



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:58 AM BST

PDB ID : 1HDS
Title : MACROMOLECULAR STRUCTURE REFINEMENT BY RESTRAINED LEAST-SQUARES AND INTERACTIVE GRAPHICS AS APPLIED TO SICKLING DEER TYPE III HEMOGLOBIN
Authors : Amma, E.L.; Girling, R.L.
Deposited on : 1979-10-01
Resolution : 1.98 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

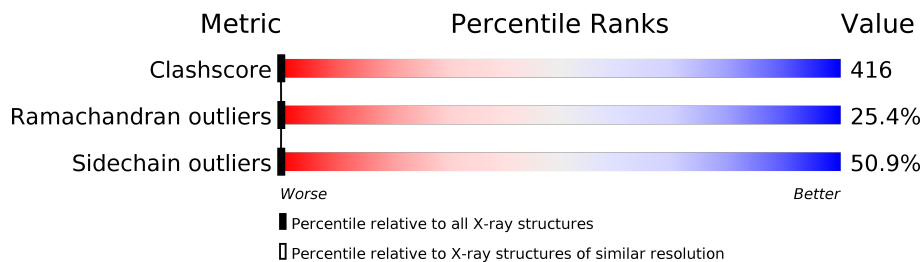
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	
1	C	141	
2	B	145	
2	D	145	

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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEM	B	146	-	-	X	-
3	HEM	C	142	-	-	X	-
3	HEM	D	146	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4556 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
			Total	C	N	O	S			
1	A	141	1076	684	199	192	1	0	0	0
1	C	141	1076	684	199	192	1	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ASN	ASP	conflict	UNP P01972
A	27	GLN	GLU	conflict	UNP P01972
A	30	GLN	GLU	conflict	UNP P01972
A	55	GLN	VAL	conflict	UNP P01972
A	60	GLN	GLU	conflict	UNP P01972
A	70	GLN	VAL	conflict	UNP P01972
A	74	ASN	ASP	conflict	UNP P01972
A	82	ASN	ASP	conflict	UNP P01972
A	85	ASN	ASP	conflict	UNP P01972
A	94	ASN	ASP	conflict	UNP P01972
A	104	SER	THR	conflict	UNP P01972
A	115	THR	SER	conflict	UNP P01972
A	116	ASN	ASP	conflict	UNP P01972
A	124	ASN	SER	conflict	UNP P01972
A	126	ASN	ASP	conflict	UNP P01972
A	132	ASP	VAL	conflict	UNP P01972
C	6	ASN	ASP	conflict	UNP P01972
C	27	GLN	GLU	conflict	UNP P01972
C	30	GLN	GLU	conflict	UNP P01972
C	55	GLN	VAL	conflict	UNP P01972
C	60	GLN	GLU	conflict	UNP P01972
C	70	GLN	VAL	conflict	UNP P01972
C	74	ASN	ASP	conflict	UNP P01972
C	82	ASN	ASP	conflict	UNP P01972
C	85	ASN	ASP	conflict	UNP P01972

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Chain	Residue	Modelled	Actual	Comment	Reference
C	94	ASN	ASP	conflict	UNP P01972
C	104	SER	THR	conflict	UNP P01972
C	115	THR	SER	conflict	UNP P01972
C	116	ASN	ASP	conflict	UNP P01972
C	124	ASN	SER	conflict	UNP P01972
C	126	ASN	ASP	conflict	UNP P01972
C	132	ASP	VAL	conflict	UNP P01972

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	145	1116	719	205	189	3	0	0	0
2	D	145	1116	719	205	189	3	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

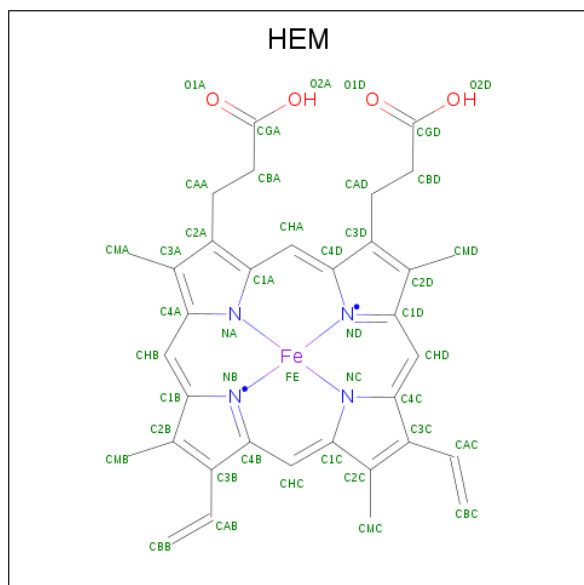
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	ASP	ASN	conflict	UNP P02074
B	25	GLN	GLU	conflict	UNP P02074
B	42	GLN	GLU	conflict	UNP P02074
B	46	ASN	ASP	conflict	UNP P02074
B	55	ASN	GLY	conflict	UNP P02074
B	71	THR	SER	conflict	UNP P02074
B	72	GLN	GLU	conflict	UNP P02074
B	86	GLN	GLU	conflict	UNP P02074
B	89	GLY	GLU	conflict	UNP P02074
B	98	ASN	ASP	conflict	UNP P02074
B	100	GLN	GLU	conflict	UNP P02074
B	110	ALA	VAL	conflict	UNP P02074
B	111	LEU	VAL	conflict	UNP P02074
B	113	VAL	LEU	conflict	UNP P02074
B	120	GLN	GLU	conflict	UNP P02074
B	124	ASN	LEU	conflict	UNP P02074
B	128	LEU	ASP	conflict	UNP P02074
B	143	LYS	ARG	conflict	UNP P02074
D	18	ASP	ASN	conflict	UNP P02074
D	25	GLN	GLU	conflict	UNP P02074
D	42	GLN	GLU	conflict	UNP P02074
D	46	ASN	ASP	conflict	UNP P02074
D	55	ASN	GLY	conflict	UNP P02074

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Chain	Residue	Modelled	Actual	Comment	Reference
D	71	THR	SER	conflict	UNP P02074
D	72	GLN	GLU	conflict	UNP P02074
D	86	GLN	GLU	conflict	UNP P02074
D	89	GLY	GLU	conflict	UNP P02074
D	98	ASN	ASP	conflict	UNP P02074
D	100	GLN	GLU	conflict	UNP P02074
D	110	ALA	VAL	conflict	UNP P02074
D	111	LEU	VAL	conflict	UNP P02074
D	113	VAL	LEU	conflict	UNP P02074
D	120	GLN	GLU	conflict	UNP P02074
D	124	ASN	LEU	conflict	UNP P02074
D	128	LEU	ASP	conflict	UNP P02074
D	143	LYS	ARG	conflict	UNP P02074

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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		

Chain D:  28% 70%

M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	M22	M23	M24	M25	M26	M27	M28	M29	M30	M31	M32	M33	M34	M35	M36	M37	M38	M39	M40	M41	M42	M43	M44	M45	M46	M47	M48	M49	M50	M51	M52	M53	M54	M55	M56	M57	M58	M59	M60
A61	A62	A63	A64	A65	A66	A67	A68	A69	A70	A71	A72	A73	A74	A75	A76	A77	A78	A79	A80	A81	A82	A83	A84	A85	A86	A87	A88	A89	A90	A91	A92	A93	A94	A95	A96	A97	A98	A99	A100	A101	A102	A103	A104	A105	A106	A107	A108	A109	A110	A111	A112	A113	A114	A115	A116	A117	A118	A119	A120
F121	F122	F123	F124	F125	F126	F127	F128	F129	F130	F131	F132	F133	F134	F135	F136	F137	F138	F139	F140	F141	F142	F143	F144	F145																																			

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.50Å 70.83Å 65.95Å 90.00° 94.15° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.98	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.98)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4556	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	10.87	704/1103 (63.8%)	9.83	796/1498 (53.1%)
1	C	10.65	668/1103 (60.6%)	9.48	847/1498 (56.5%)
2	B	11.08	695/1142 (60.9%)	10.07	841/1545 (54.4%)
2	D	11.22	702/1142 (61.5%)	11.17	890/1545 (57.6%)
All	All	10.96	2769/4490 (61.7%)	10.16	3374/6086 (55.4%)

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	9	52
1	C	2	41
2	B	2	40
2	D	6	51
All	All	19	184

