64
1:C:38:THR:CB	1:C:38:THR:HA	2.13	0.64
2:B:38:THR:CA	2:B:38:THR:OG1	2.45	0.64
1:E:20:HIS:N	1:E:21:ALA:H	1.96	0.64
2:F:4:THR:CB	2:F:7:GLU:OE2	2.46	0.64
2:B:103:PHE:CE1	2:B:141:LEU:HD12	2.32	0.64
2:B:131:GLN:NE2	2:B:131:GLN:HA	2.13	0.64
2:H:30:ARG:NE	2:H:30:ARG:HG2	2.12	0.64
2:H:92:HIS:HD2	2:H:98:VAL:HB	1.63	0.64
1:A:58:HIS:O	1:A:62:VAL:CA	2.46	0.63
2:B:128:ALA:O	2:B:131:GLN:HB2	1.98	0.63
2:D:80:ASN:HD22	2:D:83:GLY:CA	1.90	0.63
1:E:29:LEU:HD21	1:E:101:LEU:HG	1.81	0.63
1:E:47:ASP:OD1	1:E:49:SER:HB3	1.97	0.63
2:F:68:LEU:O	2:F:71:PHE:CB	2.37	0.63
1:A:109:LEU:O	1:A:113:LEU:HB2	1.99	0.63
1:A:122:HIS:O	1:A:126:ASP:N	2.18	0.63
1:C:13:ALA:N	1:C:14:TRP:H	1.95	0.63
2:D:64:GLY:O	2:D:65:LYS:C	2.38	0.63
2:B:50:THR:O	2:B:54:VAL:CB	2.46	0.63
1:C:86:LEU:HD21	3:C:142:HEM:HBA2	1.81	0.63
2:D:24:GLY:HA2	2:D:68:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:HIS:C	2:D:98:VAL:HG22	2.24	0.63
1:E:39:THR:O	1:E:39:THR:OG1	2.16	0.63
1:E:95:PRO:HG3	1:E:137:THR:CG2	2.28	0.63
1:E:106:LEU:HB2	1:E:106:LEU:HD13	1.79	0.63
2:F:106:LEU:O	2:F:110:LEU:HB3	1.98	0.63
2:B:15:TRP:O	2:B:16:GLY:C	2.40	0.63
2:B:63:HIS:O	2:B:67:VAL:HG23	1.98	0.63
2:D:44:SER:HB3	2:D:45:PHE:CE2	2.31	0.63
2:F:81:LEU:HD13	2:F:137:VAL:HA	1.79	0.63
2:D:49:SER:CA	2:D:49:SER:OG	2.45	0.63
2:D:84:THR:O	2:D:84:THR:OG1	2.14	0.63
1:G:27:GLU:O	1:G:31:ARG:CB	2.45	0.63
1:G:83:LEU:HD23	1:G:136:LEU:HD11	1.79	0.63
1:G:87:HIS:CA	1:G:91:LEU:CD1	2.42	0.63
1:A:33:PHE:CD1	1:A:40:LYS:CG	2.80	0.63
1:A:88:ALA:HB2	1:A:139:LYS:HB3	1.79	0.63
1:C:30:GLU:OE2	1:C:50:HIS:HB2	1.98	0.63
1:G:87:HIS:ND1	1:G:91:LEU:HD13	2.10	0.63
2:H:73:ASP:O	2:H:76:ALA:HB3	1.96	0.63
2:F:72:SER:O	2:F:75:LEU:CB	2.45	0.63
1:G:64:ASP:O	1:G:65:ALA:C	2.42	0.63
1:A:33:PHE:CG	1:A:40:LYS:HG2	2.34	0.63
2:B:50:THR:C	2:B:54:VAL:HG23	2.18	0.63
2:D:5:PRO:HA	2:D:8:LYS:HB3	1.81	0.63
2:D:63:HIS:HE1	3:D:147:HEM:C4D	2.16	0.63
1:E:2:LEU:HD21	1:E:131:SER:OG	1.99	0.63
1:G:121:VAL:HA	1:G:124:SER:HG	1.63	0.63
2:H:3:LEU:HD21	2:H:8:LYS:CE	2.15	0.63
2:H:39:GLN:C	2:H:41:PHE:N	2.57	0.63
2:B:17:LYS:HB2	2:B:17:LYS:CE	2.21	0.63
2:B:131:GLN:NE2	2:B:131:GLN:CA	2.60	0.63
2:D:142:ALA:CB	2:D:142:ALA:C	2.68	0.63
1:E:102:SER:HB3	1:E:129:LEU:HD21	1.78	0.63
2:H:92:HIS:CD2	2:H:98:VAL:CG2	2.82	0.63
1:C:36:PHE:N	1:C:37:PRO:HD2	2.12	0.62
2:D:34:VAL:C	2:D:36:PRO:HD3	2.23	0.62
2:D:82:LYS:O	2:D:86:ALA:HB2	1.99	0.62
1:E:105:LEU:HD22	1:E:129:LEU:HD11	1.80	0.62
2:F:6:VAL:HA	2:F:9:SER:HB2	1.81	0.62
2:F:110:LEU:CB	2:F:110:LEU:C	2.67	0.62
1:G:87:HIS:CE1	1:G:91:LEU:HD11	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:LEU:HA	2:H:81:LEU:HD23	1.81	0.62
2:B:131:GLN:O	2:B:135:ALA:HB2	1.99	0.62
1:E:29:LEU:HD21	1:E:101:LEU:HD11	1.79	0.62
1:E:36:PHE:O	1:E:39:THR:HG22	1.99	0.62
2:F:93:CYS:O	2:F:97:HIS:CA	2.47	0.62
2:F:98:VAL:O	2:F:145:TYR:CZ	2.52	0.62
2:B:50:THR:HB	2:B:53:ALA:H	1.65	0.62
1:E:47:ASP:N	1:E:54:GLN:OE1	2.32	0.62
1:E:86:LEU:O	1:E:87:HIS:C	2.39	0.62
1:E:93:VAL:CG1	3:E:142:HEM:HAC	2.29	0.62
2:H:63:HIS:O	2:H:66:LYS:HB2	1.99	0.62
1:A:3:SER:O	1:A:7:LYS:HB2	1.99	0.62
2:B:38:THR:OG1	2:B:38:THR:HG23	1.97	0.62
1:C:27:GLU:CD	1:C:108:THR:HG22	2.24	0.62
3:D:147:HEM:HHA	3:D:147:HEM:HBA2	1.81	0.62
1:E:127:LYS:HA	1:E:130:ALA:HB3	1.82	0.62
1:G:91:LEU:HD22	3:G:142:HEM:C1D	2.34	0.62
2:B:30:ARG:CG	2:B:30:ARG:CA	2.77	0.62
1:C:125:LEU:O	1:C:126:ASP:C	2.42	0.62
2:D:64:GLY:O	2:D:68:LEU:N	2.30	0.62
2:F:81:LEU:O	2:F:85:PHE:HB2	1.98	0.62
2:H:88:LEU:O	2:H:90:GLU:N	2.31	0.62
2:D:110:LEU:HD23	2:D:111:VAL:N	2.15	0.62
2:F:24:GLY:HA3	2:F:68:LEU:CD1	2.26	0.62
1:A:122:HIS:O	1:A:123:ALA:C	2.41	0.62
2:B:72:SER:HA	2:B:75:LEU:HD12	1.79	0.62
2:B:92:HIS:HD2	2:B:103:PHE:HE1	1.48	0.62
1:C:50:HIS:C	1:C:50:HIS:CD2	2.77	0.62
1:C:117:PHE:O	1:C:118:THR:CA	2.47	0.62
2:D:81:LEU:O	2:D:82:LYS:C	2.42	0.62
2:D:102:ASN:HB3	3:D:147:HEM:HMC3	1.82	0.62
1:E:52:SER:C	1:E:54:GLN:N	2.56	0.62
2:F:70:ALA:O	2:F:73:ASP:OD1	2.18	0.62
1:A:139:LYS:O	1:A:141:ARG:CG	2.31	0.62
1:C:46:PHE:HD1	1:C:48:LEU:HD23	1.65	0.62
2:F:118:PHE:O	2:F:121:GLU:HB2	2.00	0.62
1:A:76:MET:CB	1:A:76:MET:H	2.12	0.62
1:A:114:PRO:O	2:B:116:HIS:CD2	2.53	0.62
2:B:15:TRP:HA	2:B:18:VAL:H	1.64	0.62
2:B:17:LYS:CB	2:B:17:LYS:CE	2.77	0.62
1:C:38:THR:CB	1:C:38:THR:N	2.59	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:PRO:HG2	1:C:45:HIS:ND1	2.15	0.62
2:D:58:PRO:O	2:D:62:ALA:N	2.33	0.62
2:D:91:LEU:O	2:D:91:LEU:CD1	2.48	0.62
1:E:38:THR:CG2	1:E:39:THR:N	2.61	0.62
1:E:72:HIS:O	1:E:75:ASP:N	2.32	0.62
2:D:72:SER:CB	2:D:73:ASP:OD1	2.48	0.61
2:D:101:GLU:O	2:D:104:ARG:HG3	1.99	0.61
1:C:40:LYS:HE2	1:C:40:LYS:HG3	1.80	0.61
1:G:101:LEU:CD1	1:G:101:LEU:HB2	2.29	0.61
2:B:95:LYS:NZ	2:B:95:LYS:CD	2.59	0.61
1:E:11:LYS:CB	1:E:11:LYS:C	2.70	0.61
1:E:13:ALA:O	1:E:17:VAL:CG2	2.49	0.61
1:G:112:HIS:CB	1:G:112:HIS:N	2.59	0.61
2:H:68:LEU:N	2:H:68:LEU:C	2.53	0.61
1:A:20:HIS:O	1:A:21:ALA:C	2.44	0.61
1:C:99:LYS:HE2	1:C:100:LEU:HD21	1.82	0.61
1:C:123:ALA:HB2	2:D:34:VAL:HG22	1.82	0.61
1:C:134:THR:O	1:C:135:VAL:C	2.41	0.61
2:D:14:LEU:CD1	2:D:14:LEU:CA	2.78	0.61
2:D:33:VAL:CG2	2:D:54:VAL:HG21	2.29	0.61
1:E:35:SER:HA	2:F:128:ALA:HB2	1.81	0.61
1:E:35:SER:HA	2:F:128:ALA:CB	2.30	0.61
2:F:30:ARG:HH11	2:F:30:ARG:HG3	1.57	0.61
2:F:50:THR:O	2:F:54:VAL:N	2.33	0.61
2:F:63:HIS:O	2:F:67:VAL:HB	2.01	0.61
1:G:112:HIS:C	1:G:113:LEU:HD12	2.25	0.61
2:H:133:VAL:HG13	2:H:133:VAL:O	2.00	0.61
2:B:72:SER:CA	2:B:75:LEU:HD12	2.30	0.61
2:B:85:PHE:HA	2:B:88:LEU:HD13	1.82	0.61
1:C:32:MET:SD	1:C:101:LEU:HD23	2.40	0.61
2:D:3:LEU:HD11	2:D:133:VAL:CG2	2.30	0.61
1:E:132:VAL:O	1:E:136:LEU:CD1	2.44	0.61
2:F:99:ASP:OD1	1:G:42:TYR:OH	2.18	0.61
1:G:20:HIS:O	1:G:23:GLU:CB	2.48	0.61
2:B:59:LYS:CA	2:B:59:LYS:HE3	2.30	0.61
1:C:42:TYR:CD1	1:C:93:VAL:HG22	2.35	0.61
1:E:39:THR:OG1	1:E:43:PHE:CE1	2.54	0.61
1:A:36:PHE:CG	1:A:100:LEU:HD12	2.36	0.61
2:F:37:TRP:O	2:F:40:ARG:HB2	2.01	0.61
1:G:47:ASP:O	1:G:52:SER:CB	2.48	0.61
2:H:82:LYS:HD3	2:H:82:LYS:N	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:134:VAL:O	2:H:138:ALA:HB2	2.00	0.61
1:A:110:ALA:CB	2:B:115:ALA:CB	2.78	0.61
1:C:118:THR:HB	1:C:121:VAL:CG2	2.31	0.61
1:E:31:ARG:CG	2:F:124:PRO:HG3	2.30	0.61
1:E:31:ARG:HD3	2:F:127:GLN:OE1	2.00	0.61
2:F:31:LEU:HD13	2:F:109:VAL:HG22	1.83	0.61
1:G:94:ASP:O	1:G:96:VAL:N	2.34	0.61
2:H:20:VAL:C	2:H:24:GLY:H	2.02	0.61
1:A:121:VAL:N	1:A:121:VAL:C	2.56	0.61
1:C:141:ARG:CG	1:C:141:ARG:HE	2.13	0.61
2:F:91:LEU:CD2	2:F:96:LEU:HD12	2.30	0.61
1:G:30:GLU:OE2	1:G:50:HIS:CG	2.53	0.61
1:G:88:ALA:HB2	1:G:140:TYR:HD2	1.60	0.61
2:H:109:VAL:O	2:H:113:VAL:HG23	2.01	0.61
2:B:8:LYS:CG	2:B:8:LYS:CA	2.75	0.61
1:E:2:LEU:HA	1:E:127:LYS:HZ3	1.65	0.61
1:E:95:PRO:HB3	1:E:137:THR:HG21	1.83	0.61
1:G:67:THR:O	1:G:68:ASN:C	2.44	0.61
1:G:118:THR:HG22	1:G:120:ALA:CA	2.30	0.61
2:H:32:LEU:HA	2:H:38:THR:HG1	1.64	0.61
2:H:92:HIS:CD2	2:H:103:PHE:CE1	2.89	0.61
1:A:42:TYR:CE1	1:A:93:VAL:HG22	2.36	0.60
1:A:128:PHE:O	1:A:129:LEU:C	2.43	0.60
1:G:35:SER:C	1:G:37:PRO:HD3	2.26	0.60
1:G:116:GLU:O	1:G:121:VAL:HG21	2.00	0.60
1:A:17:VAL:HG13	1:A:24:TYR:CE1	2.36	0.60
1:E:2:LEU:C	1:E:3:SER:O	2.41	0.60
2:F:4:THR:OG1	2:F:7:GLU:OE2	2.20	0.60
2:F:33:VAL:HG22	2:F:51:PRO:HB3	1.80	0.60
1:A:28:ALA:O	1:A:31:ARG:HB2	2.01	0.60
1:A:42:TYR:HB2	3:A:142:HEM:HBC1	1.84	0.60
2:D:54:VAL:O	2:D:57:ASN:CB	2.42	0.60
1:G:83:LEU:CD1	3:G:142:HEM:CMA	2.73	0.60
1:A:52:SER:C	1:A:56:LYS:HD2	2.25	0.60
1:A:59:GLY:O	1:A:62:VAL:C	2.44	0.60
2:D:7:GLU:O	2:D:10:ALA:N	2.33	0.60
2:D:7:GLU:OE1	2:D:7:GLU:HA	2.01	0.60
1:E:32:MET:O	1:E:32:MET:CG	2.46	0.60
1:E:66:LEU:HD11	3:E:142:HEM:HBB2	1.83	0.60
1:E:98:PHE:CE1	3:E:142:HEM:CHC	2.84	0.60
1:G:101:LEU:CD1	1:G:101:LEU:HG	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:LEU:HD23	1:G:125:LEU:CD1	2.32	0.60
1:A:53:ALA:N	1:A:56:LYS:HD3	2.17	0.60
1:C:36:PHE:HZ	1:C:103:HIS:HE1	1.49	0.60
1:C:55:VAL:HG12	1:C:56:LYS:N	2.05	0.60
1:E:44:PRO:HG2	1:E:45:HIS:ND1	2.16	0.60
2:H:84:THR:CB	2:H:84:THR:HG1	2.08	0.60
1:A:51:GLY:O	1:A:56:LYS:NZ	2.35	0.60
1:C:7:LYS:O	1:C:10:VAL:HG12	2.01	0.60
2:D:64:GLY:O	2:D:68:LEU:CD2	2.47	0.60
2:F:136:GLY:O	2:F:140:ALA:HB2	2.00	0.60
1:G:3:SER:OG	1:G:5:ALA:HB3	2.02	0.60
1:G:29:LEU:HB2	1:G:101:LEU:CD1	2.31	0.60
2:H:80:ASN:ND2	2:H:83:GLY:CA	2.57	0.60
1:A:83:LEU:HD23	1:A:136:LEU:HD21	1.83	0.60
2:B:38:THR:CB	2:B:38:THR:HG1	2.10	0.60
1:C:97:ASN:O	1:C:98:PHE:C	2.38	0.60
2:D:42:PHE:CB	2:D:45:PHE:CG	2.84	0.60
1:G:47:ASP:OD1	1:G:49:SER:OG	2.20	0.60
1:G:66:LEU:CG	1:G:132:VAL:HG21	2.32	0.60
1:C:3:SER:CB	1:C:3:SER:HG	2.09	0.60
3:C:142:HEM:HMC2	3:C:142:HEM:CBC	2.23	0.60
2:D:100:PRO:HB2	2:D:103:PHE:CE2	2.36	0.60
1:E:52:SER:HB2	1:E:54:GLN:CB	2.31	0.60
2:F:14:LEU:HD21	2:F:118:PHE:CG	2.37	0.60
2:H:122:PHE:CE1	2:H:126:VAL:HG13	2.37	0.60
1:C:16:LYS:NZ	1:C:113:LEU:HD23	2.16	0.60
2:D:93:CYS:HB2	2:D:145:TYR:CE1	2.36	0.60
1:E:141:ARG:HG2	2:H:36:PRO:CG	2.31	0.60
1:G:27:GLU:O	1:G:31:ARG:N	2.35	0.60
2:H:87:THR:O	2:H:90:GLU:N	2.32	0.60
2:H:135:ALA:C	2:H:138:ALA:HB3	2.27	0.60
1:A:36:PHE:CD1	1:A:100:LEU:CD1	2.85	0.60
1:A:106:LEU:HD13	1:A:129:LEU:HD12	1.84	0.60
2:F:8:LYS:CG	2:F:8:LYS:HA	2.32	0.60
2:F:28:LEU:HD23	2:F:60:VAL:HG13	1.84	0.60
1:G:67:THR:C	1:G:69:ALA:N	2.54	0.60
1:C:42:TYR:CE1	1:C:93:VAL:HG22	2.37	0.59
2:D:23:VAL:CG1	2:D:23:VAL:O	2.49	0.59
2:D:128:ALA:HA	2:D:131:GLN:CG	2.31	0.59
1:E:86:LEU:O	1:E:87:HIS:O	2.19	0.59
1:E:103:HIS:HE1	2:F:131:GLN:OE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:VAL:HG21	2:F:51:PRO:CB	2.28	0.59
1:G:30:GLU:HG3	1:G:50:HIS:CE1	2.23	0.59
2:D:15:TRP:CE2	2:D:75:LEU:CD2	2.86	0.59
1:E:95:PRO:HG3	1:E:137:THR:HG21	1.84	0.59
1:G:46:PHE:CE2	3:G:142:HEM:O1D	2.43	0.59
1:G:76:MET:CE	1:G:131:SER:CB	2.80	0.59
2:H:8:LYS:HA	2:H:11:VAL:HG21	1.84	0.59
2:H:98:VAL:CG1	2:H:102:ASN:OD1	2.47	0.59
2:H:99:ASP:C	2:H:101:GLU:N	2.60	0.59
2:B:50:THR:O	2:B:54:VAL:N	2.34	0.59
2:B:73:ASP:O	2:B:77:HIS:ND1	2.35	0.59
2:B:92:HIS:CD2	2:B:103:PHE:CE1	2.89	0.59
1:C:70:VAL:HA	1:C:73:VAL:CG2	2.31	0.59
2:D:10:ALA:CB	2:D:126:VAL:HG13	2.31	0.59
1:E:127:LYS:O	1:E:130:ALA:HB3	2.02	0.59
2:F:4:THR:CG2	2:F:6:VAL:CG1	2.81	0.59
2:F:89:SER:O	2:F:90:GLU:C	2.44	0.59
2:H:31:LEU:CD2	2:H:106:LEU:HD23	2.31	0.59
2:H:33:VAL:HG11	2:H:51:PRO:HB3	1.82	0.59
2:H:122:PHE:CD1	2:H:126:VAL:CG1	2.85	0.59
2:B:15:TRP:CE3	2:B:18:VAL:CG2	2.80	0.59
1:G:33:PHE:HZ	1:G:43:PHE:CZ	2.20	0.59
2:H:78:LEU:HD23	2:H:133:VAL:HG22	1.82	0.59
2:D:3:LEU:CD1	2:D:133:VAL:CG2	2.76	0.59
2:D:113:VAL:CG1	2:D:114:LEU:N	2.64	0.59
1:E:134:THR:C	1:E:137:THR:H	2.10	0.59
1:G:94:ASP:C	1:G:96:VAL:N	2.60	0.59
1:A:4:PRO:O	1:A:7:LYS:HB3	2.03	0.59
1:A:29:LEU:CG	1:A:101:LEU:HD12	2.32	0.59
2:B:59:LYS:O	2:B:62:ALA:CB	2.50	0.59
2:B:67:VAL:O	2:B:70:ALA:HB3	2.03	0.59
1:C:70:VAL:CA	1:C:73:VAL:HG23	2.31	0.59
2:D:21:ASP:CG	2:D:65:LYS:HG2	2.28	0.59
1:E:29:LEU:CD2	1:E:101:LEU:HD11	2.32	0.59
3:G:142:HEM:HHD	3:G:142:HEM:HBC2	1.85	0.59
2:H:124:PRO:O	2:H:127:GLN:CB	2.50	0.59
1:A:87:HIS:HB3	1:A:136:LEU:HD13	1.85	0.59
1:C:43:PHE:CD2	1:C:46:PHE:CD2	2.91	0.59
1:E:100:LEU:HD23	1:E:100:LEU:N	2.17	0.59
1:E:101:LEU:HD23	1:E:104:CYS:SG	2.43	0.59
2:F:1:VAL:CG1	2:F:132:LYS:HG3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:ASP:OD2	2:H:49:SER:OG	2.15	0.59
2:H:123:THR:CB	2:H:125:PRO:HD2	2.31	0.59
1:A:113:LEU:N	1:A:114:PRO:HD3	2.18	0.59
1:C:31:ARG:HG2	1:C:31:ARG:HH11	1.67	0.59
1:E:42:TYR:HB2	1:E:43:PHE:CE1	2.38	0.59
1:C:16:LYS:NZ	1:C:116:GLU:HG3	2.14	0.59
1:E:141:ARG:CG	2:H:36:PRO:HG3	2.31	0.59
2:F:43:GLU:OE1	1:G:92:ARG:NH1	2.35	0.59
2:H:25:GLY:O	2:H:29:GLY:N	2.35	0.59
2:H:28:LEU:O	2:H:29:GLY:C	2.43	0.59
2:H:92:HIS:CA	2:H:96:LEU:HB2	2.32	0.59
2:H:123:THR:CG2	2:H:123:THR:CA	2.75	0.59
1:A:76:MET:O	1:A:77:PRO:C	2.45	0.59
1:C:129:LEU:O	1:C:133:SER:OG	2.21	0.59
2:D:40:ARG:HG2	2:D:41:PHE:CE1	2.38	0.59
2:D:127:GLN:O	2:D:127:GLN:HG2	2.02	0.59
1:E:7:LYS:HE2	1:E:74:ASP:OD1	2.03	0.59
1:G:121:VAL:C	1:G:124:SER:OG	2.46	0.59
2:H:31:LEU:HD23	2:H:106:LEU:HD22	1.83	0.59
2:H:71:PHE:CE2	2:H:75:LEU:CD1	2.86	0.59
2:H:87:THR:HG22	2:H:88:LEU:N	1.91	0.59
1:C:78:ASN:N	1:C:79:ALA:N	2.50	0.58
1:G:17:VAL:CG1	1:G:24:TYR:CD1	2.85	0.58
1:A:10:VAL:CG1	1:A:128:PHE:HB2	2.32	0.58
2:B:59:LYS:NZ	2:B:59:LYS:CA	2.65	0.58
1:C:48:LEU:HA	1:C:52:SER:HG	1.68	0.58
1:C:78:ASN:N	1:C:78:ASN:C	2.56	0.58
1:G:32:MET:CA	1:G:32:MET:HG2	2.32	0.58
1:G:87:HIS:ND1	1:G:91:LEU:HD11	2.18	0.58
1:A:20:HIS:O	1:A:23:GLU:N	2.30	0.58
1:A:72:HIS:O	1:A:75:ASP:N	2.28	0.58
1:A:88:ALA:CB	1:A:139:LYS:HB3	2.33	0.58
1:C:36:PHE:HE1	1:C:104:CYS:SG	2.26	0.58
2:D:33:VAL:HG12	2:D:33:VAL:O	2.02	0.58
1:E:36:PHE:O	1:E:38:THR:N	2.35	0.58
2:F:48:LEU:CG	2:F:48:LEU:CA	2.75	0.58
1:A:42:TYR:CD1	1:A:93:VAL:HG22	2.38	0.58
2:D:93:CYS:HB2	2:D:145:TYR:CD1	2.37	0.58
3:D:147:HEM:HHA	3:D:147:HEM:CBA	2.34	0.58
1:G:42:TYR:CE1	1:G:93:VAL:CG1	2.86	0.58
2:H:20:VAL:HG12	2:H:65:LYS:HA	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:GLU:CG	2:H:22:GLU:C	2.77	0.58
2:H:78:LEU:CB	2:H:81:LEU:HD21	2.32	0.58
2:H:124:PRO:O	2:H:127:GLN:HB3	2.04	0.58
1:A:43:PHE:HA	1:A:45:HIS:CE1	2.39	0.58
1:C:24:TYR:O	1:C:28:ALA:HB2	2.04	0.58
2:D:15:TRP:CE2	2:D:75:LEU:HD23	2.39	0.58
2:F:26:GLU:HA	2:F:55:MET:CE	2.34	0.58
2:F:26:GLU:HA	2:F:55:MET:HE2	1.85	0.58
1:G:32:MET:CB	1:G:33:PHE:N	2.67	0.58
2:B:23:VAL:CG2	2:B:24:GLY:N	2.67	0.58
2:B:111:VAL:O	2:B:111:VAL:HG12	1.97	0.58
2:D:114:LEU:O	2:D:115:ALA:C	2.41	0.58
1:E:29:LEU:HD11	1:E:58:HIS:HD2	1.69	0.58
1:G:11:LYS:O	1:G:15:GLY:N	2.37	0.58
1:C:36:PHE:HE1	1:C:104:CYS:HG	1.52	0.58
2:D:91:LEU:O	2:D:95:LYS:HB2	2.03	0.58
1:E:88:ALA:CA	1:E:140:TYR:CE2	2.82	0.58
1:G:59:GLY:O	1:G:63:ALA:N	2.33	0.58
2:H:17:LYS:CB	2:H:118:PHE:CE2	2.86	0.58
2:H:82:LYS:CD	2:H:82:LYS:N	2.64	0.58
2:B:4:THR:HG23	2:B:5:PRO:CG	2.34	0.58
2:B:39:GLN:HG3	2:B:48:LEU:HD12	1.84	0.58
2:B:92:HIS:ND1	2:B:96:LEU:CD1	2.66	0.58
1:C:99:LYS:CG	1:C:99:LYS:O	2.48	0.58
1:E:2:LEU:N	1:E:2:LEU:HD23	2.19	0.58
1:E:27:GLU:O	1:E:31:ARG:N	2.37	0.58
1:G:118:THR:HG22	1:G:121:VAL:H	1.67	0.58
2:H:35:TYR:HE2	2:H:109:VAL:HG23	1.69	0.58
2:H:81:LEU:O	2:H:85:PHE:CD1	2.57	0.58
2:B:59:LYS:CE	2:B:62:ALA:HB2	2.34	0.58
1:C:118:THR:HG22	1:C:121:VAL:CA	2.30	0.58
2:D:91:LEU:HD12	2:D:91:LEU:O	2.04	0.58
2:D:128:ALA:HA	2:D:131:GLN:HB2	1.85	0.58
2:D:128:ALA:CA	2:D:131:GLN:HB2	2.34	0.58
1:E:43:PHE:CD1	1:E:43:PHE:N	2.71	0.58
1:E:137:THR:CB	1:E:137:THR:HG1	2.10	0.58
2:F:20:VAL:CA	2:F:68:LEU:HD13	2.34	0.58
2:H:123:THR:O	2:H:126:VAL:N	2.37	0.58
2:B:136:GLY:O	2:B:140:ALA:CB	2.51	0.58
1:C:118:THR:N	1:C:118:THR:O	2.36	0.58
2:D:24:GLY:CA	2:D:68:LEU:HD23	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:VAL:C	1:E:136:LEU:HD12	2.29	0.58
2:F:34:VAL:O	1:G:141:ARG:HG2	2.04	0.58
2:H:4:THR:HG22	2:H:5:PRO:N	2.19	0.58
2:H:67:VAL:HG13	3:H:147:HEM:C1B	2.39	0.58
1:C:20:HIS:O	1:C:23:GLU:CB	2.52	0.57
1:G:112:HIS:C	1:G:113:LEU:CD1	2.77	0.57
2:H:123:THR:HG22	2:H:124:PRO:CD	2.12	0.57
1:A:83:LEU:CD1	3:A:142:HEM:HMA1	2.26	0.57
1:E:126:ASP:OD2	1:G:141:ARG:CZ	2.52	0.57
2:F:39:GLN:HG3	2:F:48:LEU:HD13	1.85	0.57
2:F:124:PRO:CD	2:F:125:PRO:CD	2.82	0.57
1:G:81:SER:CB	1:G:81:SER:HG	2.10	0.57
1:A:114:PRO:O	2:B:116:HIS:NE2	2.37	0.57
2:B:71:PHE:CE1	2:B:137:VAL:HG21	2.39	0.57
2:D:42:PHE:HB3	2:D:45:PHE:CD2	2.39	0.57
1:E:96:VAL:CG2	2:H:101:GLU:CD	2.69	0.57
2:F:4:THR:HG22	2:F:6:VAL:CG1	2.34	0.57
1:G:61:LYS:O	3:G:142:HEM:HMA3	2.04	0.57
2:B:35:TYR:C	2:B:37:TRP:H	2.13	0.57
1:C:105:LEU:O	1:C:109:LEU:HB2	2.04	0.57
2:D:103:PHE:CE1	2:D:141:LEU:HD12	2.38	0.57
1:E:106:LEU:C	1:E:110:ALA:HB2	2.27	0.57
2:F:29:GLY:C	2:F:55:MET:SD	2.86	0.57
1:G:10:VAL:HG13	1:G:125:LEU:CD2	2.34	0.57
1:G:66:LEU:CD1	1:G:132:VAL:CG2	2.54	0.57
1:G:128:PHE:CD1	1:G:128:PHE:O	2.57	0.57
1:C:93:VAL:O	1:C:94:ASP:C	2.41	0.57
1:E:29:LEU:CD1	1:E:58:HIS:HD2	2.17	0.57
1:E:86:LEU:HD11	1:E:90:LYS:CD	2.20	0.57
2:F:17:LYS:NZ	2:F:121:GLU:OE1	2.36	0.57
2:F:26:GLU:O	2:F:30:ARG:CB	2.41	0.57
2:F:58:PRO:O	2:F:62:ALA:CB	2.50	0.57
1:C:40:LYS:CE	1:C:40:LYS:HG3	2.31	0.57
2:F:1:VAL:CG2	2:F:132:LYS:O	2.53	0.57
2:F:124:PRO:CB	2:F:125:PRO:HD3	2.34	0.57
2:B:42:PHE:O	2:B:45:PHE:CB	2.51	0.57
2:D:10:ALA:HB1	2:D:126:VAL:CG1	2.32	0.57
1:G:29:LEU:CD1	1:G:33:PHE:CE2	2.86	0.57
1:G:118:THR:CG2	1:G:120:ALA:CA	2.83	0.57
1:C:17:VAL:O	1:C:19:ALA:N	2.37	0.57
1:E:123:ALA:O	1:E:126:ASP:CB	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:LEU:CD2	3:G:142:HEM:C3D	2.88	0.57
1:A:98:PHE:CZ	3:A:142:HEM:CHC	2.87	0.57
1:A:99:LYS:C	1:A:100:LEU:HD23	2.29	0.57
2:B:33:VAL:HG23	2:B:54:VAL:HG11	1.87	0.57
2:B:60:VAL:HG12	2:B:61:LYS:N	2.15	0.57
1:C:51:GLY:O	1:C:52:SER:C	2.47	0.57
1:C:118:THR:CG2	1:C:120:ALA:CB	2.75	0.57
1:E:44:PRO:CG	1:E:45:HIS:H	2.01	0.57
1:G:103:HIS:O	1:G:107:VAL:HG23	2.04	0.57
1:G:107:VAL:CG1	2:H:112:CYS:CB	2.82	0.57
1:G:129:LEU:N	1:G:129:LEU:HD23	2.10	0.57
2:H:102:ASN:C	2:H:103:PHE:C	2.73	0.57
2:H:103:PHE:N	2:H:103:PHE:C	2.56	0.57
1:A:36:PHE:CZ	1:A:100:LEU:HD13	2.40	0.57
1:C:104:CYS:CA	1:C:107:VAL:CG2	2.81	0.57
1:E:129:LEU:CD2	1:E:129:LEU:C	2.78	0.57
2:F:1:VAL:HB	2:F:132:LYS:CG	2.35	0.57
2:H:55:MET:SD	2:H:55:MET:N	2.78	0.57
2:H:69:GLY:HA2	2:H:72:SER:OG	2.05	0.57
1:A:40:LYS:O	1:A:41:THR:CA	2.52	0.56
1:A:46:PHE:CD1	1:A:54:GLN:HG2	2.40	0.56
1:A:111:ALA:HB1	2:B:119:GLY:CA	2.32	0.56
1:E:102:SER:HA	1:E:105:LEU:HD13	1.87	0.56
2:F:114:LEU:C	2:F:114:LEU:CD2	2.75	0.56
1:G:33:PHE:HZ	1:G:43:PHE:CE1	2.22	0.56
1:G:46:PHE:C	1:G:48:LEU:CD2	2.78	0.56
1:G:117:PHE:CG	1:G:117:PHE:C	2.83	0.56
2:H:114:LEU:HD23	2:H:118:PHE:HD1	1.66	0.56
2:B:1:VAL:C	2:B:2:HIS:CG	2.79	0.56
1:C:118:THR:HG22	1:C:120:ALA:C	2.22	0.56
2:F:81:LEU:HD13	2:F:137:VAL:CA	2.35	0.56
2:F:82:LYS:CD	2:F:82:LYS:NZ	2.60	0.56
2:H:20:VAL:HG12	2:H:65:LYS:HB3	1.85	0.56
2:H:35:TYR:N	2:H:36:PRO:CD	2.68	0.56
2:H:78:LEU:CD2	2:H:133:VAL:HG23	2.34	0.56
2:H:123:THR:O	2:H:127:GLN:N	2.37	0.56
1:A:118:THR:N	1:A:121:VAL:HB	2.21	0.56
2:B:20:VAL:C	2:B:22:GLU:H	2.12	0.56
1:C:47:ASP:O	1:C:52:SER:HB3	2.05	0.56
1:C:102:SER:OG	1:C:129:LEU:CD1	2.53	0.56
1:C:107:VAL:HG12	2:D:112:CYS:SG	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:THR:CB	2:D:4:THR:HG1	2.09	0.56
2:D:58:PRO:HA	2:D:61:LYS:CG	2.35	0.56
2:D:112:CYS:O	2:D:115:ALA:N	2.38	0.56
1:E:36:PHE:C	1:E:38:THR:H	2.11	0.56
1:E:55:VAL:O	1:E:56:LYS:C	2.43	0.56
2:F:24:GLY:N	2:F:68:LEU:HD11	2.20	0.56
2:F:24:GLY:CA	2:F:68:LEU:HD12	2.31	0.56
2:F:94:ASP:OD1	2:F:146:HIS:CD2	2.58	0.56
1:G:2:LEU:HB3	1:G:6:ASP:HB2	1.86	0.56
2:H:68:LEU:N	2:H:69:GLY:N	2.53	0.56
2:H:130:TYR:O	2:H:134:VAL:CG2	2.45	0.56
1:A:36:PHE:CD1	1:A:100:LEU:HD13	2.39	0.56
2:F:81:LEU:HD22	2:F:85:PHE:CE1	2.37	0.56
2:B:88:LEU:HD22	2:H:6:VAL:HG22	1.87	0.56
2:B:131:GLN:CA	2:B:131:GLN:HE21	2.18	0.56
2:D:25:GLY:CA	2:D:61:LYS:HA	2.35	0.56
1:E:29:LEU:O	1:E:32:MET:HB3	2.06	0.56
1:E:137:THR:OG1	1:E:137:THR:CG2	2.50	0.56
1:G:17:VAL:O	1:G:20:HIS:N	2.38	0.56
1:A:38:THR:O	1:A:41:THR:CB	2.53	0.56
2:D:85:PHE:CB	2:D:88:LEU:HB3	2.35	0.56
2:F:1:VAL:HG11	2:F:132:LYS:CG	2.35	0.56
2:F:91:LEU:HD23	2:F:91:LEU:C	2.31	0.56
2:H:15:TRP:O	2:H:15:TRP:CD1	2.58	0.56
1:C:130:ALA:CA	1:C:133:SER:OG	2.49	0.56
1:E:15:GLY:C	1:E:17:VAL:N	2.62	0.56
1:G:32:MET:C	1:G:32:MET:HB3	2.28	0.56
1:G:84:SER:OG	1:G:136:LEU:HG	2.06	0.56
1:G:105:LEU:O	1:G:106:LEU:C	2.48	0.56
1:A:3:SER:O	1:A:7:LYS:HG2	2.06	0.56
1:A:62:VAL:HG13	1:A:62:VAL:O	2.05	0.56
2:B:41:PHE:CZ	2:B:102:ASN:OD1	2.58	0.56
1:E:128:PHE:C	1:E:131:SER:HB2	2.31	0.56
1:G:47:ASP:C	1:G:47:ASP:OD1	2.48	0.56
2:H:67:VAL:C	2:H:69:GLY:N	2.64	0.56
2:H:79:ASP:C	2:H:79:ASP:OD2	2.49	0.56
1:A:112:HIS:C	1:A:113:LEU:HD23	2.29	0.56
1:C:36:PHE:O	1:C:39:THR:HG23	2.06	0.56
1:C:93:VAL:CG1	3:C:142:HEM:CAC	2.74	0.56
2:D:101:GLU:N	2:D:104:ARG:HH11	2.01	0.56
2:F:3:LEU:HD13	2:F:8:LYS:CA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:LEU:HD23	1:G:125:LEU:HD13	1.88	0.56
2:H:88:LEU:CD2	2:H:91:LEU:HD23	2.35	0.56
2:D:4:THR:OG1	2:D:4:THR:CA	2.49	0.56
2:D:33:VAL:HG12	2:D:34:VAL:HG22	1.87	0.56
2:D:64:GLY:O	2:D:67:VAL:N	2.38	0.56
2:F:17:LYS:HB3	2:F:118:PHE:CZ	2.40	0.56
1:G:31:ARG:HG3	2:H:127:GLN:OE1	2.06	0.56
1:G:80:LEU:HD11	1:G:132:VAL:CG1	2.31	0.56
2:H:8:LYS:HG2	2:H:78:LEU:CD1	2.36	0.56
2:H:80:ASN:OD1	2:H:83:GLY:CA	2.53	0.56
2:B:21:ASP:OD1	2:B:65:LYS:HE3	2.06	0.55
2:B:115:ALA:HA	2:B:122:PHE:CD2	2.42	0.55
2:B:146:HIS:CD2	2:B:146:HIS:H	2.13	0.55
2:D:14:LEU:HD12	2:D:14:LEU:CA	2.36	0.55
2:F:1:VAL:HG11	2:F:132:LYS:HG3	1.87	0.55
2:F:41:PHE:CE1	3:F:147:HEM:HBC1	2.40	0.55
2:H:98:VAL:O	2:H:99:ASP:CA	2.53	0.55
2:B:3:LEU:HD21	2:B:129:ALA:HB1	1.88	0.55
1:C:101:LEU:HD13	1:C:105:LEU:HD12	1.88	0.55
2:D:136:GLY:O	2:D:140:ALA:N	2.40	0.55
1:E:17:VAL:HG13	1:E:24:TYR:CE1	2.40	0.55
2:B:74:GLY:C	2:B:76:ALA:H	2.14	0.55
1:C:64:ASP:HA	1:C:64:ASP:CG	2.16	0.55
1:C:106:LEU:O	1:C:110:ALA:CA	2.54	0.55
2:D:28:LEU:HD11	2:D:32:LEU:CD1	2.36	0.55
2:D:57:ASN:HB3	2:D:60:VAL:HB	1.88	0.55
2:D:112:CYS:O	2:D:115:ALA:CB	2.52	0.55
1:G:118:THR:HG22	1:G:120:ALA:CB	2.30	0.55
1:A:112:HIS:C	1:A:113:LEU:HG	2.31	0.55
2:B:17:LYS:O	2:B:18:VAL:C	2.49	0.55
2:B:50:THR:OG1	2:B:53:ALA:CB	2.54	0.55
2:B:103:PHE:CE2	2:B:141:LEU:HD12	2.39	0.55
1:C:42:TYR:CE1	1:C:93:VAL:HG13	2.41	0.55
1:E:31:ARG:HG3	2:F:124:PRO:HG3	1.89	0.55
2:F:20:VAL:CG2	2:F:21:ASP:OD1	2.55	0.55
2:F:31:LEU:CD1	2:F:109:VAL:HG21	2.34	0.55
1:G:30:GLU:OE2	1:G:50:HIS:CD2	2.58	0.55
2:D:15:TRP:O	2:D:16:GLY:C	2.49	0.55
2:D:146:HIS:CD2	2:D:146:HIS:C	2.73	0.55
2:B:92:HIS:CA	2:B:96:LEU:CD1	2.73	0.55
2:B:101:GLU:O	2:B:104:ARG:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:ASP:C	2:F:47:ASP:OD2	2.41	0.55
2:F:50:THR:O	2:F:53:ALA:CB	2.52	0.55
1:G:20:HIS:O	1:G:23:GLU:HB2	2.07	0.55
1:A:2:LEU:N	1:A:2:LEU:CD2	2.59	0.55
1:A:8:THR:O	1:A:8:THR:HG22	2.06	0.55
2:B:12:THR:CB	2:B:12:THR:HG1	2.12	0.55
1:C:119:PRO:CD	1:C:120:ALA:H	2.19	0.55
2:D:124:PRO:CD	2:D:125:PRO:HD2	2.36	0.55
1:A:84:SER:HA	1:A:136:LEU:HD22	1.87	0.55
1:A:87:HIS:CB	1:A:136:LEU:HD13	2.35	0.55
1:A:88:ALA:CB	1:A:139:LYS:CB	2.84	0.55
2:B:32:LEU:O	2:B:39:GLN:NE2	2.40	0.55
2:B:41:PHE:CD2	2:B:98:VAL:HG12	2.41	0.55
1:C:42:TYR:CZ	1:C:93:VAL:HG13	2.42	0.55
1:C:75:ASP:O	1:C:78:ASN:N	2.39	0.55
2:D:77:HIS:HB3	2:D:84:THR:HG21	1.89	0.55
1:G:28:ALA:CA	1:G:108:THR:HG21	2.37	0.55
2:H:15:TRP:O	2:H:15:TRP:CG	2.59	0.55
1:A:31:ARG:HD3	2:B:124:PRO:HA	1.89	0.55
2:B:103:PHE:CE1	2:B:141:LEU:CD1	2.89	0.55
1:C:26:ALA:HB1	1:C:55:VAL:CG1	2.37	0.55
2:F:91:LEU:HD23	2:F:96:LEU:HD12	1.88	0.55
1:G:79:ALA:O	1:G:82:ALA:HB2	1.99	0.55
1:A:83:LEU:O	1:A:136:LEU:HD21	2.06	0.55
1:A:111:ALA:HB1	2:B:119:GLY:C	2.32	0.55
2:B:7:GLU:O	2:B:11:VAL:N	2.36	0.55
3:B:147:HEM:HBA2	3:B:147:HEM:HHA	1.89	0.55
2:D:17:LYS:H	2:D:17:LYS:CD	2.16	0.55
2:F:146:HIS:C	1:G:40:LYS:NZ	2.65	0.55
2:H:26:GLU:O	2:H:30:ARG:CD	2.55	0.55
2:B:37:TRP:HH2	1:C:141:ARG:HH21	1.55	0.54
1:C:70:VAL:HG23	1:C:128:PHE:CE1	2.41	0.54
2:F:12:THR:O	2:F:16:GLY:N	2.39	0.54
1:A:98:PHE:CE1	3:A:142:HEM:HHC	2.42	0.54
2:B:88:LEU:CD2	2:H:6:VAL:HG22	2.37	0.54
2:D:39:GLN:O	2:D:40:ARG:C	2.51	0.54
1:E:17:VAL:O	1:E:20:HIS:N	2.26	0.54
1:C:32:MET:O	1:C:36:PHE:HB2	2.08	0.54
2:D:44:SER:CB	2:D:45:PHE:HD2	2.19	0.54
2:D:68:LEU:N	2:D:68:LEU:CD1	2.54	0.54
2:F:37:TRP:HE1	1:G:94:ASP:CG	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:PHE:O	2:F:48:LEU:HD11	2.07	0.54
1:G:12:ALA:C	1:G:15:GLY:HA3	2.32	0.54
2:H:8:LYS:HA	2:H:11:VAL:CG2	2.37	0.54
1:A:86:LEU:O	1:A:87:HIS:C	2.47	0.54
1:A:137:THR:HG22	1:A:138:SER:N	2.21	0.54
1:C:58:HIS:O	1:C:61:LYS:HB3	2.06	0.54
1:C:130:ALA:HA	1:C:133:SER:HG	1.69	0.54
1:E:106:LEU:CD1	1:E:106:LEU:HD22	2.38	0.54
1:A:112:HIS:C	1:A:114:PRO:HD3	2.33	0.54
1:C:83:LEU:C	1:C:86:LEU:HB3	2.32	0.54
1:C:118:THR:HB	1:C:121:VAL:CB	2.28	0.54
1:E:36:PHE:O	1:E:39:THR:CG2	2.55	0.54
2:H:92:HIS:CG	2:H:103:PHE:HZ	2.25	0.54
1:A:112:HIS:C	1:A:113:LEU:CG	2.79	0.54
2:B:52:ASP:C	2:B:54:VAL:N	2.53	0.54
1:C:62:VAL:O	1:C:65:ALA:CB	2.38	0.54
1:C:111:ALA:HB2	2:D:115:ALA:O	2.08	0.54
2:D:31:LEU:HD13	2:D:106:LEU:HB2	1.90	0.54
2:D:123:THR:O	2:D:124:PRO:C	2.49	0.54
2:B:96:LEU:CD2	2:B:98:VAL:CG2	2.69	0.54
2:D:77:HIS:CB	2:D:77:HIS:C	2.72	0.54
1:E:13:ALA:O	1:E:16:LYS:CB	2.54	0.54
2:F:11:VAL:HA	2:F:130:TYR:CE2	2.42	0.54
2:F:37:TRP:CE2	1:G:94:ASP:OD1	2.61	0.54
1:G:126:ASP:O	1:G:129:LEU:HB2	2.07	0.54
2:H:88:LEU:HD22	2:H:91:LEU:HD23	1.90	0.54
2:H:93:CYS:HB2	2:H:145:TYR:CG	2.43	0.54
1:A:16:LYS:HG3	1:A:116:GLU:CD	2.33	0.54
1:C:118:THR:N	1:C:121:VAL:HB	2.23	0.54
1:E:83:LEU:O	1:E:87:HIS:ND1	2.34	0.54
1:E:98:PHE:CE1	3:E:142:HEM:HHC	2.43	0.54
1:G:95:PRO:HA	1:G:98:PHE:HD2	0.71	0.54
1:G:117:PHE:CD2	1:G:117:PHE:O	2.61	0.54
2:H:4:THR:CB	2:H:7:GLU:CB	2.36	0.54
2:B:51:PRO:C	2:B:54:VAL:HB	2.33	0.54
1:C:137:THR:O	1:C:137:THR:CG2	2.54	0.54
2:D:68:LEU:N	2:D:68:LEU:HD22	2.18	0.54
2:D:85:PHE:HD2	2:D:88:LEU:HD13	1.72	0.54
1:G:49:SER:C	1:G:52:SER:OG	2.51	0.54
2:H:66:LYS:O	2:H:66:LYS:HG3	2.08	0.54
2:H:85:PHE:CE2	2:H:137:VAL:HG13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:HB2	2:B:115:ALA:O	2.08	0.54
1:C:48:LEU:HA	1:C:52:SER:OG	2.08	0.54
2:D:33:VAL:C	2:D:34:VAL:HG23	2.33	0.54
2:F:100:PRO:HD3	2:F:145:TYR:CZ	2.43	0.54
1:G:111:ALA:CB	2:H:119:GLY:O	2.56	0.54
1:A:38:THR:O	1:A:41:THR:OG1	2.19	0.53
1:C:3:SER:OG	1:C:3:SER:CA	2.54	0.53
2:D:72:SER:HA	2:D:75:LEU:CD2	2.37	0.53
1:E:104:CYS:O	1:E:107:VAL:HB	2.08	0.53
2:F:124:PRO:N	2:F:125:PRO:HD2	2.23	0.53
1:G:29:LEU:CD1	1:G:33:PHE:HE2	2.20	0.53
1:G:35:SER:O	1:G:36:PHE:CD2	2.62	0.53
2:H:11:VAL:HG23	2:H:12:THR:H	1.73	0.53
2:H:66:LYS:HB3	2:H:67:VAL:CG2	2.35	0.53
2:H:99:ASP:N	2:H:99:ASP:HA	2.07	0.53
1:A:86:LEU:HD13	1:A:90:LYS:CE	2.38	0.53
1:A:118:THR:H	1:A:121:VAL:HB	1.74	0.53
2:B:38:THR:N	2:B:39:GLN:N	2.55	0.53
2:B:92:HIS:O	2:B:98:VAL:HG23	2.09	0.53
2:D:39:GLN:O	2:D:42:PHE:N	2.38	0.53
2:H:48:LEU:HD23	2:H:48:LEU:N	2.23	0.53
1:C:101:LEU:CD1	1:C:105:LEU:HD12	2.38	0.53
1:C:124:SER:C	1:C:127:LYS:HB2	2.34	0.53
2:D:107:GLY:O	2:D:111:VAL:HG21	2.04	0.53
1:E:96:VAL:HG21	2:H:101:GLU:HG2	1.81	0.53
1:E:140:TYR:O	1:E:141:ARG:HB3	2.07	0.53
1:G:83:LEU:HB3	1:G:136:LEU:HD21	1.91	0.53
2:H:112:CYS:O	2:H:115:ALA:HB3	2.08	0.53
1:A:53:ALA:HA	1:A:56:LYS:CD	2.17	0.53
2:D:93:CYS:SG	2:D:146:HIS:NE2	2.80	0.53
1:E:107:VAL:CA	1:E:110:ALA:CB	2.86	0.53
2:F:89:SER:HB2	2:F:144:LYS:HG2	1.89	0.53
1:G:93:VAL:O	1:G:140:TYR:OH	2.18	0.53
1:A:31:ARG:HH11	2:B:127:GLN:HB2	1.74	0.53
2:D:42:PHE:HB3	2:D:45:PHE:CD1	2.43	0.53
2:D:72:SER:O	2:D:75:LEU:N	2.41	0.53
2:D:117:HIS:ND1	2:D:117:HIS:N	2.51	0.53
1:E:9:ASN:HB2	1:E:124:SER:OG	2.07	0.53
1:E:10:VAL:HG13	1:E:125:LEU:CD2	2.22	0.53
1:E:127:LYS:HA	1:E:130:ALA:CB	2.38	0.53
2:F:7:GLU:HB3	2:F:129:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:TRP:CZ2	2:F:105:LEU:HD11	2.43	0.53
2:F:77:HIS:O	2:F:80:ASN:N	2.34	0.53
1:G:75:ASP:CA	1:G:77:PRO:HD2	2.39	0.53
1:A:53:ALA:N	1:A:56:LYS:CD	2.71	0.53
2:B:41:PHE:CD1	3:B:147:HEM:CAC	2.92	0.53
1:E:33:PHE:CE2	1:E:48:LEU:HD21	2.44	0.53
2:F:124:PRO:HD2	2:F:125:PRO:CD	2.38	0.53
1:G:91:LEU:CD2	3:G:142:HEM:C2D	2.91	0.53
2:B:27:ALA:O	2:B:109:VAL:HG11	2.09	0.53
1:C:95:PRO:HA	1:C:98:PHE:CD2	2.43	0.53
2:D:15:TRP:NE1	2:D:75:LEU:CD2	2.72	0.53
2:D:35:TYR:CE2	2:D:105:LEU:HD22	2.44	0.53
2:D:101:GLU:CB	2:D:104:ARG:CD	2.83	0.53
1:G:87:HIS:CG	1:G:91:LEU:HD12	2.30	0.53
1:G:90:LYS:O	1:G:91:LEU:C	2.50	0.53
1:G:91:LEU:HD21	3:G:142:HEM:C4D	2.43	0.53
1:A:4:PRO:C	1:A:7:LYS:CB	2.82	0.53
1:A:42:TYR:CE1	1:A:93:VAL:HA	2.44	0.53
1:A:76:MET:CB	1:A:77:PRO:HD3	2.39	0.53
2:B:89:SER:O	2:B:90:GLU:C	2.52	0.53
2:D:49:SER:OG	2:D:50:THR:N	2.42	0.53
1:E:106:LEU:O	1:E:110:ALA:CB	2.43	0.53
2:F:20:VAL:HG22	2:F:21:ASP:OD1	2.08	0.53
1:G:2:LEU:CA	1:G:6:ASP:OD2	2.56	0.53
1:G:93:VAL:O	1:G:98:PHE:HE2	1.92	0.53
1:G:117:PHE:CB	1:G:117:PHE:N	2.60	0.53
2:B:15:TRP:NE1	2:B:72:SER:HB3	2.21	0.53
2:B:35:TYR:HB3	2:B:37:TRP:CH2	2.43	0.53
2:B:119:GLY:C	2:B:121:GLU:H	2.16	0.53
2:D:4:THR:O	2:D:7:GLU:HB2	2.09	0.53
1:E:14:TRP:C	1:E:17:VAL:HB	2.34	0.53
1:E:141:ARG:HG3	2:H:37:TRP:HZ3	1.72	0.53
1:G:128:PHE:CD1	1:G:128:PHE:C	2.85	0.53
2:H:67:VAL:C	2:H:69:GLY:H	2.16	0.53
2:H:76:ALA:HB1	2:H:77:HIS:ND1	2.24	0.53
2:H:77:HIS:C	2:H:79:ASP:H	2.17	0.53
2:H:117:HIS:HB3	2:H:118:PHE:CD1	2.44	0.53
1:A:76:MET:HG2	1:A:76:MET:HA	1.88	0.53
1:C:70:VAL:C	1:C:72:HIS:N	2.65	0.53
2:D:63:HIS:CE1	2:D:67:VAL:HG13	2.44	0.53
2:F:89:SER:OG	2:F:141:LEU:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PHE:CE1	3:A:142:HEM:CHC	2.91	0.52
2:D:3:LEU:HA	2:D:132:LYS:HD2	1.90	0.52
2:D:20:VAL:O	2:D:20:VAL:HG12	2.07	0.52
2:D:51:PRO:O	2:D:55:MET:CB	2.53	0.52
2:F:11:VAL:HG23	2:F:130:TYR:CZ	2.44	0.52
3:G:142:HEM:HHD	3:G:142:HEM:CBC	2.39	0.52
2:H:3:LEU:CD1	2:H:78:LEU:O	2.57	0.52
2:H:48:LEU:N	2:H:48:LEU:CD2	2.73	0.52
2:B:47:ASP:C	2:B:48:LEU:HD23	2.34	0.52
1:C:39:THR:O	1:C:42:TYR:HB2	2.08	0.52
2:D:45:PHE:HB2	2:D:48:LEU:HD11	1.89	0.52
2:D:63:HIS:NE2	3:D:147:HEM:C1D	2.76	0.52
2:F:24:GLY:CA	2:F:68:LEU:CD1	2.88	0.52
2:F:80:ASN:O	2:F:80:ASN:CG	2.52	0.52
1:G:47:ASP:C	1:G:47:ASP:CB	2.64	0.52
1:G:117:PHE:CA	1:G:117:PHE:CD1	2.93	0.52
2:H:3:LEU:HD22	2:H:8:LYS:CE	2.33	0.52
2:H:32:LEU:HD13	2:H:32:LEU:H	1.74	0.52
2:H:92:HIS:HD2	2:H:98:VAL:CG2	2.22	0.52
1:A:3:SER:OG	1:A:4:PRO:N	2.37	0.52
1:A:17:VAL:O	1:A:19:ALA:N	2.42	0.52
3:A:142:HEM:HBB2	3:A:142:HEM:CMB	2.40	0.52
2:B:48:LEU:HD23	2:B:48:LEU:N	2.24	0.52
1:C:83:LEU:HD21	3:C:142:HEM:C3A	2.45	0.52
1:C:101:LEU:HD13	1:C:101:LEU:O	2.09	0.52
1:C:118:THR:HB	1:C:118:THR:H	1.74	0.52
2:D:33:VAL:HG12	2:D:34:VAL:HG23	1.90	0.52
2:D:87:THR:HG22	2:D:88:LEU:H	1.73	0.52
1:E:75:ASP:C	1:E:77:PRO:HD2	2.35	0.52
1:E:78:ASN:HA	1:E:81:SER:OG	2.10	0.52
2:F:98:VAL:HG13	2:F:102:ASN:OD1	2.09	0.52
1:A:42:TYR:C	1:A:44:PRO:HD3	2.34	0.52
1:A:135:VAL:O	1:A:136:LEU:C	2.51	0.52
1:C:102:SER:CB	1:C:129:LEU:CD1	2.88	0.52
2:D:85:PHE:O	2:D:89:SER:N	2.42	0.52
1:E:68:ASN:O	1:E:72:HIS:HD2	1.92	0.52
1:E:98:PHE:O	1:E:99:LYS:C	2.51	0.52
1:G:42:TYR:HB2	3:G:142:HEM:HBC1	1.90	0.52
2:D:31:LEU:HB3	2:D:32:LEU:HD12	1.91	0.52
1:E:38:THR:HG23	1:E:39:THR:H	1.68	0.52
1:A:17:VAL:O	1:A:17:VAL:CG1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:ALA:C	1:G:15:GLY:N	2.60	0.52
1:G:39:THR:O	1:G:43:PHE:HE1	1.92	0.52
1:G:73:VAL:HA	1:G:76:MET:HG3	1.90	0.52
1:G:103:HIS:NE2	2:H:108:ASN:HB3	2.25	0.52
1:A:4:PRO:CG	1:A:5:ALA:N	2.68	0.52
1:A:62:VAL:O	1:A:62:VAL:HG22	2.10	0.52
1:A:112:HIS:C	1:A:113:LEU:CD2	2.83	0.52
2:B:50:THR:HG22	2:B:51:PRO:CD	2.40	0.52
1:C:37:PRO:O	1:C:40:LYS:CG	2.58	0.52
2:D:49:SER:CB	2:D:49:SER:H	2.19	0.52
2:D:101:GLU:CA	2:D:104:ARG:NH1	2.34	0.52
1:E:86:LEU:HD12	1:E:90:LYS:HB2	1.92	0.52
1:C:32:MET:SD	1:C:101:LEU:CD2	2.98	0.52
1:C:119:PRO:HG3	2:D:30:ARG:CZ	2.40	0.52
2:D:131:GLN:NE2	2:D:131:GLN:O	2.43	0.52
1:G:43:PHE:N	1:G:43:PHE:HD1	2.08	0.52
1:A:38:THR:C	1:A:41:THR:H	2.17	0.52
1:C:31:ARG:NH1	1:C:31:ARG:CG	2.68	0.52
1:C:37:PRO:O	1:C:40:LYS:HE2	2.10	0.52
1:C:46:PHE:HD1	1:C:48:LEU:CD2	2.22	0.52
1:C:90:LYS:HG2	1:C:91:LEU:CG	2.40	0.52
1:C:137:THR:O	1:C:137:THR:HG22	2.10	0.52
2:F:89:SER:CB	2:F:144:LYS:HG2	2.40	0.52
1:G:75:ASP:CG	1:G:77:PRO:HD2	2.35	0.52
1:G:83:LEU:C	1:G:136:LEU:HD21	2.32	0.52
1:A:31:ARG:HD2	2:B:127:GLN:OE1	2.10	0.52
1:C:1:VAL:O	1:C:1:VAL:HG12	2.10	0.52
1:C:37:PRO:HG2	1:C:38:THR:HG22	1.91	0.52
1:C:58:HIS:O	1:C:61:LYS:CB	2.58	0.52
2:D:15:TRP:O	2:D:18:VAL:N	2.40	0.52
2:D:88:LEU:HD21	3:D:147:HEM:HMA1	1.91	0.52
2:D:123:THR:HB	2:D:125:PRO:CD	2.37	0.52
1:E:112:HIS:O	1:E:113:LEU:HG	2.06	0.52
2:F:35:TYR:CD1	2:F:37:TRP:CH2	2.98	0.52
2:H:117:HIS:CD2	2:H:118:PHE:CD2	2.97	0.52
2:B:75:LEU:HA	2:B:78:LEU:HD22	1.92	0.51
2:D:128:ALA:HA	2:D:131:GLN:CB	2.39	0.51
1:E:1:VAL:O	1:E:127:LYS:NZ	2.39	0.51
1:E:49:SER:O	1:E:50:HIS:C	2.52	0.51
1:G:101:LEU:O	1:G:105:LEU:HB2	2.11	0.51
2:H:20:VAL:CG1	2:H:65:LYS:HA	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:114:LEU:HA	2:H:117:HIS:HB2	1.92	0.51
2:H:125:PRO:CG	2:H:126:VAL:N	2.57	0.51
2:B:1:VAL:CA	2:B:2:HIS:ND1	2.74	0.51
1:E:30:GLU:OE2	1:E:50:HIS:CE1	2.64	0.51
1:E:120:ALA:O	1:E:123:ALA:CB	2.57	0.51
1:E:122:HIS:CE1	2:F:30:ARG:CD	2.92	0.51
2:H:123:THR:CB	2:H:124:PRO:HD2	2.40	0.51
1:A:36:PHE:CD1	1:A:100:LEU:HD12	2.45	0.51
1:A:126:ASP:O	1:A:129:LEU:N	2.43	0.51
2:B:18:VAL:C	2:B:18:VAL:HG12	2.33	0.51
2:B:28:LEU:HD11	2:B:32:LEU:HD21	1.89	0.51
2:B:124:PRO:O	2:B:127:GLN:HB3	2.10	0.51
1:C:20:HIS:O	1:C:23:GLU:HB3	2.10	0.51
2:D:101:GLU:CD	2:D:104:ARG:CD	2.83	0.51
1:G:11:LYS:HA	1:G:70:VAL:HG21	1.92	0.51
1:G:20:HIS:O	1:G:23:GLU:CA	2.58	0.51
2:H:86:ALA:CB	2:H:144:LYS:HE3	2.35	0.51
1:A:134:THR:O	1:A:138:SER:OG	2.25	0.51
2:B:35:TYR:C	2:B:37:TRP:N	2.68	0.51
2:B:136:GLY:O	2:B:140:ALA:HB2	2.10	0.51
2:D:50:THR:HB	2:D:51:PRO:CD	2.40	0.51
1:G:123:ALA:HB2	2:H:34:VAL:HG22	1.93	0.51
1:G:131:SER:O	1:G:134:THR:HB	2.10	0.51
2:H:38:THR:C	2:H:40:ARG:N	2.60	0.51
2:H:65:LYS:O	2:H:69:GLY:N	2.43	0.51
1:A:10:VAL:HG11	1:A:128:PHE:HB2	1.91	0.51
1:A:30:GLU:OE1	1:A:50:HIS:CE1	2.62	0.51
1:C:70:VAL:O	1:C:73:VAL:HG23	2.11	0.51
2:D:24:GLY:HA3	2:D:68:LEU:HD23	1.88	0.51
2:D:49:SER:HG	2:D:53:ALA:CB	2.23	0.51
1:G:17:VAL:C	1:G:19:ALA:N	2.69	0.51
2:H:99:ASP:O	2:H:102:ASN:OD1	2.28	0.51
2:B:45:PHE:CZ	2:B:60:VAL:HA	2.45	0.51
2:D:101:GLU:CG	2:D:104:ARG:CD	2.88	0.51
1:E:35:SER:CA	2:F:128:ALA:HB2	2.41	0.51
2:F:109:VAL:HA	2:F:112:CYS:HB2	1.92	0.51
2:D:25:GLY:HA2	2:D:61:LYS:HA	1.92	0.51
2:D:101:GLU:CG	2:D:104:ARG:HD3	2.41	0.51
1:E:19:ALA:O	1:E:20:HIS:CA	2.58	0.51
1:E:43:PHE:CE1	3:E:142:HEM:HBC1	2.45	0.51
1:G:104:CYS:C	1:G:108:THR:OG1	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:142:HEM:HBC2	3:G:142:HEM:CHD	2.40	0.51
2:B:37:TRP:HB2	1:C:92:ARG:HB3	1.92	0.51
1:C:81:SER:O	1:C:84:SER:HB3	2.11	0.51
1:C:90:LYS:CG	1:C:91:LEU:CD2	2.89	0.51
1:E:6:ASP:HA	1:E:124:SER:HG	1.75	0.51
1:E:31:ARG:HG2	2:F:124:PRO:HG3	1.92	0.51
1:E:84:SER:HB3	1:E:136:LEU:HA	1.92	0.51
2:F:11:VAL:HA	2:F:130:TYR:CZ	2.46	0.51
2:H:60:VAL:HG13	2:H:60:VAL:O	2.11	0.51
2:H:127:GLN:CG	2:H:127:GLN:HA	2.38	0.51
2:B:91:LEU:HG	2:B:91:LEU:O	2.10	0.51
2:H:45:PHE:CD1	2:H:60:VAL:HG23	2.46	0.51
2:H:45:PHE:HD1	2:H:60:VAL:HG23	1.76	0.51
1:A:121:VAL:O	1:A:125:LEU:HB2	2.10	0.51
1:C:87:HIS:O	1:C:92:ARG:HA	2.12	0.51
2:F:77:HIS:CB	2:F:84:THR:HG21	2.41	0.51
2:H:123:THR:CG2	2:H:123:THR:HA	2.40	0.51
1:A:13:ALA:O	1:A:17:VAL:HG23	2.11	0.50
2:D:24:GLY:HA2	2:D:68:LEU:CD2	2.37	0.50
2:D:77:HIS:CA	2:D:77:HIS:CG	2.84	0.50
2:F:101:GLU:OE1	2:F:101:GLU:HA	1.92	0.50
1:G:36:PHE:O	1:G:39:THR:HG23	2.11	0.50
1:G:107:VAL:HG12	2:H:112:CYS:CB	2.41	0.50
1:A:8:THR:O	1:A:8:THR:HG23	2.10	0.50
2:B:41:PHE:CD1	3:B:147:HEM:HAC	2.46	0.50
1:C:4:PRO:O	1:C:5:ALA:C	2.53	0.50
2:D:11:VAL:CG1	2:D:12:THR:H	2.16	0.50
2:D:102:ASN:HB3	3:D:147:HEM:CMC	2.40	0.50
2:D:113:VAL:CG1	2:D:114:LEU:CD2	2.77	0.50
1:E:33:PHE:CE2	1:E:48:LEU:HD23	2.41	0.50
1:E:52:SER:C	1:E:54:GLN:H	2.19	0.50
2:F:123:THR:OG1	2:F:126:VAL:HB	2.11	0.50
2:H:69:GLY:O	2:H:70:ALA:C	2.54	0.50
1:A:2:LEU:CD1	1:A:128:PHE:HA	2.41	0.50
1:A:66:LEU:O	1:A:70:VAL:CG2	2.48	0.50
1:A:86:LEU:HA	1:A:90:LYS:HE3	1.92	0.50
2:B:37:TRP:HZ3	1:C:141:ARG:HG3	1.76	0.50
1:C:97:ASN:HA	1:C:100:LEU:HB2	1.93	0.50
2:F:22:GLU:HG2	2:F:23:VAL:CA	2.38	0.50
1:G:110:ALA:CB	2:H:115:ALA:HB3	2.37	0.50
2:H:30:ARG:HD3	2:H:113:VAL:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:TRP:NE1	2:D:75:LEU:HD23	2.27	0.50
2:D:49:SER:C	2:D:49:SER:OG	2.54	0.50
1:E:88:ALA:N	1:E:140:TYR:CE2	2.79	0.50
1:E:101:LEU:O	1:E:105:LEU:CD1	2.46	0.50
2:F:31:LEU:CD1	2:F:35:TYR:CE2	2.95	0.50
1:G:24:TYR:O	1:G:28:ALA:HB2	2.12	0.50
2:H:36:PRO:O	2:H:39:GLN:HB2	2.10	0.50
1:C:66:LEU:HD23	1:C:129:LEU:HD23	1.86	0.50
2:D:9:SER:O	2:D:13:ALA:N	2.42	0.50
2:D:15:TRP:CZ2	2:D:75:LEU:HD21	2.46	0.50
2:F:29:GLY:N	2:F:55:MET:CE	2.44	0.50
2:F:48:LEU:CD2	2:F:48:LEU:HB3	2.38	0.50
1:G:12:ALA:O	1:G:15:GLY:HA3	2.10	0.50
1:G:80:LEU:O	1:G:82:ALA:C	2.55	0.50
2:H:122:PHE:CE1	2:H:126:VAL:CG1	2.95	0.50
1:A:3:SER:OG	1:A:4:PRO:HD2	2.05	0.50
1:C:10:VAL:CG2	1:C:125:LEU:CD2	2.89	0.50
1:C:31:ARG:HG3	2:D:124:PRO:HA	1.94	0.50
2:F:11:VAL:O	2:F:12:THR:C	2.52	0.50
2:F:81:LEU:HD13	2:F:137:VAL:N	2.27	0.50
2:F:118:PHE:O	2:F:121:GLU:N	2.45	0.50
1:G:28:ALA:O	1:G:31:ARG:HB3	2.11	0.50
1:G:114:PRO:O	2:H:116:HIS:NE2	2.45	0.50
2:H:32:LEU:HD13	2:H:32:LEU:N	2.26	0.50
2:H:92:HIS:CG	2:H:103:PHE:CZ	3.00	0.50
1:A:7:LYS:HD2	1:A:73:VAL:HG22	1.94	0.50
1:C:119:PRO:HD2	1:C:120:ALA:H	1.76	0.50
2:D:15:TRP:CE2	2:D:75:LEU:HD21	2.47	0.50
2:D:35:TYR:N	2:D:36:PRO:HD3	2.26	0.50
1:E:39:THR:OG1	1:E:43:PHE:HE1	1.93	0.50
2:F:20:VAL:HG23	2:F:21:ASP:N	2.19	0.50
2:H:11:VAL:CG2	2:H:12:THR:N	2.73	0.50
1:C:104:CYS:HA	1:C:107:VAL:HG23	1.89	0.50
2:D:13:ALA:C	2:D:15:TRP:N	2.69	0.50
1:E:2:LEU:CA	1:E:127:LYS:HZ3	2.24	0.50
2:H:8:LYS:O	2:H:11:VAL:HG23	2.12	0.50
1:A:17:VAL:O	1:A:20:HIS:N	2.45	0.50
2:D:37:TRP:C	2:D:39:GLN:N	2.67	0.50
1:E:102:SER:CB	1:E:129:LEU:CD2	2.66	0.50
2:F:72:SER:O	2:F:75:LEU:N	2.44	0.50
1:G:14:TRP:CA	1:G:14:TRP:HE3	2.05	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:LEU:N	2:H:69:GLY:H	2.10	0.50
2:H:124:PRO:HA	2:H:127:GLN:HB2	1.93	0.50
1:A:4:PRO:C	1:A:7:LYS:HB3	2.37	0.49
1:A:43:PHE:N	1:A:44:PRO:HD3	2.27	0.49
1:C:78:ASN:N	1:C:79:ALA:H	2.10	0.49
1:E:67:THR:CG2	1:E:68:ASN:N	2.42	0.49
1:E:122:HIS:HE2	2:F:109:VAL:HG12	1.77	0.49
1:G:17:VAL:HG13	1:G:24:TYR:CE1	2.46	0.49
1:G:98:PHE:O	1:G:102:SER:HB3	2.12	0.49
2:H:25:GLY:HA3	2:H:61:LYS:HG2	1.94	0.49
1:C:33:PHE:CD1	1:C:40:LYS:HG2	2.47	0.49
1:G:32:MET:CG	1:G:32:MET:HA	2.41	0.49
2:H:126:VAL:O	2:H:127:GLN:C	2.53	0.49
1:A:4:PRO:HA	1:A:7:LYS:CG	2.43	0.49
1:A:43:PHE:HA	1:A:45:HIS:HE1	1.75	0.49
2:B:15:TRP:CH2	2:B:71:PHE:CD2	3.01	0.49
1:C:83:LEU:HA	1:C:86:LEU:HB3	1.93	0.49
1:C:131:SER:O	1:C:132:VAL:C	2.54	0.49
2:F:35:TYR:O	2:F:36:PRO:C	2.54	0.49
1:G:3:SER:CB	1:G:4:PRO:HD2	2.32	0.49
1:G:76:MET:N	1:G:77:PRO:HD2	2.20	0.49
1:G:101:LEU:O	1:G:105:LEU:N	2.40	0.49
2:H:85:PHE:H	2:H:85:PHE:HD1	1.47	0.49
2:H:102:ASN:O	2:H:106:LEU:N	2.43	0.49
2:B:58:PRO:HG2	2:B:59:LYS:N	2.27	0.49
1:C:79:ALA:C	1:C:81:SER:H	2.21	0.49
2:D:16:GLY:C	2:D:18:VAL:H	2.21	0.49
1:E:112:HIS:O	1:E:114:PRO:HD3	2.13	0.49
2:H:80:ASN:HD21	2:H:83:GLY:HA3	1.69	0.49
1:A:38:THR:C	1:A:41:THR:HG23	2.36	0.49
1:A:85:ASP:O	1:A:89:HIS:CD2	2.65	0.49
1:A:94:ASP:OD2	1:A:96:VAL:CG2	2.60	0.49
1:A:95:PRO:HB3	1:A:137:THR:OG1	2.12	0.49
1:A:121:VAL:HG23	1:A:121:VAL:H	1.70	0.49
2:B:20:VAL:HG21	2:B:72:SER:OG	2.13	0.49
1:C:31:ARG:HD3	2:D:127:GLN:OE1	2.13	0.49
2:D:3:LEU:HD23	2:D:132:LYS:CG	2.43	0.49
2:D:32:LEU:HD21	2:D:42:PHE:CD1	2.39	0.49
2:D:42:PHE:CB	2:D:45:PHE:CD1	2.95	0.49
2:D:47:ASP:OD2	2:D:49:SER:OG	2.30	0.49
2:H:32:LEU:N	2:H:32:LEU:CD1	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:PHE:HB3	1:C:48:LEU:HD21	1.95	0.49
2:D:28:LEU:HD12	2:D:28:LEU:C	2.36	0.49
2:D:121:GLU:C	2:D:123:THR:N	2.70	0.49
1:E:35:SER:CB	1:E:35:SER:HG	2.10	0.49
2:F:124:PRO:N	2:F:125:PRO:HD3	2.26	0.49
1:G:114:PRO:HA	2:H:116:HIS:CD2	2.48	0.49
2:H:17:LYS:HB3	2:H:118:PHE:HE2	1.74	0.49
2:H:19:ASN:OD1	2:H:22:GLU:OE2	2.30	0.49
2:H:47:ASP:O	2:H:53:ALA:HB1	2.13	0.49
1:A:55:VAL:HG23	1:A:56:LYS:N	2.28	0.49
1:A:87:HIS:CD2	1:A:136:LEU:HD11	2.34	0.49
2:B:58:PRO:HG2	2:B:59:LYS:H	1.77	0.49
2:B:102:ASN:HA	2:B:105:LEU:HD12	1.93	0.49
2:B:133:VAL:C	2:B:135:ALA:H	2.17	0.49
1:C:105:LEU:O	1:C:109:LEU:N	2.46	0.49
2:D:103:PHE:CD1	2:D:141:LEU:HD12	2.48	0.49
2:F:1:VAL:CG1	2:F:132:LYS:CG	2.90	0.49
1:G:46:PHE:O	1:G:48:LEU:HD21	2.12	0.49
1:G:83:LEU:HD11	3:G:142:HEM:HMA2	1.88	0.49
2:B:98:VAL:O	2:B:145:TYR:CZ	2.65	0.49
2:D:27:ALA:O	2:D:28:LEU:C	2.55	0.49
1:E:121:VAL:O	1:E:121:VAL:HG12	2.04	0.49
2:F:124:PRO:HB2	2:F:125:PRO:HD3	1.95	0.49
1:G:121:VAL:C	1:G:124:SER:H	2.21	0.49
1:G:125:LEU:O	1:G:126:ASP:C	2.52	0.49
2:H:4:THR:HB	2:H:7:GLU:HB3	1.73	0.49
2:H:79:ASP:OD2	2:H:80:ASN:N	2.46	0.49
2:H:92:HIS:O	2:H:96:LEU:CB	2.58	0.49
2:B:14:LEU:CD1	2:B:114:LEU:CD1	2.88	0.49
2:B:41:PHE:HZ	2:B:102:ASN:OD1	1.96	0.49
3:C:142:HEM:CMC	3:C:142:HEM:CBC	2.89	0.49
2:D:81:LEU:HD13	2:D:137:VAL:HG22	1.88	0.49
2:F:7:GLU:HB3	2:F:129:ALA:CB	2.43	0.49
2:B:92:HIS:CG	2:B:96:LEU:HD11	2.48	0.49
1:C:16:LYS:HE2	1:C:16:LYS:HG3	1.90	0.49
2:D:77:HIS:CB	2:D:84:THR:HG21	2.42	0.49
2:D:85:PHE:CA	2:D:88:LEU:HB3	2.43	0.49
2:F:31:LEU:HD11	2:F:35:TYR:CE2	2.48	0.49
2:H:61:LYS:NZ	2:H:61:LYS:HD3	2.28	0.49
2:H:134:VAL:O	2:H:134:VAL:HG12	2.12	0.49
2:F:2:HIS:O	2:F:2:HIS:CG	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:LYS:CG	2:B:17:LYS:HE2	2.37	0.48
1:C:75:ASP:O	1:C:76:MET:C	2.55	0.48
2:D:82:LYS:O	2:D:83:GLY:C	2.56	0.48
1:E:87:HIS:HA	1:E:91:LEU:HD12	1.95	0.48
2:F:60:VAL:O	2:F:61:LYS:C	2.52	0.48
2:H:46:GLY:O	2:H:48:LEU:CD2	2.58	0.48
1:A:92:ARG:HG2	2:D:37:TRP:CB	2.43	0.48
2:B:111:VAL:HG13	2:B:122:PHE:HZ	1.75	0.48
1:C:102:SER:OG	1:C:129:LEU:HD13	2.14	0.48
2:D:107:GLY:HA2	2:D:134:VAL:CG2	2.33	0.48
2:F:90:GLU:OE1	2:F:90:GLU:HB3	2.13	0.48
1:G:75:ASP:OD1	1:G:77:PRO:HD2	2.13	0.48
2:H:2:HIS:O	2:H:132:LYS:CD	2.61	0.48
1:A:140:TYR:C	1:A:141:ARG:CG	2.84	0.48
1:A:141:ARG:CZ	1:A:141:ARG:HB3	2.44	0.48
2:B:15:TRP:CZ3	2:B:71:PHE:HE2	2.31	0.48
2:B:43:GLU:C	2:B:45:PHE:N	2.49	0.48
2:B:74:GLY:C	2:B:76:ALA:N	2.69	0.48
2:B:103:PHE:HB2	2:B:138:ALA:HB1	1.94	0.48
2:B:118:PHE:O	2:B:121:GLU:HB2	2.13	0.48
1:C:31:ARG:CD	2:D:127:GLN:OE1	2.61	0.48
1:C:59:GLY:C	1:C:62:VAL:H	2.20	0.48
1:C:90:LYS:HG2	1:C:91:LEU:HG	1.94	0.48
2:F:20:VAL:HG22	2:F:21:ASP:N	2.29	0.48
1:G:61:LYS:O	1:G:65:ALA:HB2	2.14	0.48
1:G:62:VAL:O	1:G:65:ALA:CB	2.58	0.48
2:H:114:LEU:CD2	2:H:118:PHE:CE1	2.87	0.48
2:B:38:THR:HB	2:B:41:PHE:HE1	1.77	0.48
1:C:88:ALA:O	1:C:92:ARG:HG2	2.13	0.48
2:D:124:PRO:HD2	2:D:125:PRO:HD2	1.95	0.48
1:E:42:TYR:C	1:E:43:PHE:CD1	2.91	0.48
1:E:139:LYS:HZ3	1:E:139:LYS:HG2	1.37	0.48
1:G:104:CYS:HA	1:G:107:VAL:HG23	1.96	0.48
2:H:101:GLU:O	2:H:104:ARG:HB2	2.13	0.48
1:C:7:LYS:NZ	1:C:74:ASP:CG	2.68	0.48
1:C:49:SER:O	1:C:50:HIS:C	2.55	0.48
2:D:50:THR:HB	2:D:51:PRO:HD2	1.95	0.48
1:E:141:ARG:CG	2:H:37:TRP:CZ3	2.85	0.48
1:E:141:ARG:O	1:G:127:LYS:HD2	2.14	0.48
2:F:107:GLY:HA2	2:F:134:VAL:CG1	2.43	0.48
2:H:14:LEU:CD2	2:H:14:LEU:HD13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TRP:CH2	1:A:66:LEU:HD22	2.49	0.48
2:B:72:SER:HA	2:B:75:LEU:HD11	1.95	0.48
2:B:130:TYR:O	2:B:134:VAL:HG12	2.14	0.48
1:C:132:VAL:CG1	1:C:132:VAL:C	2.87	0.48
2:D:7:GLU:O	2:D:8:LYS:C	2.56	0.48
2:D:42:PHE:HB2	2:D:45:PHE:CG	2.48	0.48
2:F:35:TYR:O	2:F:37:TRP:N	2.47	0.48
2:H:42:PHE:O	2:H:45:PHE:HB2	2.14	0.48
1:A:62:VAL:O	1:A:62:VAL:CG1	2.59	0.48
2:F:1:VAL:HG21	2:F:132:LYS:O	2.14	0.48
1:G:29:LEU:O	1:G:30:GLU:C	2.52	0.48
1:G:91:LEU:CD2	3:G:142:HEM:C4D	2.97	0.48
1:A:100:LEU:O	1:A:103:HIS:CB	2.44	0.48
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.19	0.48
1:C:17:VAL:C	1:C:19:ALA:N	2.71	0.48
1:C:37:PRO:O	1:C:40:LYS:HG3	2.14	0.48
1:C:121:VAL:O	1:C:125:LEU:HB2	2.14	0.48
2:F:63:HIS:HA	2:F:66:LYS:HB2	1.96	0.48
2:B:59:LYS:HE3	2:B:59:LYS:C	2.39	0.48
1:C:43:PHE:HB3	1:C:46:PHE:HB2	1.96	0.48
2:F:37:TRP:NE1	1:G:94:ASP:CG	2.67	0.48
2:F:67:VAL:HG22	3:F:147:HEM:C1B	2.49	0.48
2:H:60:VAL:HG12	2:H:61:LYS:N	2.16	0.48
1:C:27:GLU:CG	1:C:108:THR:HG22	2.39	0.47
1:C:94:ASP:HA	1:C:95:PRO:HD2	1.29	0.47
2:F:111:VAL:O	2:F:111:VAL:HG12	2.14	0.47
2:F:118:PHE:HB3	2:F:121:GLU:CB	2.44	0.47
1:C:46:PHE:HB3	1:C:48:LEU:CD2	2.44	0.47
1:C:86:LEU:HD21	3:C:142:HEM:CBA	2.44	0.47
2:D:21:ASP:CA	2:D:65:LYS:HG2	2.41	0.47
2:D:39:GLN:C	2:D:41:PHE:N	2.69	0.47
2:F:90:GLU:CB	2:F:90:GLU:OE1	2.57	0.47
2:F:118:PHE:HB3	2:F:121:GLU:HB3	1.95	0.47
1:G:66:LEU:HD12	1:G:132:VAL:CG1	2.28	0.47
2:H:6:VAL:C	2:H:8:LYS:N	2.68	0.47
2:H:36:PRO:O	2:H:39:GLN:CG	2.62	0.47
2:H:93:CYS:O	2:H:94:ASP:C	2.53	0.47
2:H:141:LEU:N	2:H:141:LEU:HD22	2.27	0.47
1:A:42:TYR:CB	3:A:142:HEM:HBC1	2.44	0.47
1:A:127:LYS:HE3	1:C:141:ARG:CB	2.43	0.47
1:A:140:TYR:C	1:A:141:ARG:HG2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:PHE:CD2	2:B:98:VAL:CG1	2.97	0.47
2:B:93:CYS:HB2	2:B:145:TYR:CD2	2.49	0.47
2:D:63:HIS:HE1	3:D:147:HEM:CHA	2.27	0.47
1:G:121:VAL:O	1:G:124:SER:N	2.46	0.47
2:H:11:VAL:H	2:H:11:VAL:HG22	0.95	0.47
2:H:31:LEU:CD2	2:H:106:LEU:CB	2.67	0.47
2:H:92:HIS:NE2	2:H:98:VAL:HG21	2.29	0.47
1:A:29:LEU:HD13	1:A:32:MET:HE2	1.96	0.47
2:B:93:CYS:HB2	2:B:145:TYR:CD1	2.49	0.47
1:E:128:PHE:O	1:E:131:SER:CB	2.52	0.47
2:H:93:CYS:HB2	2:H:145:TYR:CE2	2.50	0.47
2:B:127:GLN:O	2:B:128:ALA:C	2.58	0.47
1:C:43:PHE:CE2	1:C:46:PHE:CZ	3.02	0.47
2:D:78:LEU:HD11	2:D:133:VAL:CG2	2.44	0.47
2:D:81:LEU:C	2:D:83:GLY:N	2.67	0.47
2:D:124:PRO:N	2:D:125:PRO:CD	2.75	0.47
1:E:101:LEU:HD22	1:E:104:CYS:HB2	1.96	0.47
2:F:1:VAL:HG23	2:F:132:LYS:O	2.15	0.47
2:F:80:ASN:O	2:F:84:THR:CB	2.62	0.47
2:F:127:GLN:O	2:F:130:TYR:C	2.55	0.47
1:G:17:VAL:CG1	1:G:24:TYR:HD1	2.27	0.47
2:B:4:THR:OG1	2:B:5:PRO:HD2	2.15	0.47
2:B:77:HIS:HB2	2:B:84:THR:HG21	1.96	0.47
1:C:93:VAL:CG1	3:C:142:HEM:HAC	2.38	0.47
2:H:15:TRP:CE3	2:H:130:TYR:OH	2.67	0.47
2:H:72:SER:O	2:H:75:LEU:HB2	2.14	0.47
2:H:82:LYS:H	2:H:82:LYS:HD2	1.77	0.47
1:A:40:LYS:O	1:A:41:THR:C	2.58	0.47
1:A:103:HIS:O	1:A:107:VAL:HB	2.14	0.47
2:B:4:THR:CB	2:B:7:GLU:HB2	2.45	0.47
2:B:28:LEU:O	2:B:29:GLY:C	2.54	0.47
2:B:88:LEU:H	2:B:88:LEU:CD1	2.09	0.47
1:C:29:LEU:HD11	1:C:62:VAL:HG21	1.97	0.47
1:C:90:LYS:HG3	1:C:91:LEU:CD2	2.45	0.47
1:C:94:ASP:C	1:C:94:ASP:OD2	2.58	0.47
1:C:128:PHE:CD2	1:C:129:LEU:HB2	2.49	0.47
2:D:21:ASP:OD2	2:D:65:LYS:HE3	2.15	0.47
2:D:50:THR:CB	2:D:51:PRO:HD2	2.43	0.47
2:D:137:VAL:HG12	2:D:138:ALA:N	2.29	0.47
2:F:3:LEU:HD22	2:F:7:GLU:HB2	1.96	0.47
2:F:4:THR:HG21	2:F:6:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:24:GLY:N	2:F:68:LEU:CD1	2.78	0.47
2:F:107:GLY:CA	2:F:134:VAL:HG11	2.45	0.47
1:G:31:ARG:HH21	1:G:31:ARG:CG	2.21	0.47
3:A:142:HEM:HBB2	3:A:142:HEM:HMB1	1.95	0.47
1:C:97:ASN:O	1:C:101:LEU:N	2.44	0.47
2:D:110:LEU:O	2:D:114:LEU:HG	2.15	0.47
3:A:142:HEM:HHA	3:A:142:HEM:HAA1	1.45	0.47
2:B:7:GLU:O	2:B:11:VAL:CB	2.62	0.47
2:B:102:ASN:C	2:B:104:ARG:N	2.68	0.47
1:C:80:LEU:O	1:C:81:SER:C	2.57	0.47
2:F:26:GLU:C	2:F:55:MET:HE2	2.40	0.47
2:H:41:PHE:CD1	2:H:41:PHE:N	2.82	0.47
2:H:81:LEU:HB3	2:H:85:PHE:CE1	2.50	0.47
1:A:129:LEU:HA	1:A:129:LEU:HD23	1.43	0.47
1:C:17:VAL:CG1	1:C:21:ALA:CA	2.87	0.47
1:C:91:LEU:O	1:C:92:ARG:C	2.57	0.47