All (2769) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	SER	CB-OG	64.78	2.26	1.42
2	B	144	TYR	CE2-CZ	55.70	2.10	1.38
2	D	123	PRO	N-CD	53.15	2.22	1.47
2	B	32	VAL	CB-CG2	50.79	2.59	1.52
1	C	84	SER	CB-OG	49.53	2.06	1.42
2	B	118	GLY	N-CA	-48.47	0.73	1.46
2	D	8	ALA	C-O	44.77	2.08	1.23
2	D	65	ARG	CZ-NH1	43.81	1.90	1.33
2	B	62	HIS	CB-CG	43.44	2.28	1.50
2	D	5	GLU	N-CA	-43.16	0.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	144	TYR	CE1-CZ	43.14	1.94	1.38
1	C	138	SER	CB-OG	41.55	1.96	1.42
2	B	15	GLY	C-O	40.93	1.89	1.23
2	D	145	HIS	CD2-NE2	40.54	2.27	1.38
1	C	104	SER	CB-OG	-40.03	0.90	1.42
2	B	65	ARG	CZ-NH2	39.78	1.84	1.33
1	A	49	SER	CB-OG	39.52	1.93	1.42
2	D	70	PHE	C-O	39.31	1.98	1.23
1	C	43	PHE	CG-CD1	38.65	1.96	1.38
2	B	103	ARG	CZ-NH2	38.39	1.82	1.33
2	D	6	GLU	CD-OE2	38.04	1.67	1.25
1	A	87	HIS	CB-CG	37.10	2.16	1.50
2	D	42	GLN	CD-OE1	36.74	2.04	1.24
1	C	38	THR	C-O	36.42	1.92	1.23
1	A	140	TYR	CE2-CZ	-36.38	0.91	1.38
2	B	103	ARG	CZ-NH1	-35.75	0.86	1.33
2	D	5	GLU	CG-CD	35.26	2.04	1.51
2	D	75	LYS	C-O	35.11	1.90	1.23
2	D	34	TYR	CE2-CZ	-34.59	0.93	1.38
1	C	46	PHE	CE2-CZ	33.68	2.01	1.37
1	A	74	ASN	C-O	33.64	1.87	1.23
2	B	102	PHE	CG-CD1	33.47	1.89	1.38
1	A	140	TYR	CE1-CZ	-33.40	0.95	1.38
1	A	141	ARG	CZ-NH2	33.18	1.76	1.33
1	C	24	TYR	CD2-CE2	33.12	1.89	1.39
2	D	57	PRO	N-CD	32.63	1.93	1.47
2	B	1	MET	N-CA	32.25	2.10	1.46
1	C	141	ARG	C-O	32.11	1.84	1.23
1	A	3	SER	CB-OG	32.01	1.83	1.42
2	D	14	TRP	CG-CD1	31.90	1.81	1.36
2	B	34	TYR	CD2-CE2	-31.78	0.91	1.39
1	A	43	PHE	CG-CD2	31.77	1.86	1.38
2	B	34	TYR	CE2-CZ	31.69	1.79	1.38
1	C	46	PHE	CB-CG	31.20	2.04	1.51
1	A	52	SER	CB-OG	31.17	1.82	1.42
2	B	102	PHE	CB-CG	-31.03	0.98	1.51
2	B	115	ARG	CZ-NH1	-30.99	0.92	1.33
2	D	85	ALA	N-CA	30.97	2.08	1.46
2	D	36	TRP	NE1-CE2	-30.96	0.97	1.37
2	D	84	PHE	CG-CD1	30.77	1.84	1.38
2	D	145	HIS	CG-ND1	30.75	2.06	1.38
2	B	71	THR	N-CA	-30.58	0.85	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	84	PHE	CG-CD2	-30.55	0.93	1.38
2	B	75	LYS	N-CA	30.53	2.07	1.46
2	B	106	GLY	N-CA	-30.46	1.00	1.46
1	A	114	PRO	N-CD	30.33	1.90	1.47
1	A	78	GLY	N-CA	30.24	1.91	1.46
2	D	48	SER	CB-OG	30.23	1.81	1.42
2	D	7	LYS	CA-CB	30.18	2.20	1.53
1	A	30	GLN	CD-NE2	30.04	2.08	1.32
2	B	69	ALA	CA-CB	-29.90	0.89	1.52
1	A	77	PRO	CA-C	29.72	2.12	1.52
1	A	131	ASN	N-CA	29.66	2.05	1.46
2	B	36	TRP	CE2-CZ2	-29.21	0.90	1.39
1	C	72	HIS	CG-CD2	29.19	1.85	1.35
2	D	75	LYS	CD-CE	29.11	2.24	1.51
2	D	126	GLN	CD-OE1	28.83	1.87	1.24
2	B	45	GLY	C-O	28.75	1.69	1.23
2	B	144	TYR	CG-CD2	28.52	1.76	1.39
1	C	98	PHE	C-N	28.48	1.99	1.34
2	B	117	PHE	CG-CD1	28.32	1.81	1.38
1	A	29	LEU	CA-C	-28.26	0.79	1.52
1	A	22	PRO	N-CD	28.20	1.87	1.47
2	D	7	LYS	C-O	-28.08	0.69	1.23
1	A	124	ASN	C-O	27.97	1.76	1.23
1	C	3	SER	CA-CB	27.83	1.94	1.52
2	D	40	PHE	CE2-CZ	27.73	1.90	1.37
2	B	79	ASP	C-O	27.68	1.75	1.23
1	A	132	ASP	CG-OD2	27.64	1.89	1.25
1	C	56	LYS	CB-CG	27.45	2.26	1.52
2	D	19	VAL	CB-CG2	27.45	2.10	1.52
2	B	49	SER	C-O	27.38	1.75	1.23
1	C	98	PHE	CE1-CZ	-27.38	0.85	1.37
1	A	14	TRP	CZ3-CH2	-27.28	0.96	1.40
2	D	145	HIS	C-O	27.25	1.75	1.23
1	C	74	ASN	CB-CG	27.11	2.13	1.51
1	A	72	HIS	CE1-NE2	27.09	1.95	1.32
1	C	98	PHE	CG-CD1	26.99	1.79	1.38
2	D	68	ASP	N-CA	-26.85	0.92	1.46
2	D	54	MET	C-O	26.60	1.73	1.23
1	C	44	PRO	N-CD	26.53	1.84	1.47
2	B	92	CYS	CB-SG	26.45	2.27	1.82
1	A	11	LYS	C-O	-26.40	0.73	1.23
2	D	108	VAL	C-O	-26.34	0.73	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	ALA	CA-CB	26.29	2.07	1.52
1	C	80	LEU	C-O	26.27	1.73	1.23
1	C	75	ASP	N-CA	-26.27	0.93	1.46
2	D	103	ARG	NE-CZ	26.25	1.67	1.33
2	D	7	LYS	CE-NZ	26.24	2.14	1.49
2	B	108	VAL	CB-CG2	26.18	2.07	1.52
2	D	55	ASN	N-CA	-26.06	0.94	1.46
2	D	144	TYR	CZ-OH	26.02	1.82	1.37
2	B	42	GLN	C-N	26.00	1.93	1.34
1	C	8	SER	C-O	25.99	1.72	1.23
2	D	75	LYS	CB-CG	-25.98	0.82	1.52
2	B	23	GLY	N-CA	25.93	1.84	1.46
1	A	18	GLY	C-O	-25.88	0.82	1.23
1	A	94	ASN	C-O	-25.86	0.74	1.23
1	A	70	GLN	CD-OE1	25.83	1.80	1.24
2	B	33	VAL	CA-CB	-25.82	1.00	1.54
1	A	85	ASN	CB-CG	25.81	2.10	1.51
1	A	36	PHE	CG-CD2	-25.77	1.00	1.38
2	D	88	SER	CB-OG	-25.69	1.08	1.42
2	B	142	HIS	N-CA	-25.66	0.95	1.46
1	A	109	LEU	CA-C	25.64	2.19	1.52
2	B	41	PHE	C-O	-25.55	0.74	1.23
1	A	4	ALA	N-CA	25.54	1.97	1.46
1	C	35	SER	CB-OG	25.53	1.75	1.42
2	D	53	VAL	N-CA	-25.39	0.95	1.46
1	C	59	GLY	CA-C	25.33	1.92	1.51
1	C	137	THR	C-O	25.29	1.71	1.23
2	D	130	GLN	CB-CG	-25.27	0.84	1.52
2	B	117	PHE	CD1-CE1	-25.22	0.88	1.39
1	A	92	ARG	CZ-NH2	25.17	1.65	1.33
2	B	70	PHE	CE2-CZ	25.01	1.84	1.37
1	A	14	TRP	NE1-CE2	-24.98	1.05	1.37
2	B	59	VAL	C-O	24.93	1.70	1.23
2	D	18	ASP	C-O	-24.92	0.76	1.23
1	C	128	PHE	CE1-CZ	24.88	1.84	1.37
1	A	59	GLY	N-CA	-24.82	1.08	1.46
1	C	8	SER	CB-OG	-24.77	1.10	1.42
1	C	24	TYR	CG-CD2	-24.71	1.07	1.39
2	B	36	TRP	CG-CD2	24.70	1.85	1.43
2	D	55	ASN	CA-CB	24.69	2.17	1.53
2	D	109	LEU	N-CA	-24.64	0.97	1.46
1	C	86	LEU	CA-CB	24.57	2.10	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	115	ARG	CA-CB	24.56	2.08	1.53
1	A	50	HIS	CE1-NE2	24.50	1.89	1.32
2	B	34	TYR	CG-CD2	24.40	1.70	1.39
1	A	41	THR	CB-OG1	-24.38	0.94	1.43
2	B	81	LYS	CG-CD	24.38	2.35	1.52
2	D	76	HIS	CG-CD2	24.33	1.77	1.35
1	A	85	ASN	C-O	24.32	1.69	1.23
1	A	124	ASN	CA-CB	-24.26	0.90	1.53
1	A	77	PRO	CA-CB	-24.26	1.05	1.53
2	B	50	ALA	CA-CB	-24.25	1.01	1.52
2	D	4	ALA	N-CA	24.24	1.94	1.46
1	C	128	PHE	CG-CD1	-24.23	1.02	1.38
1	A	106	LEU	CA-CB	-24.19	0.98	1.53
1	C	87	HIS	CB-CG	-24.17	1.06	1.50
1	C	100	LEU	CA-CB	-24.16	0.98	1.53
1	A	42	TYR	C-O	-24.08	0.77	1.23
1	C	81	SER	CA-CB	23.99	1.89	1.52
1	C	33	PHE	C-O	23.99	1.69	1.23
1	A	71	GLY	N-CA	-23.77	1.10	1.46
1	A	53	ALA	C-O	23.69	1.68	1.23
2	D	16	LYS	CA-CB	23.62	2.06	1.53
1	C	141	ARG	CG-CD	23.60	2.10	1.51
1	C	98	PHE	C-O	-23.59	0.78	1.23
2	D	73	GLY	N-CA	-23.58	1.10	1.46
2	B	56	ASN	C-O	-23.57	0.78	1.23
1	A	141	ARG	NE-CZ	23.50	1.63	1.33
2	D	34	TYR	CB-CG	-23.48	1.16	1.51
1	A	3	SER	C-O	23.46	1.68	1.23
2	D	51	GLY	C-N	23.42	1.88	1.34
1	C	14	TRP	CD1-NE1	-23.38	0.98	1.38
1	A	119	PRO	CG-CD	23.36	2.27	1.50
2	B	113	VAL	CB-CG2	23.35	2.01	1.52
2	D	76	HIS	CG-ND1	-23.33	0.87	1.38
2	B	64	LYS	CD-CE	23.32	2.09	1.51
2	B	5	GLU	N-CA	23.31	1.93	1.46
1	C	24	TYR	CE2-CZ	23.29	1.68	1.38
1	C	119	PRO	CA-CB	-23.26	1.07	1.53
1	C	59	GLY	C-O	23.24	1.60	1.23
1	A	43	PHE	C-N	23.20	1.78	1.34
2	D	5	GLU	CD-OE2	23.01	1.50	1.25
2	D	13	PHE	CG-CD2	-22.99	1.04	1.38
2	B	43	HIS	ND1-CE1	22.97	1.92	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	35	PRO	N-CD	22.96	1.79	1.47
1	C	9	ASN	CB-CG	22.95	2.03	1.51
2	B	29	ARG	CZ-NH2	-22.93	1.03	1.33
1	C	44	PRO	N-CA	22.93	1.86	1.47
1	C	115	THR	C-O	22.87	1.66	1.23
2	B	36	TRP	CD2-CE2	22.85	1.68	1.41
2	B	43	HIS	CE1-NE2	22.74	1.84	1.32
1	C	12	ALA	C-O	22.70	1.66	1.23
2	B	11	THR	C-O	-22.67	0.80	1.23
1	A	135	VAL	CB-CG2	22.66	2.00	1.52
1	A	127	LYS	C-N	-22.64	0.81	1.34
2	B	133	VAL	C-O	-22.64	0.80	1.23
1	A	12	ALA	C-O	-22.64	0.80	1.23
2	B	139	ALA	C-O	22.58	1.66	1.23
2	B	41	PHE	C-N	22.54	1.85	1.34
1	A	41	THR	N-CA	-22.54	1.01	1.46
2	D	14	TRP	CE3-CZ3	22.54	1.76	1.38
1	C	53	ALA	CA-CB	22.51	1.99	1.52
2	D	56	ASN	C-O	22.50	1.66	1.23
1	C	36	PHE	C-N	22.47	1.76	1.34
2	D	55	ASN	CG-OD1	22.44	1.73	1.24
1	A	25	GLY	CA-C	22.43	1.87	1.51
1	C	11	LYS	CD-CE	22.43	2.07	1.51
1	A	14	TRP	CZ2-CH2	22.37	1.79	1.37
1	A	128	PHE	CD1-CE1	22.34	1.83	1.39
2	D	44	PHE	N-CA	-22.34	1.01	1.46
1	C	130	ALA	N-CA	22.32	1.91	1.46
1	C	117	PHE	CB-CG	-22.27	1.13	1.51
1	C	135	VAL	C-O	22.17	1.65	1.23
1	A	108	THR	C-O	-22.11	0.81	1.23
1	C	74	ASN	C-N	22.10	1.84	1.34
2	D	130	GLN	CG-CD	22.07	2.01	1.51
2	B	22	VAL	CA-CB	-22.04	1.08	1.54
1	C	117	PHE	CG-CD2	22.03	1.71	1.38
2	D	53	VAL	CB-CG2	22.02	1.99	1.52
2	D	102	PHE	N-CA	22.02	1.90	1.46
2	B	7	LYS	CE-NZ	21.98	2.04	1.49
1	C	90	LYS	N-CA	21.98	1.90	1.46
1	A	54	GLN	C-O	21.94	1.65	1.23
2	B	145	HIS	CG-CD2	21.90	1.73	1.35
1	C	93	VAL	CA-CB	21.82	2.00	1.54
2	D	57	PRO	CA-CB	21.78	1.97	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	32	VAL	N-CA	21.78	1.90	1.46
1	A	9	ASN	CG-OD1	21.75	1.71	1.24
1	C	61	LYS	CE-NZ	21.73	2.03	1.49
1	C	130	ALA	C-O	21.71	1.64	1.23
2	B	4	ALA	C-O	-21.68	0.82	1.23
1	C	9	ASN	CG-OD1	-21.68	0.76	1.24
1	A	31	ARG	C-O	21.61	1.64	1.23
1	A	8	SER	C-O	21.60	1.64	1.23
2	B	130	GLN	CD-NE2	-21.56	0.79	1.32
2	D	41	PHE	C-N	21.56	1.83	1.34
1	C	117	PHE	CD2-CE2	21.55	1.82	1.39
1	C	51	GLY	C-O	-21.55	0.89	1.23
2	D	88	SER	CA-CB	21.54	1.85	1.52
2	D	43	HIS	CG-CD2	21.53	1.72	1.35
1	C	11	LYS	CE-NZ	-21.52	0.95	1.49
1	A	74	ASN	CG-ND2	21.49	1.86	1.32
2	B	41	PHE	CE1-CZ	21.46	1.78	1.37
1	A	40	LYS	CB-CG	21.41	2.10	1.52
2	D	74	LEU	N-CA	-21.41	1.03	1.46
2	D	70	PHE	N-CA	-21.39	1.03	1.46
2	D	111	LEU	C-N	-21.39	0.84	1.34
2	B	38	GLN	C-O	-21.38	0.82	1.23
1	C	110	ALA	CA-C	21.31	2.08	1.52
1	A	99	LYS	CG-CD	21.26	2.24	1.52
1	C	24	TYR	CB-CG	21.25	1.83	1.51
1	A	58	HIS	C-N	21.25	1.71	1.33
1	A	56	LYS	C-O	21.19	1.63	1.23
2	D	6	GLU	C-O	21.18	1.63	1.23
1	A	127	LYS	C-O	21.15	1.63	1.23
2	D	144	TYR	CG-CD2	21.11	1.66	1.39
1	C	96	VAL	CB-CG2	21.10	1.97	1.52
2	D	124	ASN	CG-OD1	21.10	1.70	1.24
1	A	84	SER	CA-CB	-21.09	1.21	1.52
1	C	18	GLY	N-CA	21.09	1.77	1.46
2	B	55	ASN	CA-C	21.08	2.07	1.52
1	A	117	PHE	CD1-CE1	-21.03	0.97	1.39
1	A	114	PRO	CA-C	-21.01	1.10	1.52
2	D	25	GLN	CG-CD	21.00	1.99	1.51
1	C	61	LYS	CA-CB	20.98	2.00	1.53
2	B	76	HIS	CG-CD2	-20.98	1.00	1.35
2	B	17	VAL	C-O	20.98	1.63	1.23
2	B	145	HIS	CA-CB	20.97	2.00	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	GLN	CA-CB	20.96	2.00	1.53
1	A	37	PRO	N-CD	20.93	1.77	1.47
2	D	125	VAL	C-O	20.91	1.63	1.23
2	D	143	LYS	C-O	20.91	1.63	1.23
2	B	126	GLN	CG-CD	20.90	1.99	1.51
1	C	14	TRP	CB-CG	-20.87	1.12	1.50
1	A	40	LYS	CA-CB	-20.85	1.08	1.53
2	B	41	PHE	CE2-CZ	-20.84	0.97	1.37
2	D	135	GLY	CA-C	-20.78	1.18	1.51
2	D	64	LYS	C-O	-20.77	0.83	1.23
2	B	110	ALA	N-CA	20.74	1.87	1.46
2	D	143	LYS	CA-CB	20.72	1.99	1.53
2	D	84	PHE	CA-CB	20.71	1.99	1.53
2	D	142	HIS	CB-CG	-20.71	1.12	1.50
2	D	63	GLY	C-O	20.69	1.56	1.23
1	A	50	HIS	CB-CG	20.68	1.87	1.50
1	A	31	ARG	C-N	20.65	1.81	1.34
1	C	15	GLY	C-O	-20.60	0.90	1.23
2	B	71	THR	CA-CB	20.57	2.06	1.53
1	A	46	PHE	CG-CD2	-20.57	1.07	1.38
2	B	133	VAL	CB-CG2	20.55	1.96	1.52
1	A	131	ASN	CA-CB	-20.54	0.99	1.53
2	B	63	GLY	C-O	-20.54	0.90	1.23
2	B	70	PHE	CE1-CZ	20.53	1.76	1.37
1	C	31	ARG	NE-CZ	-20.50	1.06	1.33
2	B	41	PHE	CD1-CE1	-20.48	0.98	1.39
1	C	94	ASN	CG-OD1	20.47	1.69	1.24
2	D	48	SER	CA-CB	-20.45	1.22	1.52
1	A	45	HIS	CD2-NE2	20.45	1.84	1.42
2	B	97	VAL	CB-CG2	20.44	1.95	1.52
1	C	119	PRO	CA-C	20.44	1.93	1.52
1	A	108	THR	CB-OG1	-20.43	1.02	1.43
1	C	22	PRO	N-CA	20.39	1.81	1.47
2	D	76	HIS	CB-CG	20.37	1.86	1.50
2	B	20	ASP	CG-OD1	20.32	1.72	1.25
1	A	140	TYR	CG-CD1	-20.27	1.12	1.39
1	A	31	ARG	CA-C	-20.24	1.00	1.52
2	B	145	HIS	CE1-NE2	20.24	1.79	1.32
1	C	93	VAL	C-O	20.20	1.61	1.23
2	D	108	VAL	N-CA	20.20	1.86	1.46
1	A	32	MET	N-CA	20.19	1.86	1.46
2	D	87	LEU	N-CA	-20.19	1.05	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ASN	N-CA	20.18	1.86	1.46
1	A	32	MET	CA-CB	-20.18	1.09	1.53
1	C	30	GLN	CD-NE2	20.12	1.83	1.32
1	C	103	HIS	CG-CD2	-20.08	1.01	1.35
1	C	58	HIS	CB-CG	-20.05	1.14	1.50
1	A	2	LEU	CA-C	20.03	2.05	1.52
2	B	82	GLY	C-O	20.00	1.55	1.23
2	B	103	ARG	CG-CD	20.00	2.02	1.51
1	C	4	ALA	CA-CB	19.99	1.94	1.52
2	D	118	GLY	CA-C	-19.98	1.19	1.51
1	C	74	ASN	N-CA	19.95	1.86	1.46
2	B	98	ASN	CG-OD1	19.92	1.67	1.24
1	A	84	SER	N-CA	19.91	1.86	1.46
1	C	75	ASP	CA-C	19.91	2.04	1.52
2	D	3	THR	CB-OG1	19.91	1.83	1.43
1	A	107	VAL	CA-CB	-19.91	1.12	1.54
1	C	25	GLY	N-CA	19.89	1.75	1.46
1	C	1	VAL	CA-CB	-19.86	1.13	1.54
2	D	92	CYS	CB-SG	19.86	2.16	1.82
2	B	43	HIS	CG-CD2	19.85	1.69	1.35
2	B	46	ASN	CB-CG	19.83	1.96	1.51
2	B	121	PHE	CE2-CZ	-19.82	0.99	1.37
2	D	4	ALA	CA-C	19.81	2.04	1.52
1	C	42	TYR	CE1-CZ	19.80	1.64	1.38
1	A	77	PRO	C-N	19.79	1.68	1.33
2	B	115	ARG	CZ-NH2	-19.77	1.07	1.33
1	C	88	ALA	C-O	19.77	1.60	1.23
2	B	123	PRO	CA-CB	-19.76	1.14	1.53
1	A	141	ARG	CZ-NH1	19.75	1.58	1.33
2	D	144	TYR	CD1-CE1	19.69	1.68	1.39
1	C	116	ASN	CG-ND2	19.66	1.81	1.32
1	C	140	TYR	N-CA	-19.61	1.07	1.46
2	D	79	ASP	CA-CB	19.61	1.97	1.53
2	B	76	HIS	CG-ND1	19.51	1.81	1.38
1	C	138	SER	CA-CB	19.50	1.82	1.52
1	C	102	SER	C-N	19.46	1.78	1.34
2	D	78	ASP	CA-CB	-19.44	1.11	1.53
1	A	74	ASN	CB-CG	19.38	1.95	1.51
2	B	39	ARG	CB-CG	19.33	2.04	1.52
2	D	121	PHE	CG-CD2	-19.28	1.09	1.38
1	A	60	GLN	C-O	-19.27	0.86	1.23
1	A	117	PHE	CG-CD1	19.26	1.67	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	138	ASN	CG-OD1	19.21	1.66	1.24
2	D	103	ARG	CA-CB	19.20	1.96	1.53
2	B	57	PRO	N-CD	19.17	1.74	1.47
2	B	144	TYR	CZ-OH	19.16	1.70	1.37
2	D	42	GLN	CB-CG	19.15	2.04	1.52
2	B	55	ASN	C-N	19.15	1.78	1.34
1	C	117	PHE	C-N	-19.11	0.90	1.34
2	D	21	VAL	N-CA	-19.10	1.08	1.46
1	C	140	TYR	CG-CD1	-19.07	1.14	1.39
1	A	138	SER	CB-OG	19.07	1.67	1.42
1	A	26	ALA	C-O	19.04	1.59	1.23
1	A	25	GLY	N-CA	-19.03	1.17	1.46
1	A	139	LYS	C-O	18.95	1.59	1.23
1	C	107	VAL	CA-CB	-18.93	1.15	1.54
2	D	14	TRP	C-N	-18.93	0.98	1.33
2	D	110	ALA	CA-C	18.93	2.02	1.52
2	D	95	LEU	CB-CG	18.92	2.07	1.52
1	C	131	ASN	CG-OD1	18.89	1.65	1.24
2	D	90	LEU	C-O	-18.89	0.87	1.23
2	B	1	MET	CG-SD	18.87	2.30	1.81
1	A	38	THR	C-O	-18.86	0.87	1.23
2	D	40	PHE	CD2-CE2	-18.86	1.01	1.39
2	B	113	VAL	CB-CG1	18.81	1.92	1.52
2	D	14	TRP	N-CA	-18.80	1.08	1.46
1	C	56	LYS	CE-NZ	18.77	1.96	1.49
1	C	16	LYS	N-CA	18.73	1.83	1.46
2	D	14	TRP	CD2-CE3	-18.73	1.12	1.40
1	C	124	ASN	CG-ND2	18.72	1.79	1.32
2	B	103	ARG	N-CA	-18.71	1.08	1.46
2	B	74	LEU	C-N	-18.68	0.91	1.34
2	B	10	VAL	N-CA	18.66	1.83	1.46
2	D	56	ASN	CB-CG	-18.66	1.08	1.51
1	A	100	LEU	N-CA	-18.64	1.09	1.46
1	A	92	ARG	CZ-NH1	-18.64	1.08	1.33
2	B	138	ASN	C-O	18.63	1.58	1.23
2	B	7	LYS	CA-C	18.60	2.01	1.52
1	A	16	LYS	C-N	18.60	1.76	1.34
2	D	70	PHE	CD2-CE2	-18.59	1.02	1.39
2	D	131	LYS	CA-CB	18.59	1.94	1.53
1	A	71	GLY	C-O	-18.58	0.94	1.23
2	B	132	VAL	CB-CG2	-18.58	1.13	1.52
2	B	6	GLU	CD-OE2	18.58	1.46	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	LEU	N-CA	18.54	1.83	1.46
1	A	140	TYR	CB-CG	18.53	1.79	1.51
1	A	109	LEU	CA-CB	-18.48	1.11	1.53
1	C	120	ALA	N-CA	-18.46	1.09	1.46
2	B	131	LYS	CD-CE	18.45	1.97	1.51
1	A	78	GLY	CA-C	18.42	1.81	1.51
2	D	11	THR	N-CA	18.40	1.83	1.46
1	C	57	ALA	C-O	18.38	1.58	1.23
2	D	123	PRO	CA-C	18.34	1.89	1.52
1	A	94	ASN	CA-CB	18.31	2.00	1.53
2	B	72	GLN	C-N	-18.27	1.00	1.33
1	A	131	ASN	CB-CG	-18.21	1.09	1.51
2	B	19	VAL	C-N	-18.21	0.92	1.34
1	C	100	LEU	N-CA	18.18	1.82	1.46
1	C	49	SER	CB-OG	18.18	1.65	1.42
2	B	142	HIS	CG-CD2	18.18	1.66	1.35
2	B	141	ALA	C-O	18.16	1.57	1.23
2	B	38	GLN	CA-C	18.14	2.00	1.52
1	C	108	THR	CB-OG1	-18.14	1.06	1.43
2	D	41	PHE	CD2-CE2	18.12	1.75	1.39
2	B	110	ALA	CA-CB	18.12	1.90	1.52
1	A	95	PRO	N-CA	-18.11	1.16	1.47
2	D	57	PRO	N-CA	-18.11	1.16	1.47
1	C	10	VAL	CB-CG2	18.10	1.90	1.52
1	A	70	GLN	CG-CD	18.07	1.92	1.51
1	C	31	ARG	CA-C	18.05	1.99	1.52
2	D	94	LYS	C-N	-18.02	0.92	1.34
1	A	67	THR	N-CA	-18.02	1.10	1.46
1	A	17	VAL	CB-CG1	-18.01	1.15	1.52
1	A	78	GLY	C-O	17.98	1.52	1.23
1	C	6	ASN	C-N	17.97	1.75	1.34
2	B	45	GLY	C-N	-17.95	0.92	1.34
1	A	51	GLY	C-O	17.94	1.52	1.23
1	C	55	GLN	C-O	17.93	1.57	1.23
2	B	55	ASN	C-O	-17.92	0.89	1.23
2	D	115	ARG	CA-CB	17.92	1.93	1.53
2	D	138	ASN	N-CA	17.92	1.82	1.46
1	A	27	GLN	CD-OE1	-17.90	0.84	1.24
2	D	14	TRP	CE2-CZ2	-17.89	1.09	1.39
2	D	136	VAL	C-O	17.89	1.57	1.23
2	B	43	HIS	CD2-NE2	17.88	1.79	1.42
2	B	143	LYS	CB-CG	17.86	2.00	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	SER	N-CA	-17.85	1.10	1.46
2	D	128	LEU	CB-CG	-17.85	1.00	1.52
1	A	9	ASN	N-CA	17.84	1.82	1.46
1	C	77	PRO	CA-C	-17.81	1.17	1.52
2	D	71	THR	CB-OG1	17.79	1.78	1.43
2	D	144	TYR	CG-CD1	17.72	1.62	1.39
1	C	36	PHE	CE1-CZ	17.71	1.71	1.37
1	C	134	THR	CA-CB	17.70	1.99	1.53
1	C	84	SER	CA-CB	-17.69	1.26	1.52
2	D	120	GLN	CD-OE1	17.69	1.62	1.24
1	C	17	VAL	C-N	-17.68	1.01	1.33
2	D	11	THR	CB-OG1	17.68	1.78	1.43
2	D	65	ARG	CB-CG	17.68	2.00	1.52
1	C	135	VAL	CB-CG2	17.67	1.90	1.52
1	A	126	ASN	CG-ND2	17.67	1.77	1.32
2	D	39	ARG	CZ-NH2	17.63	1.55	1.33
2	B	75	LYS	C-O	17.62	1.56	1.23
1	C	122	HIS	CB-CG	-17.62	1.18	1.50
1	C	135	VAL	CA-CB	-17.62	1.17	1.54
2	D	3	THR	N-CA	17.62	1.81	1.46
1	C	45	HIS	N-CA	17.61	1.81	1.46
2	D	65	ARG	C-N	-17.61	0.93	1.34
1	A	17	VAL	CB-CG2	17.61	1.89	1.52
2	D	119	GLY	N-CA	17.61	1.72	1.46
2	D	44	PHE	CB-CG	-17.60	1.21	1.51
1	A	34	LEU	CA-CB	17.59	1.94	1.53
2	B	125	VAL	CB-CG1	17.59	1.89	1.52
2	B	106	GLY	CA-C	17.59	1.79	1.51
2	D	84	PHE	CE1-CZ	17.57	1.70	1.37
1	A	70	GLN	CB-CG	-17.55	1.05	1.52
2	D	101	ASN	CG-OD1	17.54	1.62	1.24
1	A	35	SER	CA-CB	17.54	1.79	1.52
2	B	29	ARG	NE-CZ	17.53	1.55	1.33
1	C	67	THR	CB-OG1	-17.52	1.08	1.43
1	C	121	VAL	C-N	17.52	1.74	1.34
1	C	29	LEU	CG-CD2	17.47	2.16	1.51
1	A	29	LEU	CB-CG	17.46	2.03	1.52
2	B	133	VAL	CA-CB	-17.45	1.18	1.54
2	B	78	ASP	CG-OD2	17.44	1.65	1.25
2	D	8	ALA	N-CA	-17.44	1.11	1.46
1	C	41	THR	CA-C	-17.43	1.07	1.52
2	B	6	GLU	CD-OE1	17.42	1.44	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	ALA	C-O	-17.40	0.90	1.23
2	B	110	ALA	C-N	17.39	1.74	1.34
2	B	95	LEU	N-CA	17.39	1.81	1.46
2	B	40	PHE	CG-CD2	-17.38	1.12	1.38
2	B	82	GLY	C-N	-17.36	0.94	1.34
2	D	42	GLN	C-N	-17.33	0.94	1.34
2	B	23	GLY	C-O	-17.31	0.95	1.23
1	C	45	HIS	CD2-NE2	17.31	1.78	1.42
1	C	133	SER	N-CA	-17.28	1.11	1.46
1	C	85	ASN	CG-ND2	17.24	1.75	1.32
1	A	116	ASN	CG-OD1	17.23	1.61	1.24
1	C	83	LEU	C-N	-17.23	0.94	1.34
2	B	96	HIS	CG-CD2	-17.22	1.06	1.35
1	A	20	ASN	CG-ND2	17.21	1.75	1.32
1	A	57	ALA	C-O	-17.21	0.90	1.23
1	C	38	THR	CB-CG2	17.21	2.09	1.52
1	C	117	PHE	CD1-CE1	-17.21	1.04	1.39
1	A	42	TYR	C-N	17.20	1.73	1.34
2	B	128	LEU	C-N	-17.19	0.94	1.34
1	C	3	SER	C-O	17.18	1.55	1.23
1	C	112	HIS	C-O	17.16	1.55	1.23
1	C	14	TRP	CG-CD1	17.15	1.60	1.36
1	A	137	THR	N-CA	-17.14	1.12	1.46
1	C	61	LYS	CB-CG	-17.13	1.06	1.52
2	B	29	ARG	CD-NE	-17.13	1.17	1.46
1	A	128	PHE	CG-CD2	17.12	1.64	1.38
2	D	96	HIS	N-CA	17.10	1.80	1.46
2	D	44	PHE	CA-C	17.09	1.97	1.52
1	A	117	PHE	CG-CD2	17.07	1.64	1.38
2	D	142	HIS	C-O	-17.06	0.91	1.23
1	A	28	ALA	N-CA	-17.05	1.12	1.46
1	C	140	TYR	CB-CG	17.03	1.77	1.51
2	D	95	LEU	CG-CD1	17.02	2.14	1.51
1	C	19	GLY	CA-C	17.02	1.79	1.51
1	C	117	PHE	CG-CD1	17.01	1.64	1.38
2	B	71	THR	C-O	17.00	1.55	1.23
1	C	112	HIS	ND1-CE1	-17.00	0.92	1.34
2	D	94	LYS	CD-CE	16.98	1.93	1.51
2	D	1	MET	N-CA	16.97	1.80	1.46
2	D	45	GLY	C-O	-16.97	0.96	1.23
1	A	70	GLN	CD-NE2	16.96	1.75	1.32
1	A	131	ASN	CG-OD1	16.96	1.61	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	87	LEU	CA-CB	16.95	1.92	1.53
1	A	29	LEU	CA-CB	16.94	1.92	1.53
1	A	19	GLY	CA-C	16.94	1.78	1.51
2	D	37	THR	CB-OG1	-16.93	1.09	1.43
2	D	36	TRP	N-CA	16.91	1.80	1.46
2	D	25	GLN	C-O	-16.91	0.91	1.23
1	A	50	HIS	CG-CD2	-16.87	1.07	1.35
2	B	142	HIS	CB-CG	-16.87	1.19	1.50
2	B	46	ASN	CA-CB	16.86	1.97	1.53
1	A	104	SER	CA-CB	16.85	1.78	1.52
2	B	137	ALA	C-O	16.84	1.55	1.23
2	D	95	LEU	C-O	16.83	1.55	1.23
1	C	1	VAL	C-O	-16.82	0.91	1.23
2	B	80	LEU	C-O	16.80	1.55	1.23
2	B	130	GLN	CD-OE1	16.79	1.60	1.24
1	A	76	LEU	C-O	16.78	1.55	1.23
2	D	36	TRP	CD1-NE1	16.77	1.66	1.38
1	A	67	THR	C-N	-16.76	0.95	1.34
2	B	34	TYR	CE1-CZ	-16.75	1.16	1.38
1	C	46	PHE	CD1-CE1	16.73	1.72	1.39
1	C	17	VAL	CB-CG2	16.71	1.88	1.52
1	A	77	PRO	N-CA	16.67	1.75	1.47
2	D	28	GLY	C-N	-16.66	0.95	1.34
2	B	12	GLY	C-O	16.66	1.50	1.23
2	B	34	TYR	CG-CD1	16.64	1.60	1.39
1	C	114	PRO	N-CD	16.63	1.71	1.47
1	C	92	ARG	C-O	16.60	1.54	1.23
2	B	70	PHE	CB-CG	-16.60	1.23	1.51
2	D	125	VAL	CA-CB	-16.58	1.20	1.54