2:D:65:LYS:NZ	2:D:65:LYS:HD2	2.27	0.47
1:E:42:TYR:OH	1:E:94:ASP:HB2	2.15	0.47
2:F:80:ASN:HD21	2:F:83:GLY:CA	2.23	0.47
2:F:96:LEU:HD22	3:F:147:HEM:CAD	2.45	0.47
1:G:6:ASP:OD2	1:G:127:LYS:HE3	2.15	0.47
1:G:24:TYR:N	1:G:24:TYR:CD2	2.79	0.47
1:G:116:GLU:O	1:G:121:VAL:HG11	2.14	0.47
1:G:127:LYS:HZ2	1:G:127:LYS:HG2	1.37	0.47
2:H:81:LEU:CA	2:H:85:PHE:HE1	2.27	0.47
2:H:86:ALA:HB1	2:H:144:LYS:HZ1	1.75	0.47
1:A:83:LEU:HD23	1:A:136:LEU:HD23	1.95	0.46
1:A:107:VAL:HG23	2:B:112:CYS:SG	2.55	0.46
2:B:32:LEU:O	2:B:36:PRO:HA	2.15	0.46
2:B:119:GLY:C	2:B:121:GLU:N	2.73	0.46
2:D:15:TRP:C	2:D:18:VAL:HG23	2.39	0.46
2:D:51:PRO:CA	2:D:54:VAL:CG2	2.84	0.46
2:D:136:GLY:HA2	2:D:139:ASN:HB3	1.96	0.46
1:E:2:LEU:HA	1:E:127:LYS:HZ2	1.78	0.46
1:G:38:THR:O	1:G:41:THR:OG1	2.25	0.46
1:G:100:LEU:C	1:G:103:HIS:H	2.23	0.46
1:G:111:ALA:HB2	2:H:119:GLY:O	2.15	0.46
1:A:42:TYR:OH	1:A:94:ASP:HB2	2.15	0.46
2:B:21:ASP:CB	2:B:65:LYS:HB2	2.42	0.46
2:B:133:VAL:O	2:B:137:VAL:HG23	2.14	0.46
1:C:55:VAL:HG12	1:C:56:LYS:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:CYS:O	1:E:108:THR:N	2.49	0.46
1:G:30:GLU:CD	1:G:50:HIS:CE1	2.94	0.46
1:A:14:TRP:CH2	1:A:66:LEU:CD2	2.98	0.46
1:A:27:GLU:O	1:A:30:GLU:N	2.48	0.46
2:B:3:LEU:CD2	2:B:3:LEU:HD13	2.43	0.46
2:B:41:PHE:CE2	2:B:98:VAL:CG1	2.99	0.46
2:B:132:LYS:O	2:B:135:ALA:HB3	2.16	0.46
1:C:4:PRO:CD	1:C:5:ALA:N	2.77	0.46
1:C:43:PHE:HE2	1:C:46:PHE:CZ	2.33	0.46
1:C:46:PHE:CD1	1:C:48:LEU:CD2	2.98	0.46
1:C:90:LYS:HG2	1:C:91:LEU:CD2	2.46	0.46
2:D:44:SER:C	2:D:45:PHE:CD2	2.72	0.46
2:D:75:LEU:N	2:D:75:LEU:CD1	2.74	0.46
2:F:24:GLY:C	2:F:26:GLU:N	2.71	0.46
2:F:115:ALA:O	2:F:116:HIS:C	2.56	0.46
1:G:20:HIS:N	1:G:20:HIS:CD2	2.83	0.46
1:G:119:PRO:HB3	2:H:55:MET:HE2	1.97	0.46
2:B:80:ASN:CG	2:B:80:ASN:O	2.58	0.46
2:D:44:SER:OG	2:D:45:PHE:CD2	2.69	0.46
2:H:96:LEU:N	2:H:96:LEU:HD23	2.23	0.46
2:H:114:LEU:HD23	2:H:118:PHE:HE1	1.74	0.46
1:A:4:PRO:C	1:A:7:LYS:HB2	2.41	0.46
1:A:98:PHE:CD1	1:A:133:SER:CB	2.98	0.46
2:B:67:VAL:HG12	2:B:68:LEU:CD2	2.45	0.46
2:F:3:LEU:HD13	2:F:8:LYS:HA	1.98	0.46
1:C:10:VAL:O	1:C:14:TRP:HB2	2.16	0.46
2:D:123:THR:C	2:D:125:PRO:HD2	2.40	0.46
3:D:147:HEM:CBC	3:D:147:HEM:CMC	2.64	0.46
1:G:36:PHE:N	1:G:37:PRO:CD	2.69	0.46
2:H:21:ASP:OD2	2:H:65:LYS:HG3	2.03	0.46
2:H:135:ALA:HA	2:H:138:ALA:HB3	1.97	0.46
2:B:97:HIS:C	2:B:98:VAL:HG22	2.40	0.46
1:C:4:PRO:CD	1:C:5:ALA:H	2.26	0.46
1:C:26:ALA:HB1	1:C:55:VAL:HG11	1.98	0.46
1:C:43:PHE:HE2	1:C:46:PHE:CE2	2.34	0.46
1:C:107:VAL:HA	1:C:110:ALA:CB	2.32	0.46
2:D:2:HIS:O	2:D:132:LYS:HD2	2.15	0.46
2:D:11:VAL:HG11	2:D:78:LEU:HD21	1.97	0.46
2:D:33:VAL:O	2:D:33:VAL:CG1	2.62	0.46
2:D:106:LEU:O	2:D:110:LEU:N	2.48	0.46
1:E:132:VAL:CG1	1:E:133:SER:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:110:LEU:CA	2:F:110:LEU:CG	2.82	0.46
1:G:114:PRO:O	2:H:116:HIS:CD2	2.69	0.46
2:H:49:SER:C	2:H:50:THR:OG1	2.50	0.46
2:B:143:HIS:O	2:B:143:HIS:CD2	2.68	0.46
1:C:32:MET:SD	1:C:101:LEU:HA	2.56	0.46
2:F:26:GLU:O	2:F:55:MET:CE	2.62	0.46
1:A:68:ASN:OD1	1:A:72:HIS:CD2	2.69	0.46
1:A:106:LEU:HD13	1:A:129:LEU:CD1	2.46	0.46
1:C:83:LEU:HD23	1:C:87:HIS:HE1	1.80	0.46
1:C:87:HIS:ND1	1:C:87:HIS:N	2.64	0.46
1:C:118:THR:O	1:C:121:VAL:CA	2.64	0.46
2:F:14:LEU:CD2	2:F:118:PHE:CD2	2.97	0.46
3:G:142:HEM:HMB1	3:G:142:HEM:CBB	2.41	0.46
1:A:86:LEU:CD1	1:A:90:LYS:NZ	2.70	0.46
1:A:134:THR:O	1:A:135:VAL:O	2.34	0.46
2:D:122:PHE:CE2	2:D:127:GLN:HG3	2.51	0.46
1:E:14:TRP:O	1:E:17:VAL:HB	2.15	0.46
2:F:3:LEU:HD13	2:F:8:LYS:HB2	1.98	0.46
2:F:50:THR:HA	2:F:51:PRO:HD3	1.78	0.46
1:G:27:GLU:O	1:G:28:ALA:C	2.59	0.46
2:B:3:LEU:HD23	2:B:7:GLU:CB	2.45	0.45
1:C:43:PHE:CE2	1:C:46:PHE:CE2	3.04	0.45
1:C:102:SER:CA	1:C:129:LEU:CD1	2.94	0.45
1:C:104:CYS:CA	1:C:107:VAL:HG22	2.44	0.45
1:E:39:THR:O	1:E:43:PHE:HE1	1.92	0.45
1:E:86:LEU:HD12	1:E:90:LYS:CB	2.46	0.45
1:G:66:LEU:O	1:G:67:THR:CA	2.63	0.45
1:A:43:PHE:N	1:A:44:PRO:CD	2.79	0.45
1:A:107:VAL:O	1:A:110:ALA:HB3	2.16	0.45
2:B:3:LEU:HD23	2:B:7:GLU:CD	2.41	0.45
2:B:123:THR:HB	2:B:124:PRO:HD2	1.98	0.45
1:C:88:ALA:O	1:C:92:ARG:CG	2.65	0.45
1:E:17:VAL:HG23	1:E:17:VAL:H	1.41	0.45
1:E:68:ASN:O	1:E:69:ALA:CA	2.64	0.45
1:E:117:PHE:CD2	1:E:117:PHE:C	2.94	0.45
1:G:95:PRO:CA	1:G:98:PHE:CD2	2.59	0.45
1:C:102:SER:CA	1:C:129:LEU:HD11	2.43	0.45
1:C:141:ARG:CD	1:C:141:ARG:NH1	2.77	0.45
2:D:8:LYS:HG3	2:D:8:LYS:O	2.15	0.45
2:D:135:ALA:O	2:D:139:ASN:CB	2.63	0.45
1:E:1:VAL:CG1	1:E:2:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ASP:OD1	1:C:124:SER:OG	2.34	0.45
1:C:16:LYS:CD	1:C:116:GLU:CG	2.85	0.45
1:C:135:VAL:HG12	1:C:136:LEU:HD23	1.97	0.45
2:D:66:LYS:O	2:D:66:LYS:CG	2.62	0.45
2:D:104:ARG:CG	2:D:104:ARG:C	2.88	0.45
2:D:129:ALA:O	2:D:130:TYR:C	2.58	0.45
1:E:127:LYS:HB3	1:E:127:LYS:HE2	1.48	0.45
1:G:47:ASP:OD1	1:G:48:LEU:N	2.49	0.45
2:B:96:LEU:CG	2:B:98:VAL:CG2	2.92	0.45
1:C:107:VAL:C	1:C:110:ALA:CB	2.87	0.45
2:D:135:ALA:O	2:D:139:ASN:HB2	2.17	0.45
2:F:75:LEU:HD22	2:F:75:LEU:N	2.32	0.45
1:G:106:LEU:HD12	1:G:125:LEU:HB2	1.99	0.45
2:H:141:LEU:HA	2:H:141:LEU:HD13	1.55	0.45
2:B:59:LYS:CE	2:B:62:ALA:HB1	2.47	0.45
1:C:105:LEU:C	1:C:109:LEU:HB2	2.42	0.45
2:D:72:SER:HB2	2:D:73:ASP:OD1	2.16	0.45
2:F:35:TYR:CE2	2:F:105:LEU:HD22	2.51	0.45
2:F:58:PRO:HA	2:F:61:LYS:HD3	1.98	0.45
2:H:76:ALA:CB	2:H:77:HIS:ND1	2.80	0.45
1:A:133:SER:O	1:A:137:THR:N	2.50	0.45
1:C:113:LEU:HD22	1:C:116:GLU:HB2	1.93	0.45
2:D:32:LEU:CD2	2:D:42:PHE:CD1	2.98	0.45
2:D:33:VAL:C	2:D:34:VAL:CG2	2.89	0.45
2:D:74:GLY:C	2:D:76:ALA:H	2.23	0.45
1:E:69:ALA:C	1:E:71:ALA:N	2.61	0.45
1:E:72:HIS:C	1:E:74:ASP:H	2.20	0.45
2:F:7:GLU:HA	2:F:10:ALA:HB3	1.98	0.45
2:F:101:GLU:O	2:F:104:ARG:CB	2.62	0.45
1:G:16:LYS:HE3	1:G:116:GLU:OE2	2.16	0.45
2:H:17:LYS:CB	2:H:118:PHE:HE2	2.26	0.45
2:H:107:GLY:HA3	2:H:134:VAL:HG11	1.97	0.45
1:A:29:LEU:O	1:A:30:GLU:C	2.60	0.45
1:A:100:LEU:HA	1:A:100:LEU:HD22	1.44	0.45
1:A:117:PHE:CD2	2:B:116:HIS:CD2	3.04	0.45
2:D:9:SER:O	2:D:10:ALA:C	2.60	0.45
2:D:60:VAL:O	2:D:61:LYS:C	2.60	0.45
2:D:63:HIS:NE2	3:D:147:HEM:ND	2.64	0.45
1:E:78:ASN:O	1:E:81:SER:OG	2.34	0.45
2:H:3:LEU:HD13	2:H:78:LEU:O	2.17	0.45
1:A:98:PHE:CZ	1:A:136:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:SER:O	1:C:127:LYS:HB2	2.17	0.45
2:D:25:GLY:HA3	2:D:61:LYS:HA	1.97	0.45
2:D:102:ASN:CB	3:D:147:HEM:HMC3	2.46	0.45
1:E:35:SER:CB	2:F:131:GLN:HG3	2.47	0.45
1:E:118:THR:O	1:E:119:PRO:C	2.59	0.45
2:F:6:VAL:HA	2:F:9:SER:CB	2.47	0.45
1:G:52:SER:O	1:G:53:ALA:C	2.58	0.45
1:C:99:LYS:HE2	1:C:100:LEU:HD23	1.98	0.45
2:D:21:ASP:OD2	2:D:65:LYS:CE	2.65	0.45
2:D:21:ASP:CB	2:D:65:LYS:HG2	2.47	0.45
2:D:93:CYS:HB2	2:D:145:TYR:CZ	2.52	0.45
2:D:105:LEU:HD23	2:D:105:LEU:HA	1.87	0.45
2:D:106:LEU:O	2:D:109:VAL:N	2.50	0.45
2:F:107:GLY:CA	2:F:134:VAL:CG1	2.95	0.45
2:H:84:THR:HB	2:H:85:PHE:CD1	2.52	0.45
1:A:94:ASP:OD2	1:A:96:VAL:HG23	2.17	0.44
2:B:38:THR:O	2:B:41:PHE:HD1	2.00	0.44
2:B:67:VAL:HG12	2:B:68:LEU:HD21	1.98	0.44
1:C:59:GLY:C	1:C:61:LYS:N	2.66	0.44
1:E:43:PHE:N	1:E:44:PRO:CD	2.77	0.44
1:E:48:LEU:O	1:E:49:SER:C	2.58	0.44
2:F:57:ASN:OD1	2:F:57:ASN:C	2.60	0.44
1:G:34:LEU:HD22	2:H:125:PRO:HA	1.99	0.44
2:H:17:LYS:HB2	2:H:118:PHE:CZ	2.51	0.44
2:H:24:GLY:O	2:H:27:ALA:HB3	2.17	0.44
2:H:133:VAL:O	2:H:137:VAL:HG23	2.17	0.44
1:A:138:SER:O	1:A:139:LYS:C	2.61	0.44
2:B:101:GLU:O	2:B:104:ARG:CA	2.65	0.44
1:C:4:PRO:HA	1:C:7:LYS:HG3	1.98	0.44
1:C:101:LEU:CD1	1:C:105:LEU:CD1	2.95	0.44
2:D:17:LYS:CD	2:D:17:LYS:N	2.80	0.44
2:D:74:GLY:HA2	2:D:84:THR:HG21	2.00	0.44
2:F:75:LEU:HD13	2:F:78:LEU:HD22	1.99	0.44
1:G:27:GLU:CD	1:G:31:ARG:HE	2.24	0.44
2:H:20:VAL:HG13	2:H:68:LEU:HD23	1.93	0.44
2:H:134:VAL:O	2:H:138:ALA:CB	2.64	0.44
2:B:7:GLU:OE1	2:B:132:LYS:HD2	2.16	0.44
1:C:86:LEU:CD2	3:C:142:HEM:CBA	2.95	0.44
1:C:118:THR:CB	1:C:121:VAL:H	2.30	0.44
1:E:11:LYS:CG	1:E:11:LYS:HA	2.46	0.44
1:E:68:ASN:OD1	1:E:72:HIS:CD2	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:HIS:CG	2:F:132:LYS:NZ	2.59	0.44
1:G:72:HIS:O	1:G:73:VAL:C	2.60	0.44
1:A:39:THR:C	1:A:41:THR:N	2.67	0.44
2:B:58:PRO:HA	2:B:61:LYS:CB	2.36	0.44
1:C:66:LEU:CD2	1:C:128:PHE:CZ	2.76	0.44
1:E:68:ASN:O	1:E:72:HIS:CD2	2.69	0.44
1:E:95:PRO:CG	1:E:137:THR:HG21	2.48	0.44
1:E:132:VAL:HG13	1:E:136:LEU:HD12	2.00	0.44
2:F:114:LEU:HD23	2:F:114:LEU:HA	1.39	0.44
1:A:86:LEU:O	1:A:91:LEU:HG	2.17	0.44
1:C:95:PRO:HA	1:C:98:PHE:HD2	1.82	0.44
2:D:101:GLU:OE1	2:D:104:ARG:NH1	2.50	0.44
1:A:117:PHE:CD2	1:A:117:PHE:C	2.89	0.44
2:B:96:LEU:HD21	3:B:147:HEM:C1D	2.53	0.44
1:C:117:PHE:O	1:C:118:THR:C	2.59	0.44
2:D:15:TRP:O	2:D:18:VAL:CG2	2.61	0.44
1:E:2:LEU:N	1:E:2:LEU:CD2	2.79	0.44
1:E:23:GLU:O	1:E:27:GLU:N	2.44	0.44
2:H:50:THR:O	2:H:51:PRO:C	2.61	0.44
2:H:137:VAL:HG12	2:H:141:LEU:HD21	2.00	0.44
1:A:121:VAL:O	1:A:124:SER:HB2	2.18	0.44
1:C:101:LEU:HD13	1:C:101:LEU:C	2.42	0.44
2:D:93:CYS:HG	2:D:146:HIS:HE2	1.59	0.44
1:E:21:ALA:O	1:E:63:ALA:CB	2.66	0.44
1:G:80:LEU:HB3	1:G:135:VAL:HG12	1.99	0.44
2:H:14:LEU:CD1	2:H:122:PHE:HE1	2.31	0.44
2:B:15:TRP:HE1	2:B:72:SER:CB	2.27	0.44
1:C:6:ASP:HA	1:C:124:SER:OG	2.17	0.44
1:C:81:SER:O	1:C:84:SER:CB	2.66	0.44
1:C:83:LEU:O	1:C:86:LEU:HB3	2.17	0.44
1:C:118:THR:H	1:C:121:VAL:HB	1.83	0.44
1:E:117:PHE:O	1:E:117:PHE:HD2	1.99	0.44
2:F:126:VAL:O	2:F:130:TYR:HD2	2.00	0.44
2:F:127:GLN:O	2:F:130:TYR:CA	2.65	0.44
2:F:131:GLN:O	2:F:135:ALA:HB2	2.18	0.44
1:G:4:PRO:HA	1:G:7:LYS:HG3	1.99	0.44
2:H:27:ALA:HB3	2:H:28:LEU:H	1.39	0.44
2:H:54:VAL:CG1	2:H:55:MET:SD	3.04	0.44
1:A:122:HIS:ND1	2:B:30:ARG:HG2	2.33	0.44
2:B:4:THR:HG21	2:B:6:VAL:HG22	1.99	0.44
2:B:37:TRP:HZ3	1:C:141:ARG:HE	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LYS:CA	2:B:59:LYS:HZ2	2.25	0.44
2:B:80:ASN:OD1	2:B:83:GLY:HA3	2.18	0.44
2:B:93:CYS:O	2:B:94:ASP:C	2.59	0.44
2:D:25:GLY:O	2:D:29:GLY:HA3	2.17	0.44
2:D:68:LEU:CD2	2:D:68:LEU:H	2.15	0.44
2:D:108:ASN:HA	2:D:111:VAL:CG2	2.47	0.44
1:E:14:TRP:CA	1:E:17:VAL:HG23	2.48	0.44
2:F:33:VAL:CG2	2:F:51:PRO:CB	2.85	0.44
1:G:4:PRO:O	1:G:6:ASP:N	2.50	0.44
1:G:11:LYS:CG	1:G:70:VAL:HG23	2.47	0.44
1:G:114:PRO:O	1:G:115:ALA:HB2	2.15	0.44
1:A:81:SER:HA	1:A:84:SER:HB3	2.00	0.43
2:B:126:VAL:O	2:B:130:TYR:HD2	2.00	0.43
1:C:103:HIS:O	1:C:107:VAL:HG22	2.17	0.43
2:D:137:VAL:O	2:D:141:LEU:N	2.47	0.43
1:G:48:LEU:CD2	1:G:48:LEU:H	2.22	0.43
1:A:46:PHE:HA	1:A:54:GLN:OE1	2.18	0.43
2:B:60:VAL:O	2:B:61:LYS:O	2.37	0.43
1:C:39:THR:CB	1:C:39:THR:HG1	2.16	0.43
2:D:14:LEU:CD1	2:D:130:TYR:HE2	2.25	0.43
2:D:20:VAL:O	2:D:20:VAL:HG13	2.18	0.43
2:D:20:VAL:C	2:D:21:ASP:OD1	2.45	0.43
2:D:99:ASP:O	2:D:102:ASN:CG	2.61	0.43
2:F:35:TYR:HB3	2:F:37:TRP:CZ3	2.53	0.43
2:F:128:ALA:O	2:F:132:LYS:HB2	2.18	0.43
1:G:94:ASP:HA	1:G:95:PRO:HD2	1.91	0.43
1:A:16:LYS:C	1:A:18:GLY:H	2.24	0.43
2:B:35:TYR:HB3	2:B:37:TRP:CE2	2.49	0.43
1:C:86:LEU:HD12	1:C:86:LEU:HA	1.36	0.43
2:D:40:ARG:HG2	2:D:41:PHE:CZ	2.52	0.43
2:D:67:VAL:CG1	3:D:147:HEM:NA	2.81	0.43
1:E:84:SER:HB2	1:E:139:LYS:HD2	2.00	0.43
1:G:1:VAL:HG13	1:G:2:LEU:O	2.18	0.43
1:G:75:ASP:C	1:G:77:PRO:N	2.71	0.43
2:H:45:PHE:CE1	2:H:60:VAL:HA	2.53	0.43
2:B:8:LYS:HA	2:B:11:VAL:HB	1.99	0.43
2:B:92:HIS:C	2:B:96:LEU:HB3	2.39	0.43
2:B:106:LEU:O	2:B:109:VAL:HB	2.19	0.43
1:C:50:HIS:CD2	1:C:50:HIS:O	2.70	0.43
1:C:83:LEU:HD21	3:C:142:HEM:HMA2	1.98	0.43
2:D:11:VAL:HG11	2:D:133:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:ALA:C	2:D:89:SER:H	2.26	0.43
1:E:6:ASP:O	1:E:10:VAL:HG23	2.18	0.43
2:F:81:LEU:CD1	2:F:136:GLY:C	2.92	0.43
2:F:129:ALA:O	2:F:132:LYS:HB3	2.18	0.43
3:F:147:HEM:HAA1	3:F:147:HEM:HHA	1.57	0.43
2:H:92:HIS:HA	2:H:96:LEU:CB	2.47	0.43
2:H:107:GLY:CA	2:H:134:VAL:HG11	2.47	0.43
2:H:117:HIS:CD2	2:H:118:PHE:CE2	3.05	0.43
1:A:135:VAL:HA	1:A:138:SER:OG	2.19	0.43
2:B:81:LEU:O	2:B:82:LYS:C	2.60	0.43
2:D:67:VAL:HG12	3:D:147:HEM:NA	2.33	0.43
3:D:147:HEM:CBA	3:D:147:HEM:CHA	2.95	0.43
2:F:121:GLU:O	2:F:123:THR:HG23	2.19	0.43
2:H:28:LEU:HD21	2:H:63:HIS:HD2	1.76	0.43
1:A:118:THR:HG22	1:A:119:PRO:CD	2.38	0.43
2:B:59:LYS:HE3	2:B:62:ALA:HB2	1.93	0.43
2:B:75:LEU:CA	2:B:78:LEU:HD22	2.48	0.43
2:B:131:GLN:O	2:B:132:LYS:C	2.60	0.43
1:C:77:PRO:O	1:C:78:ASN:C	2.61	0.43
1:C:104:CYS:CA	1:C:107:VAL:HG23	2.46	0.43
1:C:117:PHE:C	1:C:118:THR:C	2.80	0.43
1:E:16:LYS:HD3	1:E:116:GLU:OE1	2.18	0.43
1:E:129:LEU:O	1:E:132:VAL:HG12	2.18	0.43
2:F:14:LEU:HA	2:F:14:LEU:HD22	1.80	0.43
2:F:81:LEU:HD12	2:F:136:GLY:C	2.44	0.43
2:D:33:VAL:CG1	2:D:34:VAL:HG23	2.48	0.43
2:D:93:CYS:HG	2:D:146:HIS:CD2	2.36	0.43
1:E:35:SER:HB3	2:F:131:GLN:HG3	2.00	0.43
2:F:3:LEU:HA	2:F:3:LEU:HD23	1.33	0.43
2:H:20:VAL:CG1	2:H:68:LEU:HB3	2.47	0.43
2:H:45:PHE:HZ	2:H:63:HIS:HB2	1.83	0.43
1:A:19:ALA:O	1:A:20:HIS:C	2.62	0.43
1:A:73:VAL:H	1:A:73:VAL:HG12	0.71	0.43
1:A:91:LEU:HG	1:A:91:LEU:H	1.39	0.43
2:F:97:HIS:C	1:G:41:THR:HG22	2.43	0.43
1:G:109:LEU:HD22	1:G:109:LEU:HD13	1.96	0.43
2:H:133:VAL:HG13	2:H:137:VAL:HG23	2.00	0.43
2:B:28:LEU:HD12	2:B:28:LEU:O	2.18	0.43
2:D:49:SER:N	2:D:49:SER:OG	2.52	0.43
2:D:85:PHE:CE1	2:D:137:VAL:HG22	2.54	0.43
1:E:39:THR:O	1:E:43:PHE:HD1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:41:PHE:CZ	2:F:102:ASN:OD1	2.72	0.43
2:F:98:VAL:O	2:F:145:TYR:CE1	2.72	0.43
1:C:103:HIS:O	1:C:106:LEU:HB3	2.17	0.43
2:D:74:GLY:C	2:D:76:ALA:N	2.75	0.43
1:E:52:SER:OG	1:E:54:GLN:HB3	2.18	0.43
1:E:92:ARG:HB3	2:H:37:TRP:CB	2.33	0.43
2:F:35:TYR:HB3	2:F:37:TRP:CE3	2.53	0.43
2:F:131:GLN:O	2:F:135:ALA:CB	2.67	0.43
2:H:88:LEU:O	2:H:89:SER:C	2.62	0.43
2:H:88:LEU:HD23	2:H:88:LEU:HA	1.67	0.43
2:B:3:LEU:HD11	2:B:133:VAL:CG2	2.44	0.42
2:B:95:LYS:NZ	2:B:95:LYS:HD2	2.34	0.42
1:C:109:LEU:HD13	1:C:109:LEU:HA	1.98	0.42
1:C:117:PHE:O	2:D:30:ARG:NH2	2.52	0.42
1:C:118:THR:CG2	1:C:120:ALA:CA	2.97	0.42
1:E:29:LEU:HD22	1:E:32:MET:HE2	2.00	0.42
1:E:72:HIS:O	1:E:76:MET:N	2.52	0.42
1:E:72:HIS:C	1:E:74:ASP:N	2.71	0.42
1:G:2:LEU:HB3	1:G:6:ASP:CB	2.49	0.42
1:G:7:LYS:O	1:G:8:THR:C	2.55	0.42
2:H:67:VAL:HG13	3:H:147:HEM:C2B	2.54	0.42
1:A:76:MET:N	1:A:77:PRO:CD	2.83	0.42
1:C:15:GLY:O	1:C:16:LYS:C	2.61	0.42
2:D:37:TRP:O	2:D:40:ARG:CB	2.64	0.42
2:F:15:TRP:CE3	2:F:15:TRP:HA	2.53	0.42
1:G:32:MET:HG3	1:G:101:LEU:HD12	2.01	0.42
1:G:117:PHE:CG	1:G:117:PHE:O	2.72	0.42
1:A:78:ASN:C	1:A:81:SER:H	2.27	0.42
1:A:91:LEU:HA	1:A:91:LEU:HD23	1.41	0.42
2:B:75:LEU:C	2:B:78:LEU:HD22	2.45	0.42
2:B:81:LEU:HA	2:B:81:LEU:HD13	1.40	0.42
1:C:43:PHE:N	1:C:44:PRO:CD	2.82	0.42
1:C:84:SER:HB3	1:C:139:LYS:CD	2.37	0.42
2:D:113:VAL:O	2:D:116:HIS:CB	2.63	0.42
2:F:31:LEU:CD1	2:F:35:TYR:HE2	2.32	0.42
2:H:21:ASP:CA	2:H:65:LYS:CB	2.94	0.42
1:C:14:TRP:CE3	1:C:14:TRP:HA	2.54	0.42
1:C:79:ALA:C	1:C:81:SER:N	2.76	0.42
2:D:7:GLU:OE1	2:D:7:GLU:CA	2.68	0.42
2:D:108:ASN:C	2:D:110:LEU:N	2.73	0.42
1:E:123:ALA:HB3	1:E:124:SER:H	1.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:VAL:HG21	2:B:51:PRO:CB	2.46	0.42
2:B:96:LEU:CD1	2:B:98:VAL:HG21	2.49	0.42
2:F:17:LYS:NZ	2:F:17:LYS:CD	2.72	0.42
2:F:42:PHE:CD1	2:F:42:PHE:N	2.87	0.42
2:H:14:LEU:CD2	2:H:14:LEU:CA	2.96	0.42
2:H:20:VAL:HG12	2:H:65:LYS:CA	2.40	0.42
2:H:32:LEU:HA	2:H:32:LEU:HD12	1.85	0.42
2:H:88:LEU:C	2:H:90:GLU:N	2.75	0.42
2:B:88:LEU:O	2:B:92:HIS:N	2.53	0.42
1:C:2:LEU:HA	1:C:6:ASP:OD2	2.19	0.42
1:C:88:ALA:O	1:C:89:HIS:ND1	2.52	0.42
2:D:23:VAL:HG13	2:D:113:VAL:HG11	2.02	0.42
2:D:74:GLY:HA2	2:D:77:HIS:HB2	2.00	0.42
2:D:82:LYS:CA	2:D:140:ALA:CB	2.80	0.42
2:F:1:VAL:HG21	2:F:132:LYS:HA	2.02	0.42
1:G:107:VAL:CG1	2:H:112:CYS:HG	2.02	0.42
1:G:110:ALA:HB1	2:H:116:HIS:HB2	2.00	0.42
1:G:113:LEU:HG	1:G:116:GLU:HG3	2.01	0.42
2:H:36:PRO:CG	2:H:37:TRP:CZ3	2.98	0.42
2:H:90:GLU:O	2:H:94:ASP:HB2	2.18	0.42
1:A:7:LYS:CD	1:A:73:VAL:HG22	2.50	0.42
1:A:42:TYR:CG	3:A:142:HEM:HBC1	2.54	0.42
2:B:99:ASP:O	2:B:102:ASN:OD1	2.38	0.42
1:E:27:GLU:OE1	1:E:112:HIS:NE2	2.52	0.42
1:E:35:SER:OG	1:E:35:SER:N	2.53	0.42
1:E:139:LYS:CB	1:E:139:LYS:HZ2	2.29	0.42
2:F:26:GLU:OE2	2:F:117:HIS:HE1	2.01	0.42
2:F:80:ASN:CG	2:F:83:GLY:H	2.23	0.42
2:F:114:LEU:HD21	2:F:118:PHE:HE1	1.84	0.42
1:G:101:LEU:C	1:G:103:HIS:N	2.75	0.42
2:H:76:ALA:HB1	2:H:77:HIS:CE1	2.54	0.42
1:A:20:HIS:O	1:A:24:TYR:N	2.48	0.42
1:A:41:THR:O	1:A:44:PRO:HD3	2.20	0.42
1:C:38:THR:O	1:C:41:THR:OG1	2.10	0.42
1:C:84:SER:HA	1:C:136:LEU:HD22	2.01	0.42
1:A:22:GLY:HA3	1:A:60:LYS:HA	2.00	0.42
1:A:136:LEU:HD22	1:A:136:LEU:HA	1.97	0.42
2:B:5:PRO:HB2	2:B:6:VAL:HG13	2.00	0.42
2:B:28:LEU:O	2:B:32:LEU:HB2	2.20	0.42
2:B:96:LEU:HD21	3:B:147:HEM:CHD	2.49	0.42
2:B:125:PRO:HA	2:B:128:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLU:O	1:C:24:TYR:C	2.61	0.42
2:D:15:TRP:HD1	2:D:130:TYR:HH	1.44	0.42
1:E:76:MET:SD	1:E:135:VAL:CG2	2.82	0.42
2:F:26:GLU:OE1	2:F:30:ARG:NH1	2.52	0.42
1:G:8:THR:O	1:G:8:THR:HG22	2.20	0.42
1:G:93:VAL:CG1	3:G:142:HEM:CAC	2.90	0.42
2:H:25:GLY:O	2:H:29:GLY:CA	2.68	0.42
1:A:65:ALA:HB1	1:A:80:LEU:HD23	1.98	0.42
2:B:30:ARG:HB3	2:B:109:VAL:CG1	2.50	0.42
2:D:13:ALA:C	2:D:15:TRP:H	2.28	0.42
2:D:65:LYS:O	2:D:66:LYS:C	2.59	0.42
2:D:73:ASP:O	2:D:76:ALA:N	2.49	0.42
1:E:47:ASP:CG	1:E:49:SER:H	2.27	0.42
2:F:3:LEU:CD1	2:F:8:LYS:HA	2.49	0.42
1:G:48:LEU:H	1:G:48:LEU:HG	1.44	0.42
1:G:86:LEU:O	1:G:87:HIS:C	2.62	0.42
1:A:42:TYR:CD1	1:A:93:VAL:CG2	3.03	0.41
2:B:30:ARG:CB	2:B:30:ARG:HD2	2.48	0.41
1:C:20:HIS:HB3	1:C:24:TYR:CZ	2.55	0.41
2:D:3:LEU:HD23	2:D:132:LYS:CB	2.39	0.41
2:D:26:GLU:CD	2:D:30:ARG:NH1	2.62	0.41
2:D:51:PRO:O	2:D:55:MET:HG2	2.20	0.41
2:D:66:LYS:O	2:D:66:LYS:HG2	2.16	0.41
2:D:77:HIS:O	2:D:81:LEU:CD2	2.55	0.41
1:E:100:LEU:CD2	1:E:100:LEU:N	2.81	0.41
2:F:3:LEU:HD13	2:F:8:LYS:CB	2.50	0.41
2:F:120:LYS:O	2:F:121:GLU:C	2.63	0.41
2:H:26:GLU:OE1	2:H:30:ARG:CD	2.64	0.41
2:B:133:VAL:C	2:B:135:ALA:N	2.77	0.41
1:C:8:THR:O	1:C:12:ALA:CB	2.68	0.41
1:C:98:PHE:C	1:C:100:LEU:N	2.78	0.41
1:E:47:ASP:H	1:E:54:GLN:CD	2.29	0.41
2:F:29:GLY:O	2:F:33:VAL:N	2.53	0.41
2:F:31:LEU:HA	2:F:31:LEU:HD12	1.58	0.41
2:H:99:ASP:O	2:H:101:GLU:N	2.53	0.41
1:C:31:ARG:HH11	2:D:127:GLN:CD	2.21	0.41
2:F:31:LEU:HD22	2:F:106:LEU:HA	2.01	0.41
1:G:105:LEU:O	1:G:109:LEU:CB	2.52	0.41
1:G:124:SER:O	1:G:125:LEU:C	2.61	0.41
2:H:63:HIS:O	2:H:66:LYS:CB	2.68	0.41
1:A:72:HIS:C	1:A:74:ASP:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:PHE:C	1:C:100:LEU:H	2.25	0.41
1:E:101:LEU:O	1:E:104:CYS:HB2	2.20	0.41
1:G:43:PHE:CB	1:G:46:PHE:HB2	2.50	0.41
1:A:10:VAL:HG13	1:A:128:PHE:HB2	2.01	0.41
1:A:14:TRP:O	1:A:17:VAL:HG23	2.21	0.41
1:A:24:TYR:HD2	1:A:24:TYR:HA	0.98	0.41
1:A:40:LYS:HB2	1:A:40:LYS:HE3	1.62	0.41
2:D:98:VAL:O	2:D:100:PRO:HB3	2.19	0.41
1:E:99:LYS:C	1:E:100:LEU:HD23	2.46	0.41
1:E:137:THR:CG2	1:E:137:THR:O	2.69	0.41
1:A:17:VAL:HG13	1:A:24:TYR:CD1	2.55	0.41
1:A:21:ALA:C	1:A:23:GLU:H	2.28	0.41
1:A:28:ALA:HB3	1:A:29:LEU:H	1.07	0.41
1:A:42:TYR:HB2	3:A:142:HEM:CBC	2.49	0.41
1:C:12:ALA:O	1:C:13:ALA:CA	2.64	0.41
1:C:122:HIS:CD2	1:C:122:HIS:C	2.98	0.41
2:F:42:PHE:HZ	3:F:147:HEM:HBC2	1.84	0.41
2:F:136:GLY:O	2:F:140:ALA:CB	2.66	0.41
1:G:7:LYS:O	1:G:11:LYS:HD2	2.21	0.41
1:G:118:THR:O	1:G:120:ALA:N	2.49	0.41
2:H:112:CYS:O	2:H:115:ALA:CB	2.68	0.41
1:A:33:PHE:HB3	1:A:40:LYS:CG	2.50	0.41
2:B:50:THR:HG22	2:B:51:PRO:HD2	2.03	0.41
1:C:39:THR:O	1:C:42:TYR:HD2	2.03	0.41
1:C:106:LEU:CA	1:C:109:LEU:HB2	2.49	0.41
2:D:64:GLY:C	2:D:67:VAL:H	2.28	0.41
2:D:85:PHE:HA	2:D:88:LEU:CB	2.51	0.41
2:F:32:LEU:HA	2:F:32:LEU:HD12	1.27	0.41
1:G:30:GLU:OE2	1:G:50:HIS:ND1	2.52	0.41
1:G:104:CYS:SG	2:H:127:GLN:NE2	2.94	0.41
2:H:17:LYS:CB	2:H:118:PHE:CZ	3.04	0.41
1:A:76:MET:HB2	1:A:77:PRO:HD3	2.03	0.41
2:B:1:VAL:N	2:B:2:HIS:ND1	2.68	0.41
2:B:18:VAL:HG12	2:B:20:VAL:HG23	1.93	0.41
2:B:111:VAL:HG13	2:B:122:PHE:CE2	2.55	0.41
2:D:42:PHE:O	2:D:45:PHE:CB	2.62	0.41
2:D:50:THR:HG22	2:D:51:PRO:HD2	2.02	0.41
2:D:77:HIS:HB3	2:D:84:THR:CG2	2.51	0.41
1:E:42:TYR:HE2	2:H:99:ASP:OD1	2.04	0.41
2:F:146:HIS:C	1:G:40:LYS:HZ1	2.27	0.41
1:G:2:LEU:HD13	1:G:10:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:VAL:CG1	2:H:19:ASN:N	2.82	0.41
1:A:35:SER:OG	2:B:131:GLN:HG3	2.21	0.41
1:A:66:LEU:C	1:A:70:VAL:HG23	2.40	0.41
1:A:113:LEU:N	1:A:114:PRO:CD	2.83	0.41
1:A:118:THR:CG2	1:A:119:PRO:HD2	2.40	0.41
2:B:8:LYS:CA	2:B:11:VAL:HB	2.51	0.41
2:B:62:ALA:HB3	2:B:63:HIS:H	1.23	0.41
2:B:68:LEU:C	2:B:70:ALA:N	2.77	0.41
2:B:113:VAL:O	2:B:117:HIS:N	2.47	0.41
2:B:141:LEU:CD2	3:B:147:HEM:HBB2	2.40	0.41
1:C:101:LEU:CD1	1:C:101:LEU:C	2.93	0.41
1:C:102:SER:OG	1:C:129:LEU:HD12	2.21	0.41
1:C:118:THR:CG2	1:C:121:VAL:HG23	2.51	0.41
2:D:68:LEU:HA	2:D:71:PHE:HB3	2.03	0.41
1:E:29:LEU:CD2	1:E:101:LEU:CD1	2.94	0.41
1:E:127:LYS:O	1:E:131:SER:OG	2.35	0.41
2:F:69:GLY:O	2:F:70:ALA:O	2.38	0.41
2:F:77:HIS:C	2:F:79:ASP:N	2.72	0.41
2:F:123:THR:CB	2:F:125:PRO:HD2	2.51	0.41
2:H:22:GLU:OE2	2:H:22:GLU:HB3	2.19	0.41
1:C:119:PRO:CB	2:D:30:ARG:HG3	2.46	0.41
1:E:23:GLU:O	1:E:24:TYR:C	2.62	0.41
2:F:17:LYS:HB3	2:F:118:PHE:HZ	1.84	0.41
2:H:68:LEU:HA	2:H:71:PHE:HB3	2.03	0.41
2:B:123:THR:CB	2:B:124:PRO:CD	2.99	0.40
3:B:147:HEM:HHA	3:B:147:HEM:HAD1	1.68	0.40
1:C:134:THR:O	1:C:138:SER:N	2.54	0.40
2:D:63:HIS:CE1	3:D:147:HEM:ND	2.88	0.40
2:D:103:PHE:HB3	2:D:138:ALA:HA	2.03	0.40
2:F:63:HIS:CA	2:F:66:LYS:HB2	2.50	0.40
1:G:118:THR:C	1:G:120:ALA:N	2.76	0.40
1:A:86:LEU:C	1:A:91:LEU:HD12	2.46	0.40
2:B:68:LEU:HA	2:B:71:PHE:HB3	2.02	0.40
2:B:93:CYS:CB	2:B:145:TYR:CE2	3.01	0.40
2:B:141:LEU:CD2	3:B:147:HEM:HMB3	2.50	0.40
1:C:124:SER:O	1:C:127:LYS:CB	2.69	0.40
1:C:128:PHE:CE2	1:C:129:LEU:HB2	2.56	0.40
2:D:101:GLU:N	2:D:104:ARG:NH1	2.64	0.40
2:F:107:GLY:C	2:F:134:VAL:HG11	2.47	0.40
2:H:123:THR:HB	2:H:125:PRO:CD	2.38	0.40
2:H:123:THR:C	2:H:126:VAL:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:SER:C	1:A:7:LYS:HG2	2.46	0.40
1:A:134:THR:O	1:A:137:THR:CA	2.69	0.40
1:C:40:LYS:CB	1:C:40:LYS:HD2	2.17	0.40
1:C:83:LEU:HA	1:C:86:LEU:CB	2.51	0.40
1:C:86:LEU:CD2	3:C:142:HEM:HBA1	2.51	0.40
1:C:106:LEU:HD21	1:C:126:ASP:HB2	2.02	0.40
2:D:35:TYR:CD2	2:D:105:LEU:HD22	2.56	0.40
1:E:35:SER:HB3	2:F:128:ALA:HB2	2.03	0.40
1:E:76:MET:N	1:E:77:PRO:CD	2.76	0.40
1:E:96:VAL:O	1:E:100:LEU:CD2	2.69	0.40
2:F:91:LEU:O	2:F:91:LEU:CG	2.69	0.40
1:G:49:SER:N	1:G:52:SER:OG	2.54	0.40
1:G:60:LYS:NZ	1:G:60:LYS:HD2	2.35	0.40
2:H:4:THR:HB	2:H:7:GLU:CG	2.41	0.40
2:H:94:ASP:CG	2:H:146:HIS:HE2	2.24	0.40
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.56	0.40
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.86	0.40
2:B:130:TYR:O	2:B:134:VAL:N	2.51	0.40
2:D:142:ALA:CB	2:D:142:ALA:H	2.28	0.40
1:E:101:LEU:CD2	1:E:104:CYS:SG	3.09	0.40
2:F:3:LEU:CD1	2:F:8:LYS:HB2	2.51	0.40
1:A:106:LEU:O	1:A:109:LEU:HB2	2.21	0.40
2:B:88:LEU:CD2	2:H:6:VAL:HG13	2.44	0.40
2:B:137:VAL:O	2:B:140:ALA:HB3	2.20	0.40
1:C:110:ALA:CB	2:D:115:ALA:CB	2.90	0.40
2:D:50:THR:O	2:D:53:ALA:N	2.53	0.40
2:D:91:LEU:O	2:D:96:LEU:N	2.54	0.40
1:E:29:LEU:HD11	1:E:58:HIS:CD2	2.52	0.40
1:E:111:ALA:HB2	2:F:115:ALA:HB1	2.02	0.40
2:F:54:VAL:O	2:F:54:VAL:CG1	2.60	0.40
2:F:91:LEU:O	2:F:91:LEU:HG	2.21	0.40
1:G:17:VAL:HG12	1:G:21:ALA:N	2.36	0.40
1:G:31:ARG:HD3	1:G:108:THR:HG23	2.04	0.40
1:G:84:SER:CB	1:G:136:LEU:HD23	2.43	0.40
2:H:4:THR:CG2	2:H:7:GLU:N	2.78	0.40
2:H:124:PRO:HG2	2:H:125:PRO:CD	2.52	0.40