2	B	109	LEU	C-N	-16.57	0.95	1.34
2	D	55	ASN	C-N	-16.57	0.95	1.34
2	D	89	GLY	C-N	-16.54	0.96	1.34
1	C	85	ASN	CG-OD1	16.54	1.60	1.24
1	C	61	LYS	CD-CE	16.53	1.92	1.51
2	B	94	LYS	CE-NZ	16.50	1.90	1.49
2	B	43	HIS	CG-ND1	16.50	1.75	1.38
2	D	116	ASN	C-N	16.47	1.72	1.34
1	C	113	LEU	C-N	16.46	1.65	1.34
1	C	89	HIS	ND1-CE1	-16.46	0.93	1.34
1	A	100	LEU	C-O	16.44	1.54	1.23
1	C	132	ASP	CG-OD1	16.44	1.63	1.25
2	B	126	GLN	CD-OE1	16.43	1.60	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	PHE	CD2-CE2	-16.39	1.06	1.39
2	B	55	ASN	CG-OD1	16.38	1.59	1.24
2	B	58	LYS	C-N	16.38	1.71	1.34
2	D	41	PHE	CE2-CZ	16.36	1.68	1.37
2	D	21	VAL	CB-CG2	16.36	1.87	1.52
1	A	55	GLN	CD-NE2	16.35	1.73	1.32
1	A	140	TYR	CD1-CE1	16.33	1.63	1.39
2	B	6	GLU	N-CA	16.33	1.79	1.46
1	A	60	GLN	CD-OE1	16.32	1.59	1.24
1	C	20	ASN	C-N	16.31	1.71	1.34
2	D	97	VAL	CB-CG2	-16.30	1.18	1.52
1	A	122	HIS	CG-ND1	-16.30	1.02	1.38
2	B	80	LEU	C-N	16.28	1.71	1.34
2	D	70	PHE	CG-CD1	16.28	1.63	1.38
2	B	63	GLY	CA-C	-16.27	1.25	1.51
1	A	96	VAL	CB-CG2	-16.25	1.18	1.52
1	A	24	TYR	CE1-CZ	-16.25	1.17	1.38
1	A	21	ALA	C-N	-16.24	1.03	1.34
2	B	40	PHE	CE2-CZ	16.20	1.68	1.37
1	A	72	HIS	C-O	16.18	1.54	1.23
2	B	83	ALA	CA-CB	16.18	1.86	1.52
1	A	117	PHE	C-O	-16.17	0.92	1.23
1	A	141	ARG	CA-C	16.17	1.95	1.52
1	C	7	LYS	CE-NZ	16.15	1.89	1.49
1	C	14	TRP	CD2-CE3	16.14	1.64	1.40
2	B	98	ASN	CG-ND2	16.13	1.73	1.32
2	B	22	VAL	CB-CG2	16.13	1.86	1.52
1	C	55	GLN	N-CA	-16.12	1.14	1.46
2	B	139	ALA	CA-CB	-16.12	1.18	1.52
1	A	36	PHE	CB-CG	16.08	1.78	1.51
1	C	99	LYS	CB-CG	-16.07	1.09	1.52
2	D	141	ALA	C-N	16.07	1.71	1.34
1	C	110	ALA	C-N	-16.05	0.97	1.34
1	A	59	GLY	C-O	-16.05	0.97	1.23
2	D	37	THR	C-O	16.04	1.53	1.23
1	C	103	HIS	CB-CG	16.04	1.78	1.50
1	C	132	ASP	CB-CG	-16.03	1.18	1.51
1	C	75	ASP	CG-OD2	16.01	1.62	1.25
1	C	52	SER	CB-OG	-16.00	1.21	1.42
2	D	30	LEU	CA-C	16.00	1.94	1.52
1	C	114	PRO	C-O	-15.98	0.91	1.23
1	C	1	VAL	CA-C	15.98	1.94	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	140	TYR	CG-CD2	-15.96	1.18	1.39
2	D	144	TYR	C-O	15.96	1.53	1.23
2	B	65	ARG	C-O	15.96	1.53	1.23
1	C	74	ASN	C-O	-15.96	0.93	1.23
2	D	63	GLY	C-N	-15.92	0.97	1.34
1	C	100	LEU	CB-CG	15.90	1.98	1.52
2	B	78	ASP	CB-CG	-15.88	1.18	1.51
1	A	20	ASN	CB-CG	15.86	1.87	1.51
1	C	90	LYS	CD-CE	15.86	1.91	1.51
1	C	95	PRO	C-O	15.85	1.54	1.23
2	B	116	ASN	CG-OD1	-15.84	0.89	1.24
1	A	124	ASN	CB-CG	15.84	1.87	1.51
2	B	140	LEU	N-CA	-15.84	1.14	1.46
2	D	70	PHE	CD1-CE1	-15.82	1.07	1.39
1	A	91	LEU	N-CA	15.81	1.77	1.46
1	A	103	HIS	CA-CB	15.81	1.88	1.53
2	D	73	GLY	C-O	-15.80	0.98	1.23
1	A	80	LEU	CB-CG	15.79	1.98	1.52
2	D	16	LYS	CB-CG	15.79	1.95	1.52
2	D	20	ASP	C-N	15.78	1.70	1.34
2	B	17	VAL	CB-CG1	-15.77	1.19	1.52
2	B	24	ALA	CA-CB	15.77	1.85	1.52
1	C	69	ALA	N-CA	-15.76	1.14	1.46
2	D	100	GLN	CG-CD	-15.76	1.14	1.51
2	B	95	LEU	CA-CB	15.75	1.90	1.53
2	D	43	HIS	CD2-NE2	15.74	1.75	1.42
1	A	61	LYS	CA-CB	15.74	1.88	1.53
2	D	21	VAL	CB-CG1	-15.74	1.19	1.52
1	C	79	THR	CA-CB	15.72	1.94	1.53
1	A	49	SER	CA-C	-15.72	1.12	1.52
2	B	114	ALA	N-CA	-15.72	1.15	1.46
2	D	120	GLN	CD-NE2	15.72	1.72	1.32
2	D	103	ARG	CZ-NH1	-15.66	1.12	1.33
1	A	14	TRP	CD2-CE2	15.66	1.60	1.41
1	A	85	ASN	CA-CB	-15.66	1.12	1.53
2	B	34	TYR	N-CA	15.66	1.77	1.46
2	D	143	LYS	CD-CE	15.66	1.90	1.51
1	A	113	LEU	CA-C	-15.65	1.12	1.52
2	B	107	ASN	CG-ND2	15.65	1.72	1.32
1	A	61	LYS	CG-CD	-15.64	0.99	1.52
2	B	109	LEU	CB-CG	15.64	1.98	1.52
2	D	62	HIS	CE1-NE2	15.62	1.68	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	THR	C-O	15.61	1.53	1.23
2	D	6	GLU	C-N	-15.58	0.98	1.34
1	A	89	HIS	CE1-NE2	15.56	1.68	1.32
2	B	22	VAL	CA-C	15.56	1.93	1.52
2	B	40	PHE	C-O	15.55	1.52	1.23
1	A	81	SER	C-N	-15.54	0.98	1.34
1	A	119	PRO	C-N	15.52	1.69	1.34
1	C	128	PHE	CE2-CZ	15.52	1.66	1.37
1	C	75	ASP	CG-OD1	15.50	1.61	1.25
2	D	88	SER	C-N	-15.49	1.05	1.33
1	A	75	ASP	C-O	15.48	1.52	1.23
1	A	70	GLN	C-N	15.48	1.60	1.33
1	A	125	LEU	C-O	-15.47	0.94	1.23
1	A	62	VAL	CA-CB	-15.47	1.22	1.54
1	A	11	LYS	C-N	15.47	1.69	1.34
2	B	25	GLN	CB-CG	-15.46	1.10	1.52
1	C	71	GLY	CA-C	15.45	1.76	1.51
2	B	14	TRP	C-O	-15.44	0.94	1.23
2	B	121	PHE	CB-CG	-15.44	1.25	1.51
1	C	59	GLY	C-N	-15.43	0.98	1.34
1	A	31	ARG	CB-CG	-15.42	1.10	1.52
2	B	29	ARG	C-O	-15.42	0.94	1.23
2	B	58	LYS	N-CA	-15.42	1.15	1.46
1	C	41	THR	CB-CG2	15.42	2.03	1.52
1	C	82	ASN	CG-OD1	15.41	1.57	1.24
1	C	141	ARG	CZ-NH2	15.40	1.53	1.33
2	D	48	SER	C-O	15.39	1.52	1.23
2	B	96	HIS	CE1-NE2	15.38	1.68	1.32
2	B	1	MET	C-N	-15.38	0.98	1.34
1	A	7	LYS	C-N	-15.37	0.98	1.34
1	A	81	SER	CA-CB	15.37	1.76	1.52
2	B	102	PHE	CE1-CZ	-15.37	1.08	1.37
2	D	44	PHE	CE2-CZ	-15.36	1.08	1.37
1	A	32	MET	C-N	15.36	1.69	1.34
2	B	79	ASP	CG-OD2	15.35	1.60	1.25
2	D	142	HIS	CA-CB	15.35	1.87	1.53
2	D	121	PHE	CB-CG	-15.34	1.25	1.51
2	D	39	ARG	C-N	-15.33	0.98	1.34
2	D	117	PHE	CB-CG	-15.33	1.25	1.51
1	C	55	GLN	CG-CD	15.32	1.86	1.51
2	B	6	GLU	CA-CB	15.31	1.87	1.53
1	C	15	GLY	N-CA	15.29	1.69	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	140	TYR	CD1-CE1	15.28	1.62	1.39
1	A	98	PHE	CE2-CZ	-15.27	1.08	1.37
2	D	143	LYS	CA-C	-15.26	1.13	1.52
1	C	101	LEU	C-O	15.24	1.52	1.23
2	D	61	ALA	CA-CB	15.23	1.84	1.52
1	C	58	HIS	C-O	-15.21	0.94	1.23
1	A	84	SER	C-O	-15.18	0.94	1.23
1	A	78	GLY	C-N	-15.13	0.99	1.34
2	B	129	PHE	CD1-CE1	15.13	1.69	1.39
2	B	56	ASN	C-N	15.12	1.62	1.34
1	A	133	SER	CB-OG	-15.11	1.22	1.42
2	B	125	VAL	N-CA	-15.11	1.16	1.46
2	B	142	HIS	C-N	-15.10	0.99	1.34
1	C	126	ASN	CG-ND2	15.10	1.70	1.32
2	B	13	PHE	CG-CD1	15.08	1.61	1.38
1	C	98	PHE	CE2-CZ	-15.08	1.08	1.37
2	B	66	VAL	CB-CG1	15.08	1.84	1.52
1	C	10	VAL	CA-CB	-15.07	1.23	1.54
2	B	59	VAL	N-CA	-15.06	1.16	1.46
1	C	96	VAL	CA-C	-15.06	1.13	1.52
1	A	42	TYR	CG-CD1	15.05	1.58	1.39
1	A	112	HIS	CG-ND1	15.05	1.71	1.38
2	D	12	GLY	N-CA	15.05	1.68	1.46
1	C	116	ASN	C-N	-15.05	0.99	1.34
1	C	19	GLY	C-O	-15.05	0.99	1.23
2	B	64	LYS	CA-CB	-15.04	1.20	1.53
2	B	86	GLN	CD-NE2	15.03	1.70	1.32
2	D	58	LYS	CE-NZ	15.03	1.86	1.49
1	C	40	LYS	C-N	-14.99	0.99	1.34
2	D	109	LEU	CA-C	14.98	1.92	1.52
1	A	69	ALA	N-CA	14.98	1.76	1.46
2	D	129	PHE	N-CA	14.98	1.76	1.46
2	B	144	TYR	C-O	14.97	1.51	1.23
1	A	86	LEU	C-N	14.96	1.68	1.34
2	D	137	ALA	C-N	-14.96	0.99	1.34
1	C	36	PHE	CB-CG	-14.94	1.25	1.51
1	A	103	HIS	CG-ND1	14.91	1.71	1.38
2	B	124	ASN	CB-CG	-14.91	1.16	1.51
2	B	138	ASN	CG-ND2	14.90	1.70	1.32
2	B	141	ALA	C-N	14.89	1.68	1.34
2	B	18	ASP	CB-CG	14.89	1.83	1.51
2	D	78	ASP	CB-CG	14.89	1.83	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	124	ASN	C-N	14.88	1.68	1.34
2	B	2	LEU	CA-CB	14.88	1.88	1.53
2	B	25	GLN	C-N	-14.88	0.99	1.34
2	D	103	ARG	CZ-NH2	14.88	1.52	1.33
1	A	118	THR	CB-CG2	14.86	2.01	1.52
2	B	14	TRP	CE3-CZ3	-14.85	1.13	1.38
2	D	44	PHE	CA-CB	14.84	1.86	1.53
1	A	65	ALA	CA-C	-14.83	1.14	1.52
1	A	3	SER	CA-CB	14.82	1.75	1.52
1	C	37	PRO	CG-CD	14.80	1.99	1.50
1	C	39	THR	N-CA	-14.80	1.16	1.46
2	B	117	PHE	CE1-CZ	14.79	1.65	1.37
1	A	126	ASN	C-N	-14.75	1.00	1.34
2	B	20	ASP	CG-OD2	14.75	1.59	1.25
2	B	126	GLN	C-O	-14.75	0.95	1.23
1	A	77	PRO	N-CD	-14.74	1.27	1.47
2	D	44	PHE	CG-CD2	-14.74	1.16	1.38
2	B	134	ALA	CA-CB	-14.74	1.21	1.52
2	D	50	ALA	CA-C	14.73	1.91	1.52
1	A	141	ARG	C-OXT	-14.73	0.95	1.23
2	B	52	ALA	N-CA	14.73	1.75	1.46
1	A	34	LEU	C-O	14.72	1.51	1.23
2	B	16	LYS	CB-CG	-14.72	1.12	1.52
1	A	109	LEU	C-O	-14.72	0.95	1.23
2	D	73	GLY	CA-C	14.71	1.75	1.51
1	C	24	TYR	CD1-CE1	-14.71	1.17	1.39
2	D	129	PHE	CG-CD1	14.68	1.60	1.38
1	A	47	ASP	C-O	14.68	1.51	1.23
2	D	28	GLY	C-O	14.66	1.47	1.23
2	D	117	PHE	C-O	14.66	1.51	1.23
2	B	42	GLN	CD-NE2	14.63	1.69	1.32
1	C	116	ASN	CA-CB	-14.62	1.15	1.53
2	D	70	PHE	C-N	-14.62	1.00	1.34
1	C	44	PRO	CG-CD	-14.62	1.02	1.50
1	C	102	SER	CA-CB	-14.60	1.31	1.52
2	B	129	PHE	CB-CG	-14.60	1.26	1.51
1	C	44	PRO	C-O	14.60	1.52	1.23
2	D	46	ASN	C-N	-14.60	1.00	1.34
1	C	141	ARG	CD-NE	14.59	1.71	1.46
2	B	119	GLY	N-CA	14.58	1.68	1.46
1	C	131	ASN	N-CA	-14.58	1.17	1.46
2	D	84	PHE	CE2-CZ	-14.58	1.09	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	108	VAL	CB-CG2	-14.57	1.22	1.52
1	A	62	VAL	CB-CG1	14.55	1.83	1.52
1	A	107	VAL	C-O	-14.54	0.95	1.23
2	D	52	ALA	CA-CB	14.53	1.82	1.52
2	B	121	PHE	CA-CB	-14.53	1.22	1.53
2	D	124	ASN	CB-CG	14.53	1.84	1.51
1	C	139	LYS	CB-CG	14.49	1.91	1.52
2	B	84	PHE	CB-CG	14.48	1.75	1.51
1	C	24	TYR	CZ-OH	-14.48	1.13	1.37
2	B	143	LYS	C-O	14.47	1.50	1.23
2	D	123	PRO	C-O	-14.46	0.94	1.23
1	C	33	PHE	C-N	14.45	1.67	1.34
1	A	7	LYS	CA-C	14.45	1.90	1.52
1	C	133	SER	CA-CB	14.44	1.74	1.52
2	D	83	ALA	CA-C	14.42	1.90	1.52
1	A	48	LEU	CA-CB	14.41	1.86	1.53
2	D	145	HIS	CB-CG	-14.40	1.24	1.50
2	D	66	VAL	C-O	14.40	1.50	1.23
2	D	120	GLN	C-O	-14.40	0.95	1.23
2	B	55	ASN	N-CA	-14.38	1.17	1.46
2	D	105	LEU	CG-CD2	-14.38	0.98	1.51
1	C	17	VAL	N-CA	-14.38	1.17	1.46
2	B	44	PHE	CG-CD2	-14.38	1.17	1.38
1	A	94	ASN	N-CA	14.37	1.75	1.46
2	D	75	LYS	CA-CB	14.37	1.85	1.53
2	B	42	GLN	CD-OE1	14.34	1.55	1.24
2	B	100	GLN	CA-CB	-14.34	1.22	1.53
2	D	62	HIS	CG-ND1	14.34	1.70	1.38
1	C	122	HIS	CG-ND1	14.33	1.70	1.38
2	D	36	TRP	CE3-CZ3	-14.33	1.14	1.38
1	A	13	ALA	C-O	-14.33	0.96	1.23
2	B	14	TRP	C-N	14.32	1.58	1.33
2	D	110	ALA	CA-CB	-14.32	1.22	1.52
1	C	115	THR	CA-C	14.32	1.90	1.52
2	D	26	ALA	CA-C	14.32	1.90	1.52
1	C	44	PRO	CA-CB	-14.30	1.25	1.53
2	D	130	GLN	CD-OE1	14.30	1.55	1.24
2	B	45	GLY	N-CA	14.30	1.67	1.46
1	C	85	ASN	N-CA	-14.30	1.17	1.46
2	D	68	ASP	CG-OD2	14.29	1.58	1.25
2	B	39	ARG	C-O	-14.28	0.96	1.23
1	A	43	PHE	CG-CD1	-14.27	1.17	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	HIS	CA-CB	14.27	1.85	1.53
2	B	11	THR	CB-CG2	14.26	1.99	1.52
1	A	79	THR	C-O	14.26	1.50	1.23
2	D	77	LEU	CB-CG	14.25	1.93	1.52
2	D	41	PHE	CE1-CZ	14.24	1.64	1.37
2	B	8	ALA	CA-CB	14.23	1.82	1.52
2	B	39	ARG	N-CA	-14.22	1.18	1.46
1	C	12	ALA	CA-CB	-14.22	1.22	1.52
1	A	45	HIS	CA-CB	14.21	1.85	1.53
1	A	12	ALA	CA-C	14.20	1.89	1.52
2	B	129	PHE	CG-CD2	-14.20	1.17	1.38
2	B	84	PHE	CG-CD1	14.19	1.60	1.38
1	A	80	LEU	C-O	14.19	1.50	1.23
2	D	81	LYS	CG-CD	14.18	2.00	1.52
2	D	4	ALA	C-N	-14.18	1.01	1.34
2	B	126	GLN	CA-C	14.16	1.89	1.52
2	B	59	VAL	CB-CG1	14.15	1.82	1.52
1	C	47	ASP	C-O	14.14	1.50	1.23
2	B	125	VAL	CA-C	14.13	1.89	1.52
2	B	132	VAL	C-O	14.13	1.50	1.23
1	C	10	VAL	N-CA	-14.12	1.18	1.46
2	B	139	ALA	C-N	14.12	1.66	1.34
2	D	131	LYS	CE-NZ	14.10	1.84	1.49
2	B	129	PHE	CG-CD1	14.10	1.59	1.38
1	A	80	LEU	CA-C	-14.10	1.16	1.52
1	A	119	PRO	CA-CB	14.10	1.81	1.53
1	C	76	LEU	C-O	14.08	1.50	1.23
2	B	69	ALA	N-CA	-14.08	1.18	1.46
1	C	99	LYS	CA-CB	-14.05	1.23	1.53
1	C	55	GLN	CA-CB	14.03	1.84	1.53
1	A	126	ASN	C-O	14.01	1.50	1.23
2	D	33	VAL	CB-CG1	-14.01	1.23	1.52
2	D	18	ASP	CG-OD1	14.00	1.57	1.25
2	B	102	PHE	C-N	13.99	1.66	1.34
2	B	104	LEU	N-CA	13.98	1.74	1.46
2	D	39	ARG	CD-NE	13.98	1.70	1.46
1	C	87	HIS	CG-ND1	13.98	1.69	1.38
2	B	62	HIS	N-CA	13.97	1.74	1.46
2	B	117	PHE	CE2-CZ	13.97	1.63	1.37
1	A	130	ALA	C-O	-13.96	0.96	1.23
2	D	61	ALA	N-CA	-13.95	1.18	1.46
2	B	97	VAL	C-O	13.94	1.49	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	50	ALA	C-N	-13.93	1.07	1.33
2	B	5	GLU	CG-CD	13.92	1.72	1.51
2	B	99	PRO	N-CD	-13.90	1.28	1.47
1	C	8	SER	CA-CB	-13.89	1.32	1.52
1	A	79	THR	CB-OG1	-13.89	1.15	1.43
2	B	130	GLN	CA-CB	13.88	1.84	1.53
2	D	127	ALA	CA-CB	13.89	1.81	1.52
2	D	13	PHE	C-N	13.88	1.66	1.34
1	C	28	ALA	C-N	13.88	1.66	1.34
1	A	35	SER	CB-OG	13.87	1.60	1.42
2	B	99	PRO	CG-CD	13.87	1.96	1.50
2	B	54	MET	CB-CG	13.85	1.95	1.51
1	A	7	LYS	C-O	-13.84	0.97	1.23
2	B	76	HIS	N-CA	13.82	1.74	1.46
2	B	122	THR	C-O	13.82	1.49	1.23
2	D	13	PHE	CG-CD1	-13.81	1.18	1.38
2	B	136	VAL	CA-CB	-13.80	1.25	1.54
2	D	6	GLU	CG-CD	13.80	1.72	1.51
1	A	12	ALA	CA-CB	13.80	1.81	1.52
1	C	36	PHE	CA-CB	13.79	1.84	1.53
2	D	43	HIS	CA-CB	13.79	1.84	1.53
2	D	19	VAL	CA-CB	-13.78	1.25	1.54
1	A	59	GLY	CA-C	13.77	1.73	1.51
1	A	45	HIS	C-O	13.76	1.49	1.23
1	C	11	LYS	N-CA	13.71	1.73	1.46
2	D	110	ALA	C-O	13.70	1.49	1.23
2	D	113	VAL	CB-CG2	13.70	1.81	1.52
2	D	92	CYS	CA-C	13.70	1.88	1.52
2	D	68	ASP	C-N	-13.70	1.02	1.34
2	B	27	LEU	C-O	13.69	1.49	1.23
2	D	105	LEU	C-O	13.69	1.49	1.23
1	A	122	HIS	C-O	13.68	1.49	1.23
2	D	39	ARG	CA-CB	-13.66	1.24	1.53
2	D	122	THR	CB-OG1	-13.66	1.16	1.43
2	D	142	HIS	ND1-CE1	13.65	1.68	1.34
1	A	105	LEU	N-CA	13.63	1.73	1.46
1	A	115	THR	C-O	-13.63	0.97	1.23
1	C	124	ASN	CG-OD1	-13.63	0.94	1.24
1	C	30	GLN	CG-CD	13.62	1.82	1.51
1	C	117	PHE	CA-C	13.62	1.88	1.52
1	A	2	LEU	C-N	13.62	1.65	1.34
1	A	46	PHE	CE2-CZ	-13.57	1.11	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	104	LEU	CB-CG	13.57	1.91	1.52
2	B	60	LYS	CE-NZ	13.56	1.82	1.49
1	C	20	ASN	CA-C	-13.56	1.17	1.52
2	B	118	GLY	C-N	-13.55	1.08	1.33
1	C	9	ASN	CG-ND2	13.54	1.66	1.32
2	D	121	PHE	CA-CB	13.54	1.83	1.53
2	D	7	LYS	C-N	-13.54	1.02	1.34
2	D	73	GLY	C-N	13.54	1.65	1.34
1	A	17	VAL	C-O	13.53	1.49	1.23
1	A	36	PHE	CE1-CZ	-13.53	1.11	1.37
2	D	108	VAL	CA-C	-13.52	1.17	1.52
1	A	7	LYS	CB-CG	-13.51	1.16	1.52
2	B	46	ASN	CG-OD1	13.51	1.53	1.24
1	C	78	GLY	N-CA	13.50	1.66	1.46
2	D	40	PHE	CG-CD2	13.50	1.58	1.38
2	B	118	GLY	C-O	13.48	1.45	1.23
2	B	62	HIS	CG-ND1	13.48	1.68	1.38
2	D	67	LEU	CA-CB	13.47	1.84	1.53
1	A	87	HIS	CD2-NE2	13.47	1.70	1.42
1	C	111	SER	C-N	13.43	1.65	1.34
1	A	20	ASN	CG-OD1	13.42	1.53	1.24
1	A	12	ALA	C-N	13.41	1.64	1.34
1	C	82	ASN	CG-ND2	13.39	1.66	1.32
1	A	128	PHE	C-O	-13.37	0.97	1.23
1	A	90	LYS	C-O	13.37	1.48	1.23
1	C	71	GLY	C-O	-13.37	1.02	1.23
1	C	87	HIS	CA-C	-13.36	1.18	1.52
1	A	5	ALA	C-O	-13.36	0.97	1.23
1	A	44	PRO	N-CD	-13.36	1.29	1.47
2	B	36	TRP	CD2-CE3	-13.35	1.20	1.40
2	B	13	PHE	CB-CG	-13.35	1.28	1.51
1	A	36	PHE	C-N	13.34	1.59	1.34
2	D	34	TYR	N-CA	13.33	1.73	1.46
2	B	15	GLY	CA-C	13.32	1.73	1.51
1	C	45	HIS	CA-C	-13.29	1.18	1.52
2	D	128	LEU	N-CA	13.28	1.73	1.46
2	D	104	LEU	CG-CD1	13.27	2.00	1.51
1	A	1	VAL	CA-C	13.27	1.87	1.52
1	C	84	SER	CA-C	13.27	1.87	1.52
1	C	2	LEU	C-O	-13.26	0.98	1.23
2	D	66	VAL	CB-CG2	-13.25	1.25	1.52
2	D	1	MET	C-O	13.24	1.48	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	PHE	CA-CB	13.24	1.83	1.53
2	D	93	ASN	CG-ND2	13.23	1.66	1.32
1	A	36	PHE	CD1-CE1	-13.23	1.12	1.39
2	B	44	PHE	CG-CD1	13.23	1.58	1.38
2	B	133	VAL	C-N	-13.22	1.03	1.34
2	B	36	TRP	C-O	-13.21	0.98	1.23
2	D	4	ALA	C-O	13.21	1.48	1.23
1	C	111	SER	C-O	13.20	1.48	1.23
2	D	114	ALA	C-N	-13.19	1.03	1.34
2	B	66	VAL	C-N	-13.18	1.03	1.34
2	D	132	VAL	N-CA	13.18	1.72	1.46
1	C	10	VAL	C-N	13.18	1.64	1.34
2	D	67	LEU	C-N	-13.15	1.03	1.34
2	B	53	VAL	CB-CG1	-13.15	1.25	1.52
2	B	143	LYS	CD-CE	13.14	1.84	1.51
2	B	105	LEU	CA-C	13.14	1.87	1.52
2	D	57	PRO	C-O	-13.10	0.97	1.23
1	A	118	THR	CA-CB	-13.10	1.19	1.53
1	C	30	GLN	N-CA	-13.09	1.20	1.46
1	C	81	SER	C-N	13.09	1.64	1.34
2	B	92	CYS	C-N	13.06	1.64	1.34
1	C	58	HIS	C-N	-13.05	1.09	1.33
2	D	76	HIS	N-CA	13.05	1.72	1.46
1	C	128	PHE	C-O	13.03	1.48	1.23
2	B	56	ASN	CB-CG	-13.03	1.21	1.51
1	C	28	ALA	CA-C	-13.03	1.19	1.52
2	D	55	ASN	CB-CG	-13.02	1.21	1.51
1	A	96	VAL	N-CA	-13.00	1.20	1.46
2	D	17	VAL	N-CA	-12.99	1.20	1.46
1	A	102	SER	CA-C	-12.99	1.19	1.52
1	C	17	VAL	CA-C	12.99	1.86	1.52
2	D	41	PHE	CG-CD1	12.99	1.58	1.38
1	C	112	HIS	CA-CB	-12.98	1.25	1.53
1	A	6	ASN	CB-CG	-12.97	1.21	1.51
2	B	51	GLY	C-N	12.96	1.63	1.34
2	B	96	HIS	CA-C	-12.95	1.19	1.52
2	D	14	TRP	NE1-CE2	12.92	1.54	1.37
1	C	107	VAL	N-CA	-12.91	1.20	1.46
2	D	100	GLN	CA-CB	12.90	1.82	1.53
1	C	24	TYR	CG-CD1	-12.90	1.22	1.39
1	C	93	VAL	CB-CG2	-12.90	1.25	1.52
2	B	65	ARG	N-CA	12.88	1.72	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	59	VAL	CA-CB	-12.88	1.27	1.54
2	D	112	VAL	CB-CG1	12.87	1.79	1.52
1	A	119	PRO	N-CD	12.86	1.65	1.47
1	C	111	SER	CA-C	12.84	1.86	1.52
2	B	58	LYS	C-O	12.83	1.47	1.23
1	A	93	VAL	CB-CG1	12.82	1.79	1.52
2	D	23	GLY	CA-C	-12.82	1.31	1.51
2	B	54	MET	N-CA	12.81	1.72	1.46
2	B	136	VAL	CB-CG2	-12.80	1.25	1.52
2	B	33	VAL	C-N	-12.79	1.04	1.34
2	D	141	ALA	CA-C	12.79	1.86	1.52
1	C	14	TRP	N-CA	-12.78	1.20	1.46
2	D	67	LEU	CA-C	12.77	1.86	1.52
2	B	137	ALA	N-CA	12.77	1.71	1.46
2	B	115	ARG	C-N	-12.76	1.04	1.34
2	D	86	GLN	C-O	-12.76	0.99	1.23
1	A	70	GLN	C-O	-12.75	0.99	1.23
2	B	10	VAL	CB-CG1	12.74	1.79	1.52
1	C	6	ASN	CB-CG	-12.74	1.21	1.51
2	B	58	LYS	CB-CG	12.73	1.86	1.52
2	B	81	LYS	N-CA	-12.72	1.21	1.46
1	C	114	PRO	CB-CG	12.72	2.13	1.50
2	B	111	LEU	CA-CB	-12.71	1.24	1.53
1	C	42	TYR	CD1-CE1	-12.71	1.20	1.39
2	D	38	GLN	C-O	-12.70	0.99	1.23
2	B	11	THR	CB-OG1	12.70	1.68	1.43
2	B	105	LEU	C-O	12.68	1.47	1.23
2	B	128	LEU	N-CA	-12.68	1.21	1.46
1	C	93	VAL	C-N	-12.67	1.04	1.34
1	A	68	LYS	C-N	-12.66	1.04	1.34
2	B	21	VAL	CB-CG1	-12.66	1.26	1.52
2	B	19	VAL	CA-CB	12.65	1.81	1.54
2	D	126	GLN	CG-CD	-12.65	1.22	1.51
1	A	99	LYS	C-O	12.65	1.47	1.23
2	B	96	HIS	CB-CG	12.60	1.72	1.50
2	B	73	GLY	N-CA	12.60	1.65	1.46
2	D	35	PRO	C-O	-12.60	0.98	1.23
1	A	47	ASP	CG-OD2	-12.59	0.96	1.25
2	D	18	ASP	N-CA	-12.56	1.21	1.46
2	B	2	LEU	C-O	-12.56	0.99	1.23
2	D	36	TRP	CZ2-CH2	-12.55	1.13	1.37
1	A	28	ALA	CA-CB	-12.54	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	68	ASP	CB-CG	12.54	1.78	1.51
2	B	6	GLU	CB-CG	-12.54	1.28	1.52
1	C	43	PHE	N-CA	-12.53	1.21	1.46
2	D	78	ASP	CA-C	12.52	1.85	1.52
1	C	20	ASN	N-CA	12.51	1.71	1.46
2	B	65	ARG	CB-CG	-12.51	1.18	1.52
1	A	64	ASN	CG-OD1	-12.50	0.96	1.24
2	D	130	GLN	CD-NE2	-12.50	1.01	1.32
1	A	33	PHE	CD2-CE2	-12.48	1.14	1.39
1	C	27	GLN	CG-CD	-12.47	1.22	1.51
1	C	45	HIS	CA-CB	12.46	1.81	1.53
2	D	104	LEU	C-N	-12.45	1.05	1.34
2	D	111	LEU	N-CA	-12.45	1.21	1.46
1	C	85	ASN	CB-CG	12.45	1.79	1.51
1	C	122	HIS	CA-C	-12.43	1.20	1.52
2	B	66	VAL	C-O	12.42	1.47	1.23
2	B	78	ASP	C-O	-12.39	0.99	1.23
2	B	101	ASN	CA-C	12.39	1.85	1.52
1	C	106	LEU	N-CA	-12.39	1.21	1.46
1	C	108	THR	CA-C	12.38	1.85	1.52
1	C	6	ASN	CA-C	-12.38	1.20	1.52
2	B	41	PHE	CA-C	12.36	1.85	1.52
2	B	128	LEU	CA-CB	12.36	1.82	1.53
1	C	137	THR	N-CA	12.35	1.71	1.46
2	B	6	GLU	C-O	12.35	1.46	1.23
2	B	93	ASN	CB-CG	12.33	1.79	1.51
2	B	14	TRP	CG-CD2	12.33	1.64	1.43
1	A	99	LYS	CE-NZ	12.32	1.79	1.49
1	C	22	PRO	C-O	12.32	1.47	1.23
2	B	87	LEU	CB-CG	-12.31	1.16	1.52
2	D	96	HIS	CA-C	12.31	1.84	1.52
1	A	36	PHE	C-O	12.31	1.46	1.23
1	C	134	THR	N-CA	12.30	1.71	1.46
2	D	7	LYS	CA-C	-12.30	1.21	1.52
1	A	55	GLN	CA-CB	12.30	1.81	1.53
2	D	131	LYS	C-N	12.30	1.62	1.34
2	D	18	ASP	CA-CB	12.29	1.80	1.53
1	A	75	ASP	CG-OD1	12.28	1.53	1.25
2	D	6	GLU	CB-CG	-12.26	1.28	1.52
1	A	120	ALA	N-CA	-12.25	1.21	1.46
2	D	92	CYS	C-O	-12.24	1.00	1.23
2	B	83	ALA	CA-C	-12.20	1.21	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	138	ASN	CA-C	-12.20	1.21	1.52
1	C	129	LEU	CB-CG	12.18	1.87	1.52
2	D	62	HIS	C-N	12.18	1.54	1.33
2	D	11	THR	C-N	12.18	1.54	1.33
1	A	10	VAL	CA-CB	-12.18	1.29	1.54
2	B	53	VAL	C-N	-12.17	1.06	1.34
2	B	93	ASN	CG-ND2	12.17	1.63	1.32
2	D	60	LYS	C-O	12.17	1.46	1.23
2	B	85	ALA	CA-CB	-12.17	1.26	1.52
1	A	40	LYS	C-N	12.16	1.62	1.34
2	D	79	ASP	N-CA	-12.15	1.22	1.46
2	B	32	VAL	CB-CG1	-12.15	1.27	1.52
2	B	99	PRO	C-N	12.15	1.61	1.34
2	D	108	VAL	CB-CG1	-12.15	1.27	1.52
2	D	10	VAL	C-N	12.14	1.61	1.34
2	D	32	VAL	CB-CG2	-12.12	1.27	1.52
1	A	87	HIS	C-N	12.12	1.61	1.34
2	D	14	TRP	CD2-CE2	12.12	1.55	1.41
2	B	44	PHE	CE2-CZ	-12.11	1.14	1.37
1	C	53	ALA	N-CA	12.10	1.70	1.46
1	C	17	VAL	CB-CG1	12.10	1.78	1.52
2	D	71	THR	CB-CG2	12.10	1.92	1.52
2	D	54	MET	C-N	12.10	1.61	1.34
2	D	89	GLY	CA-C	12.07	1.71	1.51
1	C	114	PRO	N-CA	12.07	1.67	1.47
1	C	128	PHE	CG-CD2	-12.07	1.20	1.38
2	B	84	PHE	CE1-CZ	12.06	1.60	1.37
1	C	16	LYS	C-O	-12.06	1.00	1.23
2	D	120	GLN	CG-CD	12.05	1.78	1.51
2	B	14	TRP	N-CA	-12.03	1.22	1.46
2	D	54	MET	CG-SD	12.01	2.12	1.81
2	D	44	PHE	CE1-CZ	12.00	1.60	1.37
2	D	59	VAL	CA-C	12.00	1.84	1.52
2	B	110	ALA	C-O	-11.99	1.00	1.23
2	D	2	LEU	CA-CB	11.99	1.81	1.53
2	D	29	ARG	C-O	-11.99	1.00	1.23
2	D	140	LEU	C-O	-11.98	1.00	1.23
1	C	98	PHE	CG-CD2	11.97	1.56	1.38
2	B	72	GLN	N-CA	11.97	1.70	1.46
2	D	14	TRP	CD1-NE1	-11.97	1.17	1.38
1	A	82	ASN	CG-OD1	11.96	1.50	1.24
1	C	68	LYS	CE-NZ	11.96	1.78	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	42	TYR	CZ-OH	-11.95	1.17	1.37
1	C	47	ASP	CB-CG	11.94	1.76	1.51
2	D	115	ARG	C-N	11.94	1.61	1.34
2	B	134	ALA	C-N	11.93	1.54	1.33
2	D	86	GLN	CA-C	11.93	1.83	1.52
1	C	66	LEU	CB-CG	-11.93	1.18	1.52
2	D	121	PHE	CG-CD1	-11.93	1.20	1.38
2	B	62	HIS	CG-CD2	11.92	1.56	1.35
1	C	87	HIS	CG-CD2	-11.91	1.15	1.35
1	A	94	ASN	C-N	11.89	1.56	1.34
2	D	86	GLN	CB-CG	-11.89	1.20	1.52
2	D	59	VAL	CB-CG2	11.89	1.77	1.52
2	D	79	ASP	CG-OD1	-11.88	0.98	1.25
1	A	48	LEU	CB-CG	-11.87	1.18	1.52
2	D	31	LEU	CA-CB	11.87	1.81	1.53
1	A	95	PRO	N-CD	11.87	1.64	1.47
1	C	108	THR	C-N	-11.87	1.06	1.34
2	B	16	LYS	CD-CE	11.86	1.80	1.51
1	C	89	HIS	CD2-NE2	11.85	1.66	1.42
2	D	99	PRO	CG-CD	-11.85	1.11	1.50
1	C	77	PRO	C-O	11.82	1.46	1.23
2	D	102	PHE	CD1-CE1	-11.82	1.15	1.39
1	A	45	HIS	CE1-NE2	11.82	1.59	1.32
2	D	16	LYS	C-O	11.82	1.45	1.23
1	C	85	ASN	CA-C	11.78	1.83	1.52
2	D	107	ASN	N-CA	11.77	1.69	1.46
1	C	54	GLN	C-O	11.77	1.45	1.23
1	A	115	THR	CB-OG1	11.76	1.66	1.43
1	A	112	HIS	C-N	11.76	1.61	1.34
2	D	145	HIS	CA-C	11.75	1.83	1.52
1	A	14	TRP	C-N	-11.75	1.11	1.33
2	D	15	GLY	C-N	-11.75	1.07	1.34
1	A	6	ASN	CG-OD1	11.74	1.49	1.24
2	B	38	GLN	CB-CG	-11.74	1.20	1.52
1	A	141	ARG	N-CA	-11.74	1.22	1.46
2	B	16	LYS	CA-C	-11.73	1.22	1.52
1	C	61	LYS	C-O	11.73	1.45	1.23
1	A	121	VAL	C-N	11.73	1.61	1.34
2	B	4	ALA	N-CA	11.72	1.69	1.46
2	B	113	VAL	C-O	-11.71	1.01	1.23
1	A	33	PHE	CA-CB	-11.70	1.28	1.53
2	B	112	VAL	C-O	-11.70	1.01	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	PHE	CA-C	-11.68	1.22	1.52
2	B	73	GLY	CA-C	-11.68	1.33	1.51
2	B	102	PHE	CA-C	-11.68	1.22	1.52
1	C	79	THR	N-CA	11.67	1.69	1.46
1	A	110	ALA	C-O	11.67	1.45	1.23
1	C	95	PRO	CA-C	-11.66	1.29	1.52
1	C	110	ALA	CA-CB	-11.66	1.27	1.52
1	C	45	HIS	C-O	11.63	1.45	1.23
1	A	100	LEU	CB-CG	11.62	1.86	1.52
2	B	117	PHE	CG-CD2	-11.62	1.21	1.38
2	B	141	ALA	N-CA	11.62	1.69	1.46
2	D	144	TYR	N-CA	-11.62	1.23	1.46
2	D	124	ASN	CA-C	11.61	1.83	1.52
1	A	116	ASN	N-CA	11.60	1.69	1.46
1	C	25	GLY	CA-C	-11.60	1.33	1.51
2	D	93	ASN	N-CA	-11.59	1.23	1.46
2	D	110	ALA	N-CA	11.59	1.69	1.46
2	B	34	TYR	C-N	-11.59	1.12	1.34
1	C	134	THR	C-O	11.58	1.45	1.23
1	C	69	ALA	CA-C	11.57	1.83	1.52
2	D	67	LEU	CB-CG	-11.57	1.19	1.52
2	D	6	GLU	CA-CB	11.57	1.79	1.53
2	D	125	VAL	CA-C	-11.57	1.22	1.52
1	C	57	ALA	CA-C	-11.56	1.23	1.52
1	A	93	VAL	C-O	-11.55	1.01	1.23
1	A	116	ASN	C-N	-11.53	1.07	1.34
1	A	103	HIS	CD2-NE2	11.52	1.66	1.42
1	A	89	HIS	CG-ND1	11.51	1.64	1.38
2	B	16	LYS	C-O	11.51	1.45	1.23
1	C	28	ALA	N-CA	11.50	1.69	1.46
1	C	67	THR	C-O	-11.50	1.01	1.23
1	C	128	PHE	C-N	-11.50	1.07	1.34
1	A	7	LYS	CD-CE	11.48	1.79	1.51
1	A	60	GLN	C-N	-11.44	1.07	1.34
2	D	137	ALA	C-O	-11.44	1.01	1.23
1	A	55	GLN	C-N	-11.43	1.07	1.34
1	C	111	SER	N-CA	-11.43	1.23	1.46
1	C	19	GLY	N-CA	-11.43	1.28	1.46
1	A	8	SER	CA-C	-11.42	1.23	1.52
1	C	71	GLY	N-CA	-11.42	1.28	1.46
2	D	133	VAL	CB-CG2	-11.42	1.28	1.52
2	B	87	LEU	CG-CD1	11.42	1.94	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	79	ASP	CG-OD2	11.42	1.51	1.25
1	C	91	LEU	N-CA	11.40	1.69	1.46
1	A	97	ASN	N-CA	11.40	1.69	1.46
2	B	37	THR	N-CA	11.39	1.69	1.46
1	C	58	HIS	CG-CD2	11.39	1.55	1.35
2	D	145	HIS	ND1-CE1	11.39	1.63	1.34
1	A	67	THR	CA-C	11.38	1.82	1.52
1	A	44	PRO	CA-CB	11.37	1.76	1.53
2	D	42	GLN	CG-CD	-11.37	1.24	1.51
2	D	68	ASP	CA-C	11.37	1.82	1.52
2	D	129	PHE	CE1-CZ	11.36	1.58	1.37
1	C	6	ASN	C-O	-11.36	1.01	1.23
1	A	112	HIS	CB-CG	-11.36	1.29	1.50
1	A	108	THR	CA-CB	11.35	1.82	1.53
1	A	128	PHE	CB-CG	-11.35	1.32	1.51
1	C	64	ASN	CA-CB	11.34	1.82	1.53
2	B	144	TYR	C-N	11.33	1.60	1.34
2	D	100	GLN	CB-CG	11.32	1.83	1.52
1	C	140	TYR	C-O	11.32	1.44	1.23
1	A	50	HIS	CD2-NE2	11.30	1.65	1.42
2	B	33	VAL	C-O	-11.30	1.01	1.23
2	D	46	ASN	N-CA	11.30	1.69	1.46
1	A	136	LEU	CB-CG	-11.28	1.19	1.52
2	B	25	GLN	N-CA	11.28	1.69	1.46
2	B	140	LEU	CB-CG	-11.27	1.19	1.52
2	B	111	LEU	C-O	-11.26	1.01	1.23
1	C	83	LEU	CA-CB	11.26	1.79	1.53
1	A	24	TYR	CB-CG	-11.25	1.34	1.51
2	B	115	ARG	C-O	-11.24	1.01	1.23
2	B	74	LEU	CG-CD1	11.24	1.93	1.51
1	A	20	ASN	CA-CB	-11.23	1.24	1.53
1	A	65	ALA	CA-CB	11.22	1.76	1.52
2	B	123	PRO	N-CD	11.22	1.63	1.47
2	B	77	LEU	CA-CB	11.22	1.79	1.53
2	B	140	LEU	CG-CD2	11.21	1.93	1.51
2	B	24	ALA	N-CA	11.21	1.68	1.46
1	A	119	PRO	N-CA	11.19	1.66	1.47
1	A	74	ASN	CA-C	-11.14	1.24	1.52
1	A	23	ALA	N-CA	-11.13	1.24	1.46
2	B	136	VAL	CA-C	11.13	1.81	1.52
1	C	20	ASN	CG-OD1	11.13	1.48	1.24
2	D	68	ASP	CG-OD1	-11.13	0.99	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	PRO	CG-CD	11.12	1.87	1.50
1	C	76	LEU	N-CA	-11.12	1.24	1.46
1	A	92	ARG	C-O	11.12	1.44	1.23
1	C	115	THR	C-N	-11.11	1.08	1.34
2	D	26	ALA	CA-CB	-11.10	1.29	1.52
1	A	120	ALA	C-O	11.09	1.44	1.23
2	D	93	ASN	CB-CG	11.08	1.76	1.51
2	B	7	LYS	N-CA	-11.07	1.24	1.46
2	B	32	VAL	CA-C	-11.07	1.24	1.52
1	A	51	GLY	CA-C	11.05	1.69	1.51
2	D	71	THR	N-CA	-11.05	1.24	1.46
1	C	115	THR	N-CA	-11.05	1.24	1.46
1	A	31	ARG	CZ-NH1	-11.04	1.18	1.33
1	C	65	ALA	C-O	11.04	1.44	1.23
2	B	25	GLN	C-O	11.04	1.44	1.23
2	B	96	HIS	CD2-NE2	11.03	1.65	1.42
1	C	2	LEU	N-CA	-11.03	1.24	1.46
1	A	88	ALA	C-O	11.03	1.44	1.23
1	A	64	ASN	CA-C	11.02	1.81	1.52
2	D	90	LEU	CB-CG	11.02	1.84	1.52
1	A	19	GLY	C-O	-10.99	1.06	1.23
1	C	91	LEU	CA-CB	-10.97	1.28	1.53
2	D	101	ASN	N-CA	10.96	1.68	1.46
2	B	131	LYS	C-N	10.96	1.59	1.34
2	D	122	THR	CA-C	-10.96	1.24	1.52
2	B	21	VAL	CA-CB	10.94	1.77	1.54
1	C	23	ALA	CA-CB	10.94	1.75	1.52
2	D	31	LEU	CA-C	10.93	1.81	1.52
2	B	136	VAL	C-O	10.93	1.44	1.23
2	B	16	LYS	N-CA	10.93	1.68	1.46
2	B	39	ARG	CA-C	-10.92	1.24	1.52
1	C	132	ASP	C-O	10.92	1.44	1.23
2	D	140	LEU	CA-CB	-10.91	1.28	1.53
1	A	43	PHE	CA-CB	10.91	1.77	1.53
1	C	131	ASN	CA-CB	10.90	1.81	1.53
2	B	64	LYS	CA-C	-10.90	1.24	1.52
2	D	34	TYR	CG-CD2	-10.90	1.25	1.39
1	A	136	LEU	C-O	10.89	1.44	1.23
2	D	16	LYS	CA-C	-10.87	1.24	1.52
1	C	82	ASN	C-O	-10.87	1.02	1.23
2	D	106	GLY	C-N	10.87	1.59	1.34
1	A	1	VAL	CB-CG1	10.87	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	40	PHE	C-O	10.86	1.44	1.23
1	A	93	VAL	N-CA	-10.86	1.24	1.46
2	B	68	ASP	CB-CG	10.85	1.74	1.51
1	A	73	LEU	CA-CB	-10.84	1.28	1.53
2	B	113	VAL	CA-CB	-10.84	1.31	1.54
2	B	30	LEU	C-N	10.84	1.58	1.34
2	D	95	LEU	N-CA	-10.83	1.24	1.46
2	D	55	ASN	CG-ND2	10.83	1.59	1.32
2	D	145	HIS	N-CA	-10.81	1.24	1.46
2	B	51	GLY	C-O	10.81	1.41	1.23
2	D	35	PRO	N-CA	10.80	1.65	1.47
1	A	29	LEU	CG-CD2	10.80	1.91	1.51
2	D	41	PHE	CG-CD2	-10.78	1.22	1.38
2	B	64	LYS	N-CA	10.78	1.68	1.46
2	B	74	LEU	CB-CG	10.78	1.83	1.52
1	A	111	SER	CB-OG	-10.77	1.28	1.42
1	C	32	MET	C-O	-10.77	1.02	1.23
2	D	27	LEU	C-N	10.77	1.52	1.33
2	D	93	ASN	CA-C	10.77	1.80	1.52
1	C	125	LEU	CA-CB	-10.76	1.28	1.53
1	C	92	ARG	CG-CD	10.76	1.78	1.51
2	D	60	LYS	CD-CE	10.75	1.78	1.51
1	A	54	GLN	CA-CB	-10.75	1.30	1.53
1	A	113	LEU	C-N	10.75	1.54	1.34
2	D	118	GLY	C-O	10.74	1.40	1.23
2	B	1	MET	SD-CE	10.72	2.37	1.77
1	A	63	ALA	CA-CB	10.72	1.75	1.52
1	A	136	LEU	CA-C	10.72	1.80	1.52
1	A	82	ASN	C-O	10.71	1.43	1.23
2	D	60	LYS	CA-CB	-10.70	1.30	1.53
2	B	55	ASN	CG-ND2	10.69	1.59	1.32
1	C	136	LEU	CA-CB	10.68	1.78	1.53
2	B	14	TRP	CZ2-CH2	-10.68	1.17	1.37
2	B	136	VAL	C-N	-10.67	1.09	1.34
1	A	71	GLY	CA-C	-10.67	1.34	1.51
2	B	143	LYS	CG-CD	10.67	1.88	1.52
2	B	70	PHE	CG-CD1	-10.66	1.22	1.38
1	C	42	TYR	C-N	-10.66	1.09	1.34
2	D	97	VAL	CA-CB	-10.66	1.32	1.54
2	D	38	GLN	CG-CD	10.65	1.75	1.51
1	C	55	GLN	CD-OE1	10.65	1.47	1.24
2	D	29	ARG	CG-CD	-10.64	1.25	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	111	LEU	CG-CD1	-10.63	1.12	1.51
2	D	90	LEU	C-N	10.63	1.58	1.34
2	B	76	HIS	CE1-NE2	-10.62	1.08	1.32
2	D	102	PHE	C-N	-10.62	1.09	1.34
2	B	46	ASN	CG-ND2	-10.62	1.06	1.32
1	C	91	LEU	C-O	10.62	1.43	1.23
2	D	80	LEU	CG-CD2	-10.62	1.12	1.51
2	B	138	ASN	N-CA	-10.61	1.25	1.46
2	D	131	LYS	C-O	-10.61	1.03	1.23
2	B	99	PRO	C-O	10.61	1.44	1.23
1	C	92	ARG	NE-CZ	10.60	1.46	1.33
1	C	50	HIS	ND1-CE1	10.59	1.61	1.34
1	C	16	LYS	CG-CD	10.59	1.88	1.52
1	A	46	PHE	N-CA	-10.59	1.25	1.46
2	D	38	GLN	C-N	10.58	1.58	1.34
2	D	138	ASN	C-O	10.58	1.43	1.23
2	B	23	GLY	CA-C	-10.57	1.34	1.51
1	A	8	SER	CB-OG	10.56	1.55	1.42
2	B	70	PHE	N-CA	10.55	1.67	1.46
2	B	91	HIS	C-O	10.55	1.43	1.23
1	C	46	PHE	C-O	-10.55	1.03	1.23
1	C	92	ARG	CZ-NH1	-10.54	1.19	1.33
2	B	36	TRP	C-N	10.53	1.58	1.34
1	C	75	ASP	CA-CB	10.53	1.77	1.53
1	C	50	HIS	N-CA	10.52	1.67	1.46
1	C	13	ALA	N-CA	-10.52	1.25	1.46
1	A	16	LYS	CD-CE	10.52	1.77	1.51
2	D	117	PHE	CG-CD1	-10.50	1.23	1.38
1	A	57	ALA	CA-CB	10.49	1.74	1.52
1	C	49	SER	CA-CB	-10.49	1.37	1.52
1	C	67	THR	CB-CG2	10.49	1.86	1.52
2	D	25	GLN	C-N	10.49	1.58	1.34
2	D	62	HIS	CD2-NE2	10.49	1.64	1.42
1	A	11	LYS	CG-CD	-10.48	1.16	1.52
2	B	53	VAL	C-O	10.47	1.43	1.23
1	C	132	ASP	C-N	-10.47	1.09	1.34
1	C	29	LEU	CA-CB	10.46	1.77	1.53
2	B	82	GLY	CA-C	-10.46	1.35	1.51
1	C	11	LYS	CA-C	-10.46	1.25	1.52
2	D	95	LEU	C-N	-10.46	1.10	1.34
2	B	70	PHE	C-N	10.45	1.58	1.34
2	D	50	ALA	C-O	10.45	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	LYS	CD-CE	10.44	1.77	1.51
2	D	63	GLY	CA-C	10.43	1.68	1.51
1	A	48	LEU	CG-CD2	10.42	1.90	1.51
1	C	34	LEU	CA-CB	-10.42	1.29	1.53
1	C	122	HIS	CA-CB	-10.41	1.31	1.53
1	A	137	THR	CB-CG2	10.41	1.86	1.52
1	C	84	SER	C-O	10.40	1.43	1.23
1	A	29	LEU	N-CA	10.39	1.67	1.46
2	D	99	PRO	CA-C	-10.39	1.32	1.52
2	D	22	VAL	CB-CG1	10.39	1.74	1.52
1	A	41	THR	CA-CB	10.38	1.80	1.53
1	C	88	ALA	C-N	-10.37	1.10	1.34
1	C	45	HIS	CG-ND1	10.37	1.61	1.38
2	B	40	PHE	CA-C	10.36	1.79	1.52
2	D	22	VAL	CB-CG2	10.36	1.74	1.52
1	A	93	VAL	CB-CG2	10.36	1.74	1.52
1	C	29	LEU	CB-CG	-10.36	1.22	1.52
2	D	86	GLN	CA-CB	10.36	1.76	1.53
2	D	86	GLN	CD-OE1	10.35	1.46	1.24
2	B	61	ALA	CA-C	-10.35	1.26	1.52
1	C	43	PHE	CE1-CZ	-10.35	1.17	1.37
1	C	87	HIS	CE1-NE2	10.35	1.56	1.32
2	D	31	LEU	CG-CD1	-10.35	1.13	1.51
2	D	123	PRO	CB-CG	-10.35	0.98	1.50
2	D	44	PHE	C-N	-10.35	1.14	1.33
2	D	81	LYS	CA-CB	10.35	1.76	1.53
2	D	142	HIS	CG-ND1	10.34	1.61	1.38
1	A	48	LEU	C-O	10.34	1.43	1.23
1	A	129	LEU	C-O	-10.33	1.03	1.23
1	A	137	THR	C-O	-10.33	1.03	1.23
1	A	127	LYS	CD-CE	10.32	1.77	1.51
1	A	138	SER	C-O	10.31	1.43	1.23
2	B	119	GLY	CA-C	-10.30	1.35	1.51
2	B	13	PHE	CA-C	10.30	1.79	1.52
2	D	87	LEU	CB-CG	-10.30	1.22	1.52
1	C	125	LEU	CG-CD1	-10.29	1.13	1.51
1	C	101	LEU	CA-CB	10.29	1.77	1.53
1	C	82	ASN	C-N	10.28	1.57	1.34
1	C	26	ALA	N-CA	-10.28	1.25	1.46
1	C	45	HIS	C-N	10.28	1.57	1.34
1	A	138	SER	N-CA	10.27	1.66	1.46
1	A	89	HIS	N-CA	-10.27	1.25	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	80	LEU	N-CA	-10.27	1.25	1.46
2	B	41	PHE	N-CA	10.27	1.66	1.46
2	D	47	LEU	C-O	-10.26	1.03	1.23
2	D	96	HIS	CB-CG	-10.26	1.31	1.50
2	B	88	SER	CA-C	-10.26	1.26	1.52
2	D	1	MET	C-N	10.25	1.57	1.34
1	A	10	VAL	C-O	10.25	1.42	1.23
1	A	6	ASN	CG-ND2	10.24	1.58	1.32
1	C	32	MET	CA-CB	10.24	1.76	1.53
2	D	11	THR	CA-C	10.24	1.79	1.52
2	B	5	GLU	C-N	-10.24	1.10	1.34
1	C	141	ARG	CA-CB	-10.24	1.31	1.53
2	B	75	LYS	CG-CD	10.23	1.87	1.52
2	D	76	HIS	CE1-NE2	10.23	1.56	1.32
2	D	93	ASN	CA-CB	-10.22	1.26	1.53
1	A	36	PHE	CD2-CE2	10.22	1.59	1.39
2	B	11	THR	CA-CB	10.22	1.79	1.53
2	B	36	TRP	CE3-CZ3	-10.21	1.21	1.38
1	C	105	LEU	CG-CD1	10.19	1.89	1.51
2	B	145	HIS	CD2-NE2	-10.18	1.15	1.38
1	A	137	THR	C-N	10.17	1.57	1.34
2	B	20	ASP	CA-C	-10.16	1.26	1.52
2	B	2	LEU	CG-CD2	10.16	1.89	1.51
2	D	97	VAL	C-N	-10.15	1.10	1.34
2	B	33	VAL	CB-CG1	10.15	1.74	1.52
2	D	36	TRP	CA-C	10.13	1.79	1.52
2	D	49	SER	N-CA	10.12	1.66	1.46
1	C	83	LEU	C-O	10.12	1.42	1.23
1	C	108	THR	C-O	10.12	1.42	1.23
1	C	61	LYS	C-N	-10.12	1.10	1.34
1	C	118	THR	CB-OG1	10.12	1.63	1.43
2	D	47	LEU	CA-CB	10.11	1.77	1.53
2	B	128	LEU	CG-CD2	10.10	1.89	1.51
1	A	63	ALA	CA-C	-10.09	1.26	1.52
1	A	126	ASN	CA-C	10.06	1.79	1.52
1	A	73	LEU	C-N	-10.06	1.10	1.34
1	A	117	PHE	CE2-CZ	10.06	1.56	1.37
1	A	139	LYS	N-CA	-10.06	1.26	1.46
2	D	32	VAL	C-O	-10.05	1.04	1.23
1	A	137	THR	CA-CB	10.04	1.79	1.53
2	D	109	LEU	CG-CD2	10.04	1.89	1.51
2	D	142	HIS	N-CA	10.04	1.66	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	48	LEU	CG-CD1	-10.04	1.14	1.51
1	A	83	LEU	C-O	10.03	1.42	1.23
2	D	5	GLU	CB-CG	-10.02	1.33	1.52
2	B	27	LEU	C-N	-10.02	1.15	1.33
2	B	23	GLY	C-N	-10.02	1.11	1.34
1	C	16	LYS	C-N	10.01	1.57	1.34
2	D	81	LYS	C-O	-10.01	1.04	1.23
1	A	112	HIS	CD2-NE2	10.00	1.62	1.42
1	C	9	ASN	C-N	9.99	1.57	1.34
2	B	61	ALA	N-CA	9.98	1.66	1.46
2	B	116	ASN	C-O	9.98	1.42	1.23
1	A	10	VAL	C-N	-9.96	1.11	1.34
2	D	119	GLY	C-N	9.95	1.56	1.34
2	B	10	VAL	C-O	-9.95	1.04	1.23
1	C	106	LEU	CG-CD1	-9.95	1.15	1.51
1	A	33	PHE	CE2-CZ	-9.94	1.18	1.37
1	C	38	THR	CA-CB	-9.94	1.27	1.53
1	A	2	LEU	CA-CB	9.93	1.76	1.53
2	B	120	GLN	CD-OE1	9.93	1.45	1.24
1	C	119	PRO	C-O	-9.92	1.03	1.23
1	C	79	THR	C-N	9.92	1.56	1.34
2	D	63	GLY	N-CA	-9.91	1.31	1.46
2	D	145	HIS	C-OXT	9.91	1.42	1.23
1	A	54	GLN	CD-NE2	9.91	1.57	1.32
2	D	88	SER	CA-C	-9.90	1.27	1.52
2	D	91	HIS	CD2-NE2	-9.89	1.16	1.38
1	C	16	LYS	CA-CB	-9.89	1.32	1.53
2	B	13	PHE	C-O	-9.88	1.04	1.23
1	C	10	VAL	C-O	-9.88	1.04	1.23
1	C	130	ALA	CA-C	-9.88	1.27	1.52
2	B	112	VAL	CB-CG1	-9.88	1.32	1.52
1	A	69	ALA	CA-C	-9.87	1.27	1.52
2	B	109	LEU	CG-CD1	-9.87	1.15	1.51
1	C	40	LYS	CA-CB	-9.85	1.32	1.53
2	B	14	TRP	CZ3-CH2	-9.85	1.24	1.40
2	B	116	ASN	CB-CG	-9.83	1.28	1.51
2	B	112	VAL	CB-CG2	-9.83	1.32	1.52
2	B	43	HIS	CA-C	9.82	1.78	1.52
2	D	83	ALA	CA-CB	9.82	1.73	1.52
2	D	129	PHE	CB-CG	-9.82	1.34	1.51
1	A	13	ALA	N-CA	9.81	1.66	1.46
2	D	36	TRP	CG-CD2	9.79	1.60	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	94	LYS	N-CA	-9.79	1.26	1.46
1	C	33	PHE	CE1-CZ	9.79	1.55	1.37
2	B	61	ALA	CA-CB	-9.79	1.31	1.52
2	D	100	GLN	C-N	-9.78	1.11	1.34
1	A	68	LYS	CD-CE	-9.77	1.26	1.51
2	D	81	LYS	CD-CE	9.77	1.75	1.51
2	D	131	LYS	CB-CG	9.76	1.78	1.52
2	D	121	PHE	CE1-CZ	9.76	1.55	1.37
2	D	121	PHE	C-O	-9.76	1.04	1.23
1	A	127	LYS	CB-CG	9.74	1.78	1.52
1	A	43	PHE	CD1-CE1	-9.74	1.19	1.39
2	D	120	GLN	CB-CG	9.74	1.78	1.52
2	B	7	LYS	C-O	-9.73	1.04	1.23
1	A	121	VAL	N-CA	-9.71	1.26	1.46
2	B	97	VAL	CA-CB	9.71	1.75	1.54
2	D	89	GLY	C-O	-9.71	1.08	1.23
1	A	99	LYS	C-N	-9.70	1.11	1.34
2	B	26	ALA	CA-CB	-9.70	1.32	1.52
1	A	54	GLN	CD-OE1	-9.70	1.02	1.24
2	D	116	ASN	N-CA	-9.69	1.26	1.46
2	B	49	SER	CA-CB	9.69	1.67	1.52
2	D	52	ALA	C-O	9.68	1.41	1.23
2	B	52	ALA	C-N	9.66	1.56	1.34
1	C	22	PRO	CG-CD	9.66	1.82	1.50
2	B	18	ASP	C-O	-9.66	1.05	1.23
2	B	65	ARG	CA-C	-9.66	1.27	1.52
2	D	144	TYR	CE2-CZ	9.65	1.51	1.38
1	A	112	HIS	CE1-NE2	9.65	1.54	1.32
2	D	102	PHE	CG-CD1	9.64	1.53	1.38
2	D	10	VAL	C-O	-9.63	1.05	1.23
2	D	59	VAL	C-O	9.63	1.41	1.23
2	D	143	LYS	CB-CG	-9.63	1.26	1.52
2	B	38	GLN	C-N	-9.62	1.11	1.34
2	B	104	LEU	CA-C	-9.61	1.27	1.52
1	A	2	LEU	CG-CD1	9.61	1.87	1.51
2	B	121	PHE	CE1-CZ	-9.61	1.19	1.37
2	D	36	TRP	CA-CB	-9.61	1.32	1.53
1	C	140	TYR	CZ-OH	-9.61	1.21	1.37
1	A	83	LEU	C-N	-9.61	1.11	1.34
1	C	133	SER	CB-OG	-9.60	1.29	1.42
2	B	57	PRO	CA-C	9.60	1.72	1.52
1	A	135	VAL	CA-C	9.59	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	32	VAL	C-N	-9.59	1.11	1.34
1	A	128	PHE	C-N	9.59	1.56	1.34
1	A	85	ASN	N-CA	9.59	1.65	1.46
2	D	53	VAL	CB-CG1	9.58	1.73	1.52
2	D	91	HIS	N-CA	9.56	1.65	1.46
2	D	14	TRP	CB-CG	-9.56	1.33	1.50
2	B	103	ARG	CB-CG	9.55	1.78	1.52
2	B	103	ARG	CA-CB	-9.53	1.32	1.53
1	A	8	SER	N-CA	9.52	1.65	1.46
2	D	34	TYR	CD2-CE2	9.52	1.53	1.39
1	C	30	GLN	CD-OE1	9.52	1.44	1.24
1	C	10	VAL	CB-CG1	9.51	1.72	1.52
2	D	14	TRP	CA-C	9.51	1.77	1.52
1	A	27	GLN	CA-CB	-9.51	1.33	1.53
2	D	102	PHE	CG-CD2	9.50	1.53	1.38
1	C	116	ASN	CA-C	9.50	1.77	1.52
1	A	39	THR	CA-CB	-9.49	1.28	1.53
2	B	31	LEU	C-N	9.49	1.55	1.34
1	C	140	TYR	C-N	9.49	1.55	1.34
1	C	37	PRO	N-CA	9.48	1.63	1.47
2	B	47	LEU	CG-CD2	-9.48	1.16	1.51
1	C	101	LEU	N-CA	9.48	1.65	1.46
1	C	27	GLN	C-O	-9.48	1.05	1.23
1	C	107	VAL	C-O	9.47	1.41	1.23
2	D	98	ASN	N-CA	-9.47	1.27	1.46
1	C	133	SER	CA-C	9.47	1.77	1.52
1	A	114	PRO	CG-CD	9.46	1.81	1.50
2	D	135	GLY	C-O	-9.46	1.08	1.23
2	D	65	ARG	N-CA	-9.45	1.27	1.46
1	C	77	PRO	N-CA	9.45	1.63	1.47
2	D	80	LEU	C-O	-9.44	1.05	1.23
2	D	98	ASN	CG-ND2	-9.44	1.09	1.32
2	B	116	ASN	CA-CB	9.44	1.77	1.53
1	C	41	THR	N-CA	9.44	1.65	1.46
1	C	136	LEU	C-N	-9.43	1.12	1.34
1	A	60	GLN	CA-C	9.43	1.77	1.52
2	B	90	LEU	CA-CB	-9.41	1.32	1.53
2	B	105	LEU	C-N	9.41	1.50	1.33
1	A	92	ARG	CD-NE	9.41	1.62	1.46
2	D	20	ASP	CA-CB	-9.41	1.33	1.53
1	C	114	PRO	C-N	9.40	1.55	1.34
1	A	87	HIS	CG-ND1	9.40	1.59	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	HIS	ND1-CE1	9.40	1.58	1.34
1	A	134	THR	C-N	-9.39	1.12	1.34
1	A	24	TYR	CA-C	-9.39	1.28	1.52
1	C	36	PHE	CA-C	-9.39	1.28	1.52
2	B	40	PHE	N-CA	9.39	1.65	1.46
1	A	75	ASP	CB-CG	9.38	1.71	1.51
2	B	80	LEU	CB-CG	-9.38	1.25	1.52
2	B	25	GLN	CA-CB	-9.38	1.33	1.53
1	A	35	SER	C-O	-9.38	1.05	1.23
2	B	83	ALA	C-O	9.37	1.41	1.23
1	A	14	TRP	CA-C	-9.36	1.28	1.52
1	A	73	LEU	CG-CD1	9.36	1.86	1.51
1	C	22	PRO	CA-C	-9.36	1.34	1.52
2	D	6	GLU	CD-OE1	9.36	1.35	1.25
1	C	69	ALA	C-N	-9.35	1.12	1.34
2	B	13	PHE	CD1-CE1	9.34	1.57	1.39
2	B	88	SER	C-O	9.34	1.41	1.23
1	A	36	PHE	CG-CD1	-9.33	1.24	1.38
1	C	77	PRO	N-CD	9.32	1.60	1.47
2	D	112	VAL	CB-CG2	-9.32	1.33	1.52
2	D	22	VAL	CA-CB	-9.31	1.35	1.54
2	D	14	TRP	C-O	-9.31	1.05	1.23
1	C	101	LEU	C-N	-9.31	1.12	1.34
2	D	103	ARG	CG-CD	9.30	1.75	1.51
2	B	13	PHE	N-CA	9.29	1.65	1.46
2	B	88	SER	CA-CB	-9.29	1.39	1.52
1	A	44	PRO	C-N	-9.28	1.12	1.34
1	A	39	THR	CA-C	-9.28	1.28	1.52
2	D	16	LYS	CD-CE	9.28	1.74	1.51
1	C	104	SER	CA-C	9.28	1.77	1.52
1	A	92	ARG	NE-CZ	9.27	1.45	1.33
2	D	55	ASN	C-O	9.27	1.41	1.23
1	A	129	LEU	N-CA	9.25	1.64	1.46
2	B	76	HIS	C-O	9.25	1.41	1.23
2	D	10	VAL	CA-C	9.25	1.76	1.52
1	C	87	HIS	C-O	9.24	1.41	1.23
2	B	44	PHE	C-N	9.24	1.49	1.33
2	D	107	ASN	C-O	-9.24	1.05	1.23
1	C	62	VAL	C-O	-9.24	1.05	1.23
1	A	110	ALA	CA-CB	9.23	1.71	1.52
1	A	62	VAL	C-O	9.23	1.40	1.23
1	C	89	HIS	C-O	-9.23	1.05	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	97	VAL	CB-CG1	9.23	1.72	1.52
1	C	97	ASN	CA-C	9.23	1.76	1.52
1	C	126	ASN	C-N	-9.22	1.12	1.34
2	D	30	LEU	N-CA	-9.22	1.27	1.46
1	A	11	LYS	CE-NZ	9.22	1.72	1.49
2	D	84	PHE	CG-CD2	-9.22	1.25	1.38
1	A	71	GLY	C-N	9.20	1.55	1.34
1	A	106	LEU	CG-CD2	9.20	1.85	1.51
2	B	62	HIS	ND1-CE1	9.20	1.57	1.34
1	A	30	GLN	CA-CB	-9.20	1.33	1.53
1	A	3	SER	N-CA	9.19	1.64	1.46
1	C	50	HIS	CE1-NE2	9.19	1.53	1.32
2	B	87	LEU	CA-C	9.18	1.76	1.52
1	C	77	PRO	CB-CG	9.17	1.95	1.50
2	B	116	ASN	C-N	-9.16	1.12	1.34
2	D	142	HIS	CE1-NE2	9.16	1.53	1.32
2	B	14	TRP	CD1-NE1	-9.16	1.22	1.38
1	C	62	VAL	CB-CG1	9.15	1.72	1.52
1	C	97	ASN	CG-OD1	-9.15	1.03	1.24
2	B	25	GLN	CD-NE2	9.15	1.55	1.32
2	D	71	THR	C-O	-9.15	1.05	1.23
2	B	71	THR	C-N	-9.14	1.13	1.34
1	C	131	ASN	CB-CG	9.14	1.72	1.51
2	B	86	GLN	CD-OE1	9.14	1.44	1.24
2	B	140	LEU	C-N	9.13	1.55	1.34
2	B	9	ALA	CA-CB	-9.12	1.33	1.52
1	C	35	SER	N-CA	-9.12	1.28	1.46
2	D	78	ASP	C-O	-9.11	1.06	1.23
2	B	35	PRO	C-O	-9.11	1.05	1.23
1	A	135	VAL	N-CA	-9.10	1.28	1.46
2	D	41	PHE	CA-C	-9.10	1.29	1.52
1	C	54	GLN	CA-C	9.09	1.76	1.52
1	A	61	LYS	C-O	9.09	1.40	1.23
1	A	80	LEU	CG-CD2	9.08	1.85	1.51
2	D	75	LYS	CE-NZ	9.08	1.71	1.49