All (5) 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:53:ALA:CB	2:F:43:GLU:O[1_454]	1.28	0.92
2:D:6:VAL:CG2	2:F:73:ASP:OD2[1_455]	1.92	0.28
1:C:54:GLN:OE1	2:F:46:GLY:CA[1_454]	1.94	0.26
1:C:85:ASP:OD2	2:D:83:GLY:O[1_554]	2.00	0.20
2:D:9:SER:OG	3:F:147:HEM:O2A[1_455]	2.08	0.12

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%)	121 (87%)	15 (11%)	3 (2%)	5 26
1	C	139/141 (99%)	116 (84%)	13 (9%)	10 (7%)	1 4
1	E	139/141 (99%)	113 (81%)	20 (14%)	6 (4%)	2 12
1	G	139/141 (99%)	105 (76%)	24 (17%)	10 (7%)	1 4
2	B	144/146 (99%)	120 (83%)	23 (16%)	1 (1%)	18 53
2	D	144/146 (99%)	120 (83%)	17 (12%)	7 (5%)	1 10
2	F	144/146 (99%)	123 (85%)	14 (10%)	7 (5%)	1 10
2	H	144/146 (99%)	114 (79%)	22 (15%)	8 (6%)	1 8
All	All	1132/1148 (99%)	932 (82%)	148 (13%)	52 (5%)	2 11

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	C	73	VAL
2	D	11	VAL
2	D	40	ARG
2	D	54	VAL
2	F	24	GLY
2	F	80	ASN
1	G	18	GLY

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Mol	Chain	Res	Type
1	G	81	SER
1	G	82	ALA
2	H	15	TRP
2	H	88	LEU
2	H	89	SER
1	C	18	GLY
1	C	81	SER
2	D	17	LYS
1	E	18	GLY
1	E	21	ALA
2	F	67	VAL
2	F	73	ASP
1	G	28	ALA
1	G	50	HIS
2	H	40	ARG
2	H	117	HIS
1	A	28	ALA
1	C	21	ALA
1	C	106	LEU
2	D	8	LYS
1	E	123	ALA
2	F	40	ARG
1	G	52	SER
2	H	97	HIS
1	C	28	ALA
1	C	32	MET
1	E	87	HIS
1	E	106	LEU
2	F	36	PRO
2	H	119	GLY
1	A	21	ALA
1	C	86	LEU
1	C	92	ARG
1	E	114	PRO
1	G	95	PRO
1	C	52	SER
2	D	16	GLY
2	F	2	HIS
1	G	73	VAL
2	H	115	ALA
2	D	36	PRO
1	G	15	GLY

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Mol	Chain	Res	Type
2	B	36	PRO
1	G	114	PRO

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%)	78 (69%)	35 (31%)	0	1
1	C	113/113 (100%)	66 (58%)	47 (42%)	0	0
1	E	113/113 (100%)	64 (57%)	49 (43%)	0	0
1	G	113/113 (100%)	65 (58%)	48 (42%)	0	0
2	B	118/118 (100%)	70 (59%)	48 (41%)	0	0
2	D	118/118 (100%)	79 (67%)	39 (33%)	0	1
2	F	118/118 (100%)	73 (62%)	45 (38%)	0	1
2	H	118/118 (100%)	62 (52%)	56 (48%)	0	0
All	All	924/924 (100%)	557 (60%)	367 (40%)	0	1

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	2	LEU
1	A	3	SER
1	A	4	PRO
1	A	7	LYS
1	A	10	VAL
1	A	20	HIS
1	A	23	GLU
1	A	29	LEU
1	A	37	PRO
1	A	38	THR
1	A	45	HIS
1	A	47	ASP

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Mol	Chain	Res	Type
1	A	48	LEU
1	A	60	LYS
1	A	61	LYS
1	A	62	VAL
1	A	73	VAL
1	A	75	ASP
1	A	76	MET
1	A	77	PRO
1	A	86	LEU
1	A	90	LYS
1	A	93	VAL
1	A	99	LYS
1	A	100	LEU
1	A	102	SER
1	A	105	LEU
1	A	118	THR
1	A	124	SER
1	A	127	LYS
1	A	136	LEU
1	A	137	THR
1	A	138	SER
1	A	139	LYS
2	B	2	HIS
2	B	4	THR
2	B	8	LYS
2	B	11	VAL
2	B	14	LEU
2	B	17	LYS
2	B	18	VAL
2	B	21	ASP
2	B	26	GLU
2	B	28	LEU
2	B	30	ARG
2	B	33	VAL
2	B	35	TYR
2	B	44	SER
2	B	48	LEU
2	B	49	SER
2	B	58	PRO
2	B	59	LYS
2	B	60	VAL
2	B	61	LYS

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Mol	Chain	Res	Type
2	B	65	LYS
2	B	66	LYS
2	B	68	LEU
2	B	72	SER
2	B	73	ASP
2	B	75	LEU
2	B	78	LEU
2	B	79	ASP
2	B	81	LEU
2	B	82	LYS
2	B	88	LEU
2	B	89	SER
2	B	91	LEU
2	B	95	LYS
2	B	96	LEU
2	B	98	VAL
2	B	101	GLU
2	B	104	ARG
2	B	111	VAL
2	B	113	VAL
2	B	114	LEU
2	B	120	LYS
2	B	121	GLU
2	B	131	GLN
2	B	132	LYS
2	B	139	ASN
2	B	144	LYS
2	B	146	HIS
1	C	2	LEU
1	C	3	SER
1	C	8	THR
1	C	10	VAL
1	C	31	ARG
1	C	32	MET
1	C	34	LEU
1	C	35	SER
1	C	40	LYS
1	C	41	THR
1	C	46	PHE
1	C	47	ASP
1	C	48	LEU
1	C	50	HIS

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Mol	Chain	Res	Type
1	C	52	SER
1	C	54	GLN
1	C	55	VAL
1	C	60	LYS
1	C	61	LYS
1	C	70	VAL
1	C	76	MET
1	C	80	LEU
1	C	83	LEU
1	C	90	LYS
1	C	91	LEU
1	C	92	ARG
1	C	94	ASP
1	C	96	VAL
1	C	99	LYS
1	C	100	LEU
1	C	101	LEU
1	C	102	SER
1	C	104	CYS
1	C	105	LEU
1	C	106	LEU
1	C	108	THR
1	C	109	LEU
1	C	118	THR
1	C	124	SER
1	C	125	LEU
1	C	126	ASP
1	C	127	LYS
1	C	128	PHE
1	C	129	LEU
1	C	134	THR
1	C	136	LEU
1	C	138	SER
2	D	1	VAL
2	D	4	THR
2	D	7	GLU
2	D	8	LYS
2	D	9	SER
2	D	11	VAL
2	D	12	THR
2	D	14	LEU
2	D	15	TRP

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Mol	Chain	Res	Type
2	D	17	LYS
2	D	22	GLU
2	D	26	GLU
2	D	40	ARG
2	D	42	PHE
2	D	45	PHE
2	D	48	LEU
2	D	54	VAL
2	D	60	VAL
2	D	65	LYS
2	D	66	LYS
2	D	68	LEU
2	D	72	SER
2	D	75	LEU
2	D	81	LEU
2	D	90	GLU
2	D	93	CYS
2	D	100	PRO
2	D	106	LEU
2	D	109	VAL
2	D	111	VAL
2	D	113	VAL
2	D	123	THR
2	D	125	PRO
2	D	131	GLN
2	D	133	VAL
2	D	137	VAL
2	D	141	LEU
2	D	143	HIS
2	D	146	HIS
1	E	1	VAL
1	E	2	LEU
1	E	6	ASP
1	E	10	VAL
1	E	11	LYS
1	E	16	LYS
1	E	27	GLU
1	E	29	LEU
1	E	31	ARG
1	E	34	LEU
1	E	36	PHE
1	E	39	THR

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Mol	Chain	Res	Type
1	E	41	THR
1	E	43	PHE
1	E	44	PRO
1	E	45	HIS
1	E	49	SER
1	E	52	SER
1	E	60	LYS
1	E	62	VAL
1	E	67	THR
1	E	73	VAL
1	E	76	MET
1	E	83	LEU
1	E	84	SER
1	E	91	LEU
1	E	92	ARG
1	E	96	VAL
1	E	99	LYS
1	E	100	LEU
1	E	101	LEU
1	E	102	SER
1	E	105	LEU
1	E	107	VAL
1	E	109	LEU
1	E	113	LEU
1	E	114	PRO
1	E	117	PHE
1	E	119	PRO
1	E	124	SER
1	E	125	LEU
1	E	127	LYS
1	E	128	PHE
1	E	129	LEU
1	E	132	VAL
1	E	134	THR
1	E	138	SER
1	E	139	LYS
1	E	141	ARG
2	F	1	VAL
2	F	3	LEU
2	F	5	PRO
2	F	6	VAL
2	F	7	GLU

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Mol	Chain	Res	Type
2	F	11	VAL
2	F	12	THR
2	F	15	TRP
2	F	18	VAL
2	F	22	GLU
2	F	23	VAL
2	F	26	GLU
2	F	30	ARG
2	F	32	LEU
2	F	33	VAL
2	F	38	THR
2	F	39	GLN
2	F	41	PHE
2	F	42	PHE
2	F	48	LEU
2	F	54	VAL
2	F	55	MET
2	F	59	LYS
2	F	65	LYS
2	F	66	LYS
2	F	67	VAL
2	F	73	ASP
2	F	78	LEU
2	F	79	ASP
2	F	80	ASN
2	F	88	LEU
2	F	89	SER
2	F	95	LYS
2	F	96	LEU
2	F	97	HIS
2	F	112	CYS
2	F	114	LEU
2	F	120	LYS
2	F	121	GLU
2	F	126	VAL
2	F	132	LYS
2	F	133	VAL
2	F	137	VAL
2	F	144	LYS
2	F	146	HIS
1	G	1	VAL
1	G	4	PRO