1	A	100	LEU	CG-CD1	-9.07	1.18	1.51
2	B	130	GLN	CB-CG	9.07	1.77	1.52
2	B	77	LEU	CA-C	-9.06	1.29	1.52
2	D	24	ALA	CA-C	-9.06	1.29	1.52
1	C	122	HIS	ND1-CE1	9.06	1.57	1.34
1	C	70	GLN	C-O	9.03	1.40	1.23
1	A	10	VAL	CA-C	9.02	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	TRP	CA-CB	9.01	1.73	1.53
1	C	87	HIS	CD2-NE2	-9.01	1.18	1.38
1	A	31	ARG	CG-CD	9.01	1.74	1.51
1	C	103	HIS	CD2-NE2	-9.01	1.18	1.38
1	A	22	PRO	C-O	9.01	1.41	1.23
1	C	60	GLN	CD-OE1	9.00	1.43	1.24
1	A	83	LEU	N-CA	-9.00	1.28	1.46
1	C	7	LYS	C-O	9.00	1.40	1.23
1	A	122	HIS	C-N	-8.99	1.13	1.34
1	A	70	GLN	CA-CB	-8.99	1.34	1.53
1	A	88	ALA	CA-C	8.98	1.76	1.52
1	A	90	LYS	CG-CD	-8.97	1.22	1.52
1	C	79	THR	CB-OG1	-8.96	1.25	1.43
1	C	1	VAL	C-N	8.96	1.54	1.34
2	B	74	LEU	C-O	8.95	1.40	1.23
2	D	140	LEU	CG-CD1	8.95	1.84	1.51
1	A	39	THR	C-O	8.94	1.40	1.23
1	C	37	PRO	CA-CB	8.94	1.71	1.53
1	A	85	ASN	CA-C	8.94	1.76	1.52
2	B	115	ARG	CD-NE	-8.93	1.31	1.46
1	A	61	LYS	C-N	8.93	1.54	1.34
2	B	17	VAL	CA-C	8.93	1.76	1.52
2	B	131	LYS	CG-CD	8.93	1.82	1.52
2	D	34	TYR	CD1-CE1	8.93	1.52	1.39
2	D	97	VAL	C-O	-8.92	1.06	1.23
1	A	56	LYS	CE-NZ	8.91	1.71	1.49
1	C	105	LEU	C-O	8.91	1.40	1.23
1	C	36	PHE	CE2-CZ	-8.91	1.20	1.37
2	D	27	LEU	CG-CD1	8.91	1.84	1.51
2	D	94	LYS	C-O	8.91	1.40	1.23
2	D	17	VAL	CB-CG1	8.90	1.71	1.52
1	A	91	LEU	C-O	8.89	1.40	1.23
2	B	130	GLN	CG-CD	8.89	1.71	1.51
1	A	103	HIS	C-N	-8.89	1.13	1.34
1	A	42	TYR	CD2-CE2	-8.88	1.26	1.39
1	A	132	ASP	C-O	8.88	1.40	1.23
1	C	21	ALA	CA-CB	8.88	1.71	1.52
1	A	86	LEU	CG-CD2	8.88	1.84	1.51
2	D	108	VAL	C-N	8.88	1.54	1.34
2	B	21	VAL	CA-C	-8.88	1.29	1.52
1	C	113	LEU	CG-CD2	8.88	1.84	1.51
2	D	102	PHE	C-O	8.88	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	GLN	CB-CG	-8.88	1.28	1.52
1	A	89	HIS	CB-CG	-8.87	1.34	1.50
2	D	2	LEU	C-N	-8.87	1.13	1.34
2	D	70	PHE	CG-CD2	8.87	1.52	1.38
1	C	26	ALA	CA-CB	8.86	1.71	1.52
1	A	79	THR	CA-CB	8.86	1.76	1.53
1	A	116	ASN	CB-CG	-8.86	1.30	1.51
1	C	126	ASN	CA-C	8.85	1.75	1.52
2	B	79	ASP	CG-OD1	8.85	1.45	1.25
1	C	63	ALA	N-CA	-8.85	1.28	1.46
1	C	39	THR	CA-CB	8.85	1.76	1.53
1	A	105	LEU	C-N	8.84	1.54	1.34
1	C	47	ASP	C-N	-8.83	1.13	1.34
2	B	130	GLN	C-N	-8.83	1.13	1.34
1	A	86	LEU	C-O	-8.83	1.06	1.23
2	D	99	PRO	N-CA	8.83	1.62	1.47
1	A	14	TRP	CG-CD2	-8.82	1.28	1.43
2	B	128	LEU	CA-C	8.82	1.75	1.52
2	B	50	ALA	C-N	8.82	1.49	1.33
2	B	76	HIS	CB-CG	8.82	1.66	1.50
1	C	92	ARG	CB-CG	-8.82	1.28	1.52
1	A	117	PHE	CD2-CE2	-8.81	1.21	1.39
1	C	60	GLN	C-N	-8.81	1.13	1.34
1	A	2	LEU	N-CA	8.80	1.64	1.46
1	C	48	LEU	C-N	8.80	1.54	1.34
1	C	53	ALA	C-N	8.80	1.54	1.34
1	C	60	GLN	CB-CG	8.80	1.76	1.52
1	A	75	ASP	N-CA	8.79	1.64	1.46
1	A	3	SER	CA-C	-8.79	1.30	1.52
1	A	9	ASN	CA-CB	-8.78	1.30	1.53
2	B	138	ASN	CA-C	-8.78	1.30	1.52
1	A	30	GLN	CD-OE1	-8.78	1.04	1.24
1	A	125	LEU	CB-CG	-8.77	1.27	1.52
1	C	99	LYS	CG-CD	8.76	1.82	1.52
2	D	62	HIS	CA-CB	8.76	1.73	1.53
2	B	67	LEU	N-CA	8.75	1.63	1.46
1	C	58	HIS	CE1-NE2	-8.75	1.12	1.32
2	D	31	LEU	C-N	-8.74	1.14	1.34
1	C	94	ASN	CB-CG	8.72	1.71	1.51
2	D	65	ARG	CG-CD	8.72	1.73	1.51
2	B	37	THR	CA-CB	-8.71	1.30	1.53
2	D	81	LYS	N-CA	8.71	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	PRO	CB-CG	-8.70	1.06	1.50
2	D	76	HIS	CA-CB	8.70	1.73	1.53
1	C	56	LYS	C-O	8.69	1.39	1.23
1	C	72	HIS	CD2-NE2	8.69	1.60	1.42
2	B	117	PHE	C-O	-8.69	1.06	1.23
1	A	132	ASP	N-CA	8.69	1.63	1.46
1	A	124	ASN	CG-OD1	8.68	1.43	1.24
1	C	100	LEU	C-O	8.68	1.39	1.23
2	B	49	SER	CA-C	8.68	1.75	1.52
2	B	145	HIS	CB-CG	8.67	1.65	1.50
1	C	81	SER	N-CA	-8.66	1.29	1.46
2	B	86	GLN	CB-CG	8.66	1.75	1.52
1	A	103	HIS	CB-CG	-8.66	1.34	1.50
1	C	13	ALA	CA-CB	8.64	1.70	1.52
1	C	42	TYR	CA-CB	8.64	1.73	1.53
1	C	107	VAL	C-N	-8.64	1.14	1.34
2	B	119	GLY	C-O	8.63	1.37	1.23
2	D	65	ARG	CA-C	8.63	1.75	1.52
2	D	102	PHE	CA-CB	-8.63	1.34	1.53
2	B	84	PHE	CA-CB	8.63	1.73	1.53
1	C	80	LEU	CA-C	8.63	1.75	1.52
1	A	37	PRO	C-N	-8.62	1.14	1.34
2	D	33	VAL	CA-CB	8.62	1.72	1.54
1	C	1	VAL	N-CA	8.61	1.63	1.46
2	D	47	LEU	CB-CG	-8.61	1.27	1.52
2	B	66	VAL	N-CA	-8.61	1.29	1.46
2	D	122	THR	N-CA	8.61	1.63	1.46
1	C	134	THR	C-N	-8.61	1.14	1.34
2	B	3	THR	CB-OG1	8.60	1.60	1.43
1	C	48	LEU	C-O	-8.59	1.07	1.23
1	A	61	LYS	CD-CE	8.58	1.72	1.51
2	B	39	ARG	NE-CZ	-8.58	1.22	1.33
1	C	42	TYR	CB-CG	8.57	1.64	1.51
1	C	80	LEU	CG-CD1	8.57	1.83	1.51
2	D	132	VAL	C-N	-8.57	1.14	1.34
2	B	47	LEU	C-O	8.56	1.39	1.23
1	C	94	ASN	CA-C	-8.56	1.30	1.52
2	D	33	VAL	N-CA	-8.56	1.29	1.46
2	B	94	LYS	C-N	8.56	1.53	1.34
1	A	45	HIS	CG-ND1	8.56	1.57	1.38
1	C	109	LEU	CA-CB	-8.55	1.34	1.53
2	B	144	TYR	CG-CD1	8.55	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	94	ASN	N-CA	8.55	1.63	1.46
2	D	141	ALA	C-O	8.54	1.39	1.23
1	A	41	THR	CA-C	-8.53	1.30	1.52
2	D	81	LYS	C-N	8.54	1.48	1.33
1	A	53	ALA	CA-CB	8.53	1.70	1.52
2	B	91	HIS	CD2-NE2	8.53	1.59	1.42
2	D	115	ARG	NE-CZ	8.53	1.44	1.33
2	B	41	PHE	CA-CB	8.53	1.72	1.53
1	A	81	SER	N-CA	-8.53	1.29	1.46
2	D	56	ASN	C-N	-8.53	1.18	1.34
1	A	10	VAL	N-CA	8.52	1.63	1.46
1	C	70	GLN	N-CA	-8.52	1.29	1.46
2	B	44	PHE	CE1-CZ	8.51	1.53	1.37
2	D	19	VAL	C-N	-8.51	1.14	1.34
1	A	92	ARG	CA-CB	8.51	1.72	1.53
1	C	90	LYS	CE-NZ	8.51	1.70	1.49
2	B	101	ASN	C-N	-8.49	1.14	1.34
1	C	141	ARG	C-OXT	8.49	1.39	1.23
2	D	17	VAL	CA-C	8.48	1.75	1.52
2	D	25	GLN	CA-C	-8.48	1.30	1.52
1	C	68	LYS	CB-CG	8.48	1.75	1.52
2	D	100	GLN	CD-NE2	8.48	1.54	1.32
1	C	7	LYS	CB-CG	8.47	1.75	1.52
2	B	4	ALA	CA-C	8.47	1.75	1.52
1	C	127	LYS	CG-CD	-8.46	1.23	1.52
2	B	134	ALA	C-O	-8.46	1.07	1.23
1	C	33	PHE	CE2-CZ	8.46	1.53	1.37
1	C	47	ASP	CG-OD1	8.46	1.44	1.25
1	A	119	PRO	CA-C	-8.45	1.35	1.52
2	B	142	HIS	ND1-CE1	8.45	1.55	1.34
1	A	136	LEU	C-N	8.45	1.53	1.34
2	B	87	LEU	C-O	8.44	1.39	1.23
1	A	112	HIS	N-CA	-8.43	1.29	1.46
1	A	122	HIS	CA-C	8.43	1.74	1.52
2	B	57	PRO	C-O	8.43	1.40	1.23
2	D	29	ARG	CA-CB	-8.43	1.35	1.53
2	D	114	ALA	N-CA	8.42	1.63	1.46
2	D	67	LEU	N-CA	8.42	1.63	1.46
2	B	93	ASN	C-N	-8.41	1.14	1.34
2	D	72	GLN	CD-NE2	8.41	1.53	1.32
1	A	107	VAL	N-CA	8.40	1.63	1.46
2	B	70	PHE	CA-C	-8.40	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	42	TYR	C-O	8.40	1.39	1.23
2	B	26	ALA	CA-C	8.40	1.74	1.52
1	C	14	TRP	NE1-CE2	-8.38	1.26	1.37
1	C	137	THR	C-N	-8.37	1.14	1.34
2	B	79	ASP	CA-C	-8.36	1.31	1.52
2	B	127	ALA	CA-CB	-8.36	1.34	1.52
1	C	33	PHE	CA-CB	-8.36	1.35	1.53
2	B	138	ASN	CG-OD1	8.35	1.42	1.24
2	B	72	GLN	CA-CB	-8.35	1.35	1.53
2	B	94	LYS	CA-C	8.34	1.74	1.52
2	D	31	LEU	C-O	8.34	1.39	1.23
2	D	2	LEU	CB-CG	8.34	1.76	1.52
1	A	133	SER	C-O	-8.34	1.07	1.23
2	D	127	ALA	C-O	8.34	1.39	1.23
1	C	3	SER	CA-C	8.34	1.74	1.52
1	A	17	VAL	N-CA	-8.32	1.29	1.46
1	C	127	LYS	C-N	8.32	1.53	1.34
1	A	38	THR	N-CA	8.32	1.62	1.46
1	C	24	TYR	CE1-CZ	8.32	1.49	1.38
2	D	69	ALA	CA-C	8.32	1.74	1.52
2	B	104	LEU	C-N	-8.31	1.15	1.34
2	B	102	PHE	CD1-CE1	-8.31	1.22	1.39
1	C	54	GLN	CB-CG	8.31	1.75	1.52
1	C	58	HIS	N-CA	8.30	1.62	1.46
1	A	112	HIS	CG-CD2	-8.30	1.21	1.35
2	B	43	HIS	N-CA	-8.30	1.29	1.46
1	A	42	TYR	CD1-CE1	8.29	1.51	1.39
2	D	61	ALA	CA-C	-8.29	1.31	1.52
2	D	41	PHE	C-O	-8.28	1.07	1.23
2	B	30	LEU	CG-CD1	-8.27	1.21	1.51
1	A	59	GLY	C-N	-8.26	1.15	1.34
1	C	44	PRO	CB-CG	8.26	1.91	1.50
2	D	43	HIS	CE1-NE2	-8.26	1.13	1.32
1	A	64	ASN	C-N	8.25	1.53	1.34
1	A	60	GLN	CD-NE2	8.24	1.53	1.32
2	B	5	GLU	CB-CG	8.24	1.67	1.52
1	C	59	GLY	N-CA	-8.23	1.33	1.46
1	A	98	PHE	CA-C	-8.23	1.31	1.52
2	D	115	ARG	CA-C	-8.23	1.31	1.52
1	A	83	LEU	CA-C	-8.22	1.31	1.52
2	B	27	LEU	CA-CB	-8.22	1.34	1.53
1	C	134	THR	CB-OG1	-8.21	1.26	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	PHE	CG-CD2	-8.20	1.26	1.38
1	A	139	LYS	CE-NZ	8.20	1.69	1.49
1	C	54	GLN	CG-CD	-8.20	1.32	1.51
2	D	115	ARG	CG-CD	-8.19	1.31	1.51
2	B	81	LYS	CA-CB	8.19	1.72	1.53
2	D	136	VAL	N-CA	-8.19	1.29	1.46
1	A	49	SER	C-O	8.19	1.39	1.23
1	A	14	TRP	C-O	-8.18	1.07	1.23
1	C	62	VAL	CA-C	-8.18	1.31	1.52
1	A	122	HIS	CG-CD2	-8.18	1.21	1.35
2	D	7	LYS	CD-CE	-8.17	1.30	1.51
2	D	112	VAL	CA-C	8.17	1.74	1.52
1	A	116	ASN	C-O	-8.17	1.07	1.23
2	D	32	VAL	CA-C	8.17	1.74	1.52
2	D	74	LEU	CA-C	8.17	1.74	1.52
1	C	64	ASN	CG-ND2	8.16	1.53	1.32
1	A	52	SER	CA-CB	8.16	1.65	1.52
1	C	129	LEU	C-N	-8.16	1.15	1.34
1	A	105	LEU	CA-C	-8.15	1.31	1.52
1	C	66	LEU	C-N	8.14	1.52	1.34
2	D	47	LEU	CA-C	8.14	1.74	1.52
2	B	10	VAL	CA-CB	8.14	1.71	1.54
1	A	14	TRP	CG-CD1	8.14	1.48	1.36
1	A	130	ALA	C-N	8.13	1.52	1.34
1	C	31	ARG	CG-CD	8.13	1.72	1.51
1	C	32	MET	C-N	8.12	1.52	1.34
1	C	58	HIS	CA-CB	8.12	1.71	1.53
2	B	75	LYS	CA-CB	8.12	1.71	1.53
1	C	72	HIS	CA-C	8.11	1.74	1.52
1	C	14	TRP	CZ3-CH2	8.11	1.53	1.40
2	D	90	LEU	N-CA	8.11	1.62	1.46
1	C	121	VAL	CB-CG2	-8.11	1.35	1.52
1	A	11	LYS	CA-C	8.10	1.74	1.52
2	D	31	LEU	CG-CD2	-8.10	1.21	1.51
2	D	96	HIS	CA-CB	8.10	1.71	1.53
2	B	145	HIS	CA-C	-8.10	1.31	1.52
1	A	15	GLY	C-N	8.10	1.52	1.34
1	C	16	LYS	CB-CG	8.10	1.74	1.52
2	B	110	ALA	CA-C	8.09	1.74	1.52
1	C	17	VAL	CA-CB	-8.09	1.37	1.54
1	C	22	PRO	CA-CB	8.09	1.69	1.53
2	B	116	ASN	CA-C	8.08	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	86	GLN	CD-NE2	8.08	1.53	1.32
2	B	56	ASN	CG-ND2	8.07	1.53	1.32
1	A	98	PHE	CD1-CE1	-8.07	1.23	1.39
1	C	66	LEU	CG-CD2	8.07	1.81	1.51
2	D	111	LEU	C-O	-8.06	1.08	1.23
1	C	33	PHE	CG-CD1	-8.05	1.26	1.38
1	C	66	LEU	CA-CB	8.05	1.72	1.53
2	B	96	HIS	CA-CB	8.05	1.71	1.53
1	C	33	PHE	CD2-CE2	8.04	1.55	1.39
1	C	38	THR	N-CA	-8.02	1.30	1.46
1	A	44	PRO	CB-CG	-8.01	1.09	1.50
1	A	53	ALA	N-CA	8.01	1.62	1.46
2	D	101	ASN	CA-C	-8.01	1.32	1.52
1	C	91	LEU	CB-CG	8.01	1.75	1.52
2	D	29	ARG	CD-NE	-8.01	1.32	1.46
1	A	101	LEU	CA-C	8.01	1.73	1.52
2	B	76	HIS	CA-C	8.01	1.73	1.52
1	C	126	ASN	CB-CG	-8.01	1.32	1.51
1	A	73	LEU	CG-CD2	8.00	1.81	1.51
2	B	88	SER	C-N	8.00	1.47	1.33
2	B	32	VAL	CA-CB	-8.00	1.38	1.54
2	D	106	GLY	N-CA	-8.00	1.34	1.46
2	D	1	MET	SD-CE	7.99	2.22	1.77
2	B	143	LYS	CA-C	-7.98	1.32	1.52
2	B	129	PHE	CA-CB	-7.98	1.36	1.53
2	B	90	LEU	C-O	-7.98	1.08	1.23
2	B	80	LEU	CG-CD2	7.97	1.81	1.51
1	C	101	LEU	CB-CG	-7.97	1.29	1.52
2	B	137	ALA	CA-CB	-7.97	1.35	1.52
2	D	96	HIS	C-O	7.97	1.38	1.23
1	C	35	SER	C-N	-7.96	1.15	1.34
2	D	5	GLU	CA-CB	7.96	1.71	1.53
2	D	13	PHE	N-CA	7.95	1.62	1.46
1	A	134	THR	CA-C	7.95	1.73	1.52
1	A	58	HIS	N-CA	7.94	1.62	1.46
1	C	130	ALA	CA-CB	-7.94	1.35	1.52
2	B	71	THR	CB-CG2	7.92	1.78	1.52
2	B	101	ASN	CG-OD1	-7.92	1.06	1.24
2	B	145	HIS	N-CA	7.91	1.62	1.46
2	D	126	GLN	CB-CG	7.91	1.74	1.52
2	B	54	MET	CA-CB	7.91	1.71	1.53
2	D	13	PHE	CE1-CZ	7.91	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	ASN	C-O	-7.90	1.08	1.23
2	B	53	VAL	N-CA	7.90	1.62	1.46
2	D	56	ASN	N-CA	-7.90	1.30	1.46
1	C	67	THR	N-CA	7.90	1.62	1.46
1	C	109	LEU	CG-CD2	-7.90	1.22	1.51
1	C	27	GLN	C-N	7.90	1.52	1.34
2	D	50	ALA	CA-CB	-7.89	1.35	1.52
2	D	86	GLN	CG-CD	7.89	1.69	1.51
2	B	49	SER	CB-OG	-7.89	1.31	1.42
2	D	76	HIS	C-O	7.88	1.38	1.23
1	A	130	ALA	CA-CB	-7.87	1.35	1.52
1	C	6	ASN	N-CA	-7.87	1.30	1.46
1	A	84	SER	CA-C	-7.86	1.32	1.52
2	B	13	PHE	CA-CB	7.86	1.71	1.53
1	C	108	THR	CB-CG2	7.86	1.78	1.52
1	A	45	HIS	C-N	-7.86	1.16	1.34
2	B	18	ASP	CA-C	7.86	1.73	1.52
2	B	143	LYS	C-N	-7.85	1.16	1.34
1	A	31	ARG	CZ-NH2	7.85	1.43	1.33
2	B	109	LEU	CA-CB	-7.84	1.35	1.53
2	D	44	PHE	C-O	7.84	1.38	1.23
2	B	48	SER	C-O	7.83	1.38	1.23
1	C	116	ASN	CB-CG	-7.83	1.33	1.51
1	A	11	LYS	CD-CE	-7.83	1.31	1.51
1	A	90	LYS	CD-CE	7.82	1.70	1.51
1	A	87	HIS	ND1-CE1	7.81	1.54	1.34
1	C	120	ALA	CA-CB	-7.81	1.36	1.52
2	D	77	LEU	N-CA	-7.81	1.30	1.46
2	D	124	ASN	C-N	7.81	1.52	1.34
1	C	129	LEU	C-O	-7.81	1.08	1.23
2	B	64	LYS	C-O	-7.80	1.08	1.23
2	D	14	TRP	CG-CD2	7.80	1.56	1.43
1	A	135	VAL	CB-CG1	-7.79	1.36	1.52
2	D	7	LYS	CB-CG	-7.79	1.31	1.52
1	C	136	LEU	C-O	7.79	1.38	1.23
2	D	91	HIS	CG-ND1	-7.78	1.21	1.38
2	D	49	SER	C-N	7.78	1.51	1.34
1	C	73	LEU	CG-CD1	-7.77	1.23	1.51
2	D	118	GLY	N-CA	7.77	1.57	1.46
2	D	130	GLN	CA-C	7.77	1.73	1.52
1	C	89	HIS	CB-CG	-7.77	1.36	1.50
2	D	128	LEU	CA-C	7.75	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASN	CG-OD1	-7.74	1.06	1.24
2	B	60	LYS	CD-CE	7.73	1.70	1.51
2	D	32	VAL	N-CA	7.73	1.61	1.46
2	D	64	LYS	N-CA	7.73	1.61	1.46
1	A	114	PRO	N-CA	7.72	1.60	1.47
1	A	134	THR	C-O	-7.72	1.08	1.23
2	D	70	PHE	CB-CG	7.71	1.64	1.51
1	C	135	VAL	C-N	7.70	1.51	1.34
2	D	29	ARG	NE-CZ	-7.70	1.23	1.33
1	A	116	ASN	CG-ND2	7.70	1.52	1.32
2	B	77	LEU	N-CA	-7.70	1.30	1.46
2	D	93	ASN	C-O	7.70	1.38	1.23
1	A	55	GLN	CA-C	7.70	1.73	1.52
1	C	115	THR	CB-CG2	7.69	1.77	1.52
1	C	123	ALA	CA-CB	7.69	1.68	1.52
2	B	57	PRO	N-CA	-7.69	1.34	1.47
1	A	41	THR	CB-CG2	7.68	1.77	1.52
2	D	144	TYR	C-N	7.68	1.51	1.34
1	C	138	SER	CA-C	-7.67	1.33	1.52
2	B	74	LEU	CA-CB	7.67	1.71	1.53
1	C	19	GLY	C-N	-7.66	1.16	1.34
1	C	18	GLY	CA-C	-7.66	1.39	1.51
1	C	103	HIS	N-CA	-7.66	1.31	1.46
2	B	82	GLY	N-CA	-7.66	1.34	1.46
2	D	117	PHE	CG-CD2	-7.66	1.27	1.38
1	A	43	PHE	CE2-CZ	7.65	1.51	1.37
1	C	32	MET	CB-CG	-7.65	1.26	1.51
2	D	29	ARG	CB-CG	7.65	1.73	1.52
2	B	91	HIS	CA-CB	-7.64	1.37	1.53
1	C	13	ALA	C-N	-7.64	1.16	1.34
1	A	138	SER	CA-CB	-7.64	1.41	1.52
1	A	60	GLN	CB-CG	-7.63	1.31	1.52
1	A	2	LEU	C-O	7.62	1.37	1.23
2	D	90	LEU	CA-C	-7.62	1.33	1.52
1	C	39	THR	C-N	7.62	1.51	1.34
1	A	4	ALA	CA-C	-7.61	1.33	1.52
1	A	2	LEU	CB-CG	7.61	1.74	1.52
2	B	64	LYS	CE-NZ	7.61	1.68	1.49
1	C	7	LYS	N-CA	7.61	1.61	1.46
1	C	136	LEU	CG-CD1	-7.60	1.23	1.51
2	D	34	TYR	C-N	-7.59	1.19	1.34
1	A	86	LEU	N-CA	-7.58	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	GLN	CD-OE1	-7.58	1.07	1.24
2	D	89	GLY	N-CA	7.58	1.57	1.46
1	A	91	LEU	CG-CD1	7.58	1.79	1.51
2	B	125	VAL	C-N	-7.57	1.16	1.34
2	D	133	VAL	CA-CB	7.57	1.70	1.54
2	D	23	GLY	N-CA	7.57	1.57	1.46
2	D	62	HIS	C-O	-7.57	1.08	1.23
2	D	67	LEU	C-O	7.57	1.37	1.23
2	B	104	LEU	CA-CB	7.57	1.71	1.53
1	A	34	LEU	CB-CG	-7.55	1.30	1.52
1	A	72	HIS	CG-CD2	7.55	1.48	1.35
2	B	35	PRO	C-N	7.54	1.51	1.34
2	B	124	ASN	N-CA	-7.54	1.31	1.46
2	B	62	HIS	CD2-NE2	7.54	1.57	1.42
1	C	7	LYS	CG-CD	-7.54	1.26	1.52
2	B	116	ASN	N-CA	-7.53	1.31	1.46
1	A	36	PHE	CA-C	-7.53	1.33	1.52
1	A	130	ALA	CA-C	7.52	1.72	1.52
1	A	24	TYR	CG-CD2	-7.52	1.29	1.39
2	D	136	VAL	C-N	7.52	1.51	1.34
2	D	41	PHE	N-CA	7.51	1.61	1.46
2	D	126	GLN	CA-CB	-7.51	1.37	1.53
1	A	56	LYS	CA-CB	-7.50	1.37	1.53
2	B	84	PHE	C-N	7.50	1.51	1.34
1	A	122	HIS	N-CA	-7.50	1.31	1.46
2	D	132	VAL	CA-CB	-7.50	1.39	1.54
1	A	105	LEU	CB-CG	-7.49	1.30	1.52
1	C	98	PHE	N-CA	7.49	1.61	1.46
2	D	72	GLN	CA-CB	-7.49	1.37	1.53
1	A	104	SER	N-CA	-7.48	1.31	1.46
1	A	65	ALA	N-CA	-7.48	1.31	1.46
2	D	109	LEU	C-N	-7.47	1.16	1.34
1	A	107	VAL	C-N	-7.46	1.16	1.34
1	C	11	LYS	CB-CG	-7.46	1.32	1.52
1	C	131	ASN	C-O	-7.46	1.09	1.23
2	D	18	ASP	C-N	7.45	1.51	1.34
1	A	77	PRO	C-O	7.45	1.38	1.23
1	C	68	LYS	C-O	-7.45	1.09	1.23
2	B	81	LYS	CE-NZ	-7.45	1.30	1.49
2	D	96	HIS	ND1-CE1	-7.44	1.16	1.34
2	D	99	PRO	N-CD	7.44	1.58	1.47
2	B	16	LYS	CE-NZ	7.43	1.67	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	113	VAL	CA-C	-7.43	1.33	1.52
1	C	113	LEU	C-O	7.42	1.37	1.23
2	D	46	ASN	CG-OD1	7.42	1.40	1.24
1	A	61	LYS	N-CA	7.42	1.61	1.46
1	C	128	PHE	N-CA	-7.41	1.31	1.46
1	C	118	THR	C-O	7.41	1.37	1.23
1	A	64	ASN	C-O	-7.41	1.09	1.23
1	C	91	LEU	CG-CD1	7.39	1.79	1.51
1	A	93	VAL	CA-CB	-7.38	1.39	1.54
1	A	118	THR	C-O	7.38	1.37	1.23
1	C	8	SER	N-CA	7.37	1.61	1.46
1	A	1	VAL	C-O	-7.37	1.09	1.23
1	A	106	LEU	CA-C	-7.37	1.33	1.52
1	A	140	TYR	N-CA	-7.37	1.31	1.46
1	C	54	GLN	CA-CB	-7.37	1.37	1.53
2	B	121	PHE	CD2-CE2	7.36	1.53	1.39
2	B	24	ALA	C-O	7.36	1.37	1.23
2	B	99	PRO	N-CA	-7.35	1.34	1.47
1	A	54	GLN	CG-CD	7.35	1.68	1.51
1	C	93	VAL	CB-CG1	7.35	1.68	1.52
2	D	65	ARG	C-O	7.35	1.37	1.23
1	A	132	ASP	C-N	-7.34	1.17	1.34
2	B	77	LEU	C-N	-7.34	1.17	1.34
1	A	74	ASN	C-N	-7.34	1.17	1.34
2	D	15	GLY	CA-C	7.33	1.63	1.51
1	A	136	LEU	CG-CD1	7.33	1.78	1.51
1	A	125	LEU	CG-CD2	-7.32	1.24	1.51
2	B	65	ARG	CA-CB	7.31	1.70	1.53
1	A	122	HIS	CE1-NE2	-7.31	1.15	1.32
2	B	34	TYR	CD1-CE1	-7.30	1.28	1.39
1	C	53	ALA	C-O	7.29	1.37	1.23
2	B	66	VAL	CA-CB	-7.29	1.39	1.54
1	A	82	ASN	CA-C	7.29	1.71	1.52
1	A	132	ASP	CG-OD1	7.27	1.42	1.25
2	B	109	LEU	N-CA	7.27	1.60	1.46
1	A	87	HIS	CG-CD2	-7.27	1.23	1.35
2	B	20	ASP	N-CA	7.26	1.60	1.46
1	C	82	ASN	CB-CG	-7.26	1.34	1.51
2	D	39	ARG	CA-C	7.26	1.71	1.52
1	A	130	ALA	N-CA	7.26	1.60	1.46
1	A	101	LEU	CB-CG	7.25	1.73	1.52
2	D	119	GLY	CA-C	-7.25	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	GLY	CA-C	7.24	1.63	1.51
1	C	74	ASN	CA-C	-7.24	1.34	1.52
2	B	132	VAL	N-CA	-7.24	1.31	1.46
1	A	69	ALA	C-O	7.24	1.37	1.23
1	C	83	LEU	CG-CD2	7.24	1.78	1.51
2	D	129	PHE	C-O	-7.24	1.09	1.23
2	B	120	GLN	C-O	7.23	1.37	1.23
2	D	38	GLN	CD-NE2	-7.23	1.14	1.32
1	A	23	ALA	CA-C	-7.23	1.34	1.52
2	B	47	LEU	CA-CB	-7.22	1.37	1.53
1	A	132	ASP	CB-CG	-7.22	1.36	1.51
2	D	123	PRO	CG-CD	7.21	1.74	1.50
1	A	65	ALA	C-O	7.21	1.37	1.23
1	A	74	ASN	N-CA	7.21	1.60	1.46
1	A	66	LEU	N-CA	-7.20	1.31	1.46
2	B	95	LEU	CB-CG	7.20	1.73	1.52
1	A	58	HIS	CE1-NE2	7.18	1.49	1.32
2	B	14	TRP	CD2-CE2	7.18	1.50	1.41
1	C	77	PRO	C-N	7.18	1.46	1.33
1	A	48	LEU	N-CA	-7.16	1.32	1.46
2	B	108	VAL	CA-C	7.16	1.71	1.52
2	D	56	ASN	CG-OD1	7.16	1.39	1.24
1	A	126	ASN	CA-CB	-7.16	1.34	1.53
2	D	57	PRO	CA-C	-7.15	1.38	1.52
2	D	132	VAL	CB-CG1	7.15	1.67	1.52
2	D	20	ASP	CB-CG	7.15	1.66	1.51
1	A	24	TYR	CE2-CZ	-7.14	1.29	1.38
2	B	124	ASN	C-O	7.14	1.36	1.23
1	C	124	ASN	CB-CG	-7.14	1.34	1.51
1	A	82	ASN	CG-ND2	-7.13	1.15	1.32
2	D	129	PHE	C-N	7.13	1.50	1.34
2	D	4	ALA	CA-CB	-7.13	1.37	1.52
2	D	44	PHE	CD2-CE2	7.13	1.53	1.39
2	D	42	GLN	CD-NE2	7.13	1.50	1.32
2	D	40	PHE	CA-CB	7.12	1.69	1.53
2	D	104	LEU	N-CA	-7.11	1.32	1.46
2	B	126	GLN	CD-NE2	7.11	1.50	1.32
1	A	39	THR	C-N	-7.10	1.17	1.34
1	C	76	LEU	CG-CD1	7.09	1.78	1.51
1	C	119	PRO	CB-CG	7.09	1.85	1.50
1	A	46	PHE	CD1-CE1	-7.09	1.25	1.39
2	D	8	ALA	CA-C	-7.09	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	ALA	C-N	7.08	1.50	1.34
1	A	28	ALA	C-O	7.08	1.36	1.23
2	B	64	LYS	CB-CG	7.08	1.71	1.52
1	A	74	ASN	CA-CB	-7.08	1.34	1.53
1	A	91	LEU	CG-CD2	7.07	1.78	1.51
2	B	7	LYS	CD-CE	7.07	1.69	1.51
1	C	58	HIS	CA-C	7.07	1.71	1.52
2	D	57	PRO	C-N	-7.07	1.17	1.34
1	A	69	ALA	CA-CB	-7.06	1.37	1.52
1	A	82	ASN	CA-CB	-7.06	1.34	1.53
1	C	46	PHE	CA-CB	7.06	1.69	1.53
2	B	37	THR	C-O	7.05	1.36	1.23
1	A	95	PRO	CA-CB	7.05	1.67	1.53
1	A	131	ASN	C-O	7.05	1.36	1.23
1	A	141	ARG	CA-CB	7.04	1.69	1.53
2	D	33	VAL	CA-C	7.04	1.71	1.52
2	B	99	PRO	CA-C	-7.04	1.38	1.52
2	D	66	VAL	CA-CB	7.04	1.69	1.54
1	A	73	LEU	N-CA	7.02	1.60	1.46
1	A	89	HIS	CA-CB	-7.01	1.38	1.53
2	B	138	ASN	CB-CG	-7.01	1.34	1.51
2	D	140	LEU	CG-CD2	-7.01	1.25	1.51
1	A	45	HIS	CG-CD2	7.00	1.47	1.35
2	D	71	THR	C-N	-6.99	1.18	1.34
1	A	23	ALA	C-O	-6.99	1.10	1.23
2	D	84	PHE	CD2-CE2	6.99	1.53	1.39
1	A	35	SER	C-N	6.99	1.50	1.34
2	B	37	THR	CB-OG1	-6.98	1.29	1.43
2	D	42	GLN	CA-C	-6.98	1.34	1.52
1	A	90	LYS	N-CA	-6.98	1.32	1.46
1	A	40	LYS	CA-C	-6.98	1.34	1.52
2	B	11	THR	CA-C	6.97	1.71	1.52
1	C	48	LEU	CB-CG	6.97	1.72	1.52
1	A	11	LYS	N-CA	-6.96	1.32	1.46
1	A	106	LEU	CG-CD1	-6.95	1.26	1.51
1	C	97	ASN	N-CA	-6.95	1.32	1.46
1	C	98	PHE	CA-CB	-6.95	1.38	1.53
2	D	75	LYS	CG-CD	6.95	1.76	1.52
2	D	52	ALA	C-N	6.95	1.50	1.34
2	B	86	GLN	N-CA	-6.94	1.32	1.46
2	D	36	TRP	C-N	6.94	1.50	1.34
1	A	128	PHE	CA-C	6.94	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	89	HIS	CG-CD2	6.94	1.47	1.35
2	D	61	ALA	C-N	6.94	1.50	1.34
2	B	114	ALA	C-O	-6.93	1.10	1.23
1	C	61	LYS	CG-CD	6.93	1.76	1.52
2	B	2	LEU	N-CA	-6.92	1.32	1.46
2	B	19	VAL	CA-C	-6.92	1.34	1.52
1	A	123	ALA	C-N	6.91	1.50	1.34
1	A	37	PRO	CA-CB	-6.91	1.39	1.53
1	C	89	HIS	CG-ND1	6.91	1.53	1.38
2	B	107	ASN	CB-CG	-6.90	1.35	1.51
1	C	36	PHE	CD2-CE2	-6.90	1.25	1.39