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Mol	Chain	Res	Type
1	G	8	THR
1	G	10	VAL
1	G	11	LYS
1	G	16	LYS
1	G	23	GLU
1	G	27	GLU
1	G	29	LEU
1	G	31	ARG
1	G	32	MET
1	G	34	LEU
1	G	35	SER
1	G	38	THR
1	G	41	THR
1	G	43	PHE
1	G	48	LEU
1	G	49	SER
1	G	52	SER
1	G	55	VAL
1	G	60	LYS
1	G	66	LEU
1	G	67	THR
1	G	70	VAL
1	G	73	VAL
1	G	76	MET
1	G	80	LEU
1	G	84	SER
1	G	85	ASP
1	G	91	LEU
1	G	93	VAL
1	G	96	VAL
1	G	101	LEU
1	G	102	SER
1	G	105	LEU
1	G	106	LEU
1	G	107	VAL
1	G	108	THR
1	G	118	THR
1	G	124	SER
1	G	126	ASP
1	G	127	LYS
1	G	129	LEU
1	G	131	SER

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Mol	Chain	Res	Type
1	G	134	THR
1	G	136	LEU
1	G	139	LYS
1	G	141	ARG
2	H	2	HIS
2	H	3	LEU
2	H	6	VAL
2	H	8	LYS
2	H	11	VAL
2	H	14	LEU
2	H	17	LYS
2	H	22	GLU
2	H	26	GLU
2	H	28	LEU
2	H	32	LEU
2	H	33	VAL
2	H	38	THR
2	H	39	GLN
2	H	42	PHE
2	H	43	GLU
2	H	44	SER
2	H	48	LEU
2	H	49	SER
2	H	50	THR
2	H	54	VAL
2	H	58	PRO
2	H	60	VAL
2	H	65	LYS
2	H	66	LYS
2	H	68	LEU
2	H	72	SER
2	H	75	LEU
2	H	78	LEU
2	H	80	ASN
2	H	82	LYS
2	H	84	THR
2	H	85	PHE
2	H	87	THR
2	H	89	SER
2	H	91	LEU
2	H	92	HIS
2	H	96	LEU

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Mol	Chain	Res	Type
2	H	101	GLU
2	H	104	ARG
2	H	106	LEU
2	H	109	VAL
2	H	110	LEU
2	H	112	CYS
2	H	113	VAL
2	H	114	LEU
2	H	120	LYS
2	H	121	GLU
2	H	122	PHE
2	H	123	THR
2	H	125	PRO
2	H	126	VAL
2	H	130	TYR
2	H	131	GLN
2	H	133	VAL
2	H	146	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	20	HIS
1	A	58	HIS
1	A	78	ASN
1	A	89	HIS
2	B	77	HIS
2	B	97	HIS
2	B	102	ASN
2	B	116	HIS
2	B	139	ASN
2	B	143	HIS
1	C	50	HIS
1	C	58	HIS
1	C	72	HIS
1	C	103	HIS
1	C	122	HIS
2	D	57	ASN
2	D	63	HIS
2	D	80	ASN
2	D	108	ASN

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Mol	Chain	Res	Type
2	D	131	GLN
1	E	58	HIS
1	E	78	ASN
1	E	97	ASN
1	E	103	HIS
2	F	39	GLN
2	F	63	HIS
2	F	80	ASN
2	F	108	ASN
2	F	143	HIS
1	G	20	HIS
1	G	58	HIS
1	G	72	HIS
1	G	97	ASN
1	G	112	HIS
2	H	39	GLN
2	H	63	HIS
2	H	80	ASN
2	H	92	HIS
2	H	117	HIS
2	H	131	GLN
2	H	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	G	142	1	50,50,50	3.64	28 (56%)	67,82,82	3.66	38 (56%)
3	HEM	A	142	1	50,50,50	3.69	26 (52%)	67,82,82	4.52	41 (61%)
3	HEM	B	147	2	50,50,50	3.94	37 (74%)	67,82,82	5.10	39 (58%)
3	HEM	E	142	1	50,50,50	3.51	30 (60%)	67,82,82	4.59	50 (74%)
3	HEM	F	147	2	50,50,50	3.57	28 (56%)	67,82,82	4.72	45 (67%)
3	HEM	D	147	2	50,50,50	2.96	25 (50%)	67,82,82	3.74	42 (62%)
3	HEM	H	147	2	50,50,50	3.65	29 (58%)	67,82,82	4.39	42 (62%)
3	HEM	C	142	1	50,50,50	3.10	25 (50%)	67,82,82	3.95	34 (50%)

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	G	142	1	-	3/14/54/54	-
3	HEM	A	142	1	-	4/14/54/54	-
3	HEM	B	147	2	-	5/14/54/54	-
3	HEM	E	142	1	-	4/14/54/54	-
3	HEM	F	147	2	-	7/14/54/54	-
3	HEM	D	147	2	-	5/14/54/54	-
3	HEM	H	147	2	-	8/14/54/54	-
3	HEM	C	142	1	-	4/14/54/54	-

All (228) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	142	HEM	C3C-C2C	11.24	1.60	1.37
3	E	142	HEM	CMC-C2C	10.43	1.72	1.50
3	F	147	HEM	CBD-CGD	10.12	1.74	1.50
3	D	147	HEM	C4D-C3D	10.09	1.62	1.45
3	G	142	HEM	FE-NB	10.08	2.25	1.94
3	A	142	HEM	O1A-CGA	9.33	1.52	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C3C-C2C	-9.02	1.18	1.37
3	B	147	HEM	FE-ND	8.94	2.22	1.94
3	F	147	HEM	FE-NA	8.90	2.24	1.95
3	A	142	HEM	C1C-NC	8.70	1.56	1.39
3	A	142	HEM	C4A-C3A	8.29	1.62	1.43
3	A	142	HEM	CBD-CAD	8.10	1.80	1.51
3	H	147	HEM	CBA-CGA	8.06	1.69	1.50
3	G	142	HEM	C1D-C2D	7.82	1.60	1.44
3	F	147	HEM	C1A-NA	-7.75	1.25	1.39
3	F	147	HEM	CMA-C3A	7.44	1.66	1.50
3	E	142	HEM	CBD-CGD	7.41	1.67	1.50
3	H	147	HEM	C4A-NA	-7.35	1.25	1.39
3	H	147	HEM	C1A-NA	7.31	1.53	1.39
3	E	142	HEM	CHB-C1B	-7.25	1.24	1.38
3	B	147	HEM	CMC-C2C	7.09	1.65	1.50
3	E	142	HEM	CAD-C3D	6.99	1.69	1.51
3	C	142	HEM	C1D-ND	-6.98	1.25	1.38
3	H	147	HEM	CHC-C1C	-6.96	1.24	1.38
3	C	142	HEM	CMD-C2D	6.82	1.64	1.50
3	B	147	HEM	CAD-C3D	6.62	1.68	1.51
3	A	142	HEM	FE-NA	6.59	2.16	1.95
3	D	147	HEM	FE-ND	6.48	2.14	1.94
3	B	147	HEM	FE-NB	6.43	2.14	1.94
3	C	142	HEM	O1D-CGD	6.17	1.42	1.22
3	B	147	HEM	CBA-CGA	6.16	1.64	1.50
3	E	142	HEM	CMD-C2D	6.16	1.63	1.50
3	A	142	HEM	CMC-C2C	6.06	1.63	1.50
3	F	147	HEM	CBD-CAD	5.82	1.72	1.51
3	B	147	HEM	CHD-C4C	5.82	1.49	1.38
3	H	147	HEM	CMC-C2C	5.80	1.62	1.50
3	H	147	HEM	FE-ND	5.80	2.12	1.94
3	A	142	HEM	C1C-C2C	-5.76	1.33	1.45
3	G	142	HEM	CBC-CAC	5.72	1.57	1.30
3	B	147	HEM	CAA-C2A	5.61	1.65	1.51
3	D	147	HEM	C4D-ND	-5.58	1.30	1.40
3	E	142	HEM	CBD-CAD	5.56	1.71	1.51
3	G	142	HEM	C4D-C3D	5.53	1.54	1.45
3	C	142	HEM	CBD-CAD	5.47	1.70	1.51
3	F	147	HEM	C1A-C2A	5.44	1.55	1.44
3	B	147	HEM	C3C-C4C	5.35	1.55	1.46
3	H	147	HEM	CHA-C1A	-5.28	1.27	1.39
3	B	147	HEM	CMA-C3A	5.27	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	147	HEM	CMD-C2D	5.23	1.61	1.50
3	C	142	HEM	FE-ND	5.22	2.11	1.94
3	H	147	HEM	C3C-C2C	5.21	1.47	1.37
3	C	142	HEM	FE-NB	5.20	2.10	1.94
3	G	142	HEM	CAB-C3B	5.18	1.61	1.47
3	H	147	HEM	CAB-C3B	5.18	1.61	1.47
3	D	147	HEM	C4C-NC	5.12	1.49	1.39
3	H	147	HEM	O1D-CGD	5.06	1.38	1.22
3	A	142	HEM	CHB-C1B	5.02	1.48	1.38
3	F	147	HEM	C4A-NA	5.00	1.49	1.39
3	A	142	HEM	C1D-ND	4.99	1.48	1.38
3	D	147	HEM	FE-NA	4.98	2.11	1.95
3	F	147	HEM	CHC-C4B	4.90	1.50	1.39
3	G	142	HEM	FE-ND	4.90	2.10	1.94
3	A	142	HEM	CBD-CGD	4.84	1.61	1.50
3	E	142	HEM	FE-NB	4.77	2.09	1.94
3	G	142	HEM	C4D-ND	-4.73	1.32	1.40
3	C	142	HEM	FE-NA	4.73	2.10	1.95
3	A	142	HEM	C3C-C2C	-4.72	1.27	1.37
3	G	142	HEM	CBA-CAA	4.71	1.68	1.51
3	D	147	HEM	FE-NB	4.70	2.09	1.94
3	E	142	HEM	C3B-C4B	-4.66	1.35	1.44
3	B	147	HEM	CBC-CAC	4.63	1.52	1.30
3	B	147	HEM	C3D-C2D	-4.61	1.26	1.36
3	E	142	HEM	FE-ND	4.61	2.09	1.94
3	G	142	HEM	C3B-C4B	-4.48	1.36	1.44
3	D	147	HEM	CBB-CAB	4.43	1.51	1.30
3	B	147	HEM	C1D-ND	4.39	1.47	1.38
3	H	147	HEM	FE-NC	4.37	2.09	1.95
3	G	142	HEM	C1A-NA	-4.37	1.31	1.39
3	H	147	HEM	CBD-CGD	4.36	1.60	1.50
3	F	147	HEM	C3C-C4C	4.33	1.53	1.46
3	H	147	HEM	CHB-C4A	4.32	1.49	1.39
3	B	147	HEM	CBD-CAD	4.29	1.66	1.51
3	H	147	HEM	FE-NA	4.29	2.09	1.95
3	B	147	HEM	C1A-C2A	-4.27	1.36	1.44
3	C	142	HEM	FE-NC	4.26	2.09	1.95
3	A	142	HEM	C3C-C4C	4.21	1.53	1.46
3	C	142	HEM	CAC-C3C	4.13	1.58	1.47
3	E	142	HEM	C3D-C2D	-4.12	1.27	1.36
3	C	142	HEM	CBD-CGD	-4.11	1.41	1.50
3	E	142	HEM	C3C-C2C	-4.10	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	147	HEM	C1D-C2D	4.08	1.52	1.44
3	A	142	HEM	C1A-NA	-4.05	1.32	1.39
3	F	147	HEM	C3C-C2C	-3.96	1.29	1.37
3	H	147	HEM	CHC-C4B	-3.94	1.30	1.39
3	C	142	HEM	O1A-CGA	3.92	1.34	1.22
3	H	147	HEM	C4D-ND	-3.92	1.33	1.40
3	F	147	HEM	C3B-C2B	-3.91	1.29	1.37
3	F	147	HEM	CBA-CGA	3.90	1.59	1.50
3	C	142	HEM	C1A-NA	-3.90	1.32	1.39
3	B	147	HEM	C1C-C2C	-3.88	1.37	1.45
3	C	142	HEM	O2D-CGD	-3.87	1.18	1.30
3	C	142	HEM	CMA-C3A	3.84	1.58	1.50
3	A	142	HEM	CMB-C2B	3.80	1.58	1.50
3	C	142	HEM	C1C-C2C	-3.78	1.37	1.45
3	F	147	HEM	CBB-CAB	3.78	1.48	1.30
3	E	142	HEM	FE-NA	3.78	2.07	1.95
3	F	147	HEM	C1C-C2C	3.77	1.52	1.45
3	D	147	HEM	FE-NC	3.75	2.07	1.95
3	B	147	HEM	CHA-C1A	-3.71	1.31	1.39
3	A	142	HEM	CAB-C3B	3.70	1.57	1.47
3	B	147	HEM	C1A-NA	3.70	1.46	1.39
3	B	147	HEM	CAC-C3C	3.68	1.57	1.47
3	E	142	HEM	C1B-C2B	3.68	1.52	1.44
3	H	147	HEM	CHA-C4D	-3.67	1.31	1.38
3	F	147	HEM	CHB-C4A	3.65	1.47	1.39
3	H	147	HEM	C1C-C2C	-3.64	1.38	1.45
3	G	142	HEM	CMC-C2C	-3.62	1.43	1.50
3	F	147	HEM	CBA-CAA	3.61	1.64	1.51
3	G	142	HEM	O1A-CGA	3.61	1.33	1.22
3	C	142	HEM	CHA-C1A	3.58	1.47	1.39
3	C	142	HEM	CMC-C2C	3.58	1.58	1.50
3	G	142	HEM	C4A-C3A	3.56	1.51	1.43
3	H	147	HEM	C1D-ND	-3.51	1.31	1.38
3	B	147	HEM	C2A-C3A	-3.51	1.29	1.38
3	G	142	HEM	CHD-C4C	-3.50	1.31	1.38
3	C	142	HEM	C1B-NB	-3.49	1.34	1.40
3	A	142	HEM	C2A-C3A	-3.45	1.29	1.38
3	A	142	HEM	C3D-C2D	-3.45	1.29	1.36
3	G	142	HEM	C1D-ND	-3.44	1.32	1.38
3	A	142	HEM	FE-ND	3.42	2.05	1.94
3	D	147	HEM	C3C-C4C	-3.42	1.40	1.46
3	G	142	HEM	C4A-NA	3.40	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	147	HEM	C1C-NC	-3.39	1.33	1.39
3	G	142	HEM	O1D-CGD	3.39	1.33	1.22
3	F	147	HEM	C2A-C3A	3.36	1.47	1.38
3	E	142	HEM	C4A-NA	-3.31	1.33	1.39
3	B	147	HEM	CHB-C4A	-3.30	1.32	1.39
3	G	142	HEM	CMA-C3A	-3.29	1.44	1.50
3	A	142	HEM	FE-NB	3.26	2.04	1.94
3	H	147	HEM	CBC-CAC	3.26	1.46	1.30
3	E	142	HEM	CMB-C2B	3.24	1.57	1.50
3	C	142	HEM	CHB-C4A	3.22	1.46	1.39
3	B	147	HEM	O1D-CGD	3.21	1.32	1.22
3	B	147	HEM	CAB-C3B	3.21	1.56	1.47
3	B	147	HEM	O2D-CGD	3.20	1.41	1.30
3	H	147	HEM	C4D-C3D	3.19	1.50	1.45
3	C	142	HEM	C1B-C2B	3.15	1.50	1.44
3	G	142	HEM	CHA-C1A	3.13	1.46	1.39
3	D	147	HEM	C1D-C2D	3.11	1.50	1.44
3	F	147	HEM	FE-NC	3.11	2.05	1.95
3	E	142	HEM	CMA-C3A	3.10	1.57	1.50
3	E	142	HEM	C1A-C2A	3.09	1.50	1.44
3	H	147	HEM	FE-NB	3.08	2.04	1.94
3	B	147	HEM	C3B-C2B	3.07	1.43	1.37
3	B	147	HEM	CMB-C2B	3.05	1.57	1.50
3	D	147	HEM	CBD-CGD	3.00	1.57	1.50
3	B	147	HEM	CHD-C1D	-2.97	1.32	1.39
3	F	147	HEM	CAA-C2A	-2.93	1.43	1.51
3	F	147	HEM	CHA-C1A	-2.90	1.32	1.39
3	D	147	HEM	C4B-NB	-2.89	1.33	1.38
3	D	147	HEM	CAC-C3C	2.88	1.55	1.47
3	E	142	HEM	CHA-C4D	-2.88	1.32	1.38
3	F	147	HEM	CAB-C3B	2.86	1.55	1.47
3	D	147	HEM	CHD-C1D	2.86	1.45	1.39
3	C	142	HEM	C4A-NA	-2.85	1.34	1.39
3	A	142	HEM	C1A-C2A	2.84	1.50	1.44
3	E	142	HEM	C1C-C2C	-2.84	1.39	1.45
3	D	147	HEM	O1A-CGA	2.81	1.31	1.22
3	E	142	HEM	CBB-CAB	2.80	1.43	1.30
3	G	142	HEM	CHD-C1D	-2.77	1.32	1.39
3	G	142	HEM	C1C-NC	2.76	1.44	1.39
3	D	147	HEM	C3D-C2D	-2.74	1.30	1.36
3	B	147	HEM	CHC-C4B	-2.73	1.33	1.39
3	D	147	HEM	CMA-C3A	2.72	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	C3C-C2C	-2.72	1.31	1.37
3	G	142	HEM	CMD-C2D	-2.69	1.45	1.50
3	D	147	HEM	CAB-C3B	2.69	1.54	1.47
3	B	147	HEM	C4A-C3A	2.68	1.49	1.43
3	F	147	HEM	CMC-C2C	2.67	1.56	1.50
3	E	142	HEM	C4A-C3A	2.66	1.49	1.43
3	D	147	HEM	CHC-C1C	2.66	1.43	1.38
3	D	147	HEM	C4A-NA	-2.64	1.34	1.39
3	H	147	HEM	C3C-C4C	-2.63	1.41	1.46
3	B	147	HEM	C3B-C4B	-2.61	1.39	1.44
3	H	147	HEM	CHD-C4C	-2.57	1.33	1.38
3	E	142	HEM	C2A-C3A	-2.56	1.32	1.38
3	E	142	HEM	CAC-C3C	2.54	1.54	1.47
3	G	142	HEM	C1B-NB	2.54	1.44	1.40
3	D	147	HEM	C3B-C4B	-2.54	1.40	1.44
3	E	142	HEM	C4B-NB	2.54	1.43	1.38
3	B	147	HEM	C1D-C2D	2.52	1.49	1.44
3	E	142	HEM	CHC-C1C	-2.52	1.33	1.38
3	D	147	HEM	CBC-CAC	2.52	1.42	1.30
3	B	147	HEM	CBA-CAA	2.51	1.60	1.51
3	B	147	HEM	C4A-NA	-2.49	1.34	1.39
3	F	147	HEM	C4A-C3A	-2.49	1.37	1.43
3	G	142	HEM	C1C-C2C	-2.47	1.40	1.45
3	H	147	HEM	C3B-C4B	-2.44	1.40	1.44
3	D	147	HEM	CBD-CAD	-2.43	1.43	1.51
3	A	142	HEM	CHD-C4C	2.41	1.43	1.38
3	A	142	HEM	CBA-CGA	-2.40	1.45	1.50
3	B	147	HEM	CBB-CAB	2.37	1.41	1.30
3	F	147	HEM	C1D-C2D	-2.30	1.39	1.44
3	D	147	HEM	CMB-C2B	2.30	1.55	1.50
3	B	147	HEM	CMD-C2D	2.29	1.55	1.50
3	F	147	HEM	CHD-C1D	2.24	1.44	1.39
3	B	147	HEM	C4D-ND	-2.23	1.36	1.40
3	D	147	HEM	O2D-CGD	-2.20	1.23	1.30
3	G	142	HEM	C3B-C2B	2.20	1.41	1.37
3	F	147	HEM	CMB-C2B	2.19	1.55	1.50
3	E	142	HEM	CHD-C1D	-2.19	1.34	1.39
3	E	142	HEM	C1C-NC	2.18	1.43	1.39
3	F	147	HEM	C1B-C2B	2.18	1.48	1.44
3	G	142	HEM	CMB-C2B	2.17	1.55	1.50
3	E	142	HEM	C1D-C2D	2.17	1.48	1.44
3	B	147	HEM	O2A-CGA	-2.16	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	142	HEM	C1D-ND	-2.16	1.34	1.38
3	A	142	HEM	FE-NC	2.16	2.02	1.95
3	A	142	HEM	CHC-C4B	2.13	1.44	1.39
3	A	142	HEM	CHD-C1D	-2.12	1.34	1.39
3	H	147	HEM	CBB-CAB	2.12	1.40	1.30
3	A	142	HEM	CMD-C2D	-2.12	1.46	1.50
3	C	142	HEM	CHC-C1C	2.07	1.42	1.38
3	C	142	HEM	C3B-C2B	-2.07	1.33	1.37
3	C	142	HEM	C4D-C3D	-2.06	1.41	1.45
3	H	147	HEM	O2D-CGD	-2.03	1.24	1.30
3	E	142	HEM	C4D-ND	2.02	1.43	1.40
3	G	142	HEM	CHC-C1C	-2.01	1.34	1.38