2	B	29	ARG	CG-CD	6.90	1.69	1.51
1	A	13	ALA	CA-CB	6.89	1.67	1.52
2	B	100	GLN	CD-NE2	6.89	1.50	1.32
2	D	59	VAL	N-CA	6.89	1.60	1.46
2	B	64	LYS	CG-CD	6.89	1.75	1.52
2	B	124	ASN	CG-OD1	6.88	1.39	1.24
2	D	69	ALA	CA-CB	-6.88	1.38	1.52
1	C	50	HIS	C-O	6.88	1.36	1.23
1	A	136	LEU	CA-CB	6.87	1.69	1.53
1	C	90	LYS	C-O	-6.87	1.10	1.23
1	A	12	ALA	N-CA	6.87	1.60	1.46
2	B	134	ALA	CA-C	6.85	1.70	1.52
2	B	59	VAL	CA-CB	6.84	1.69	1.54
1	C	125	LEU	C-O	6.84	1.36	1.23
2	B	11	THR	N-CA	-6.84	1.32	1.46
2	D	110	ALA	C-N	-6.84	1.18	1.34
1	C	93	VAL	N-CA	6.82	1.59	1.46
2	B	107	ASN	CG-OD1	-6.81	1.08	1.24
2	B	90	LEU	CA-C	6.81	1.70	1.52
1	C	78	GLY	C-N	-6.81	1.18	1.34
2	D	124	ASN	C-O	6.81	1.36	1.23
1	A	42	TYR	CE1-CZ	-6.81	1.29	1.38
2	D	114	ALA	C-O	6.81	1.36	1.23
2	B	129	PHE	C-O	6.80	1.36	1.23
2	B	31	LEU	CG-CD1	6.80	1.77	1.51
2	D	109	LEU	CA-CB	-6.80	1.38	1.53
1	C	62	VAL	CB-CG2	-6.80	1.38	1.52
2	D	21	VAL	C-O	6.80	1.36	1.23
1	C	34	LEU	C-O	6.79	1.36	1.23
1	A	68	LYS	CE-NZ	6.79	1.66	1.49
2	D	129	PHE	CA-C	-6.79	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	PRO	CB-CG	-6.79	1.16	1.50
2	B	29	ARG	CA-C	-6.79	1.35	1.52
1	C	31	ARG	CA-CB	-6.78	1.39	1.53
1	A	42	TYR	CZ-OH	-6.78	1.26	1.37
2	B	52	ALA	C-O	6.77	1.36	1.23
2	B	94	LYS	CG-CD	6.76	1.75	1.52
2	B	108	VAL	CB-CG1	-6.75	1.38	1.52
2	D	22	VAL	N-CA	-6.75	1.32	1.46
1	A	33	PHE	CA-C	6.75	1.70	1.52
2	B	36	TRP	CZ2-CH2	6.75	1.50	1.37
2	B	72	GLN	CD-NE2	6.74	1.49	1.32
2	B	44	PHE	CD1-CE1	6.73	1.52	1.39
1	A	14	TRP	N-CA	-6.73	1.32	1.46
1	C	100	LEU	CA-C	-6.73	1.35	1.52
1	C	131	ASN	C-N	-6.73	1.18	1.34
1	A	92	ARG	CG-CD	-6.72	1.35	1.51
2	B	69	ALA	C-O	6.70	1.36	1.23
2	D	105	LEU	CG-CD1	6.69	1.76	1.51
1	A	95	PRO	CB-CG	-6.69	1.16	1.50
1	C	134	THR	CA-C	-6.69	1.35	1.52
2	B	144	TYR	CA-C	-6.68	1.35	1.52
2	D	5	GLU	CA-C	6.68	1.70	1.52
2	D	27	LEU	CB-CG	-6.68	1.33	1.52
2	B	8	ALA	C-O	-6.67	1.10	1.23
2	D	54	MET	CA-CB	6.67	1.68	1.53
1	C	116	ASN	N-CA	-6.66	1.33	1.46
1	C	95	PRO	N-CA	6.66	1.58	1.47
1	A	85	ASN	CG-ND2	6.65	1.49	1.32
2	B	20	ASP	C-O	6.65	1.35	1.23
1	A	9	ASN	C-O	-6.64	1.10	1.23
2	D	127	ALA	C-N	-6.64	1.18	1.34
1	A	99	LYS	CA-C	6.63	1.70	1.52
1	A	31	ARG	CD-NE	6.63	1.57	1.46
2	B	137	ALA	CA-C	-6.63	1.35	1.52
2	B	116	ASN	CG-ND2	6.63	1.49	1.32
1	A	44	PRO	C-O	6.62	1.36	1.23
2	D	136	VAL	CA-C	6.62	1.70	1.52
1	A	10	VAL	CB-CG1	-6.62	1.39	1.52
2	B	144	TYR	N-CA	6.62	1.59	1.46
1	A	46	PHE	C-O	6.60	1.35	1.23
2	B	58	LYS	CA-CB	-6.60	1.39	1.53
1	C	97	ASN	CG-ND2	-6.60	1.16	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	LEU	C-O	6.59	1.35	1.23
2	D	108	VAL	CA-CB	6.59	1.68	1.54
2	B	89	GLY	CA-C	6.59	1.62	1.51
2	B	104	LEU	C-O	6.59	1.35	1.23
2	D	131	LYS	CG-CD	-6.58	1.30	1.52
2	B	36	TRP	CB-CG	-6.58	1.38	1.50
1	A	47	ASP	CA-C	6.58	1.70	1.52
1	C	14	TRP	CA-CB	6.57	1.68	1.53
2	B	58	LYS	CA-C	-6.57	1.35	1.52
2	D	121	PHE	CE2-CZ	-6.56	1.24	1.37
2	B	78	ASP	CG-OD1	-6.56	1.10	1.25
1	C	80	LEU	N-CA	-6.56	1.33	1.46
2	D	131	LYS	CA-C	6.56	1.70	1.52
1	C	76	LEU	CG-CD2	6.55	1.76	1.51
1	C	139	LYS	N-CA	-6.55	1.33	1.46
2	D	64	LYS	CG-CD	6.55	1.74	1.52
1	A	60	GLN	N-CA	6.55	1.59	1.46
1	A	28	ALA	C-N	-6.55	1.19	1.34
1	A	105	LEU	CG-CD1	6.55	1.76	1.51
1	A	11	LYS	CA-CB	6.54	1.68	1.53
1	C	48	LEU	N-CA	-6.54	1.33	1.46
1	C	62	VAL	C-N	-6.53	1.19	1.34
2	D	85	ALA	C-N	-6.53	1.19	1.34
1	C	37	PRO	CB-CG	-6.52	1.17	1.50
1	C	128	PHE	CD2-CE2	-6.52	1.26	1.39
1	C	4	ALA	N-CA	6.51	1.59	1.46
1	C	123	ALA	C-O	-6.51	1.10	1.23
1	A	97	ASN	CG-OD1	6.50	1.38	1.24
1	C	36	PHE	C-O	-6.50	1.11	1.23
1	A	43	PHE	CD2-CE2	6.50	1.52	1.39
1	C	7	LYS	CA-CB	-6.50	1.39	1.53
1	A	117	PHE	CA-C	6.50	1.69	1.52
2	B	67	LEU	C-N	-6.49	1.19	1.34
2	B	145	HIS	CG-ND1	6.49	1.53	1.38
2	D	117	PHE	CE1-CZ	6.48	1.49	1.37
2	D	128	LEU	CA-CB	6.47	1.68	1.53
1	A	5	ALA	N-CA	6.47	1.59	1.46
2	B	86	GLN	C-N	6.47	1.49	1.34
1	A	109	LEU	C-N	-6.46	1.19	1.34
2	B	67	LEU	CG-CD2	-6.46	1.27	1.51
2	D	66	VAL	CB-CG1	6.46	1.66	1.52
2	B	140	LEU	CG-CD1	6.46	1.75	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	LEU	CB-CG	-6.46	1.33	1.52
2	B	124	ASN	CA-CB	-6.45	1.36	1.53
1	A	88	ALA	N-CA	-6.45	1.33	1.46
2	D	2	LEU	CG-CD2	-6.45	1.28	1.51
2	B	60	LYS	CA-C	6.44	1.69	1.52
1	A	55	GLN	CG-CD	6.44	1.65	1.51
1	C	118	THR	N-CA	6.44	1.59	1.46
1	C	136	LEU	N-CA	6.44	1.59	1.46
1	A	76	LEU	CA-C	-6.43	1.36	1.52
1	A	125	LEU	CA-C	6.42	1.69	1.52
2	D	100	GLN	CD-OE1	-6.42	1.09	1.24
1	A	70	GLN	CA-C	6.42	1.69	1.52
1	A	106	LEU	C-O	6.42	1.35	1.23
1	C	86	LEU	CG-CD2	6.42	1.75	1.51
2	D	74	LEU	CA-CB	-6.42	1.39	1.53
1	A	38	THR	C-N	6.42	1.48	1.34
1	C	104	SER	N-CA	-6.42	1.33	1.46
1	C	49	SER	N-CA	-6.41	1.33	1.46
2	B	132	VAL	CA-CB	-6.40	1.41	1.54
1	C	129	LEU	N-CA	-6.40	1.33	1.46
1	C	103	HIS	ND1-CE1	-6.38	1.18	1.34
1	A	44	PRO	CA-C	6.37	1.65	1.52
1	A	50	HIS	CA-C	-6.36	1.36	1.52
2	B	54	MET	C-O	6.36	1.35	1.23
2	D	54	MET	CA-C	-6.36	1.36	1.52
1	C	11	LYS	C-N	6.35	1.48	1.34
1	C	92	ARG	CZ-NH2	6.35	1.41	1.33
1	C	102	SER	C-O	-6.35	1.11	1.23
1	A	27	GLN	CA-C	6.34	1.69	1.52
2	D	3	THR	C-O	6.34	1.35	1.23
2	B	139	ALA	CA-C	-6.32	1.36	1.52
1	A	35	SER	CA-C	-6.32	1.36	1.52
2	D	141	ALA	N-CA	6.32	1.58	1.46
1	C	14	TRP	CA-C	6.31	1.69	1.52
2	D	132	VAL	C-O	6.31	1.35	1.23
2	B	101	ASN	CG-ND2	6.30	1.48	1.32
1	C	141	ARG	CZ-NH1	6.30	1.41	1.33
1	C	7	LYS	CD-CE	6.30	1.67	1.51
2	D	122	THR	CB-CG2	6.30	1.73	1.52
1	C	76	LEU	CB-CG	6.29	1.70	1.52
1	C	86	LEU	CG-CD1	6.29	1.75	1.51
2	B	91	HIS	CA-C	6.29	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	VAL	CB-CG1	6.29	1.66	1.52
1	C	72	HIS	CE1-NE2	6.29	1.47	1.32
1	A	101	LEU	N-CA	6.28	1.58	1.46
2	B	70	PHE	CD2-CE2	6.28	1.51	1.39
2	B	78	ASP	N-CA	-6.28	1.33	1.46
1	C	1	VAL	CB-CG2	6.28	1.66	1.52
2	D	27	LEU	N-CA	-6.28	1.33	1.46
1	C	115	THR	CA-CB	6.27	1.69	1.53
1	A	54	GLN	C-N	6.27	1.48	1.34
2	D	72	GLN	CB-CG	6.27	1.69	1.52
2	B	98	ASN	CB-CG	-6.26	1.36	1.51
1	C	86	LEU	C-N	6.26	1.48	1.34
2	D	107	ASN	C-N	6.26	1.48	1.34
1	A	131	ASN	C-N	-6.26	1.19	1.34
1	C	68	LYS	N-CA	-6.26	1.33	1.46
2	D	40	PHE	CG-CD1	6.26	1.48	1.38
2	B	25	GLN	CG-CD	6.25	1.65	1.51
1	A	129	LEU	CB-CG	-6.25	1.34	1.52
2	B	97	VAL	C-N	6.24	1.48	1.34
2	D	60	LYS	CA-C	6.24	1.69	1.52
2	B	68	ASP	CG-OD2	6.24	1.39	1.25
2	B	131	LYS	N-CA	6.24	1.58	1.46
2	D	65	ARG	NE-CZ	6.24	1.41	1.33
2	D	123	PRO	N-CA	-6.24	1.36	1.47
2	B	33	VAL	N-CA	-6.23	1.33	1.46
2	B	43	HIS	C-N	6.23	1.48	1.34
1	C	74	ASN	CG-OD1	6.22	1.37	1.24
2	B	81	LYS	C-N	-6.21	1.21	1.33
2	B	88	SER	N-CA	-6.21	1.33	1.46
2	B	128	LEU	CG-CD1	6.21	1.74	1.51
2	B	71	THR	CB-OG1	6.21	1.55	1.43
1	A	81	SER	C-O	-6.21	1.11	1.23
1	C	72	HIS	CB-CG	-6.20	1.38	1.50
1	C	72	HIS	C-O	-6.20	1.11	1.23
1	A	118	THR	CA-C	6.20	1.69	1.52
1	C	89	HIS	C-N	6.20	1.48	1.34
1	C	76	LEU	CA-CB	-6.19	1.39	1.53
2	D	35	PRO	C-N	-6.19	1.19	1.34
2	B	105	LEU	CG-CD2	-6.18	1.28	1.51
2	B	113	VAL	N-CA	6.18	1.58	1.46
2	B	31	LEU	C-O	-6.18	1.11	1.23
2	D	134	ALA	CA-C	6.18	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	133	SER	C-N	-6.17	1.19	1.34
2	B	72	GLN	CG-CD	-6.16	1.36	1.51
1	C	82	ASN	CA-C	-6.16	1.36	1.52
1	C	47	ASP	CA-C	-6.15	1.36	1.52
1	A	7	LYS	CA-CB	6.15	1.67	1.53
2	B	139	ALA	N-CA	6.14	1.58	1.46
2	B	117	PHE	CB-CG	-6.14	1.41	1.51
2	B	8	ALA	N-CA	-6.14	1.34	1.46
2	D	40	PHE	CD1-CE1	-6.13	1.26	1.39
2	B	122	THR	N-CA	6.13	1.58	1.46
1	A	65	ALA	C-N	6.12	1.48	1.34
2	D	114	ALA	CA-CB	-6.11	1.39	1.52
1	C	102	SER	N-CA	-6.11	1.34	1.46
1	A	3	SER	C-N	-6.11	1.20	1.34
2	B	123	PRO	C-O	-6.10	1.11	1.23
1	A	107	VAL	CB-CG2	6.10	1.65	1.52
1	C	77	PRO	CG-CD	-6.10	1.30	1.50
2	B	144	TYR	CB-CG	6.08	1.60	1.51
2	B	7	LYS	C-N	-6.08	1.20	1.34
1	A	139	LYS	C-N	-6.08	1.20	1.34
2	D	57	PRO	CG-CD	6.08	1.70	1.50
2	B	55	ASN	CA-CB	-6.08	1.37	1.53
1	A	87	HIS	C-O	-6.07	1.11	1.23
1	A	136	LEU	CG-CD2	-6.07	1.29	1.51
1	A	27	GLN	CG-CD	6.07	1.65	1.51
1	C	31	ARG	CZ-NH2	6.07	1.41	1.33
1	A	127	LYS	CA-C	6.07	1.68	1.52
1	A	18	GLY	C-N	-6.06	1.22	1.33
2	B	93	ASN	C-O	-6.05	1.11	1.23
1	A	24	TYR	CZ-OH	6.05	1.48	1.37
2	D	60	LYS	CE-NZ	6.05	1.64	1.49
2	D	96	HIS	CG-ND1	-6.04	1.25	1.38
1	C	105	LEU	CG-CD2	6.03	1.74	1.51
1	A	10	VAL	CB-CG2	6.03	1.65	1.52
2	B	34	TYR	CA-CB	-6.03	1.40	1.53
2	B	96	HIS	C-O	-6.03	1.11	1.23
1	C	139	LYS	C-O	6.03	1.34	1.23
1	C	68	LYS	CA-C	6.02	1.68	1.52
1	C	42	TYR	CD2-CE2	-6.01	1.30	1.39
1	C	50	HIS	C-N	6.01	1.43	1.33
2	D	16	LYS	CG-CD	6.01	1.72	1.52
1	C	141	ARG	NE-CZ	6.00	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	33	VAL	CB-CG2	-5.99	1.40	1.52
1	C	27	GLN	CA-CB	5.99	1.67	1.53
2	B	70	PHE	CD1-CE1	-5.98	1.27	1.39
2	B	117	PHE	N-CA	5.98	1.58	1.46
1	A	103	HIS	CA-C	5.98	1.68	1.52
2	B	123	PRO	CB-CG	5.97	1.79	1.50
2	D	38	GLN	CB-CG	5.97	1.68	1.52
1	A	87	HIS	CA-C	5.97	1.68	1.52
1	C	108	THR	CA-CB	-5.97	1.37	1.53
2	B	126	GLN	CB-CG	5.96	1.68	1.52
1	C	74	ASN	CA-CB	5.96	1.68	1.53
1	A	62	VAL	N-CA	-5.96	1.34	1.46
2	D	113	VAL	N-CA	5.96	1.58	1.46
1	A	91	LEU	C-N	-5.96	1.20	1.34
2	D	38	GLN	CA-CB	-5.95	1.40	1.53
1	A	108	THR	C-N	5.95	1.47	1.34
1	A	134	THR	CB-CG2	5.95	1.72	1.52
1	A	109	LEU	N-CA	-5.95	1.34	1.46
1	A	139	LYS	CA-CB	-5.95	1.40	1.53
1	C	33	PHE	CD1-CE1	-5.95	1.27	1.39
1	C	103	HIS	CA-CB	5.95	1.67	1.53
1	A	87	HIS	CE1-NE2	-5.94	1.19	1.32
1	C	52	SER	N-CA	5.94	1.58	1.46
1	C	73	LEU	CB-CG	5.94	1.69	1.52
1	C	122	HIS	CG-CD2	5.94	1.45	1.35
1	C	46	PHE	CE1-CZ	-5.94	1.26	1.37
1	C	75	ASP	C-N	5.94	1.47	1.34
2	D	103	ARG	CD-NE	5.94	1.56	1.46
1	A	66	LEU	C-O	-5.93	1.12	1.23
2	B	75	LYS	CE-NZ	-5.93	1.34	1.49
1	A	140	TYR	CA-CB	-5.93	1.41	1.53
1	C	66	LEU	CA-C	-5.93	1.37	1.52
2	D	102	PHE	CB-CG	-5.93	1.41	1.51
1	A	131	ASN	CG-ND2	-5.92	1.18	1.32
2	D	111	LEU	CA-C	5.92	1.68	1.52
1	C	3	SER	C-N	-5.92	1.20	1.34
1	A	21	ALA	C-O	5.92	1.34	1.23
2	D	47	LEU	CG-CD1	5.92	1.73	1.51
1	A	106	LEU	C-N	-5.92	1.20	1.34
2	B	51	GLY	CA-C	5.92	1.61	1.51
2	B	135	GLY	C-O	5.91	1.33	1.23
1	C	54	GLN	C-N	-5.91	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	17	VAL	CB-CG2	5.91	1.65	1.52
2	B	38	GLN	CD-NE2	-5.90	1.18	1.32
2	B	52	ALA	CA-C	5.90	1.68	1.52
1	C	92	ARG	N-CA	5.90	1.58	1.46
2	B	80	LEU	CA-CB	-5.89	1.40	1.53
1	C	97	ASN	C-N	5.88	1.47	1.34
1	A	102	SER	CB-OG	5.88	1.49	1.42
1	C	50	HIS	CG-CD2	-5.87	1.25	1.35
2	B	129	PHE	C-N	5.87	1.47	1.34
2	D	20	ASP	CG-OD1	5.86	1.38	1.25
1	A	136	LEU	N-CA	5.85	1.58	1.46
2	D	74	LEU	C-O	5.85	1.34	1.23
2	B	60	LYS	CG-CD	-5.85	1.32	1.52
2	B	131	LYS	CE-NZ	5.85	1.63	1.49
1	C	65	ALA	CA-CB	-5.85	1.40	1.52
1	C	70	GLN	C-N	-5.84	1.22	1.33
2	D	69	ALA	N-CA	-5.84	1.34	1.46
1	C	47	ASP	CA-CB	5.84	1.66	1.53
1	C	73	LEU	CA-C	5.84	1.68	1.52
1	A	21	ALA	CA-C	5.83	1.68	1.52
2	B	86	GLN	C-O	-5.83	1.12	1.23
2	D	96	HIS	CG-CD2	5.83	1.45	1.35
2	B	80	LEU	CG-CD1	5.83	1.73	1.51
2	B	83	ALA	N-CA	5.83	1.58	1.46
1	C	31	ARG	CZ-NH1	5.82	1.40	1.33
2	B	27	LEU	CG-CD1	-5.82	1.30	1.51
2	D	112	VAL	N-CA	-5.82	1.34	1.46
2	B	11	THR	C-N	-5.82	1.22	1.33
2	D	101	ASN	CB-CG	5.81	1.64	1.51
1	A	28	ALA	CA-C	-5.81	1.37	1.52
2	D	66	VAL	C-N	-5.81	1.20	1.34
1	A	115	THR	CA-CB	5.80	1.68	1.53
2	B	20	ASP	C-N	-5.80	1.20	1.34
1	A	120	ALA	C-N	5.80	1.47	1.34
2	D	10	VAL	CB-CG2	5.80	1.65	1.52
2	D	81	LYS	CB-CG	-5.80	1.36	1.52
2	D	140	LEU	CA-C	5.79	1.68	1.52
2	B	46	ASN	N-CA	5.77	1.57	1.46
1	C	56	LYS	CG-CD	5.77	1.72	1.52
1	A	45	HIS	N-CA	-5.77	1.34	1.46
1	A	38	THR	CB-CG2	5.76	1.71	1.52
1	C	92	ARG	CA-CB	5.76	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	106	GLY	C-O	-5.76	1.14	1.23
2	B	73	GLY	C-N	-5.75	1.20	1.34
1	C	22	PRO	N-CD	5.75	1.55	1.47
1	A	102	SER	C-O	5.75	1.34	1.23
2	B	54	MET	CG-SD	-5.75	1.66	1.81
1	C	64	ASN	N-CA	-5.75	1.34	1.46
1	A	1	VAL	CB-CG2	5.75	1.65	1.52
2	B	27	LEU	N-CA	5.74	1.57	1.46
2	B	65	ARG	CZ-NH1	5.73	1.40	1.33
2	B	80	LEU	CA-C	5.73	1.67	1.52
1	A	133	SER	CA-C	-5.73	1.38	1.52
1	A	94	ASN	CG-OD1	5.73	1.36	1.24
2	B	6	GLU	CA-C	-5.72	1.38	1.52
1	C	43	PHE	C-N	-5.72	1.23	1.34
1	C	80	LEU	C-N	-5.72	1.20	1.34
1	A	47	ASP	N-CA	5.72	1.57	1.46
2	D	85	ALA	CA-C	-5.71	1.38	1.52
1	C	76	LEU	CA-C	5.71	1.67	1.52
2	B	89	GLY	C-N	-5.71	1.21	1.34
1	A	46	PHE	CE1-CZ	5.70	1.48	1.37
1	A	89	HIS	CD2-NE2	-5.70	1.25	1.38
1	A	87	HIS	N-CA	-5.70	1.34	1.46
1	C	13	ALA	CA-C	5.70	1.67	1.52
1	C	101	LEU	CG-CD2	-5.70	1.30	1.51
1	A	90	LYS	C-N	-5.69	1.21	1.34
2	D	19	VAL	N-CA	-5.69	1.34	1.46
2	D	2	LEU	N-CA	-5.69	1.34	1.46
1	A	61	LYS	CB-CG	5.68	1.67	1.52
1	A	79	THR	N-CA	-5.68	1.34	1.46
2	B	39	ARG	CD-NE	-5.68	1.36	1.46
2	B	129	PHE	CE2-CZ	5.67	1.48	1.37
1	A	22	PRO	CA-CB	5.66	1.64	1.53
1	C	96	VAL	N-CA	5.66	1.57	1.46
1	A	24	TYR	CD1-CE1	-5.65	1.30	1.39
2	D	56	ASN	CG-ND2	5.65	1.47	1.32
1	C	112	HIS	CA-C	5.65	1.67	1.52
2	D	8	ALA	C-N	5.64	1.47	1.34
1	C	72	HIS	CA-CB	-5.63	1.41	1.53
1	C	6	ASN	CG-OD1	5.63	1.36	1.24
1	A	58	HIS	CD2-NE2	-5.63	1.25	1.38
2	B	41	PHE	CB-CG	-5.63	1.41	1.51
1	C	5	ALA	CA-C	5.62	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	LEU	CA-CB	5.62	1.66	1.53
2	D	130	GLN	N-CA	5.62	1.57	1.46
1	A	132	ASP	CA-C	5.61	1.67	1.52
2	B	34	TYR	CB-CG	-5.61	1.43	1.51
2	B	30	LEU	N-CA	-5.61	1.35	1.46
1	A	50	HIS	N-CA	-5.61	1.35	1.46
2	D	94	LYS	CB-CG	5.61	1.67	1.52
2	D	7	LYS	N-CA	5.61	1.57	1.46
2	D	91	HIS	ND1-CE1	-5.61	1.20	1.34
1	C	23	ALA	CA-C	5.60	1.67	1.52
2	B	8	ALA	C-N	5.60	1.47	1.34
1	C	94	ASN	C-O	5.60	1.33	1.23
2	B	132	VAL	C-N	-5.59	1.21	1.34
2	D	87	LEU	C-O	5.59	1.33	1.23
1	A	112	HIS	CA-CB	5.59	1.66	1.53
2	B	77	LEU	CG-CD1	5.59	1.72	1.51
2	B	138	ASN	CA-CB	5.58	1.67	1.53
2	D	75	LYS	N-CA	-5.58	1.35	1.46
2	D	90	LEU	CA-CB	5.58	1.66	1.53
2	B	15	GLY	N-CA	-5.58	1.37	1.46
2	D	16	LYS	CE-NZ	5.58	1.62	1.49
1	C	131	ASN	CG-ND2	-5.58	1.19	1.32
2	D	142	HIS	CA-C	-5.57	1.38	1.52
2	B	79	ASP	N-CA	5.56	1.57	1.46
1	C	119	PRO	N-CD	5.56	1.55	1.47
1	C	139	LYS	CG-CD	-5.56	1.33	1.52
1	C	80	LEU	CB-CG	5.56	1.68	1.52
2	B	107	ASN	CA-C	-5.55	1.38	1.52
1	C	40	LYS	CA-C	5.55	1.67	1.52
2	D	60	LYS	N-CA	-5.55	1.35	1.46
1	C	41	THR	CB-OG1	-5.55	1.32	1.43
1	C	64	ASN	C-O	5.53	1.33	1.23
2	D	138	ASN	C-N	-5.53	1.21	1.34
2	B	43	HIS	C-O	5.53	1.33	1.23
1	A	72	HIS	CA-CB	-5.53	1.41	1.53
2	D	97	VAL	N-CA	-5.53	1.35	1.46
1	C	56	LYS	C-N	5.52	1.46	1.34
1	A	5	ALA	C-N	5.52	1.46	1.34
2	D	81	LYS	CA-C	-5.52	1.38	1.52
2	B	19	VAL	C-O	5.51	1.33	1.23
1	A	122	HIS	CB-CG	5.51	1.59	1.50
1	C	112	HIS	CE1-NE2	-5.50	1.20	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	ALA	C-O	-5.50	1.12	1.23
1	A	9	ASN	CG-ND2	-5.50	1.19	1.32
2	D	96	HIS	C-N	-5.50	1.21	1.34
1	A	22	PRO	CB-CG	5.49	1.77	1.50
2	D	130	GLN	CA-CB	-5.49	1.41	1.53
1	A	89	HIS	CA-C	5.48	1.67	1.52
1	A	134	THR	N-CA	5.48	1.57	1.46
1	A	24	TYR	C-N	5.48	1.43	1.33
2	D	43	HIS	C-N	5.46	1.46	1.34
2	B	12	GLY	N-CA	5.45	1.54	1.46
1	C	138	SER	C-O	-5.44	1.13	1.23
2	D	14	TRP	CA-CB	5.44	1.66	1.53
1	A	68	LYS	CB-CG	5.44	1.67	1.52
1	A	84	SER	C-N	-5.44	1.21	1.34
2	D	18	ASP	CB-CG	-5.44	1.40	1.51
2	B	26	ALA	C-O	5.43	1.33	1.23
1	C	49	SER	C-N	-5.43	1.21	1.34
1	A	17	VAL	CA-CB	-5.43	1.43	1.54
1	C	46	PHE	N-CA	5.43	1.57	1.46
1	A	81	SER	CA-C	5.42	1.67	1.52
1	C	67	THR	CA-CB	-5.42	1.39	1.53
1	A	89	HIS	ND1-CE1	-5.42	1.21	1.34
1	C	70	GLN	CB-CG	-5.41	1.38	1.52
1	C	124	ASN	C-O	5.41	1.33	1.23
2	D	94	LYS	CE-NZ	5.41	1.62	1.49
1	C	120	ALA	C-N	5.41	1.46	1.34
2	D	98	ASN	CA-C	5.41	1.67	1.52
1	A	45	HIS	CA-C	-5.41	1.38	1.52
2	B	44	PHE	CD2-CE2	-5.40	1.28	1.39
1	A	69	ALA	C-N	5.40	1.46	1.34
1	C	141	ARG	CB-CG	5.39	1.67	1.52
2	D	145	HIS	CA-CB	5.39	1.65	1.53
1	A	97	ASN	C-N	-5.38	1.21	1.34
1	C	92	ARG	CA-C	5.38	1.67	1.52
2	B	73	GLY	C-O	5.38	1.32	1.23
2	D	18	ASP	CG-OD2	-5.38	1.12	1.25
1	A	74	ASN	CG-OD1	-5.38	1.12	1.24
2	B	115	ARG	N-CA	-5.37	1.35	1.46
2	D	72	GLN	CA-C	-5.37	1.39	1.52
1	C	96	VAL	C-N	-5.37	1.21	1.34
2	D	5	GLU	CD-OE1	5.36	1.31	1.25
2	D	48	SER	N-CA	5.36	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	HIS	N-CA	5.35	1.57	1.46
1	A	129	LEU	CA-C	-5.35	1.39	1.52
2	B	36	TRP	CZ3-CH2	5.35	1.48	1.40
2	D	46	ASN	CB-CG	-5.35	1.38	1.51
2	D	94	LYS	CG-CD	5.35	1.70	1.52
2	D	116	ASN	CG-ND2	5.34	1.46	1.32
1	C	65	ALA	N-CA	5.34	1.57	1.46
2	D	16	LYS	N-CA	-5.34	1.35	1.46
1	A	51	GLY	C-N	-5.33	1.21	1.34
2	D	126	GLN	N-CA	5.33	1.56	1.46
1	C	64	ASN	CA-C	5.32	1.66	1.52
1	C	114	PRO	CA-C	5.32	1.63	1.52
2	B	76	HIS	C-N	5.31	1.46	1.34
1	C	99	LYS	CE-NZ	-5.31	1.35	1.49
2	D	91	HIS	C-N	-5.31	1.21	1.34
2	D	134	ALA	C-N	-5.30	1.23	1.33
1	A	22	PRO	CA-C	-5.30	1.42	1.52
1	C	32	MET	CG-SD	-5.30	1.67	1.81
2	B	135	GLY	N-CA	-5.29	1.38	1.46
2	D	84	PHE	CD1-CE1	5.29	1.49	1.39
2	D	99	PRO	CB-CG	5.29	1.76	1.50
1	A	110	ALA	N-CA	5.29	1.56	1.46
2	B	62	HIS	C-O	5.28	1.33	1.23
1	A	127	LYS	CA-CB	-5.28	1.42	1.53
1	C	65	ALA	CA-C	-5.28	1.39	1.52
1	C	32	MET	CA-C	5.27	1.66	1.52
2	D	125	VAL	C-N	5.27	1.46	1.34
2	D	42	GLN	CA-CB	-5.26	1.42	1.53
1	C	140	TYR	CD2-CE2	5.25	1.47	1.39
2	B	87	LEU	CG-CD2	-5.25	1.32	1.51
1	C	108	THR	N-CA	-5.24	1.35	1.46
1	A	95	PRO	C-N	5.23	1.46	1.34
1	C	4	ALA	C-N	-5.23	1.22	1.34
1	A	129	LEU	CG-CD1	-5.23	1.32	1.51
2	D	100	GLN	N-CA	5.23	1.56	1.46
1	A	75	ASP	CG-OD2	5.22	1.37	1.25
1	A	98	PHE	C-O	5.22	1.33	1.23
1	A	128	PHE	N-CA	-5.22	1.35	1.46
2	B	105	LEU	N-CA	-5.22	1.35	1.46
1	C	62	VAL	N-CA	5.22	1.56	1.46
2	B	37	THR	C-N	-5.21	1.22	1.34
2	D	101	ASN	CA-CB	5.21	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	THR	CB-CG2	-5.20	1.35	1.52
2	D	59	VAL	CB-CG1	5.20	1.63	1.52
1	A	34	LEU	CG-CD2	5.19	1.71	1.51
1	A	112	HIS	ND1-CE1	5.18	1.47	1.34
2	B	44	PHE	CB-CG	5.18	1.60	1.51
2	D	105	LEU	CB-CG	-5.18	1.37	1.52
2	D	117	PHE	CD2-CE2	-5.18	1.28	1.39
2	D	134	ALA	C-O	-5.18	1.13	1.23
1	A	103	HIS	N-CA	-5.17	1.36	1.46
1	A	11	LYS	CB-CG	5.17	1.66	1.52
2	B	41	PHE	CG-CD1	5.17	1.46	1.38
2	B	117	PHE	CA-CB	-5.17	1.42	1.53
1	A	133	SER	C-N	5.17	1.46	1.34
2	B	26	ALA	N-CA	5.17	1.56	1.46
2	B	68	ASP	CA-C	5.17	1.66	1.52
1	A	29	LEU	C-N	5.17	1.46	1.34
1	A	122	HIS	CD2-NE2	5.17	1.52	1.42
2	B	104	LEU	CB-CG	-5.17	1.37	1.52
2	B	33	VAL	CA-C	5.16	1.66	1.52
2	B	60	LYS	CA-CB	-5.15	1.42	1.53
1	A	100	LEU	CA-CB	-5.15	1.42	1.53
1	C	128	PHE	CB-CG	-5.15	1.42	1.51
2	D	41	PHE	CD1-CE1	5.14	1.49	1.39
2	B	16	LYS	CA-CB	-5.14	1.42	1.53
1	C	50	HIS	CA-CB	5.14	1.65	1.53
1	C	57	ALA	C-N	5.14	1.45	1.34
1	A	75	ASP	C-N	5.13	1.45	1.34
2	B	10	VAL	CB-CG2	5.13	1.63	1.52
1	A	89	HIS	C-O	5.13	1.33	1.23
1	A	141	ARG	CD-NE	5.13	1.55	1.46
2	D	143	LYS	CG-CD	-5.13	1.35	1.52
1	A	31	ARG	NE-CZ	-5.13	1.26	1.33
1	A	77	PRO	CG-CD	-5.13	1.33	1.50
1	A	101	LEU	CG-CD2	5.12	1.70	1.51
2	D	72	GLN	N-CA	5.12	1.56	1.46
2	D	125	VAL	N-CA	5.12	1.56	1.46
1	A	46	PHE	CG-CD1	5.12	1.46	1.38
2	B	111	LEU	CG-CD1	5.11	1.70	1.51
2	D	11	THR	CA-CB	-5.11	1.40	1.53
1	A	66	LEU	CG-CD1	5.10	1.70	1.51
2	D	14	TRP	CZ2-CH2	-5.10	1.27	1.37
1	A	38	THR	CB-OG1	-5.09	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	LEU	CB-CG	5.09	1.67	1.52
1	A	114	PRO	C-N	5.09	1.45	1.34
2	B	102	PHE	CD2-CE2	-5.09	1.29	1.39
1	C	40	LYS	CD-CE	5.08	1.64	1.51
1	C	21	ALA	N-CA	5.08	1.56	1.46
1	A	123	ALA	N-CA	-5.08	1.36	1.46
1	C	81	SER	C-O	-5.08	1.13	1.23
2	B	42	GLN	C-O	5.07	1.32	1.23
2	B	27	LEU	CG-CD2	5.07	1.70	1.51
2	D	80	LEU	C-N	5.07	1.45	1.34
2	D	83	ALA	C-N	5.07	1.45	1.34
2	B	35	PRO	CA-CB	5.06	1.63	1.53
1	A	88	ALA	CA-CB	5.06	1.63	1.52
1	A	44	PRO	N-CA	-5.06	1.38	1.47
2	D	11	THR	C-O	-5.06	1.13	1.23
1	C	81	SER	CB-OG	-5.04	1.35	1.42
1	C	123	ALA	CA-C	5.04	1.66	1.52
2	B	72	GLN	CD-OE1	5.04	1.35	1.24
1	A	103	HIS	ND1-CE1	5.04	1.47	1.34
1	C	126	ASN	C-O	5.04	1.32	1.23
1	A	22	PRO	CG-CD	-5.03	1.34	1.50
2	B	121	PHE	CA-C	-5.02	1.39	1.52
2	B	48	SER	CA-C	5.02	1.66	1.52
1	A	39	THR	CB-CG2	5.02	1.69	1.52
1	A	141	ARG	CG-CD	5.02	1.64	1.51
2	D	92	CYS	CA-CB	5.01	1.65	1.53
1	A	24	TYR	C-O	-5.01	1.13	1.23
1	C	62	VAL	CA-CB	-5.01	1.44	1.54
2	B	35	PRO	N-CA	-5.01	1.38	1.47

All (3374) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	70	PHE	CB-CG-CD2	71.93	171.15	120.80
1	A	92	ARG	NE-CZ-NH2	-65.06	87.77	120.30
1	A	141	ARG	NE-CZ-NH1	61.72	151.16	120.30
2	D	44	PHE	CB-CG-CD2	60.92	163.44	120.80
2	D	84	PHE	CB-CG-CD1	-60.50	78.45	120.80
2	D	65	ARG	NE-CZ-NH2	57.73	149.16	120.30
2	B	84	PHE	CB-CG-CD1	-56.87	80.99	120.80
2	B	65	ARG	NE-CZ-NH1	55.24	147.92	120.30
1	A	140	TYR	CZ-CE2-CD2	54.60	168.94	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	PHE	CB-CG-CD2	53.01	157.90	120.80
2	D	115	ARG	NE-CZ-NH1	52.80	146.70	120.30
1	C	141	ARG	NE-CZ-NH1	-51.22	94.69	120.30
1	A	98	PHE	CB-CG-CD2	50.59	156.21	120.80
2	B	79	ASP	CB-CG-OD2	50.11	163.40	118.30
1	C	31	ARG	NE-CZ-NH1	49.88	145.24	120.30
2	B	103	ARG	NE-CZ-NH2	-49.14	95.73	120.30
1	C	36	PHE	CB-CG-CD2	48.97	155.08	120.80
2	B	144	TYR	CB-CG-CD2	-48.49	91.91	121.00
1	A	75	ASP	CB-CG-OD2	48.46	161.91	118.30
2	B	40	PHE	CB-CG-CD2	48.23	154.56	120.80
2	D	7	LYS	O-C-N	-47.19	47.19	122.70
1	C	36	PHE	CG-CD2-CE2	46.87	172.36	120.80
2	B	129	PHE	CB-CG-CD1	-46.81	88.03	120.80
2	D	70	PHE	CG-CD2-CE2	46.62	172.08	120.80
2	B	13	PHE	CB-CG-CD2	45.22	152.46	120.80
2	D	144	TYR	CB-CG-CD1	-45.09	93.94	121.00
2	D	121	PHE	CB-CG-CD1	44.24	151.77	120.80
1	C	92	ARG	NE-CZ-NH2	43.96	142.28	120.30
2	D	29	ARG	NE-CZ-NH2	43.71	142.15	120.30
2	D	84	PHE	CB-CG-CD2	43.46	151.22	120.80
1	A	43	PHE	CB-CG-CD1	42.43	150.50	120.80
2	D	144	TYR	CD1-CE1-CZ	-42.38	81.66	119.80
2	D	103	ARG	NE-CZ-NH1	42.14	141.37	120.30
2	D	34	TYR	CB-CG-CD2	41.74	146.04	121.00
2	D	121	PHE	CG-CD1-CE1	40.18	165.00	120.80
1	A	132	ASP	CB-CG-OD2	-38.65	83.51	118.30
2	B	70	PHE	CZ-CE2-CD2	-38.48	73.93	120.10
1	A	42	TYR	CB-CG-CD2	37.88	143.73	121.00
1	A	132	ASP	CB-CG-OD1	37.78	152.30	118.30
1	C	46	PHE	CG-CD1-CE1	-37.71	79.32	120.80
2	B	65	ARG	NH1-CZ-NH2	-37.03	78.67	119.40
1	C	128	PHE	CG-CD2-CE2	36.77	161.25	120.80
1	C	46	PHE	CZ-CE2-CD2	-36.07	76.81	120.10
2	D	14	TRP	CG-CD2-CE3	-36.05	101.45	133.90
2	B	39	ARG	NE-CZ-NH1	-35.95	102.32	120.30
2	B	14	TRP	CG-CD1-NE1	35.89	145.99	110.10
2	B	70	PHE	CG-CD2-CE2	35.78	160.16	120.80
2	D	70	PHE	CD1-CG-CD2	-35.27	72.45	118.30
1	C	46	PHE	CG-CD2-CE2	34.81	159.09	120.80
2	D	102	PHE	CB-CG-CD1	34.76	145.13	120.80
1	A	140	TYR	CG-CD2-CE2	-34.68	93.56	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	113	VAL	CG1-CB-CG2	-34.65	55.46	110.90
2	D	11	THR	O-C-N	-34.52	64.52	123.20
1	A	43	PHE	CB-CG-CD2	-34.34	96.76	120.80
1	C	14	TRP	CD1-CG-CD2	-34.27	78.88	106.30
2	D	19	VAL	CA-CB-CG1	34.10	162.05	110.90
2	B	29	ARG	NE-CZ-NH1	33.88	137.24	120.30
1	A	46	PHE	CB-CG-CD2	33.70	144.39	120.80
1	A	110	ALA	N-CA-CB	33.46	156.95	110.10
2	B	103	ARG	NE-CZ-NH1	33.38	136.99	120.30
2	B	40	PHE	CG-CD2-CE2	33.09	157.21	120.80
1	A	141	ARG	NE-CZ-NH2	-32.97	103.82	120.30
1	A	29	LEU	O-C-N	-32.94	69.99	122.70
1	C	122	HIS	CA-CB-CG	32.88	169.50	113.60
2	D	121	PHE	CD1-CE1-CZ	-32.41	81.21	120.10
2	D	77	LEU	O-C-N	-32.17	71.22	122.70
2	D	110	ALA	N-CA-CB	31.37	154.02	110.10
1	A	92	ARG	NH1-CZ-NH2	31.24	153.76	119.40
1	C	112	HIS	ND1-CG-CD2	-31.18	62.34	106.00
2	B	13	PHE	CG-CD2-CE2	31.14	155.06	120.80
2	B	14	TRP	CD1-NE1-CE2	-30.93	81.16	109.00
2	D	43	HIS	CG-ND1-CE1	30.84	151.38	108.20
2	B	16	LYS	O-C-N	-30.73	73.53	122.70
2	B	79	ASP	OD1-CG-OD2	-30.38	65.58	123.30
1	C	115	THR	CA-CB-CG2	30.26	154.76	112.40
2	D	44	PHE	CG-CD1-CE1	30.22	154.05	120.80
1	C	42	TYR	CZ-CE2-CD2	30.22	147.00	119.80
1	A	42	TYR	CG-CD2-CE2	30.10	145.38	121.30
2	B	102	PHE	CD1-CG-CD2	-29.90	79.43	118.30
2	D	21	VAL	CG1-CB-CG2	-29.88	63.10	110.90
2	D	129	PHE	CB-CG-CD1	29.78	141.65	120.80
1	A	33	PHE	CB-CG-CD2	29.56	141.49	120.80
1	C	49	SER	O-C-N	-29.48	75.53	122.70
2	D	144	TYR	CD1-CG-CD2	29.29	150.12	117.90
1	C	92	ARG	NH1-CZ-NH2	-29.27	87.21	119.40
2	D	18	ASP	O-C-N	-29.04	76.24	122.70
2	B	94	LYS	CD-CE-NZ	28.89	178.14	111.70
2	B	33	VAL	CG1-CB-CG2	-28.72	64.95	110.90
1	A	87	HIS	ND1-CG-CD2	28.62	148.87	108.80
2	B	113	VAL	CA-CB-CG2	28.60	153.81	110.90
2	D	129	PHE	CG-CD2-CE2	28.57	152.22	120.80
2	D	129	PHE	CD1-CG-CD2	-28.55	81.19	118.30
1	A	140	TYR	CG-CD1-CE1	-28.47	98.52	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	LEU	CB-CG-CD1	28.25	159.03	111.00
2	D	65	ARG	NE-CZ-NH1	-28.21	106.19	120.30
2	B	70	PHE	O-C-N	-28.19	77.59	122.70
1	A	140	TYR	CB-CG-CD1	-28.13	104.12	121.00
2	D	14	TRP	CD1-CG-CD2	-28.10	83.82	106.30
2	D	44	PHE	CD1-CE1-CZ	-28.04	86.45	120.10
1	C	110	ALA	N-CA-CB	27.99	149.29	110.10
2	B	121	PHE	CZ-CE2-CD2	27.93	153.62	120.10
1	C	24	TYR	CB-CG-CD1	27.86	137.71	121.00
1	A	36	PHE	CG-CD1-CE1	27.79	151.37	120.80
2	B	44	PHE	CB-CG-CD2	27.77	140.24	120.80
2	D	143	LYS	O-C-N	-27.59	78.56	122.70
2	B	102	PHE	CG-CD2-CE2	27.52	151.08	120.80
2	D	144	TYR	CG-CD2-CE2	-27.43	99.35	121.30
2	D	57	PRO	N-CD-CG	-27.35	62.17	103.20
2	B	6	GLU	OE1-CD-OE2	-27.34	90.49	123.30
2	B	144	TYR	CB-CG-CD1	27.23	137.34	121.00
2	D	14	TRP	CB-CG-CD2	27.20	161.96	126.60
1	A	24	TYR	CB-CG-CD2	26.74	137.04	121.00
2	B	95	LEU	N-CA-CB	-26.72	56.96	110.40
2	B	77	LEU	O-C-N	-26.70	79.98	122.70
1	C	108	THR	N-CA-CB	26.64	160.92	110.30
2	D	21	VAL	CA-CB-CG1	26.50	150.65	110.90
1	A	62	VAL	CG1-CB-CG2	-26.39	68.68	110.90
1	C	103	HIS	CG-ND1-CE1	-26.33	71.33	108.20
2	D	103	ARG	NE-CZ-NH2	-26.32	107.14	120.30
2	B	20	ASP	O-C-N	-26.32	80.59	122.70
1	C	46	PHE	CB-CG-CD1	-26.31	102.38	120.80
2	D	6	GLU	O-C-N	26.25	164.70	122.70
2	B	65	ARG	NE-CZ-NH2	26.06	133.33	120.30
1	C	4	ALA	N-CA-CB	-26.01	73.69	110.10
2	B	121	PHE	CB-CG-CD2	25.99	139.00	120.80
2	D	115	ARG	NE-CZ-NH2	-25.97	107.32	120.30
1	C	98	PHE	CD1-CE1-CZ	25.96	151.26	120.10
1	A	140	TYR	CD1-CE1-CZ	25.89	143.10	119.80
2	D	2	LEU	CA-C-O	-25.46	66.64	120.10
2	D	144	TYR	CE1-CZ-CE2	25.39	160.43	119.80
1	A	29	LEU	CB-CA-C	25.33	158.33	110.20
2	D	41	PHE	CB-CG-CD2	-25.08	103.25	120.80
1	A	52	SER	O-C-N	25.08	162.82	122.70
2	D	1	MET	O-C-N	-25.06	82.60	122.70
1	A	42	TYR	CD1-CG-CD2	-25.02	90.38	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	GLN	CB-CG-CD	24.91	176.37	111.60
2	B	13	PHE	CD1-CG-CD2	-24.85	86.00	118.30
1	C	128	PHE	CB-CG-CD2	24.80	138.16	120.80
1	C	29	LEU	CA-CB-CG	24.74	172.20	115.30
2	B	67	LEU	CA-C-O	-24.73	68.17	120.10
2	B	79	ASP	O-C-N	-24.72	83.15	122.70
2	D	91	HIS	O-C-N	24.57	162.02	122.70
1	C	85	ASN	O-C-N	-24.55	83.41	122.70
1	C	66	LEU	CA-CB-CG	24.51	171.67	115.30
2	D	96	HIS	CG-ND1-CE1	24.46	142.44	108.20
1	C	46	PHE	CD1-CE1-CZ	24.39	149.37	120.10
2	B	144	TYR	CG-CD2-CE2	-24.34	101.83	121.30
1	A	47	ASP	CB-CG-OD1	24.33	140.20	118.30
1	A	8	SER	CA-C-N	24.26	170.57	117.20
1	A	40	LYS	O-C-N	-24.25	83.90	122.70
2	B	114	ALA	N-CA-CB	24.11	143.85	110.10
2	D	96	HIS	ND1-CG-CD2	-24.11	72.25	106.00
2	B	123	PRO	O-C-N	-24.10	84.14	122.70
1	A	40	LYS	CD-CE-NZ	24.08	167.09	111.70
1	C	33	PHE	CG-CD1-CE1	24.05	147.26	120.80
2	D	2	LEU	CB-CG-CD1	-24.03	70.15	111.00
2	D	11	THR	CA-C-N	23.96	164.12	116.20
2	D	29	ARG	NH1-CZ-NH2	-23.91	93.09	119.40
2	B	70	PHE	CA-C-O	23.91	170.30	120.10
2	D	70	PHE	CA-C-O	-23.78	70.17	120.10
2	B	84	PHE	CZ-CE2-CD2	23.77	148.63	120.10
2	D	3	THR	C-N-CA	-23.76	62.29	121.70
1	A	46	PHE	CB-CG-CD1	-23.74	104.19	120.80
2	B	57	PRO	CA-N-CD	-23.65	78.39	111.50
2	D	128	LEU	O-C-N	23.64	160.52	122.70
2	B	73	GLY	O-C-N	23.60	160.46	122.70
2	B	32	VAL	O-C-N	-23.57	84.98	122.70
2	D	117	PHE	CZ-CE2-CD2	-23.51	91.89	120.10
2	D	133	VAL	CG1-CB-CG2	-23.50	73.30	110.90
1	A	98	PHE	CB-CG-CD1	-23.49	104.36	120.80
1	C	14	TRP	CG-CD1-NE1	23.49	133.59	110.10
1	C	85	ASN	CA-C-O	-23.49	70.78	120.10
2	D	128	LEU	CB-CA-C	23.48	154.81	110.20
1	A	62	VAL	CA-CB-CG2	23.45	146.07	110.90
2	D	44	PHE	CD1-CG-CD2	-23.43	87.84	118.30
2	B	6	GLU	CG-CD-OE1	23.37	165.04	118.30
1	A	120	ALA	CA-C-N	23.37	168.61	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	THR	CA-CB-CG2	-23.36	79.70	112.40
1	C	36	PHE	CD1-CG-CD2	-23.32	87.98	118.30
2	B	109	LEU	CB-CG-CD2	-23.28	71.42	111.00
2	D	7	LYS	CA-C-O	23.27	168.97	120.10
2	B	1	MET	CB-CA-C	23.25	156.89	110.40
2	D	11	THR	CB-CA-C	23.20	174.25	111.60
2	D	103	ARG	N-CA-CB	23.20	152.35	110.60
1	A	38	THR	CA-CB-CG2	23.07	144.69	112.40
2	B	84	PHE	CD1-CG-CD2	23.04	148.25	118.30
2	B	84	PHE	CG-CD2-CE2	-23.02	95.48	120.80
2	B	76	HIS	CA-C-N	23.00	167.80	117.20
1	A	53	ALA	CB-CA-C	23.00	144.59	110.10
2	D	140	LEU	CB-CG-CD2	22.98	150.06	111.00
2	B	20	ASP	CB-CG-OD1	-22.89	97.70	118.30
1	C	43	PHE	CB-CG-CD2	22.83	136.78	120.80
2	D	72	GLN	CG-CD-OE1	-22.77	76.07	121.60
1	A	70	GLN	CB-CG-CD	22.70	170.63	111.60
1	A	105	LEU	CA-CB-CG	22.67	167.44	115.30
2	B	77	LEU	CA-C-O	22.63	167.61	120.10
1	A	77	PRO	O-C-N	22.57	161.56	123.20
2	D	2	LEU	CA-C-N	22.50	166.70	117.20
2	D	125	VAL	CA-CB-CG1	22.45	144.57	110.90
2	B	44	PHE	CB-CG-CD1	-22.44	105.09	120.80
1	C	137	THR	CA-C-N	22.44	166.56	117.20
2	D	18	ASP	CA-C-O	22.33	166.98	120.10
1	A	29	LEU	CA-C-N	22.27	166.19	117.20
2	B	123	PRO	N-CD-CG	-22.25	69.82	103.20
2	D	129	PHE	CG-CD1-CE1	22.12	145.14	120.80
1	C	109	LEU	C-N-CA	22.11	176.98	121.70
2	D	34	TYR	CD1-CG-CD2	-22.06	93.63	117.90
2	D	42	GLN	CA-CB-CG	-22.01	64.97	113.40
1	A	127	LYS	CA-C-O	-21.97	73.96	120.10
2	D	105	LEU	CB-CG-CD1	-21.96	73.67	111.00
2	B	75	LYS	N-CA-CB	21.95	150.11	110.60
2	D	100	GLN	OE1-CD-NE2	-21.89	71.54	121.90
1	A	36	PHE	CB-CG-CD1	21.88	136.12	120.80
2	B	121	PHE	C-N-CA	21.88	176.40	121.70
1	C	107	VAL	CA-C-N	21.85	165.27	117.20
1	A	85	ASN	CA-C-O	-21.84	74.24	120.10
2	B	76	HIS	O-C-N	-21.83	87.77	122.70
2	D	51	GLY	O-C-N	-21.82	87.78	122.70
2	B	102	PHE	O-C-N	-21.82	87.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	93	ASN	O-C-N	21.75	157.50	122.70
1	A	46	PHE	CZ-CE2-CD2	-21.72	94.04	120.10
1	C	84	SER	O-C-N	-21.71	87.96	122.70
2	D	14	TRP	CG-CD1-NE1	21.66	131.76	110.10
2	D	68	ASP	CB-CG-OD1	21.65	137.79	118.30
2	D	43	HIS	ND1-CG-CD2	-21.58	75.79	106.00
2	D	100	GLN	CG-CD-NE2	21.57	168.48	116.70
2	D	82	GLY	CA-C-O	21.54	159.37	120.60
2	B	37	THR	O-C-N	-21.51	88.29	122.70
2	D	113	VAL	CA-CB-CG2	21.47	143.10	110.90
2	B	14	TRP	CD1-CG-CD2	-21.41	89.17	106.30
1	A	117	PHE	CG-CD2-CE2	-21.40	97.26	120.80
2	D	128	LEU	CB-CG-CD2	21.40	147.38	111.00
2	D	115	ARG	O-C-N	-21.39	88.48	122.70
1	A	94	ASN	CB-CG-ND2	21.31	167.84	116.70
2	B	51	GLY	CA-C-O	21.28	158.90	120.60
2	B	129	PHE	CZ-CE2-CD2	-21.21	94.64	120.10
1	C	47	ASP	C-N-CA	21.21	174.72	121.70
2	D	39	ARG	CB-CG-CD	21.20	166.73	111.60
2	D	65	ARG	O-C-N	21.18	156.59	122.70
2	B	129	PHE	CB-CG-CD2	21.15	135.61	120.80
1	C	117	PHE	CB-CG-CD1	21.15	135.60	120.80
2	B	76	HIS	C-N-CA	21.13	174.53	121.70
1	C	24	TYR	CG-CD1-CE1	21.09	138.18	121.30
1	A	1	VAL	O-C-N	-21.06	89.00	122.70
2	B	143	LYS	CB-CA-C	21.03	152.45	110.40
1	A	122	HIS	CA-CB-CG	21.02	149.34	113.60
2	D	125	VAL	CB-CA-C	21.02	151.34	111.40
1	C	2	LEU	O-C-N	-20.98	89.12	122.70
1	A	76	LEU	CB-CG-CD1	20.92	146.56	111.00
1	A	87	HIS	CG-ND1-CE1	-20.83	78.63	105.70
1	C	112	HIS	CG-CD2-NE2	20.81	148.74	109.20
1	C	13	ALA	N-CA-CB	20.80	139.22	110.10
1	A	140	TYR	CE1-CZ-CE2	-20.77	86.56	119.80
1	A	29	LEU	C-N-CA	20.75	173.57	121.70
2	D	144	TYR	N-CA-CB	-20.73	73.28	110.60
2	D	139	ALA	N-CA-CB	20.73	139.12	110.10
1	C	37	PRO	C-N-CA	20.72	173.51	121.70
1	C	120	ALA	O-C-N	-20.66	89.64	122.70
1	A	141	ARG	CG-CD-NE	-20.65	68.43	111.80
1	A	133	SER	O-C-N	-20.62	89.71	122.70
1	A	75	ASP	OD1-CG-OD2	-20.55	84.25	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	44	PHE	CG-CD2-CE2	20.55	143.41	120.80
2	D	36	TRP	CD1-CG-CD2	-20.51	89.89	106.30
1	A	16	LYS	CD-CE-NZ	-20.46	64.64	111.70
1	C	36	PHE	CZ-CE2-CD2	-20.41	95.61	120.10
2	B	96	HIS	O-C-N	-20.40	90.05	122.70
2	D	14	TRP	CE2-CD2-CE3	20.39	143.16	118.70
2	D	127	ALA	CA-C-O	-20.31	77.45	120.10
2	B	54	MET	CA-CB-CG	-20.27	78.83	113.30
2	B	42	GLN	O-C-N	-20.18	90.41	122.70
2	B	129	PHE	CG-CD1-CE1	-20.18	98.61	120.80
2	D	11	THR	CA-CB-CG2	20.15	140.61	112.40
2	B	44	PHE	CG-CD2-CE2	20.13	142.94	120.80
2	D	47	LEU	CA-CB-CG	20.11	161.56	115.30
1	C	2	LEU	CA-CB-CG	20.10	161.52	115.30
1	C	139	LYS	O-C-N	-20.08	90.58	122.70
1	A	46	PHE	CG-CD2-CE2	20.07	142.88	120.80
1	A	15	GLY	CA-C-N	20.05	161.32	117.20
1	C	47	ASP	CB-CG-OD1	-20.02	100.28	118.30
2	D	117	PHE	CD1-CE1-CZ	-20.00	96.10	120.10
2	D	77	LEU	C-N-CA	19.99	171.67	121.70
2	D	81	LYS	N-CA-CB	-19.98	74.64	110.60
1	C	137	THR	O-C-N	-19.98	90.74	122.70
2	D	4	ALA	C-N-CA	19.96	171.60	121.70
2	D	14	TRP	N-CA-CB	19.95	146.50	110.60
2	B	78	ASP	CB-CA-C	19.93	150.26	110.40
1	C	135	VAL	CA-CB-CG2	19.93	140.79	110.90
1	A	76	LEU	CA-CB-CG	19.92	161.12	115.30
2	D	123	PRO	N-CD-CG	-19.92	73.32	103.20
1	C	129	LEU	CB-CG-CD1	19.87	144.79	111.00
2	D	19	VAL	C-N-CA	19.84	171.30	121.70
2	D	99	PRO	CA-N-CD	-19.82	83.76	111.50
1	A	14	TRP	C-N-CA	19.79	163.86	122.30
2	D	16	LYS	CB-CG-CD	-19.79	60.15	111.60
1	A	33	PHE	CD1-CE1-CZ	-19.77	96.37	120.10
1	A	97	ASN	CB-CG-ND2	19.77	164.16	116.70
2	D	115	ARG	CB-CG-CD	19.73	162.91	111.60
2	D	9	ALA	CA-C-N	19.67	160.48	117.20
2	D	5	GLU	C-N-CA	19.67	170.88	121.70
2	D	99	PRO	O-C-N	-19.66	91.25	122.70
2	D	136	VAL	CA-CB-CG1	19.61	140.31	110.90
1	C	83	LEU	C-N-CA	19.60	170.69	121.70
2	B	77	LEU	C-N-CA	19.58	170.66	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	GLN	C-N-CA	19.57	170.63	121.70
2	B	77	LEU	CB-CG-CD1	-19.57	77.74	111.00
2	D	22	VAL	O-C-N	-19.56	89.95	123.20
1	C	24	TYR	CB-CG-CD2	-19.54	109.28	121.00
1	A	24	TYR	CA-C-N	19.52	155.24	116.20
1	C	46	PHE	CA-C-O	19.51	161.07	120.10
2	B	81	LYS	N-CA-CB	-19.49	75.52	110.60
2	B	41	PHE	CZ-CE2-CD2	19.49	143.48	120.10
2	D	121	PHE	CD1-CG-CD2	-19.45	93.02	118.30
2	D	144	TYR	CA-C-O	-19.44	79.27	120.10
2	B	129	PHE	N-CA-CB	19.42	145.56	110.60
2	B	87	LEU	CA-C-N	19.41	159.90	117.20
1	A	131	ASN	OD1-CG-ND2	-19.41	77.27	121.90
2	D	142	HIS	N-CA-CB	19.39	145.49	110.60
1	A	20	ASN	CB-CG-ND2	19.37	163.18	116.70
2	B	21	VAL	CB-CA-C	-19.35	74.63	111.40
2	D	51	GLY	CA-C-O	19.34	155.40	120.60
1	C	44	PRO	CA-N-CD	-19.33	84.44	111.50
1	C	31	ARG	NH1-CZ-NH2	-19.32	98.15	119.40
1	A	117	PHE	CB-CG-CD2	-19.31	107.29	120.80
2	B	8	ALA	C-N-CA	19.30	169.95	121.70
2	D	102	PHE	CG-CD1-CE1	19.29	142.01	120.80
1	C	139	LYS	CA-C-O	19.28	160.59	120.10
1	C	81	SER	CA-C-O	19.26	160.54	120.10
2	D	143	LYS	C-N-CA	19.24	169.81	121.70
1	A	84	SER	C-N-CA	19.23	169.79	121.70
2	B	14	TRP	CE3-CZ3-CH2	19.23	142.35	121.20
1	A	29	LEU	CB-CG-CD1	19.19	143.63	111.00
1	A	61	LYS	CB-CG-CD	19.18	161.48	111.60
2	D	40	PHE	CB-CG-CD1	-19.18	107.37	120.80
2	D	72	GLN	CA-C-O	-19.18	79.82	120.10
2	B	4	ALA	O-C-N	19.16	153.35	122.70
1	A	8	SER	CA-C-O	-19.11	79.97	120.10
2	D	2	LEU	CB-CG-CD2	19.05	143.39	111.00
1	A	77	PRO	C-N-CA	-19.05	82.30	122.30
1	C	43	PHE	CB-CG-CD1	-19.04	107.47	120.80
2	B	68	ASP	C-N-CA	19.03	169.28	121.70
2	B	40	PHE	CD1-CG-CD2	-18.88	93.76	118.30
1	C	56	LYS	CB-CA-C	18.85	148.11	110.40
2	D	14	TRP	CD2-CE3-CZ3	-18.84	94.31	118.80
2	B	95	LEU	CA-CB-CG	-18.82	72.00	115.30
2	B	144	TYR	CG-CD1-CE1	18.82	136.35	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	80	LEU	O-C-N	18.82	152.81	122.70
2	D	1	MET	CA-C-O	18.81	159.60	120.10
1	A	92	ARG	C-N-CA	18.77	168.62	121.70
2	D	61	ALA	CA-C-O	18.77	159.51	120.10
1	A	7	LYS	CB-CG-CD	18.77	160.39	111.60
1	C	32	MET	CA-CB-CG	18.77	145.20	113.30
1	C	35	SER	CA-C-N	18.74	158.42	117.20
1	A	97	ASN	CB-CG-OD1	-18.68	84.23	121.60
2	D	61	ALA	O-C-N	-18.68	92.81	122.70
2	B	79	ASP	CA-C-O	18.67	159.31	120.10
1	C	128	PHE	N-CA-CB	18.66	144.19	110.60
2	B	32	VAL	CA-C-N	18.65	158.23	117.20
1	A	81	SER	CA-C-O	-18.64	80.95	120.10
1	C	135	VAL	CG1-CB-CG2	-18.57	81.18	110.90
2	D	30	LEU	CA-CB-CG	18.57	158.00	115.30
1	A	114	PRO	O-C-N	-18.55	93.01	122.70
1	C	82	ASN	O-C-N	18.55	152.37	122.70
1	C	75	ASP	CB-CG-OD1	-18.51	101.64	118.30
2	B	14	TRP	CD2-CE2-CZ2	-18.49	100.12	122.30
1	A	131	ASN	CA-CB-CG	18.48	154.07	113.40
2	B	118	GLY	CA-C-O	-18.48	87.34	120.60
1	C	112	HIS	CA-C-O	-18.43	81.40	120.10
1	A	119	PRO	N-CD-CG	-18.41	75.59	103.20
1	A	128	PHE	CB-CG-CD1	-18.39	107.92	120.80
2	D	9	ALA	CB-CA-C	18.39	137.69	110.10
1	A	27	GLN	CA-CB-CG	18.38	153.84	113.40
2	D	137	ALA	CB-CA-C	18.38	137.67	110.10
2	B	34	TYR	CB-CA-C	18.37	147.15	110.40
2	B	42	GLN	C-N-CA	18.37	167.62	121.70
1	A	107	VAL	C-N-CA	18.34	167.56	121.70
1	A	16	LYS	CA-C-O	18.33	158.60	120.10
1	C	3	SER	N-CA-CB	18.33	138.00	110.50
2	B	65	ARG	CA-C-N	18.33	157.52	117.20
2	D	33	VAL	CA-CB-CG1	18.31	138.37	110.90
2	D	40	PHE	CG-CD1-CE1	-18.29	100.69	120.80
2	B	142	HIS	O-C-N	-18.28	93.46	122.70
1	A	81	SER	O-C-N	18.27	151.94	122.70
2	D	70	PHE	CZ-CE2-CD2	-18.27	98.18	120.10
1	A	30	GLN	C-N-CA	18.26	167.36	121.70
1	C	95	PRO	O-C-N	-18.26	93.48	122.70
2	B	62	HIS	CA-CB-CG	-18.26	82.56	113.60
1	C	87	HIS	CA-C-O	-18.26	81.76	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	HIS	O-C-N	-18.25	93.51	122.70
2	D	43	HIS	CA-CB-CG	18.22	144.57	113.60
2	D	41	PHE	O-C-N	-18.20	93.58	122.70
2	D	59	VAL	CA-CB-CG1	18.20	138.20	110.90
2	D	137	ALA	C-N-CA	18.20	167.19	121.70
1	C	11	LYS	CB-CG-CD	18.18	158.88	111.60
2	D	7	LYS	C-N-CA	18.17	167.13	121.70
1	C	95	PRO	CA-C-N	18.17	157.17	117.20
2	B	25	GLN	N-CA-CB	18.15	143.27	110.60
2	D	34	TYR	CG-CD1-CE1	18.15	135.82	121.30
1	A	84	SER	O-C-N	-18.14	93.67	122.70
1	A	43	PHE	CG-CD1-CE1	18.13	140.74	120.80
2	B	71	THR	C-N-CA	18.10	166.94	121.70
2	D	91	HIS	CA-C-O	-18.09	82.10	120.10
1	A	128	PHE	CB-CG-CD2	18.08	133.46	120.80
2	B	14	TRP	CD2-CE3-CZ3	-18.04	95.35	118.80
2	D	103	ARG	CA-C-O	18.03	157.97	120.10
2	D	115	ARG	CD-NE-CZ	18.02	148.83	123.60
2	D	50	ALA	C-N-CA	18.01	160.12	122.30
1	A	139	LYS	N-CA-CB	17.99	142.98	110.60
2	B	14	TRP	CE2-CD2-CG	-17.97	92.92	107.30
2	B	13	PHE	CD1-CE1-CZ	-17.96	98.55	120.10
1	C	55	GLN	CG-CD-NE2	17.96	159.80	116.70
2	D	105	LEU	CA-C-N	17.95	152.10	116.20
1	A	28	ALA	N-CA-CB	17.94	135.21	110.10
1	A	24	TYR	CB-CA-C	17.93	146.26	110.40
2	B	40	PHE	CZ-CE2-CD2	-17.92	98.60	120.10
1	C	30	GLN	CG-CD-OE1	-17.91	85.77	121.60
1	A	106	LEU	CB-CG-CD1	17.89	141.42	111.00
1	C	106	LEU	C-N-CA	17.89	166.42	121.70
2	D	130	GLN	OE1-CD-NE2	17.88	163.03	121.90
1	C	104	SER	N-CA-CB	17.88	137.32	110.50
2	B	33	VAL	CA-CB-CG2	-17.88	84.09	110.90
2	B	13	PHE	CZ-CE2-CD2	-17.86	98.67	120.10
2	B	46	ASN	CB-CG-OD1	-17.85	85.90	121.60
2	D	126	GLN	CA-CB-CG	17.85	152.66	113.40
1	A	67	THR	CA-CB-CG2	17.82	137.34	112.40
2	D	59	VAL	CG1-CB-CG2	-17.82	82.39	110.90
2	B	47	LEU	CB-CA-C	17.81	144.04	110.20
2	D	142	HIS	O-C-N	17.77	151.13	122.70
1	A	94	ASN	OD1-CG-ND2	-17.77	81.04	121.90
1	A	31	ARG	CA-CB-CG	17.76	152.47	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	40	PHE	CD1-CG-CD2	17.75	141.37	118.30
2	D	84	PHE	N-CA-CB	-17.74	78.67	110.60
2	B	14	TRP	NE1-CE2-CD2	17.72	125.02	107.30
1	A	50	HIS	ND1-CG-CD2	17.70	133.59	108.80
2	B	7	LYS	CA-CB-CG	17.69	152.32	113.40
2	B	129	PHE	CE1-CZ-CE2	17.69	151.84	120.00
1	C	35	SER	CA-C-O	-17.68	82.97	120.10
2	D	10	VAL	CB-CA-C	-17.67	77.83	111.40
1	A	34	LEU	CB-CG-CD1	-17.66	80.98	111.00
1	A	49	SER	N-CA-CB	17.65	136.97	110.50
1	C	84	SER	CB-CA-C	-17.63	76.60	110.10
2	B	93	ASN	OD1-CG-ND2	-17.63	81.34	121.90
2	D	102	PHE	CB-CA-C	17.63	145.66	110.40
1	C	69	ALA	CB-CA-C	-17.63	83.65	110.10
2	B	115	ARG	CA-C-N	17.61	155.94	117.20
1	C	10	VAL	CG1-CB-CG2	-17.61	82.73	110.90
2	D	103	ARG	CB-CA-C	-17.59	75.22	110.40
1	A	60	GLN	CA-CB-CG	17.58	152.08	113.40
1	C	37	PRO	O-C-N	-17.58	94.57	122.70
1	C	14	TRP	CB-CG-CD2	17.57	149.45	126.60
2	D	127	ALA	CA-C-N	17.53	155.78	117.20
1	A	87	HIS	CG-CD2-NE2	-17.53	75.89	109.20
1	A	49	SER	C-N-CA	17.53	165.52	121.70
2	D	72	GLN	CA-C-N	17.51	151.21	116.20
1	C	5	ALA	N-CA-CB	-17.48	85.63	110.10
2	B	103	ARG	CA-CB-CG	17.47	151.84	113.40
1	A	102	SER	CA-C-N	17.47	155.63	117.20
1	A	72	HIS	CG-ND1-CE1	17.46	132.65	108.20
1	C	141	ARG	NH1-CZ-NH2	17.46	138.61	119.40
1	C	42	TYR	CE1-CZ-CE2	-17.45	91.88	119.80
2	D	25	GLN	CG-CD-OE1	-17.44	86.73	121.60
1	A	22	PRO	C-N-CA	17.43	165.28	121.70
1	C	1	VAL	O-C-N	-17.43	94.81	122.70
2	B	116	ASN	OD1-CG-ND2	-17.43	81.82	121.90
1	C	107	VAL	C-N-CA	17.34	165.05	121.70
2	D	72	GLN	C-N-CA	17.34	158.71	122.30
2	D	109	LEU	CB-CG-CD1	17.33	140.46	111.00
1	A	118	THR	CA-CB-CG2	-17.32	88.15	112.40
1	A	57	ALA	N-CA-CB	-17.32	85.86	110.10
2	D	7	LYS	CB-CA-C	-17.30	75.80	110.40
2	D	124	ASN	CB-CG-OD1	-17.30	87.00	121.60
1	A	116	ASN	CB-CG-ND2	17.29	158.20	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	HIS	CG-ND1-CE1	17.29	132.41	108.20
1	A	14	TRP	O-C-N	-17.28	93.83	123.20
2	B	80	LEU	O-C-N	-17.28	95.06	122.70
2	B	63	GLY	C-N-CA	17.26	164.86	121.70
2	D	44	PHE	CB-CG-CD1	-17.26	108.72	120.80
2	B	139	ALA	N-CA-CB	-17.25	85.94	110.10
2	D	127	ALA	N-CA-CB	17.25	134.25	110.10
2	D	142	HIS	C-N-CA	17.20	164.69	121.70
1	A	62	VAL	CA-CB-CG1	17.19	136.69	110.90
2	B	108	VAL	CA-CB-CG1	17.18	136.67	110.90
1	C	81	SER	O-C-N	-17.15	95.25	122.70
2	D	59	VAL	CA-CB-CG2	-17.15	85.18	110.90
1	A	114	PRO	N-CD-CG	-17.14	77.49	103.20
2	D	43	HIS	CB-CG-ND1	17.13	166.03	123.20
1	A	8	SER	O-C-N	-17.13	95.30	122.70
1	C	80	LEU	N-CA-CB	-17.12	76.16	110.40
1	C	34	LEU	CB-CG-CD1	17.11	140.09	111.00
2	D	130	GLN	CG-CD-OE1	-17.11	87.38	121.60
1	A	140	TYR	OH-CZ-CE2	17.11	166.29	120.10
1	A	138	SER	CA-C-O	-17.10	84.18	120.10
2	B	145	HIS	N-CA-CB	-17.07	79.87	110.60
2	D	138	ASN	CA-C-N	17.07	154.76	117.20
2	B	46	ASN	CA-CB-CG	-17.07	75.85	113.40
2	D	73	GLY	C-N-CA	17.05	164.34	121.70
1	C	1	VAL	CB-CA-C	17.05	143.79	111.40
2	B	10	VAL	CA-CB-CG2	17.05	136.47	110.90
1	A	137	THR	CA-CB-OG1	-17.04	73.21	109.00
1	C	43	PHE	C-N-CD	17.01	164.12	128.40
1	A	74	ASN	CB-CG-OD1	16.99	155.58	121.60
1	A	127	LYS	CD-CE-NZ	-16.95	72.71	111.70
2	D	126	GLN	OE1-CD-NE2	-16.95	82.92	121.90
1	C	23	ALA	CB-CA-C	-16.93	84.71	110.10
2	D	34	TYR	CG-CD2-CE2	16.91	134.83	121.30
2	D	33	VAL	CA-CB-CG2	-16.91	85.53	110.90
2	B	80	LEU	CB-CG-CD1	16.90	139.74	111.00
1	A	106	LEU	O-C-N	-16.89	95.68	122.70
2	D	103	ARG	CD-NE-CZ	16.88	147.23	123.60
1	C	103	HIS	ND1-CE1-NE2	16.88	147.03	109.90
1	C	83	LEU	CB-CG-CD1	16.86	139.66	111.00
1	C	57	ALA	CB-CA-C	16.86	135.38	110.10
2	B	20	ASP	CA-C-N	16.85	154.27	117.20
2	D	71	THR	C-N-CA	16.84	163.79	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	CD-NE-CZ	16.82	147.15	123.60
2	D	115	ARG	C-N-CA	16.80	163.71	121.70
1	C	127	LYS	O-C-N	-16.77	95.87	122.70
2	D	13	PHE	CG-CD2-CE2	16.77	139.25	120.80
1	C	109	LEU	O-C-N	-16.77	95.87	122.70
1	C	63	ALA	N-CA-CB	16.76	133.56	110.10
1	A	102	SER	O-C-N	-16.75	95.90	122.70
1	A	116	ASN	OD1-CG-ND2	-16.73	83.42	121.90
1	C	85	ASN	CA-C-N	16.72	153.98	117.20
1	C	117	PHE	CG-CD1-CE1	16.70	139.17	120.80
1	A	24	TYR	CD1-CG-CD2	-16.69	99.54	117.90
2	D	58	LYS	CB-CG-CD	16.67	154.94	111.60
1	C	22	PRO	CA-N-CD	-16.66	88.18	111.50
1	C	120	ALA	N-CA-CB	16.64	133.40	110.10
1	A	121	VAL	N-CA-CB	16.63	148.08	111.50
2	D	125	VAL	CG1-CB-CG2	-16.61	84.32	110.90
1	C	72	HIS	CA-C-O	16.61	154.98	120.10
1	A	89	HIS	O-C-N	-16.60	96.14	122.70