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	147	HEM	CHD-C4C-NC	18.84	144.97	124.45
3	C	142	HEM	CMA-C3A-C4A	16.59	150.68	125.42
3	B	147	HEM	CHA-C4D-ND	15.21	143.19	124.37
3	F	147	HEM	CHC-C4B-NB	14.74	140.28	124.42
3	H	147	HEM	O2A-CGA-O1A	14.22	159.90	123.33
3	F	147	HEM	CHD-C4C-NC	14.15	139.86	124.45
3	A	142	HEM	CHD-C1D-ND	-13.07	110.36	124.42
3	B	147	HEM	C3C-C2C-C1C	11.92	118.32	107.05
3	B	147	HEM	O2A-CGA-O1A	10.99	151.58	123.33
3	E	142	HEM	CHD-C4C-NC	-10.62	112.89	124.45
3	F	147	HEM	CHB-C4A-NA	-10.31	105.17	123.86
3	C	142	HEM	O2D-CGD-O1D	-10.20	97.11	123.33
3	A	142	HEM	CAD-CBD-CGD	-10.14	86.77	113.67
3	A	142	HEM	CHD-C1D-C2D	9.94	140.73	125.03
3	H	147	HEM	CHD-C1D-ND	9.87	135.05	124.42
3	E	142	HEM	CHD-C4C-C3C	9.81	141.74	125.21
3	C	142	HEM	CMA-C3A-C2A	-9.38	105.72	125.62
3	A	142	HEM	CBA-CAA-C2A	9.32	138.31	112.53
3	A	142	HEM	CHC-C4B-NB	9.21	134.34	124.42
3	C	142	HEM	O1D-CGD-CBD	9.16	152.14	123.09
3	B	147	HEM	C4C-CHD-C1D	-9.08	106.72	126.02
3	A	142	HEM	CHC-C1C-NC	-9.05	114.59	124.45
3	B	147	HEM	CHD-C4C-C3C	-8.84	110.30	125.21
3	F	147	HEM	CHD-C4C-C3C	-8.74	110.47	125.21
3	D	147	HEM	O1D-CGD-CBD	-8.67	95.59	123.09
3	E	142	HEM	CAA-CBA-CGA	8.59	136.45	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	147	HEM	CHA-C4D-C3D	-8.51	109.54	125.23
3	D	147	HEM	CHA-C4D-ND	8.49	134.86	124.37
3	B	147	HEM	CHD-C1D-C2D	8.39	138.27	125.03
3	G	142	HEM	O2A-CGA-CBA	8.36	140.41	114.00
3	B	147	HEM	CHC-C4B-NB	-8.32	115.47	124.42
3	F	147	HEM	C3B-C2B-C1B	8.27	112.62	106.41
3	D	147	HEM	CHD-C1D-ND	8.24	133.29	124.42
3	H	147	HEM	CAA-CBA-CGA	-8.20	91.92	113.67
3	G	142	HEM	O2D-CGD-O1D	-8.15	102.36	123.33
3	D	147	HEM	CHB-C1B-NB	8.04	134.31	124.37
3	D	147	HEM	O2D-CGD-CBD	7.91	138.99	114.00
3	G	142	HEM	C4D-ND-C1D	7.90	114.56	105.21
3	E	142	HEM	C2A-C1A-NA	7.80	118.81	110.15
3	E	142	HEM	CMB-C2B-C1B	-7.72	112.98	125.03
3	H	147	HEM	CAC-C3C-C4C	7.65	143.09	124.82
3	C	142	HEM	CAD-C3D-C4D	7.50	137.78	124.70
3	F	147	HEM	CMA-C3A-C4A	7.49	136.82	125.42
3	H	147	HEM	CMD-C2D-C1D	7.49	136.73	125.03
3	F	147	HEM	CHD-C1D-ND	-7.36	116.51	124.42
3	D	147	HEM	CAD-CBD-CGD	7.28	132.97	113.67
3	E	142	HEM	CAC-C3C-C4C	-7.28	107.45	124.82
3	F	147	HEM	CHC-C4B-C3B	-7.19	110.72	125.07
3	G	142	HEM	CMA-C3A-C4A	7.02	136.11	125.42
3	G	142	HEM	CHC-C4B-NB	-6.99	116.90	124.42
3	F	147	HEM	C1C-CHC-C4B	-6.94	111.27	126.02
3	H	147	HEM	C2A-C1A-NA	-6.93	102.47	110.15
3	F	147	HEM	CAA-C2A-C3A	6.87	142.48	127.07
3	A	142	HEM	C3C-C2C-C1C	6.87	113.55	107.05
3	H	147	HEM	CBA-CAA-C2A	6.85	131.47	112.53
3	E	142	HEM	C4C-CHD-C1D	6.79	140.45	126.02
3	H	147	HEM	O2D-CGD-CBD	-6.76	92.63	114.00
3	D	147	HEM	C4D-ND-C1D	6.74	113.19	105.21
3	H	147	HEM	O2D-CGD-O1D	6.69	140.53	123.33
3	C	142	HEM	CAA-C2A-C3A	6.64	141.96	127.07
3	H	147	HEM	CHC-C4B-NB	-6.62	117.30	124.42
3	E	142	HEM	C2B-C1B-NB	-6.61	102.24	109.84
3	H	147	HEM	O1A-CGA-CBA	-6.54	102.34	123.09
3	A	142	HEM	CAA-C2A-C1A	-6.51	112.22	124.94
3	E	142	HEM	C3B-C4B-NB	-6.45	104.84	109.47
3	E	142	HEM	C1B-NB-C4B	6.43	112.82	105.21
3	C	142	HEM	CAA-C2A-C1A	-6.29	112.66	124.94
3	B	147	HEM	CHD-C1D-ND	-6.27	117.68	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	142	HEM	CAA-C2A-C3A	6.25	141.08	127.07
3	A	142	HEM	C4C-CHD-C1D	6.25	139.29	126.02
3	C	142	HEM	CAD-C3D-C2D	-6.20	116.26	127.87
3	B	147	HEM	O2A-CGA-CBA	-6.17	94.52	114.00
3	E	142	HEM	CHB-C4A-C3A	-6.13	109.64	127.43
3	E	142	HEM	C3D-C4D-ND	-6.08	103.50	110.17
3	E	142	HEM	CHB-C1B-NB	6.05	131.84	124.37
3	E	142	HEM	CAD-CBD-CGD	-5.99	97.78	113.67
3	F	147	HEM	CHB-C4A-C3A	5.95	144.70	127.43
3	B	147	HEM	CBC-CAC-C3C	-5.92	97.94	127.53
3	A	142	HEM	CHA-C4D-ND	5.90	131.67	124.37
3	F	147	HEM	CMA-C3A-C2A	-5.88	113.16	125.62
3	E	142	HEM	C4B-C3B-C2B	5.86	112.66	107.28
3	A	142	HEM	C4C-NC-C1C	-5.80	96.37	105.82
3	G	142	HEM	CMC-C2C-C1C	5.80	134.94	124.73
3	H	147	HEM	C3C-C2C-C1C	5.80	112.53	107.05
3	G	142	HEM	O2D-CGD-CBD	5.78	132.25	114.00
3	F	147	HEM	C2D-C1D-ND	5.77	116.58	109.90
3	F	147	HEM	C2A-C1A-NA	5.74	116.52	110.15
3	A	142	HEM	CBD-CAD-C3D	-5.71	96.74	112.53
3	A	142	HEM	O2A-CGA-CBA	5.70	132.01	114.00
3	H	147	HEM	CHD-C1D-C2D	-5.70	116.03	125.03
3	A	142	HEM	O2A-CGA-O1A	-5.68	108.72	123.33
3	D	147	HEM	C3B-C4B-NB	-5.67	105.40	109.47
3	F	147	HEM	C1A-C2A-C3A	-5.64	98.14	106.87
3	F	147	HEM	CAD-CBD-CGD	-5.56	98.91	113.67
3	E	142	HEM	CHB-C4A-NA	5.55	133.93	123.86
3	G	142	HEM	C4A-C3A-C2A	-5.47	100.56	106.82
3	G	142	HEM	C4C-C3C-C2C	-5.46	102.08	106.81
3	D	147	HEM	O2A-CGA-CBA	5.46	131.25	114.00
3	F	147	HEM	CAA-CBA-CGA	5.44	128.10	113.67
3	H	147	HEM	C1C-CHC-C4B	5.43	137.55	126.02
3	A	142	HEM	CMA-C3A-C2A	5.43	137.13	125.62
3	H	147	HEM	CBD-CAD-C3D	5.41	127.50	112.53
3	G	142	HEM	CAD-CBD-CGD	5.41	128.00	113.67
3	F	147	HEM	C2B-C1B-NB	-5.38	103.66	109.84
3	A	142	HEM	C4D-C3D-C2D	5.36	114.69	106.89
3	D	147	HEM	CBB-CAB-C3B	-5.34	100.84	127.53
3	E	142	HEM	CMC-C2C-C3C	-5.34	115.51	128.43
3	E	142	HEM	C4A-NA-C1A	-5.29	97.19	105.82
3	H	147	HEM	CHC-C1C-NC	5.27	130.19	124.45
3	D	147	HEM	C1B-NB-C4B	5.22	111.39	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	142	HEM	C3B-C2B-C1B	5.22	110.33	106.41
3	H	147	HEM	O2A-CGA-CBA	-5.14	97.76	114.00
3	F	147	HEM	C4A-CHB-C1B	5.13	138.31	126.25
3	B	147	HEM	C2D-C1D-ND	-5.10	104.00	109.90
3	E	142	HEM	CAA-C2A-C1A	5.10	134.91	124.94
3	E	142	HEM	CAD-C3D-C4D	-5.09	115.83	124.70
3	G	142	HEM	C4A-CHB-C1B	-5.09	114.29	126.25
3	G	142	HEM	CHC-C1C-NC	5.08	129.98	124.45
3	E	142	HEM	CHC-C1C-NC	5.08	129.98	124.45
3	C	142	HEM	O2A-CGA-CBA	5.07	130.03	114.00
3	B	147	HEM	CAD-CBD-CGD	5.06	127.10	113.67
3	B	147	HEM	O1D-CGD-CBD	5.00	138.94	123.09
3	A	142	HEM	CAD-C3D-C4D	-4.99	116.01	124.70
3	A	142	HEM	CMA-C3A-C4A	-4.96	117.87	125.42
3	D	147	HEM	C3D-C4D-ND	-4.94	104.75	110.17
3	B	147	HEM	C3B-C2B-C1B	-4.91	102.73	106.41
3	E	142	HEM	CBB-CAB-C3B	-4.89	103.11	127.53
3	G	142	HEM	CMD-C2D-C1D	-4.84	117.47	125.03
3	E	142	HEM	C3C-C2C-C1C	4.84	111.62	107.05
3	G	142	HEM	C3B-C4B-NB	4.83	112.94	109.47
3	G	142	HEM	CAC-C3C-C4C	4.83	136.35	124.82
3	H	147	HEM	C4C-NC-C1C	4.82	113.67	105.82
3	B	147	HEM	CHB-C4A-NA	4.82	132.60	123.86
3	G	142	HEM	O1A-CGA-CBA	-4.81	107.84	123.09
3	D	147	HEM	C4B-C3B-C2B	4.80	111.70	107.28
3	E	142	HEM	C4D-ND-C1D	4.80	110.89	105.21
3	F	147	HEM	CHA-C1A-C2A	-4.80	114.79	125.30
3	E	142	HEM	CBA-CAA-C2A	4.80	125.80	112.53
3	H	147	HEM	CHC-C4B-C3B	4.78	134.62	125.07
3	D	147	HEM	O2A-CGA-O1A	-4.75	111.11	123.33
3	H	147	HEM	CAC-C3C-C2C	-4.73	113.05	128.43
3	A	142	HEM	CMB-C2B-C1B	-4.70	117.70	125.03
3	B	147	HEM	C4D-C3D-C2D	4.66	113.68	106.89
3	C	142	HEM	CHD-C1D-C2D	-4.62	117.73	125.03
3	E	142	HEM	CMB-C2B-C3B	4.62	139.60	128.43
3	E	142	HEM	CMD-C2D-C1D	-4.62	117.82	125.03
3	D	147	HEM	CMA-C3A-C4A	4.61	132.44	125.42
3	E	142	HEM	CMC-C2C-C1C	4.59	132.82	124.73
3	E	142	HEM	CMA-C3A-C4A	-4.56	118.48	125.42
3	G	142	HEM	CBC-CAC-C3C	-4.55	104.80	127.53
3	G	142	HEM	CHA-C4D-C3D	4.55	133.61	125.23
3	H	147	HEM	C3B-C2B-C1B	4.55	109.82	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	142	HEM	O2A-CGA-O1A	-4.51	111.73	123.33
3	E	142	HEM	CAC-C3C-C2C	4.49	143.02	128.43
3	E	142	HEM	C1A-C2A-C3A	-4.48	99.94	106.87
3	B	147	HEM	C3B-C4B-NB	4.46	112.67	109.47
3	H	147	HEM	C2B-C1B-NB	-4.43	104.75	109.84
3	H	147	HEM	CAA-C2A-C1A	4.40	133.53	124.94
3	C	142	HEM	CMB-C2B-C1B	-4.40	118.16	125.03
3	A	142	HEM	C1B-NB-C4B	4.38	110.40	105.21
3	E	142	HEM	C4A-CHB-C1B	-4.36	115.99	126.25
3	B	147	HEM	O2D-CGD-O1D	-4.34	112.16	123.33
3	H	147	HEM	CHD-C4C-C3C	4.27	132.41	125.21
3	F	147	HEM	C4D-ND-C1D	-4.27	100.16	105.21
3	B	147	HEM	C2B-C1B-NB	4.26	114.73	109.84
3	G	142	HEM	CHB-C4A-NA	4.25	131.57	123.86
3	A	142	HEM	C2A-C1A-NA	4.25	114.87	110.15
3	D	147	HEM	C4C-C3C-C2C	4.23	110.48	106.81
3	C	142	HEM	C2D-C1D-ND	4.23	114.79	109.90
3	C	142	HEM	C1D-C2D-C3D	-4.21	102.55	106.98
3	G	142	HEM	CMD-C2D-C3D	4.20	137.51	126.15
3	A	142	HEM	C2B-C1B-NB	-4.19	105.02	109.84
3	H	147	HEM	CHA-C1A-NA	4.19	131.45	123.86
3	D	147	HEM	CBC-CAC-C3C	-4.19	106.61	127.53
3	C	142	HEM	CHB-C4A-NA	-4.18	116.29	123.86
3	B	147	HEM	C4A-CHB-C1B	-4.15	116.48	126.25
3	F	147	HEM	C3C-C2C-C1C	4.14	110.96	107.05
3	E	142	HEM	CHD-C1D-C2D	4.10	131.50	125.03
3	D	147	HEM	CHD-C1D-C2D	-4.08	118.58	125.03
3	E	142	HEM	CHA-C4D-C3D	4.07	132.73	125.23
3	G	142	HEM	CHA-C4D-ND	-4.03	119.38	124.37
3	C	142	HEM	CBC-CAC-C3C	-4.03	107.39	127.53
3	H	147	HEM	CMD-C2D-C3D	-4.03	115.25	126.15
3	C	142	HEM	CHD-C4C-NC	3.99	128.80	124.45
3	D	147	HEM	CHC-C1C-NC	-3.97	120.13	124.45
3	A	142	HEM	CMC-C2C-C1C	-3.96	117.76	124.73
3	H	147	HEM	CAD-CBD-CGD	3.89	123.98	113.67
3	E	142	HEM	C3A-C4A-NA	3.88	116.37	110.14
3	G	142	HEM	CHC-C1C-C2C	-3.88	117.41	125.49
3	E	142	HEM	CMA-C3A-C2A	3.87	133.84	125.62
3	A	142	HEM	C3B-C4B-NB	-3.87	106.69	109.47
3	H	147	HEM	CMC-C2C-C3C	-3.83	119.16	128.43
3	A	142	HEM	CHC-C1C-C2C	3.80	133.40	125.49
3	E	142	HEM	C2D-C1D-ND	-3.79	105.52	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	147	HEM	C4C-C3C-C2C	-3.79	103.53	106.81
3	H	147	HEM	CHD-C4C-NC	-3.79	120.33	124.45
3	F	147	HEM	O2D-CGD-O1D	3.77	133.02	123.33
3	H	147	HEM	C2C-C1C-NC	-3.76	102.69	109.64
3	G	142	HEM	CBD-CAD-C3D	3.74	122.89	112.53
3	A	142	HEM	CHA-C1A-C2A	-3.74	117.11	125.30
3	D	147	HEM	CHA-C1A-C2A	-3.74	117.11	125.30
3	A	142	HEM	C3D-C4D-ND	-3.71	106.10	110.17
3	H	147	HEM	C1B-NB-C4B	3.70	109.59	105.21
3	G	142	HEM	C2D-C1D-ND	-3.68	105.65	109.90
3	A	142	HEM	CHD-C4C-NC	-3.68	120.45	124.45
3	F	147	HEM	CMC-C2C-C1C	-3.65	118.30	124.73
3	C	142	HEM	CMD-C2D-C1D	3.65	130.73	125.03
3	F	147	HEM	CHA-C4D-C3D	-3.58	118.62	125.23
3	H	147	HEM	CAA-C2A-C3A	-3.58	119.03	127.07
3	D	147	HEM	C1A-CHA-C4D	-3.56	117.86	126.25
3	B	147	HEM	CHB-C1B-C2B	-3.56	116.83	126.95
3	G	142	HEM	CMC-C2C-C3C	-3.56	119.82	128.43
3	B	147	HEM	CMA-C3A-C4A	-3.51	120.07	125.42
3	D	147	HEM	C2B-C1B-NB	-3.49	105.83	109.84
3	F	147	HEM	CBD-CAD-C3D	3.47	122.12	112.53
3	F	147	HEM	CBC-CAC-C3C	3.45	144.79	127.53
3	B	147	HEM	C1A-CHA-C4D	-3.45	118.13	126.25
3	A	142	HEM	O2D-CGD-O1D	3.44	132.19	123.33
3	E	142	HEM	CAB-C3B-C2B	-3.43	117.29	128.43
3	H	147	HEM	C4C-C3C-C2C	-3.43	103.84	106.81
3	E	142	HEM	O2D-CGD-CBD	3.39	124.72	114.00
3	B	147	HEM	CHC-C4B-C3B	3.34	131.74	125.07
3	F	147	HEM	O2D-CGD-CBD	-3.32	103.50	114.00
3	F	147	HEM	C1B-NB-C4B	3.32	109.13	105.21
3	C	142	HEM	C4C-C3C-C2C	3.31	109.69	106.81
3	D	147	HEM	C4C-NC-C1C	-3.30	100.44	105.82
3	B	147	HEM	CMC-C2C-C3C	-3.29	120.47	128.43
3	B	147	HEM	CHB-C1B-NB	3.29	128.43	124.37
3	F	147	HEM	C4C-CHD-C1D	-3.27	119.07	126.02
3	A	142	HEM	C4C-C3C-C2C	-3.24	104.00	106.81
3	F	147	HEM	CHA-C4D-ND	3.23	128.37	124.37
3	C	142	HEM	CHA-C4D-ND	3.20	128.32	124.37
3	E	142	HEM	CAD-C3D-C2D	3.16	133.79	127.87
3	D	147	HEM	C3C-C2C-C1C	-3.15	104.06	107.05
3	B	147	HEM	CMA-C3A-C2A	3.15	132.30	125.62
3	B	147	HEM	CBD-CAD-C3D	-3.14	103.85	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	147	HEM	C4C-CHD-C1D	-3.13	119.37	126.02
3	D	147	HEM	CAB-C3B-C2B	-3.12	118.27	128.43
3	C	142	HEM	O2A-CGA-O1A	-3.12	115.30	123.33
3	E	142	HEM	C4C-C3C-C2C	3.12	109.52	106.81
3	F	147	HEM	CBA-CAA-C2A	3.12	121.15	112.53
3	G	142	HEM	C1A-C2A-C3A	3.12	111.69	106.87
3	G	142	HEM	CHB-C4A-C3A	-3.08	118.48	127.43
3	A	142	HEM	CHC-C4B-C3B	-3.06	118.97	125.07
3	E	142	HEM	C2C-C1C-NC	-3.05	103.98	109.64
3	D	147	HEM	CHA-C1A-NA	3.05	129.39	123.86
3	D	147	HEM	C2A-C1A-NA	3.01	113.49	110.15
3	G	142	HEM	CHB-C1B-NB	2.99	128.06	124.37
3	H	147	HEM	CHB-C1B-NB	2.99	128.06	124.37
3	B	147	HEM	C1A-C2A-C3A	2.96	111.45	106.87
3	D	147	HEM	CAA-C2A-C3A	2.93	133.65	127.07
3	B	147	HEM	CMB-C2B-C1B	2.93	129.61	125.03
3	D	147	HEM	C3A-C4A-NA	2.92	114.82	110.14
3	B	147	HEM	O1A-CGA-CBA	-2.91	113.85	123.09
3	D	147	HEM	C2C-C1C-NC	2.91	115.01	109.64
3	F	147	HEM	CMD-C2D-C1D	2.90	129.57	125.03
3	G	142	HEM	C3D-C4D-ND	-2.90	106.99	110.17
3	C	142	HEM	C4A-CHB-C1B	2.89	133.05	126.25
3	E	142	HEM	O2A-CGA-O1A	2.88	130.74	123.33
3	C	142	HEM	C4A-C3A-C2A	-2.88	103.52	106.82
3	A	142	HEM	O2D-CGD-CBD	-2.88	104.91	114.00
3	H	147	HEM	CBB-CAB-C3B	-2.86	113.23	127.53
3	F	147	HEM	CAA-C2A-C1A	-2.85	119.38	124.94
3	D	147	HEM	CMD-C2D-C1D	-2.84	120.60	125.03
3	D	147	HEM	CBD-CAD-C3D	2.83	120.36	112.53
3	C	142	HEM	CHD-C1D-ND	2.83	127.47	124.42
3	C	142	HEM	CBA-CAA-C2A	2.81	120.31	112.53
3	G	142	HEM	C1A-CHA-C4D	2.79	132.80	126.25
3	F	147	HEM	C4A-C3A-C2A	2.78	110.00	106.82
3	B	147	HEM	CBB-CAB-C3B	-2.76	113.74	127.53
3	H	147	HEM	C4D-C3D-C2D	-2.74	102.91	106.89
3	C	142	HEM	C1B-NB-C4B	2.73	108.43	105.21
3	D	147	HEM	CHC-C4B-C3B	2.71	130.49	125.07
3	E	142	HEM	CHC-C4B-C3B	2.69	130.44	125.07
3	C	142	HEM	CMB-C2B-C3B	2.69	134.94	128.43
3	E	142	HEM	CHA-C1A-NA	-2.67	119.03	123.86
3	D	147	HEM	CAC-C3C-C2C	-2.66	119.77	128.43
3	C	142	HEM	O1A-CGA-CBA	-2.66	114.67	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	142	HEM	CAA-CBA-CGA	2.65	120.70	113.67
3	C	142	HEM	CHA-C1A-NA	2.65	128.66	123.86
3	B	147	HEM	C3D-C4D-ND	-2.65	107.27	110.17
3	D	147	HEM	CHA-C4D-C3D	-2.63	120.37	125.23
3	H	147	HEM	CAD-C3D-C2D	2.62	132.78	127.87
3	F	147	HEM	CMB-C2B-C1B	-2.61	120.95	125.03
3	B	147	HEM	CAD-C3D-C2D	-2.61	122.98	127.87
3	E	142	HEM	C1D-C2D-C3D	2.59	109.70	106.98
3	A	142	HEM	CBC-CAC-C3C	2.57	140.35	127.53
3	F	147	HEM	CHA-C1A-NA	2.56	128.51	123.86
3	A	142	HEM	CBB-CAB-C3B	-2.55	114.81	127.53
3	F	147	HEM	C3D-C4D-ND	2.54	112.96	110.17
3	C	142	HEM	CHA-C1A-C2A	-2.54	119.73	125.30
3	G	142	HEM	CHA-C1A-NA	2.52	128.42	123.86
3	H	147	HEM	CMA-C3A-C4A	-2.51	121.60	125.42
3	D	147	HEM	CHB-C1B-C2B	-2.51	119.81	126.95
3	G	142	HEM	CHC-C4B-C3B	2.50	130.06	125.07
3	F	147	HEM	O1A-CGA-CBA	2.46	130.90	123.09
3	C	142	HEM	CHA-C4D-C3D	-2.45	120.72	125.23
3	B	147	HEM	CHB-C4A-C3A	-2.42	120.39	127.43
3	H	147	HEM	C3D-C4D-ND	2.41	112.82	110.17
3	E	142	HEM	C4D-C3D-C2D	2.38	110.36	106.89
3	C	142	HEM	C2B-C1B-NB	-2.35	107.14	109.84
3	E	142	HEM	CMD-C2D-C3D	2.34	132.48	126.15
3	G	142	HEM	CHA-C1A-C2A	-2.32	120.21	125.30
3	D	147	HEM	C4A-C3A-C2A	-2.32	104.16	106.82
3	F	147	HEM	CAD-C3D-C4D	2.32	128.73	124.70
3	F	147	HEM	CBB-CAB-C3B	-2.29	116.08	127.53
3	A	142	HEM	CHA-C1A-NA	2.27	127.97	123.86
3	E	142	HEM	O2D-CGD-O1D	-2.27	117.51	123.33
3	G	142	HEM	CHD-C1D-C2D	2.26	128.60	125.03
3	H	147	HEM	CMA-C3A-C2A	2.26	130.42	125.62
3	E	142	HEM	C4C-NC-C1C	2.25	109.50	105.82
3	C	142	HEM	C3A-C4A-NA	2.25	113.74	110.14
3	B	147	HEM	C2A-C1A-NA	-2.23	107.68	110.15
3	C	142	HEM	CBB-CAB-C3B	-2.22	116.42	127.53
3	C	142	HEM	C4C-CHD-C1D	-2.21	121.33	126.02
3	A	142	HEM	CHB-C4A-NA	-2.18	119.90	123.86
3	G	142	HEM	C1C-CHC-C4B	2.18	130.66	126.02
3	H	147	HEM	C3A-C4A-NA	2.17	113.62	110.14
3	D	147	HEM	C4A-NA-C1A	-2.15	102.31	105.82
3	F	147	HEM	C4D-C3D-C2D	-2.14	103.78	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	142	HEM	CAC-C3C-C2C	-2.13	121.50	128.43
3	D	147	HEM	CMD-C2D-C3D	2.09	131.80	126.15
3	D	147	HEM	CAC-C3C-C4C	2.06	129.74	124.82
3	F	147	HEM	C4C-NC-C1C	2.05	109.17	105.82
3	A	142	HEM	C1C-CHC-C4B	-2.05	121.67	126.02
3	H	147	HEM	CMC-C2C-C1C	2.03	128.31	124.73
3	B	147	HEM	CMC-C2C-C1C	-2.03	121.15	124.73
3	D	147	HEM	CHB-C4A-NA	-2.02	120.19	123.86
3	F	147	HEM	CHB-C1B-C2B	2.02	132.70	126.95
3	A	142	HEM	CAC-C3C-C2C	2.02	134.99	128.43
3	A	142	HEM	C1A-CHA-C4D	-2.00	121.54	126.25

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	147	HEM	C1A-C2A-CAA-CBA
3	F	147	HEM	C2B-C3B-CAB-CBB
3	F	147	HEM	C4B-C3B-CAB-CBB
3	F	147	HEM	C2C-C3C-CAC-CBC
3	F	147	HEM	C4C-C3C-CAC-CBC
3	H	147	HEM	C2B-C3B-CAB-CBB
3	H	147	HEM	C4B-C3B-CAB-CBB
3	H	147	HEM	C2A-CAA-CBA-CGA
3	H	147	HEM	C3D-CAD-CBD-CGD
3	H	147	HEM	C4D-C3D-CAD-CBD
3	F	147	HEM	C2A-CAA-CBA-CGA
3	H	147	HEM	C2D-C3D-CAD-CBD
3	D	147	HEM	C1A-C2A-CAA-CBA
3	B	147	HEM	C3A-C2A-CAA-CBA
3	G	142	HEM	C2A-CAA-CBA-CGA
3	B	147	HEM	C3D-CAD-CBD-CGD
3	D	147	HEM	C2A-CAA-CBA-CGA
3	E	142	HEM	C2C-C3C-CAC-CBC
3	E	142	HEM	C4C-C3C-CAC-CBC
3	D	147	HEM	C3A-C2A-CAA-CBA
3	C	142	HEM	C2A-CAA-CBA-CGA
3	E	142	HEM	CAA-CBA-CGA-O2A
3	E	142	HEM	CAA-CBA-CGA-O1A
3	D	147	HEM	CAA-CBA-CGA-O1A
3	H	147	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	C	142	HEM	CAA-CBA-CGA-O2A
3	H	147	HEM	CAD-CBD-CGD-O1D
3	D	147	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAA-CBA-CGA-O1A
3	G	142	HEM	CAA-CBA-CGA-O2A
3	C	142	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAD-CBD-CGD-O2D
3	B	147	HEM	CAA-CBA-CGA-O1A
3	B	147	HEM	CAA-CBA-CGA-O2A
3	F	147	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAD-CBD-CGD-O1D
3	F	147	HEM	CAA-CBA-CGA-O1A
3	G	142	HEM	CAA-CBA-CGA-O1A

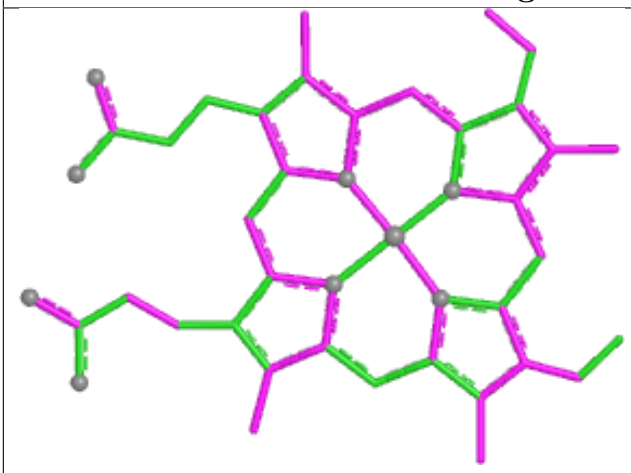
There are no ring outliers.

8 monomers are involved in 146 short contacts:

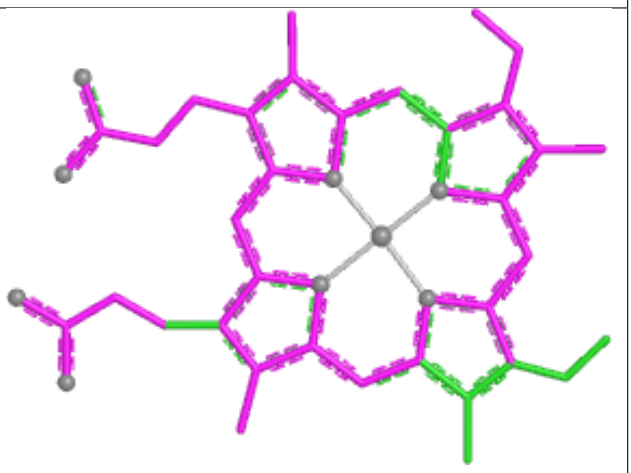
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	142	HEM	21	0
3	A	142	HEM	23	0
3	B	147	HEM	14	0
3	E	142	HEM	24	0
3	F	147	HEM	16	1
3	D	147	HEM	25	0
3	H	147	HEM	7	0
3	C	142	HEM	15	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

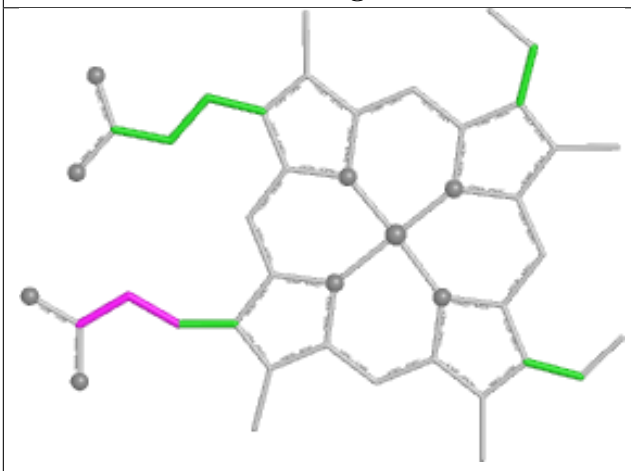
Ligand HEM G 142



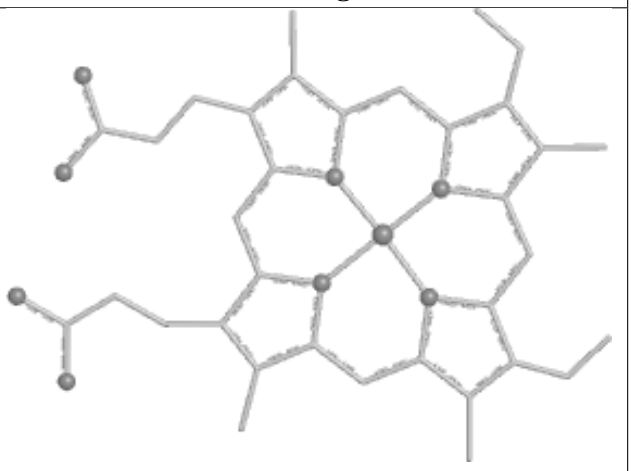
Bond lengths



Bond angles

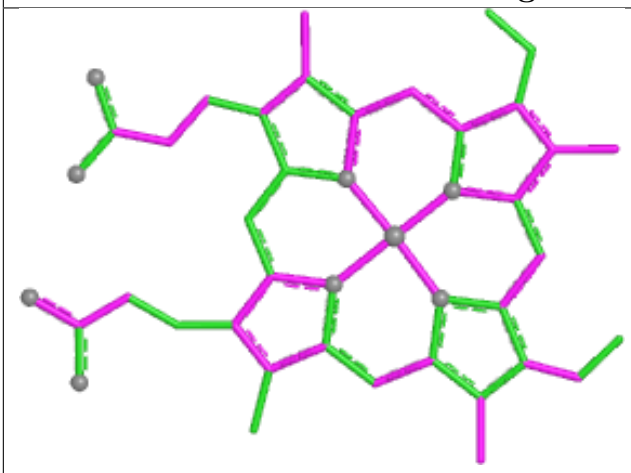


Torsions

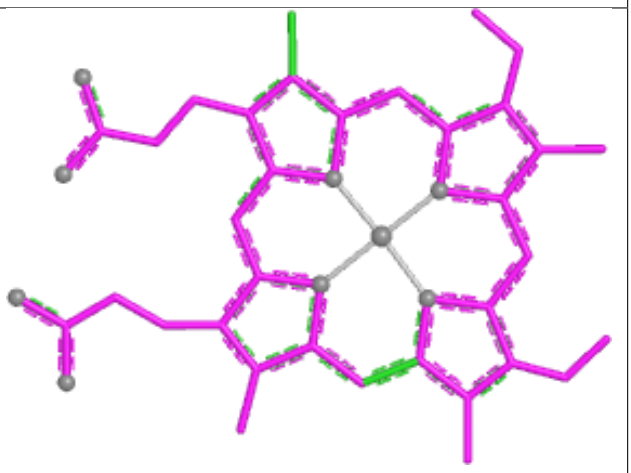


Rings

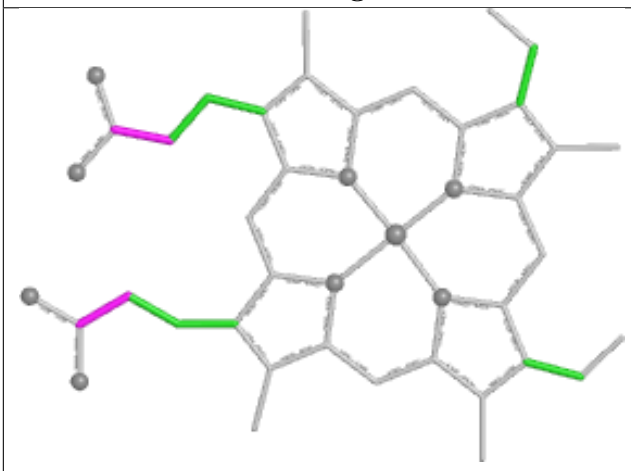
Ligand HEM A 142



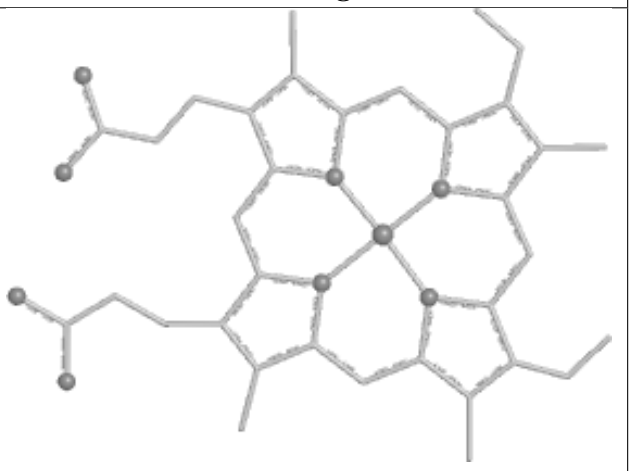
Bond lengths



Bond angles

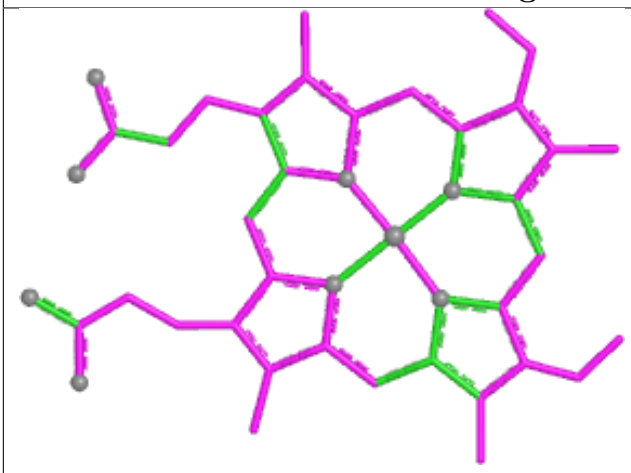


Torsions

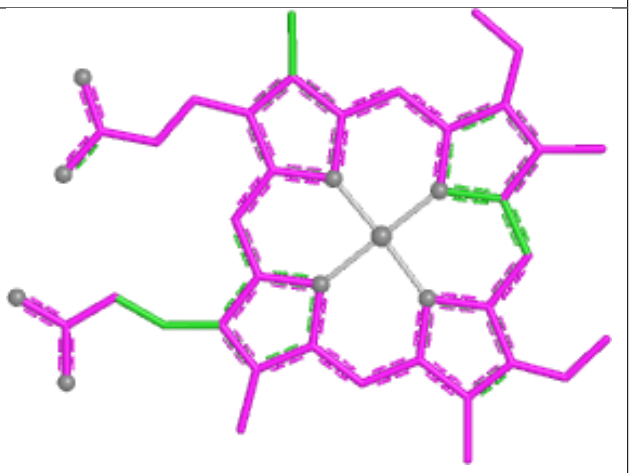


Rings

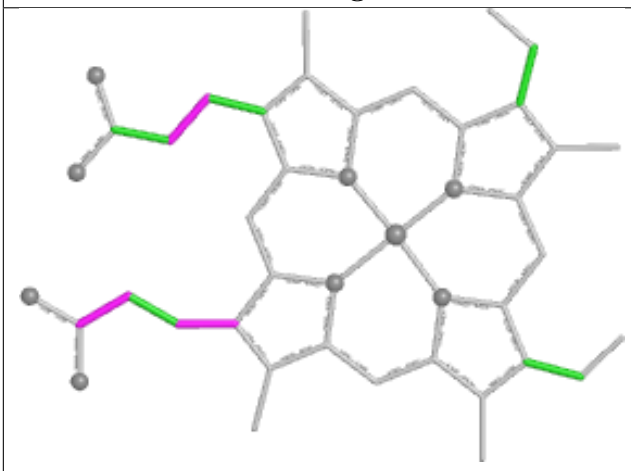
Ligand HEM B 147



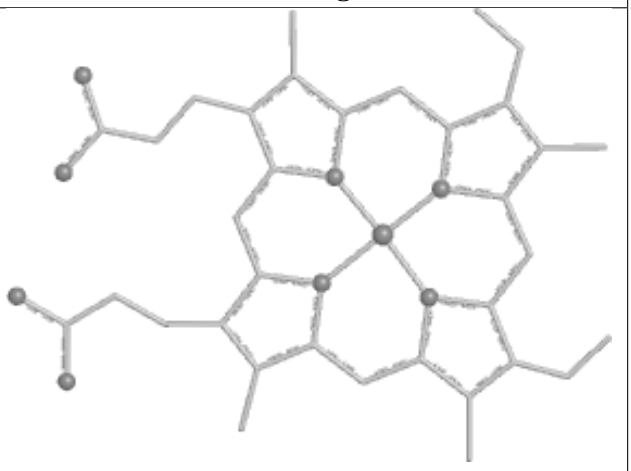
Bond lengths



Bond angles

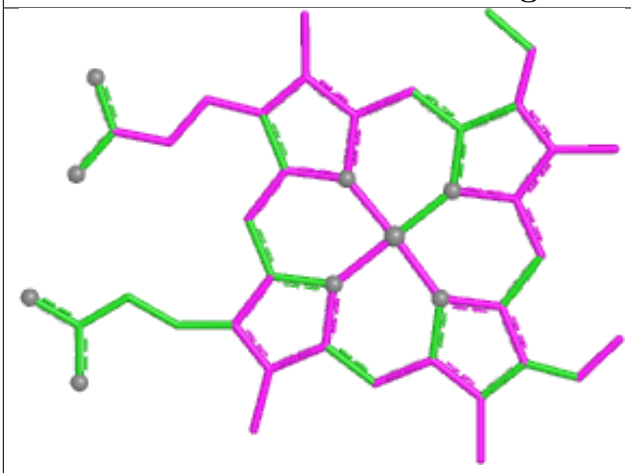


Torsions

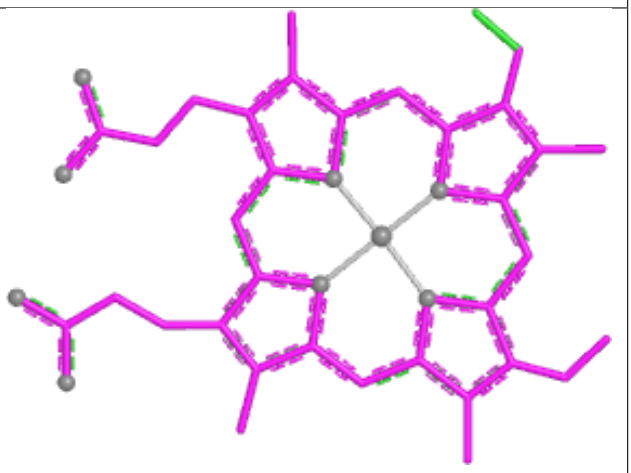


Rings

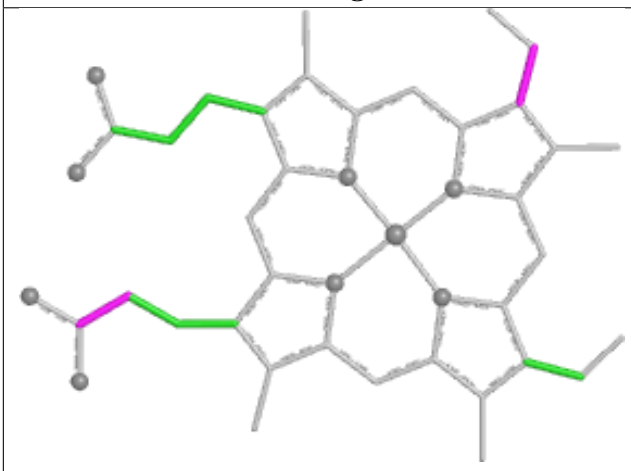
Ligand HEM E 142



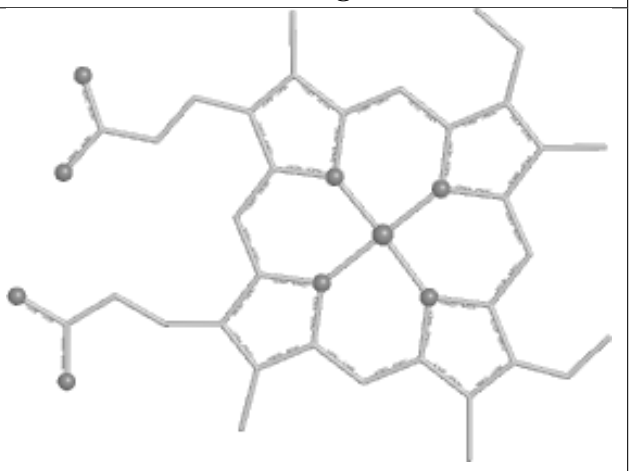
Bond lengths



Bond angles

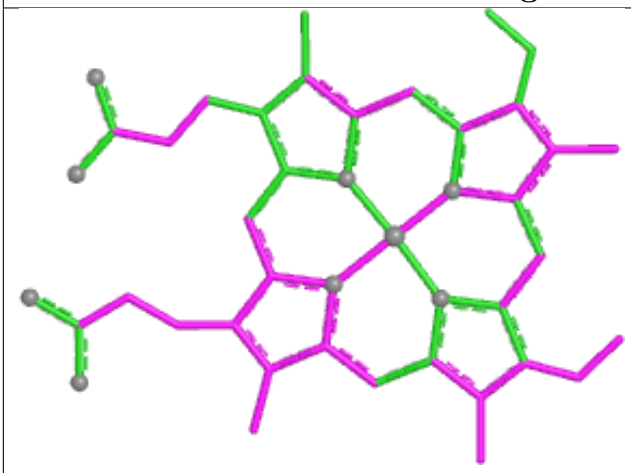


Torsions

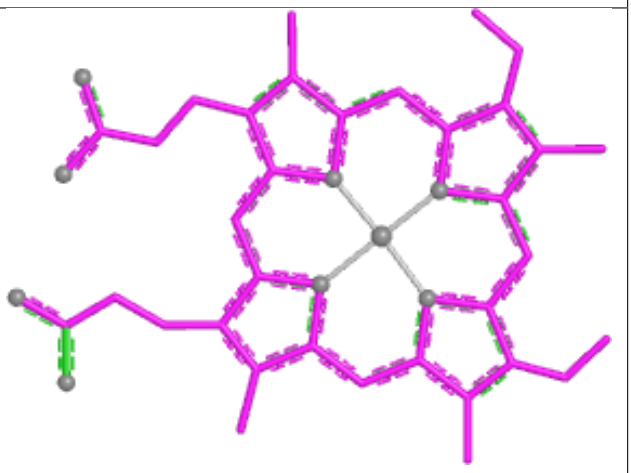


Rings

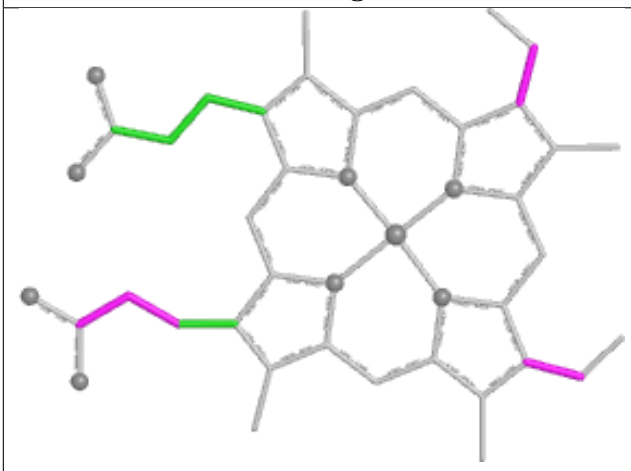
Ligand HEM F 147



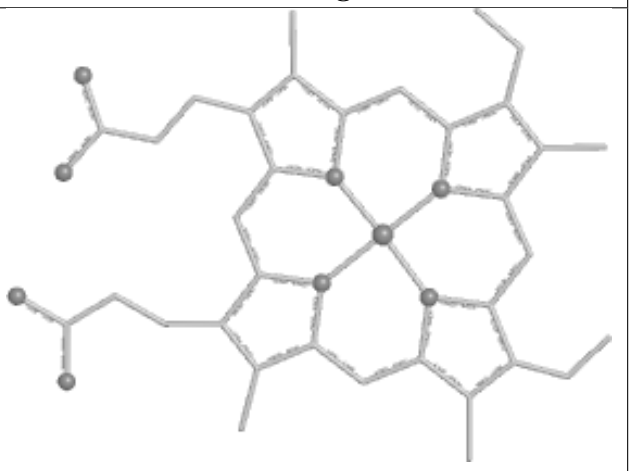
Bond lengths



Bond angles

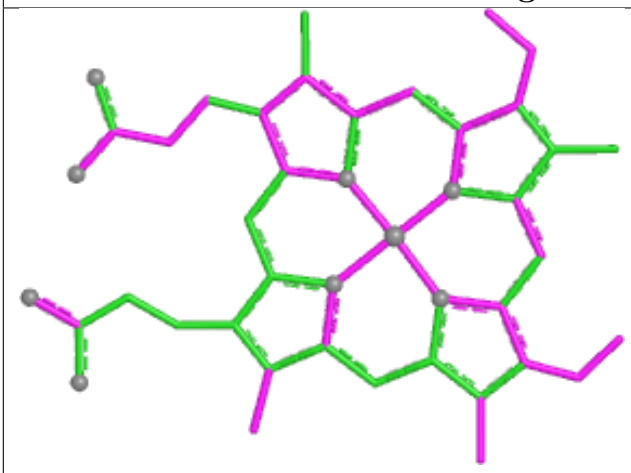


Torsions

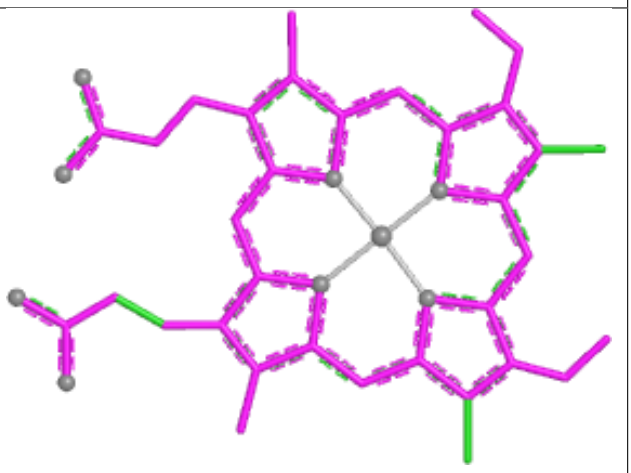


Rings

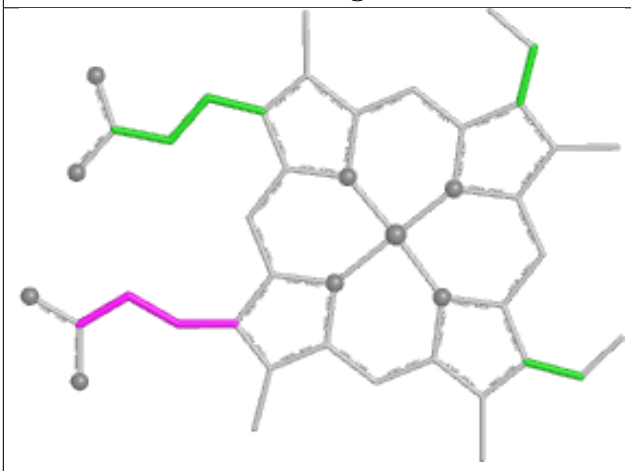
Ligand HEM D 147



Bond lengths



Bond angles



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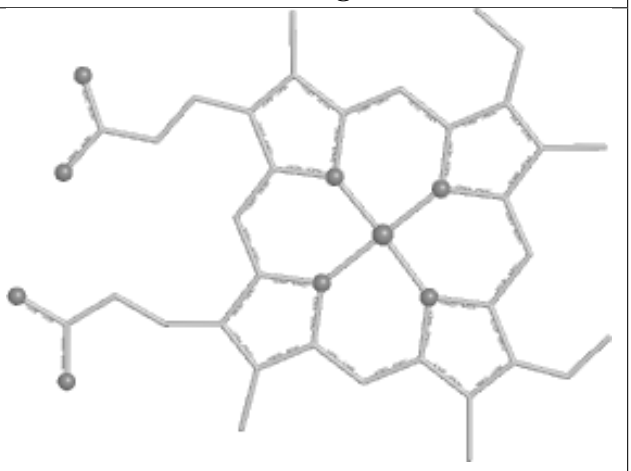
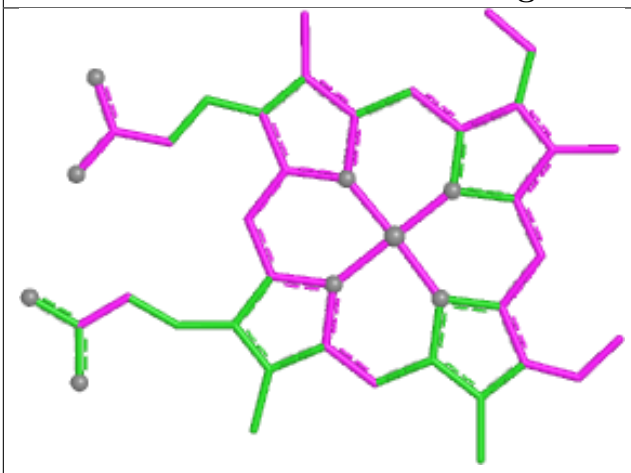
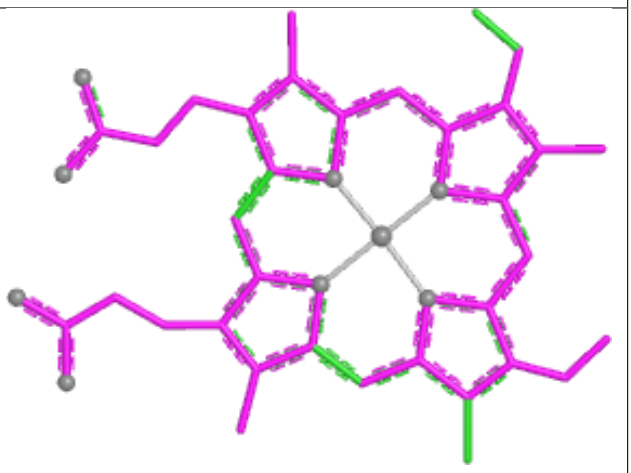


Rings

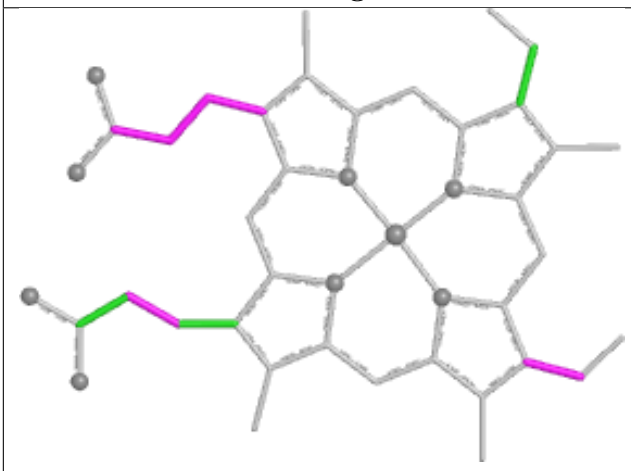
Ligand HEM H 147



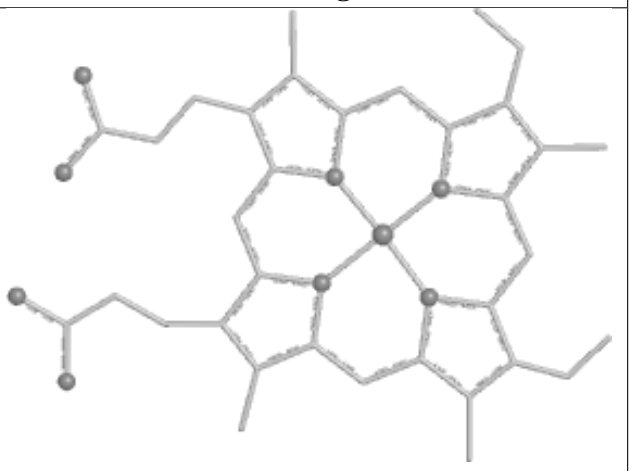
Bond lengths



Bond angles

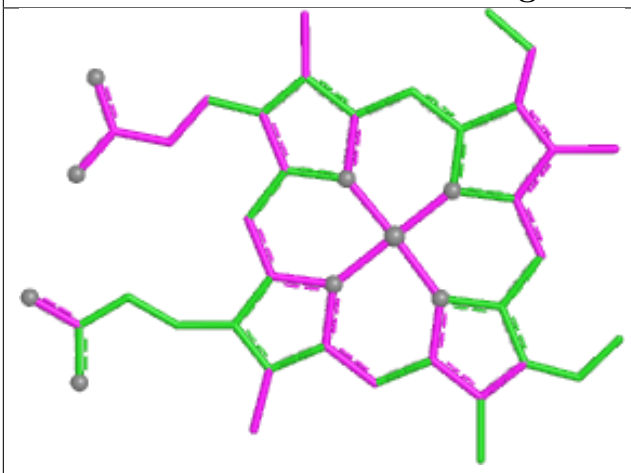


Torsions

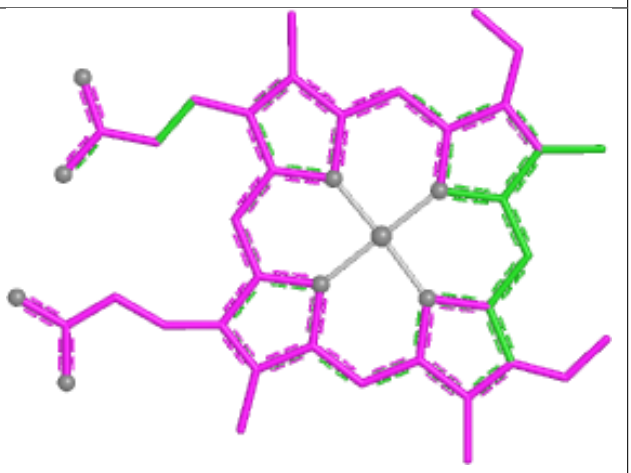


Rings

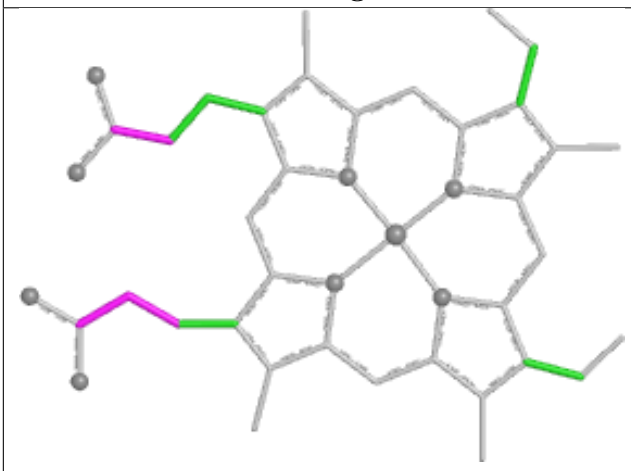
Ligand HEM C 142



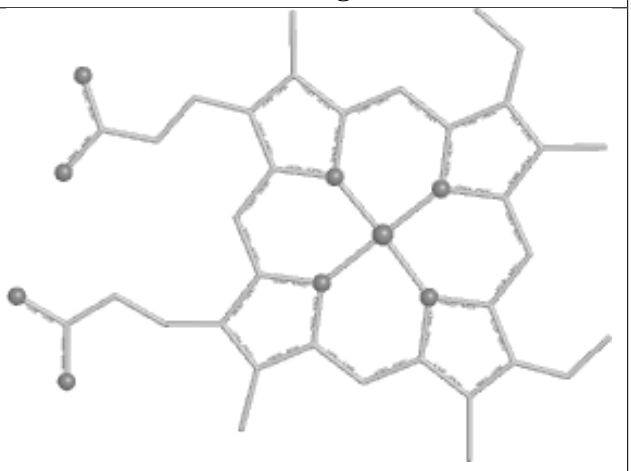
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	12
2	D	12
1	C	12
2	F	11
1	G	11
1	E	10
2	H	10

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Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	125:LEU	C	126:ASP	N	1.62
1	F	145:TYR	C	146:HIS	N	1.62
1	D	129:ALA	C	130:TYR	N	1.61
1	C	37:PRO	C	38:THR	N	1.20
1	C	135:VAL	C	136:LEU	N	1.20
1	D	1:VAL	C	2:HIS	N	1.20
1	D	72:SER	C	73:ASP	N	1.20
1	D	119:GLY	C	120:LYS	N	1.20
1	G	45:HIS	C	46:PHE	N	1.20
1	A	57:GLY	C	58:HIS	N	1.19
1	C	63:ALA	C	64:ASP	N	1.19
1	C	103:HIS	C	104:CYS	N	1.19
1	C	124:SER	C	125:LEU	N	1.19
1	C	128:PHE	C	129:LEU	N	1.19
1	D	3:LEU	C	4:THR	N	1.19
1	D	43:GLU	C	44:SER	N	1.19
1	D	134:VAL	C	135:ALA	N	1.19
1	E	54:GLN	C	55:VAL	N	1.19
1	E	132:VAL	C	133:SER	N	1.19
1	F	116:HIS	C	117:HIS	N	1.19
1	G	67:THR	C	68:ASN	N	1.19
1	A	79:ALA	C	80:LEU	N	1.18
1	A	100:LEU	C	101:LEU	N	1.18
1	A	129:LEU	C	130:ALA	N	1.18
1	C	35:SER	C	36:PHE	N	1.18
1	C	58:HIS	C	59:GLY	N	1.18
1	C	90:LYS	C	91:LEU	N	1.18
1	D	15:TRP	C	16:GLY	N	1.18
1	D	31:LEU	C	32:LEU	N	1.18
1	E	121:VAL	C	122:HIS	N	1.18
1	G	107:VAL	C	108:THR	N	1.18
1	H	4:THR	C	5:PRO	N	1.18
1	H	15:TRP	C	16:GLY	N	1.18
1	H	90:GLU	C	91:LEU	N	1.18
1	H	95:LYS	C	96:LEU	N	1.18
1	H	115:ALA	C	116:HIS	N	1.18
1	A	6:ASP	C	7:LYS	N	1.17
1	A	55:VAL	C	56:LYS	N	1.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	7:GLU	C	8:LYS	N	1.17
1	B	63:HIS	C	64:GLY	N	1.17
1	C	36:PHE	C	37:PRO	N	1.17
1	E	4:PRO	C	5:ALA	N	1.17
1	E	41:THR	C	42:TYR	N	1.17
1	E	102:SER	C	103:HIS	N	1.17
1	F	34:VAL	C	35:TYR	N	1.17
1	G	50:HIS	C	51:GLY	N	1.17
1	G	90:LYS	C	91:LEU	N	1.17
1	A	35:SER	C	36:PHE	N	1.16
1	D	127:GLN	C	128:ALA	N	1.16
1	E	134:THR	C	135:VAL	N	1.16
1	F	16:GLY	C	17:LYS	N	1.16
1	F	48:LEU	C	49:SER	N	1.16
1	F	83:GLY	C	84:THR	N	1.16
1	G	81:SER	C	82:ALA	N	1.16
1	H	101:GLU	C	102:ASN	N	1.16
1	C	81:SER	C	82:ALA	N	1.15
1	F	134:VAL	C	135:ALA	N	1.15
1	G	40:LYS	C	41:THR	N	1.15
1	A	89:HIS	C	90:LYS	N	1.14
1	D	117:HIS	C	118:PHE	N	1.14
1	D	131:GLN	C	132:LYS	N	1.14
1	E	119:PRO	C	120:ALA	N	1.14
1	F	12:THR	C	13:ALA	N	1.14
1	F	78:LEU	C	79:ASP	N	1.14
1	C	110:ALA	C	111:ALA	N	1.13
1	H	143:HIS	C	144:LYS	N	1.13
1	A	138:SER	C	139:LYS	N	1.12
1	E	105:LEU	C	106:LEU	N	1.12
1	E	109:LEU	C	110:ALA	N	1.12
1	F	112:CYS	C	113:VAL	N	1.12
1	H	55:MET	C	56:GLY	N	1.12
1	A	95:PRO	C	96:VAL	N	1.11
1	H	135:ALA	C	136:GLY	N	1.11
1	F	137:VAL	C	138:ALA	N	1.10
1	G	37:PRO	C	38:THR	N	1.10
1	G	63:ALA	C	64:ASP	N	1.10
1	H	96:LEU	C	97:HIS	N	1.10
1	A	70:VAL	C	71:ALA	N	1.09
1	G	30:GLU	C	31:ARG	N	1.09
1	G	23:GLU	C	24:TYR	N	1.06

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.