1	C	10	VAL	CA-C-O	16.59	154.94	120.10
1	C	6	ASN	OD1-CG-ND2	-16.59	83.74	121.90
1	A	14	TRP	N-CA-CB	16.57	140.42	110.60
1	C	42	TYR	CB-CG-CD1	-16.57	111.06	121.00
2	B	14	TRP	CB-CG-CD1	16.56	148.53	127.00
2	B	142	HIS	C-N-CA	16.55	163.06	121.70
1	C	98	PHE	CB-CG-CD1	16.54	132.38	120.80
1	A	127	LYS	O-C-N	16.53	149.15	122.70
1	C	24	TYR	CD1-CE1-CZ	16.53	134.68	119.80
2	B	144	TYR	CA-C-O	16.51	154.78	120.10
1	A	44	PRO	C-N-CA	16.51	162.98	121.70
2	D	42	GLN	C-N-CA	16.51	162.97	121.70
2	B	54	MET	C-N-CA	16.51	162.97	121.70
2	D	72	GLN	OE1-CD-NE2	16.49	159.82	121.90
1	A	137	THR	OG1-CB-CG2	-16.47	72.11	110.00
2	D	37	THR	CA-CB-CG2	16.45	135.44	112.40
2	D	9	ALA	CA-C-O	-16.44	85.58	120.10
1	A	120	ALA	CA-C-O	-16.43	85.59	120.10
2	B	115	ARG	CA-C-O	-16.41	85.65	120.10
2	D	68	ASP	O-C-N	-16.41	96.45	122.70
2	D	19	VAL	CA-CB-CG2	-16.40	86.30	110.90
2	D	11	THR	CA-CB-OG1	-16.37	74.63	109.00
1	C	79	THR	CA-CB-CG2	16.33	135.26	112.40
2	D	11	THR	N-CA-CB	-16.33	79.27	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	ASN	OD1-CG-ND2	-16.30	84.41	121.90
1	A	46	PHE	N-CA-CB	16.30	139.94	110.60
2	B	127	ALA	N-CA-CB	16.29	132.91	110.10
1	C	124	ASN	OD1-CG-ND2	-16.29	84.44	121.90
2	D	38	GLN	O-C-N	16.29	148.76	122.70
1	C	68	LYS	C-N-CA	16.28	162.39	121.70
2	D	71	THR	CA-CB-CG2	-16.27	89.63	112.40
1	A	109	LEU	CA-CB-CG	16.25	152.68	115.30
2	D	13	PHE	CZ-CE2-CD2	-16.25	100.60	120.10
1	A	62	VAL	CA-C-N	16.24	152.93	117.20
2	B	74	LEU	CA-C-N	16.23	152.92	117.20
2	D	1	MET	N-CA-CB	16.23	139.82	110.60
1	A	42	TYR	CD1-CE1-CZ	16.23	134.41	119.80
1	C	48	LEU	CB-CG-CD2	-16.21	83.44	111.00
2	B	55	ASN	CA-C-N	-16.21	81.53	117.20
1	A	24	TYR	CA-CB-CG	16.20	144.18	113.40
1	C	117	PHE	C-N-CA	16.17	162.14	121.70
2	D	2	LEU	N-CA-C	-16.17	67.34	111.00
2	D	119	GLY	O-C-N	-16.17	96.83	122.70
1	A	31	ARG	NE-CZ-NH1	16.15	128.38	120.30
1	C	42	TYR	O-C-N	-16.14	96.87	122.70
2	B	1	MET	CA-C-O	-16.14	86.20	120.10
2	B	28	GLY	O-C-N	16.14	148.52	122.70
2	D	34	TYR	CD1-CE1-CZ	-16.12	105.30	119.80
1	A	79	THR	CA-CB-CG2	-16.11	89.84	112.40
1	C	61	LYS	N-CA-CB	16.11	139.59	110.60
1	A	41	THR	CA-CB-OG1	16.10	142.81	109.00
1	A	33	PHE	CG-CD1-CE1	16.09	138.50	120.80
1	A	141	ARG	CD-NE-CZ	-16.09	101.08	123.60
2	D	135	GLY	CA-C-O	-16.09	91.64	120.60
1	C	47	ASP	O-C-N	-16.07	97.00	122.70
2	B	36	TRP	CH2-CZ2-CE2	-16.06	101.34	117.40
1	A	31	ARG	N-CA-CB	16.06	139.51	110.60
1	C	70	GLN	N-CA-CB	-16.05	81.70	110.60
2	B	13	PHE	CG-CD1-CE1	16.05	138.46	120.80
2	D	138	ASN	CA-C-O	-16.05	86.40	120.10
1	A	28	ALA	C-N-CA	16.05	161.82	121.70
1	C	55	GLN	CA-C-N	16.04	152.49	117.20
1	C	42	TYR	CA-C-N	16.04	152.49	117.20
1	A	131	ASN	CB-CA-C	16.03	142.47	110.40
2	B	144	TYR	CA-C-N	-16.03	81.94	117.20
2	B	123	PRO	CA-N-CD	16.01	134.12	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	LEU	O-C-N	16.00	148.31	122.70
1	A	46	PHE	C-N-CA	15.98	161.65	121.70
2	D	90	LEU	CB-CG-CD1	-15.98	83.84	111.00
2	B	38	GLN	CG-CD-NE2	15.95	154.99	116.70
1	A	131	ASN	CB-CG-OD1	15.95	153.50	121.60
2	B	32	VAL	C-N-CA	15.91	161.47	121.70
2	D	71	THR	CA-C-O	15.88	153.44	120.10
2	B	26	ALA	O-C-N	15.86	148.08	122.70
2	D	126	GLN	O-C-N	-15.85	97.35	122.70
1	C	129	LEU	CA-C-N	15.84	152.04	117.20
1	A	41	THR	O-C-N	-15.83	97.37	122.70
2	B	98	ASN	CB-CA-C	-15.82	78.75	110.40
2	B	109	LEU	CA-CB-CG	15.80	151.65	115.30
2	D	55	ASN	C-N-CA	15.80	161.20	121.70
2	D	13	PHE	N-CA-CB	15.79	139.02	110.60
2	D	100	GLN	CA-CB-CG	-15.77	78.71	113.40
2	D	113	VAL	CB-CA-C	15.76	141.34	111.40
2	B	34	TYR	CZ-CE2-CD2	-15.75	105.63	119.80
2	D	35	PRO	O-C-N	15.74	147.89	122.70
2	D	30	LEU	N-CA-CB	15.74	141.88	110.40
2	D	33	VAL	CG1-CB-CG2	15.73	136.07	110.90
2	B	83	ALA	C-N-CA	15.73	161.01	121.70
2	B	39	ARG	CG-CD-NE	15.72	144.82	111.80
2	B	141	ALA	N-CA-CB	-15.72	88.09	110.10
2	B	79	ASP	CA-CB-CG	-15.72	78.83	113.40
2	B	52	ALA	CB-CA-C	15.71	133.66	110.10
1	A	132	ASP	CB-CA-C	15.70	141.80	110.40
2	B	65	ARG	CA-CB-CG	15.69	147.93	113.40
1	A	98	PHE	CD1-CG-CD2	-15.67	97.93	118.30
1	A	31	ARG	CG-CD-NE	-15.67	78.89	111.80
2	B	121	PHE	CD1-CG-CD2	-15.66	97.94	118.30
1	A	102	SER	C-N-CA	15.65	160.83	121.70
1	A	126	ASN	N-CA-CB	15.64	138.76	110.60
1	A	46	PHE	CD1-CE1-CZ	-15.63	101.34	120.10
2	D	71	THR	CA-C-N	-15.63	82.82	117.20
2	D	38	GLN	CA-CB-CG	15.62	147.76	113.40
1	C	62	VAL	CA-CB-CG1	15.62	134.32	110.90
1	C	114	PRO	N-CD-CG	-15.58	79.82	103.20
2	D	39	ARG	NH1-CZ-NH2	-15.58	102.26	119.40
2	B	55	ASN	O-C-N	15.58	147.62	122.70
2	B	106	GLY	C-N-CA	15.58	160.64	121.70
2	D	34	TYR	CB-CA-C	15.57	141.53	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	GLY	C-N-CA	15.56	160.59	121.70
2	B	12	GLY	CA-C-O	15.55	148.58	120.60
1	C	84	SER	CA-C-N	15.54	151.40	117.20
1	C	56	LYS	O-C-N	-15.53	97.85	122.70
2	D	143	LYS	CA-C-O	15.53	152.71	120.10
2	B	37	THR	CA-C-O	15.52	152.69	120.10
2	B	47	LEU	CA-CB-CG	15.52	151.00	115.30
1	A	85	ASN	CA-C-N	15.51	151.32	117.20
1	A	16	LYS	O-C-N	-15.49	97.92	122.70
1	A	47	ASP	N-CA-CB	15.48	138.47	110.60
2	B	34	TYR	CG-CD2-CE2	15.48	133.69	121.30
1	A	131	ASN	O-C-N	-15.48	97.94	122.70
2	D	118	GLY	O-C-N	-15.46	96.92	123.20
2	B	44	PHE	CD1-CG-CD2	-15.45	98.22	118.30
2	B	66	VAL	CA-CB-CG2	15.44	134.05	110.90
1	C	86	LEU	O-C-N	-15.43	98.02	122.70
1	A	44	PRO	N-CD-CG	15.42	126.33	103.20
1	C	87	HIS	CA-C-N	15.42	151.12	117.20
1	C	62	VAL	C-N-CA	15.41	160.23	121.70
1	C	134	THR	OG1-CB-CG2	15.41	145.44	110.00
2	D	78	ASP	N-CA-CB	15.41	138.33	110.60
2	D	59	VAL	O-C-N	15.39	147.32	122.70
2	B	92	CYS	O-C-N	15.36	147.27	122.70
1	C	46	PHE	CD1-CG-CD2	15.35	138.25	118.30
2	B	87	LEU	CB-CG-CD1	15.34	137.08	111.00
2	D	19	VAL	O-C-N	-15.34	98.16	122.70
1	C	34	LEU	C-N-CA	15.32	160.01	121.70
2	B	65	ARG	CA-C-O	-15.32	87.93	120.10
1	C	26	ALA	O-C-N	-15.32	98.19	122.70
1	C	115	THR	C-N-CA	15.31	159.97	121.70
2	D	104	LEU	O-C-N	-15.31	98.21	122.70
1	A	82	ASN	CB-CA-C	15.29	140.97	110.40
2	D	129	PHE	CB-CG-CD2	15.28	131.50	120.80
2	D	70	PHE	C-N-CA	15.28	159.89	121.70
1	A	130	ALA	N-CA-CB	15.27	131.48	110.10
2	D	105	LEU	CB-CG-CD2	15.27	136.96	111.00
2	B	95	LEU	C-N-CA	15.26	159.85	121.70
2	B	121	PHE	CE1-CZ-CE2	-15.25	92.55	120.00
2	D	24	ALA	C-N-CA	15.25	159.83	121.70
2	D	35	PRO	N-CD-CG	-15.25	80.33	103.20
1	A	82	ASN	CA-CB-CG	15.24	146.94	113.40
2	B	126	GLN	OE1-CD-NE2	-15.24	86.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	20	ASP	CB-CA-C	15.24	140.88	110.40
2	B	121	PHE	CB-CA-C	15.23	140.86	110.40
1	C	33	PHE	CB-CG-CD1	15.22	131.45	120.80
1	C	60	GLN	C-N-CA	15.21	159.73	121.70
1	C	80	LEU	O-C-N	-15.21	98.37	122.70
1	A	14	TRP	CD2-CE2-CZ2	-15.20	104.06	122.30
1	A	31	ARG	NH1-CZ-NH2	-15.20	102.68	119.40
1	A	66	LEU	CB-CG-CD1	-15.19	85.18	111.00
1	A	118	THR	CA-CB-OG1	15.18	140.89	109.00
1	A	48	LEU	CB-CG-CD2	15.17	136.79	111.00
2	B	28	GLY	CA-C-O	-15.17	93.29	120.60
1	C	78	GLY	CA-C-O	-15.17	93.29	120.60
1	C	14	TRP	CG-CD2-CE3	-15.16	120.25	133.90
2	D	8	ALA	C-N-CA	15.16	159.60	121.70
1	A	16	LYS	CA-CB-CG	15.15	146.73	113.40
1	A	65	ALA	O-C-N	-15.14	98.47	122.70
2	D	130	GLN	N-CA-CB	15.14	137.86	110.60
2	D	15	GLY	C-N-CA	15.13	159.53	121.70
1	C	9	ASN	N-CA-CB	-15.11	83.40	110.60
2	B	103	ARG	CG-CD-NE	-15.11	80.07	111.80
1	A	39	THR	O-C-N	-15.11	98.53	122.70
1	A	54	GLN	CB-CA-C	15.10	140.60	110.40
1	C	39	THR	CA-CB-CG2	15.10	133.54	112.40
1	A	20	ASN	CB-CG-OD1	-15.09	91.43	121.60
2	D	88	SER	O-C-N	-15.09	97.55	123.20
1	A	111	SER	CA-C-N	15.09	150.39	117.20
1	A	100	LEU	N-CA-CB	15.08	140.56	110.40
1	C	89	HIS	O-C-N	-15.07	98.59	122.70
1	A	48	LEU	CB-CG-CD1	-15.05	85.42	111.00
1	C	80	LEU	CA-CB-CG	15.04	149.90	115.30
1	A	41	THR	C-N-CA	15.03	159.27	121.70
1	A	15	GLY	CA-C-O	-15.03	93.55	120.60
2	D	39	ARG	CG-CD-NE	-15.02	80.25	111.80
2	B	59	VAL	CA-CB-CG1	-15.01	88.39	110.90
2	B	71	THR	O-C-N	-15.01	98.69	122.70
2	B	6	GLU	CA-C-O	-15.00	88.59	120.10
1	C	132	ASP	C-N-CA	15.00	159.20	121.70
2	B	29	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	C	122	HIS	O-C-N	-15.00	98.71	122.70
2	B	32	VAL	CA-CB-CG1	14.98	133.38	110.90
2	B	85	ALA	C-N-CA	14.98	159.15	121.70
1	A	31	ARG	CB-CG-CD	14.97	150.52	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	100	GLN	CB-CA-C	14.97	140.34	110.40
1	A	70	GLN	OE1-CD-NE2	-14.94	87.53	121.90
2	B	59	VAL	CA-C-O	-14.93	88.75	120.10
1	C	70	GLN	CB-CA-C	-14.92	80.55	110.40
2	D	109	LEU	O-C-N	14.91	146.56	122.70
1	A	35	SER	N-CA-CB	14.91	132.86	110.50
1	A	49	SER	O-C-N	-14.90	98.86	122.70
2	D	102	PHE	CD1-CG-CD2	-14.89	98.94	118.30
2	D	102	PHE	CA-C-O	-14.89	88.82	120.10
2	D	111	LEU	CA-C-O	-14.89	88.83	120.10
2	D	67	LEU	CA-C-O	-14.89	88.84	120.10
2	D	25	GLN	N-CA-CB	14.88	137.38	110.60
2	D	122	THR	OG1-CB-CG2	14.88	144.21	110.00
2	D	139	ALA	CB-CA-C	-14.87	87.80	110.10
1	C	23	ALA	O-C-N	14.84	146.44	122.70
2	D	3	THR	N-CA-CB	14.81	138.45	110.30
2	B	64	LYS	O-C-N	-14.81	99.00	122.70
1	A	46	PHE	CE1-CZ-CE2	14.80	146.63	120.00
2	D	89	GLY	C-N-CA	14.76	158.59	121.70
2	D	117	PHE	CB-CG-CD2	-14.76	110.47	120.80
2	D	128	LEU	CA-CB-CG	14.74	149.21	115.30
2	D	117	PHE	CA-C-N	14.73	145.67	116.20
2	D	90	LEU	O-C-N	14.73	146.27	122.70
2	B	128	LEU	CB-CA-C	14.73	138.19	110.20
2	D	78	ASP	CB-CG-OD1	14.73	131.56	118.30
1	C	43	PHE	CE1-CZ-CE2	14.72	146.50	120.00
2	B	92	CYS	CA-C-O	-14.72	89.20	120.10
1	A	132	ASP	CA-CB-CG	-14.71	81.04	113.40
1	A	89	HIS	N-CA-CB	14.71	137.07	110.60
1	C	73	LEU	CB-CG-CD2	-14.69	86.02	111.00
2	B	87	LEU	CA-C-O	-14.67	89.30	120.10
2	B	14	TRP	CE2-CD2-CE3	14.65	136.28	118.70
1	C	98	PHE	CA-C-O	14.64	150.85	120.10
1	A	52	SER	CA-C-O	-14.63	89.37	120.10
2	B	138	ASN	CA-CB-CG	14.63	145.58	113.40
2	D	133	VAL	CA-CB-CG2	14.62	132.83	110.90
2	B	79	ASP	N-CA-CB	-14.60	84.32	110.60
2	D	9	ALA	N-CA-CB	-14.60	89.67	110.10
2	D	65	ARG	NH1-CZ-NH2	-14.58	103.36	119.40
1	C	98	PHE	CZ-CE2-CD2	14.57	137.59	120.10
1	C	102	SER	N-CA-CB	14.56	132.34	110.50
1	C	122	HIS	ND1-CG-CD2	-14.55	85.63	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	16	LYS	C-N-CA	14.54	158.05	121.70
2	D	22	VAL	CB-CA-C	14.53	139.01	111.40
2	B	80	LEU	CB-CA-C	14.52	137.79	110.20
1	C	100	LEU	CA-C-O	-14.52	89.61	120.10
2	D	39	ARG	CD-NE-CZ	14.51	143.92	123.60
1	C	25	GLY	CA-C-O	-14.51	94.48	120.60
1	C	56	LYS	CA-CB-CG	-14.51	81.47	113.40
2	D	81	LYS	C-N-CA	14.51	152.77	122.30
2	D	117	PHE	CE1-CZ-CE2	14.51	146.11	120.00
1	A	68	LYS	CA-CB-CG	14.49	145.28	113.40
1	C	50	HIS	CG-ND1-CE1	14.49	128.48	108.20
2	D	32	VAL	CA-C-O	-14.46	89.73	120.10
2	D	142	HIS	ND1-CE1-NE2	-14.43	78.15	109.90
2	B	93	ASN	CA-CB-CG	-14.42	81.67	113.40
1	C	107	VAL	O-C-N	-14.39	99.67	122.70
2	B	69	ALA	CA-C-O	14.38	150.30	120.10
2	D	50	ALA	CA-C-N	14.38	144.96	116.20
1	A	111	SER	C-N-CA	14.37	157.63	121.70
2	D	52	ALA	N-CA-CB	-14.38	89.97	110.10
1	C	127	LYS	C-N-CA	14.37	157.62	121.70
2	B	82	GLY	C-N-CA	14.37	157.61	121.70
1	A	111	SER	CA-CB-OG	-14.36	72.43	111.20
1	A	124	ASN	CB-CG-OD1	-14.35	92.90	121.60
2	D	95	LEU	O-C-N	-14.35	99.75	122.70
2	B	90	LEU	CB-CG-CD1	14.34	135.37	111.00
2	B	102	PHE	C-N-CA	14.32	157.49	121.70
2	D	144	TYR	O-C-N	14.32	145.61	122.70
1	C	95	PRO	N-CD-CG	14.30	124.66	103.20
2	D	51	GLY	N-CA-C	-14.29	77.39	113.10
2	B	76	HIS	N-CA-CB	-14.28	84.90	110.60
1	C	58	HIS	CA-CB-CG	14.28	137.87	113.60
2	B	62	HIS	CG-ND1-CE1	-14.26	87.16	105.70
1	C	99	LYS	CA-CB-CG	14.26	144.77	113.40
2	D	50	ALA	CA-C-O	-14.25	90.17	120.10
1	A	70	GLN	O-C-N	-14.25	98.98	123.20
2	D	82	GLY	O-C-N	-14.24	99.91	122.70
1	C	114	PRO	N-CA-CB	-14.23	86.22	103.30
2	B	94	LYS	CA-CB-CG	14.22	144.69	113.40
1	A	91	LEU	CB-CG-CD1	14.22	135.17	111.00
1	C	123	ALA	N-CA-CB	14.21	129.99	110.10
1	C	19	GLY	O-C-N	-14.18	100.00	122.70
1	A	57	ALA	CB-CA-C	14.17	131.35	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	LYS	O-C-N	14.17	145.37	122.70
2	B	4	ALA	CA-C-N	-14.16	86.04	117.20
1	C	132	ASP	O-C-N	-14.15	100.06	122.70
2	B	78	ASP	CB-CG-OD1	14.15	131.03	118.30
2	D	126	GLN	CB-CG-CD	-14.12	74.90	111.60
1	A	34	LEU	C-N-CA	-14.11	86.42	121.70
2	B	22	VAL	C-N-CA	-14.10	92.69	122.30
2	D	86	GLN	O-C-N	14.09	145.24	122.70
1	C	100	LEU	O-C-N	14.08	145.23	122.70
1	C	49	SER	CA-C-O	14.07	149.65	120.10
1	C	72	HIS	CA-C-N	-14.07	86.25	117.20
2	B	31	LEU	C-N-CA	-14.06	86.54	121.70
2	D	97	VAL	CA-C-O	-14.06	90.58	120.10
1	A	89	HIS	CA-C-N	14.04	148.10	117.20
1	C	60	GLN	CG-CD-OE1	-14.04	93.51	121.60
2	B	57	PRO	N-CD-CG	-14.03	82.15	103.20
2	B	34	TYR	CD1-CE1-CZ	-14.03	107.17	119.80
2	B	50	ALA	O-C-N	-14.02	99.36	123.20
1	A	70	GLN	CB-CA-C	14.02	138.44	110.40
2	D	7	LYS	N-CA-CB	14.02	135.83	110.60
2	D	40	PHE	CB-CG-CD2	-14.01	110.99	120.80
1	C	134	THR	O-C-N	-14.00	100.29	122.70
2	B	76	HIS	CA-CB-CG	13.99	137.38	113.60
2	D	128	LEU	CA-C-O	-13.99	90.72	120.10
2	D	137	ALA	O-C-N	-13.98	100.34	122.70
2	D	52	ALA	C-N-CA	13.95	156.59	121.70
1	C	57	ALA	N-CA-CB	-13.94	90.59	110.10
1	A	2	LEU	N-CA-CB	13.94	138.27	110.40
2	D	75	LYS	CB-CG-CD	13.93	147.82	111.60
2	B	102	PHE	CA-CB-CG	13.91	147.29	113.90
2	B	114	ALA	CB-CA-C	-13.91	89.24	110.10
1	C	119	PRO	N-CA-CB	13.91	119.99	103.30
1	C	98	PHE	CD1-CG-CD2	-13.89	100.24	118.30
1	C	24	TYR	CE1-CZ-CE2	-13.88	97.59	119.80
1	A	54	GLN	CG-CD-NE2	-13.88	83.39	116.70
2	B	122	THR	C-N-CD	-13.86	90.12	120.60
2	D	7	LYS	CA-CB-CG	13.86	143.88	113.40
2	B	39	ARG	NH1-CZ-NH2	13.84	134.63	119.40
2	D	17	VAL	N-CA-CB	13.83	141.92	111.50
2	D	138	ASN	CB-CA-C	13.83	138.06	110.40
1	A	28	ALA	O-C-N	-13.81	100.60	122.70
2	D	95	LEU	CB-CG-CD1	-13.81	87.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	LEU	CA-CB-CG	13.80	147.03	115.30
1	C	14	TRP	N-CA-CB	13.80	135.44	110.60
2	B	14	TRP	CA-CB-CG	13.79	139.91	113.70
1	A	80	LEU	O-C-N	-13.79	100.63	122.70
2	B	144	TYR	CD1-CE1-CZ	-13.79	107.39	119.80
1	C	128	PHE	CZ-CE2-CD2	-13.79	103.55	120.10
2	B	66	VAL	CG1-CB-CG2	-13.78	88.86	110.90
1	A	72	HIS	ND1-CE1-NE2	-13.77	79.62	109.90
2	B	115	ARG	NE-CZ-NH2	-13.76	113.42	120.30
1	C	135	VAL	O-C-N	-13.76	100.69	122.70
1	C	55	GLN	OE1-CD-NE2	-13.75	90.27	121.90
1	A	100	LEU	CB-CG-CD2	-13.73	87.66	111.00
2	D	68	ASP	C-N-CA	13.72	156.01	121.70
1	A	13	ALA	C-N-CA	13.71	155.98	121.70
1	A	141	ARG	NH1-CZ-NH2	-13.70	104.33	119.40
1	C	46	PHE	CB-CA-C	-13.70	83.00	110.40
1	A	39	THR	C-N-CA	13.69	155.93	121.70
2	B	132	VAL	N-CA-CB	13.69	141.61	111.50
1	C	5	ALA	CA-C-O	-13.66	91.40	120.10
1	C	130	ALA	CA-C-N	13.66	147.25	117.20
1	C	135	VAL	CA-CB-CG1	13.65	131.38	110.90
1	C	112	HIS	O-C-N	13.64	144.52	122.70
2	D	55	ASN	O-C-N	-13.62	100.92	122.70
2	D	6	GLU	CA-C-N	-13.61	87.25	117.20
2	D	76	HIS	ND1-CG-CD2	13.60	127.84	108.80
2	D	70	PHE	CA-C-N	13.60	147.12	117.20
2	D	99	PRO	C-N-CA	13.60	155.70	121.70
2	B	105	LEU	N-CA-CB	13.59	137.59	110.40
2	B	122	THR	N-CA-CB	13.59	136.13	110.30
1	A	91	LEU	CB-CG-CD2	13.58	134.09	111.00
2	D	103	ARG	O-C-N	-13.58	100.97	122.70
2	B	100	GLN	N-CA-CB	13.58	135.04	110.60
1	A	138	SER	CA-CB-OG	13.57	147.84	111.20
2	D	35	PRO	CA-C-O	-13.57	87.64	120.20
2	D	30	LEU	CB-CA-C	-13.55	84.45	110.20
1	C	50	HIS	CA-C-O	-13.54	91.67	120.10
2	B	126	GLN	N-CA-CB	13.53	134.96	110.60
2	D	15	GLY	O-C-N	13.53	144.34	122.70
2	D	124	ASN	N-CA-CB	13.53	134.95	110.60
1	C	62	VAL	CA-C-N	13.52	146.94	117.20
2	B	60	LYS	CD-CE-NZ	-13.51	80.63	111.70
1	A	55	GLN	OE1-CD-NE2	-13.50	90.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	LEU	CB-CG-CD2	-13.50	88.05	111.00
2	B	113	VAL	CA-CB-CG1	-13.49	90.66	110.90
2	B	129	PHE	CD1-CG-CD2	13.49	135.84	118.30
1	C	89	HIS	CA-C-O	13.49	148.42	120.10
2	D	127	ALA	CB-CA-C	-13.48	89.88	110.10
1	A	2	LEU	CB-CG-CD2	13.48	133.91	111.00
2	B	37	THR	CA-CB-CG2	13.48	131.27	112.40
1	C	117	PHE	CD1-CG-CD2	-13.47	100.78	118.30
2	B	96	HIS	CA-C-O	13.47	148.39	120.10
1	C	37	PRO	N-CA-C	13.47	147.12	112.10
2	B	62	HIS	CG-CD2-NE2	-13.46	83.62	109.20
1	C	42	TYR	CG-CD2-CE2	-13.45	110.54	121.30
2	B	124	ASN	CA-C-N	13.45	146.80	117.20
1	A	114	PRO	CA-N-CD	-13.44	92.68	111.50
1	C	45	HIS	N-CA-CB	-13.43	86.42	110.60
2	D	20	ASP	CB-CG-OD1	-13.43	106.21	118.30
2	B	16	LYS	C-N-CA	13.42	155.25	121.70
1	A	131	ASN	CA-C-N	13.39	146.67	117.20
1	C	98	PHE	CA-C-N	-13.39	87.73	117.20
1	A	72	HIS	CA-CB-CG	-13.39	90.84	113.60
1	C	2	LEU	CB-CG-CD2	-13.37	88.27	111.00
1	A	99	LYS	CD-CE-NZ	13.37	142.45	111.70
2	D	103	ARG	CA-CB-CG	13.36	142.79	113.40
2	D	117	PHE	N-CA-CB	-13.35	86.56	110.60
2	B	6	GLU	CA-C-N	13.33	146.52	117.20
2	D	34	TYR	O-C-N	13.33	146.42	121.10
2	B	51	GLY	CA-C-N	-13.30	87.94	117.20
1	C	92	ARG	NE-CZ-NH1	13.30	126.95	120.30
1	C	46	PHE	CA-C-N	-13.30	87.95	117.20
1	A	126	ASN	OD1-CG-ND2	-13.29	91.33	121.90
2	D	13	PHE	CD1-CE1-CZ	-13.27	104.18	120.10
2	D	131	LYS	CD-CE-NZ	-13.27	81.18	111.70
2	D	48	SER	N-CA-CB	13.26	130.39	110.50
1	A	105	LEU	CB-CG-CD2	13.25	133.53	111.00
1	C	124	ASN	CB-CG-ND2	13.25	148.50	116.70
2	B	112	VAL	CA-C-O	13.22	147.87	120.10
2	D	69	ALA	O-C-N	13.22	143.85	122.70
2	D	62	HIS	ND1-CG-CD2	13.22	127.31	108.80
2	B	40	PHE	CB-CG-CD1	-13.21	111.55	120.80
1	C	55	GLN	CA-C-O	-13.20	92.38	120.10
1	C	108	THR	CA-CB-CG2	13.20	130.88	112.40
1	C	112	HIS	CE1-NE2-CD2	-13.20	73.60	106.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	145	HIS	N-CA-C	13.19	146.62	111.00
2	B	74	LEU	CA-C-O	-13.18	92.43	120.10
2	D	44	PHE	CA-C-N	13.18	142.56	116.20
2	D	36	TRP	NE1-CE2-CD2	13.18	120.48	107.30
2	D	84	PHE	CG-CD1-CE1	-13.18	106.31	120.80
1	C	113	LEU	CA-C-O	13.17	147.75	120.10
2	D	84	PHE	CA-C-O	13.15	147.72	120.10
2	B	20	ASP	C-N-CA	13.14	154.56	121.70
2	B	136	VAL	CA-C-N	13.14	146.11	117.20
2	D	17	VAL	CA-CB-CG1	-13.13	91.20	110.90
1	A	108	THR	N-CA-CB	13.13	135.24	110.30
2	B	75	LYS	N-CA-C	-13.12	75.56	111.00
2	B	49	SER	CA-C-N	13.11	146.05	117.20
1	C	26	ALA	N-CA-CB	13.11	128.46	110.10
2	D	16	LYS	O-C-N	13.10	143.66	122.70
1	C	11	LYS	CD-CE-NZ	13.10	141.83	111.70
1	C	24	TYR	CZ-CE2-CD2	-13.09	108.02	119.80
1	A	32	MET	CB-CA-C	13.08	136.56	110.40
1	C	131	ASN	CB-CG-OD1	-13.08	95.43	121.60
2	D	129	PHE	O-C-N	-13.08	101.77	122.70
1	C	92	ARG	CA-C-O	13.08	147.57	120.10
2	D	145	HIS	CB-CA-C	-13.08	84.24	110.40
2	D	3	THR	CA-C-N	-13.07	88.45	117.20
2	B	114	ALA	O-C-N	-13.06	101.80	122.70
2	D	105	LEU	O-C-N	-13.05	101.02	123.20
2	D	109	LEU	N-CA-CB	13.05	136.49	110.40
1	C	42	TYR	CD1-CE1-CZ	13.04	131.54	119.80
2	D	74	LEU	N-CA-CB	13.04	136.48	110.40
1	C	63	ALA	CA-C-O	-13.03	92.75	120.10
2	D	116	ASN	N-CA-CB	13.03	134.04	110.60
2	B	131	LYS	CD-CE-NZ	-13.02	81.76	111.70
1	C	20	ASN	CB-CG-OD1	-13.01	95.57	121.60
2	D	94	LYS	CA-C-O	-13.01	92.79	120.10
1	A	108	THR	CA-CB-OG1	12.99	136.29	109.00
2	B	136	VAL	CA-C-O	-12.99	92.81	120.10
1	A	24	TYR	CG-CD1-CE1	12.99	131.69	121.30
1	C	20	ASN	CB-CA-C	12.99	136.38	110.40
1	A	136	LEU	CA-C-O	12.99	147.37	120.10
2	D	39	ARG	CA-CB-CG	12.98	141.97	113.40
2	D	18	ASP	N-CA-CB	-12.98	87.23	110.60
1	C	92	ARG	CD-NE-CZ	-12.97	105.44	123.60
2	B	68	ASP	CA-C-O	-12.96	92.88	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	LYS	CA-C-O	12.96	147.32	120.10
1	C	3	SER	CB-CA-C	-12.94	85.52	110.10
1	A	45	HIS	CG-ND1-CE1	12.93	126.31	108.20
2	D	70	PHE	CG-CD1-CE1	12.93	135.02	120.80
1	C	117	PHE	CA-C-O	-12.93	92.95	120.10
2	D	32	VAL	CA-C-N	12.91	145.61	117.20
2	D	131	LYS	CA-CB-CG	-12.91	85.01	113.40
1	A	89	HIS	C-N-CA	12.90	153.94	121.70
1	C	128	PHE	CE1-CZ-CE2	-12.90	96.79	120.00
1	A	101	LEU	CB-CG-CD2	-12.89	89.08	111.00
2	B	81	LYS	CA-CB-CG	-12.89	85.05	113.40
2	B	91	HIS	ND1-CG-CD2	-12.88	87.96	106.00
1	A	109	LEU	C-N-CA	12.88	153.89	121.70
2	D	140	LEU	N-CA-CB	12.88	136.15	110.40
1	A	134	THR	CA-C-O	-12.87	93.07	120.10
2	D	99	PRO	CA-C-O	12.87	151.09	120.20
2	D	1	MET	N-CA-C	-12.86	76.28	111.00
1	A	31	ARG	NE-CZ-NH2	12.86	126.73	120.30
1	C	138	SER	N-CA-C	12.84	145.68	111.00
1	C	12	ALA	CA-C-N	12.84	145.45	117.20
2	B	14	TRP	CA-C-O	12.83	147.05	120.10
2	D	136	VAL	N-CA-CB	12.83	139.72	111.50
2	B	14	TRP	O-C-N	-12.82	101.40	123.20
1	A	130	ALA	CA-C-N	-12.81	89.02	117.20
2	D	93	ASN	N-CA-CB	12.80	133.63	110.60
1	C	68	LYS	O-C-N	-12.79	102.23	122.70
1	C	20	ASN	CB-CG-ND2	12.78	147.38	116.70
2	B	19	VAL	CG1-CB-CG2	12.77	131.34	110.90
2	D	121	PHE	CG-CD2-CE2	12.77	134.85	120.80
2	B	16	LYS	CA-C-O	12.77	146.91	120.10
2	B	112	VAL	N-CA-CB	12.74	139.54	111.50
1	A	73	LEU	CB-CA-C	12.74	134.41	110.20
1	A	122	HIS	N-CA-CB	12.74	133.53	110.60
2	B	112	VAL	CA-C-N	-12.73	89.19	117.20
1	C	115	THR	CA-CB-OG1	-12.73	82.26	109.00
1	A	126	ASN	O-C-N	12.73	143.07	122.70
1	C	16	LYS	CA-CB-CG	-12.72	85.40	113.40
2	B	128	LEU	CA-C-O	-12.72	93.39	120.10
1	A	115	THR	CA-CB-OG1	-12.71	82.30	109.00
2	D	111	LEU	O-C-N	12.71	143.04	122.70
2	D	140	LEU	CB-CG-CD1	-12.70	89.42	111.00
2	B	62	HIS	ND1-CG-CD2	12.69	126.57	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	SER	N-CA-C	-12.69	76.74	111.00
2	B	33	VAL	CA-CB-CG1	12.69	129.93	110.90
1	A	1	VAL	CG1-CB-CG2	-12.68	90.61	110.90
2	B	17	VAL	CG1-CB-CG2	12.66	131.16	110.90
2	D	124	ASN	OD1-CG-ND2	12.65	151.00	121.90
1	C	140	TYR	CE1-CZ-CE2	-12.65	99.56	119.80
2	D	142	HIS	CG-ND1-CE1	12.65	125.91	108.20
2	D	97	VAL	CA-CB-CG2	12.65	129.87	110.90
1	A	128	PHE	CE1-CZ-CE2	12.63	142.73	120.00
2	B	43	HIS	N-CA-CB	12.62	133.32	110.60
1	C	57	ALA	O-C-N	-12.62	102.50	122.70
2	D	22	VAL	CA-C-O	12.62	146.61	120.10
2	D	43	HIS	CB-CG-CD2	-12.62	91.67	130.80
2	D	118	GLY	CA-C-O	12.62	143.32	120.60
2	B	14	TRP	N-CA-CB	12.62	133.31	110.60
2	B	36	TRP	CD1-NE1-CE2	12.61	120.35	109.00
2	D	84	PHE	CA-C-N	-12.61	89.46	117.20
1	C	24	TYR	N-CA-CB	12.61	133.29	110.60
1	A	103	HIS	CG-ND1-CE1	12.61	125.85	108.20
2	B	35	PRO	O-C-N	-12.59	102.56	122.70
1	C	77	PRO	CA-CB-CG	-12.57	80.11	104.00
1	A	107	VAL	CA-CB-CG1	12.57	129.75	110.90
1	C	107	VAL	N-CA-CB	12.56	139.13	111.50
1	A	106	LEU	CA-C-N	12.56	144.82	117.20
1	A	55	GLN	CG-CD-OE1	12.55	146.71	121.60
1	C	91	LEU	CB-CG-CD2	12.53	132.29	111.00
1	A	42	TYR	CE1-CZ-CE2	-12.53	99.76	119.80
2	D	21	VAL	CA-C-N	12.53	144.75	117.20
1	C	98	PHE	CG-CD1-CE1	-12.52	107.02	120.80
2	B	56	ASN	CB-CA-C	12.51	135.42	110.40
1	C	9	ASN	CB-CA-C	12.51	135.42	110.40
2	D	70	PHE	O-C-N	12.51	142.71	122.70
1	A	113	LEU	CB-CG-CD1	-12.50	89.75	111.00
2	B	25	GLN	CB-CG-CD	12.50	144.09	111.60
2	B	88	SER	N-CA-CB	12.50	129.25	110.50
2	D	77	LEU	CA-C-O	12.50	146.34	120.10
1	A	110	ALA	CA-C-N	12.47	144.64	117.20
2	B	76	HIS	CB-CA-C	-12.47	85.45	110.40
1	C	115	THR	N-CA-CB	12.47	133.99	110.30
1	C	113	LEU	CB-CG-CD1	-12.46	89.81	111.00
2	D	37	THR	O-C-N	-12.43	102.81	122.70
2	D	115	ARG	NH1-CZ-NH2	-12.43	105.73	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	131	LYS	C-N-CA	-12.43	90.63	121.70
1	A	73	LEU	N-CA-C	-12.43	77.45	111.00
2	D	86	GLN	CG-CD-OE1	-12.42	96.75	121.60
2	D	88	SER	CA-C-N	12.42	141.05	116.20
1	A	95	PRO	N-CA-CB	12.41	118.19	103.30
2	D	107	ASN	N-CA-CB	-12.41	88.26	110.60
2	B	124	ASN	CA-C-O	-12.41	94.05	120.10
2	D	102	PHE	CB-CG-CD2	-12.40	112.12	120.80
1	A	90	LYS	CG-CD-CE	12.40	149.09	111.90
2	D	40	PHE	CG-CD2-CE2	-12.40	107.16	120.80
2	D	41	PHE	N-CA-CB	12.40	132.92	110.60
2	D	142	HIS	CA-C-N	-12.39	89.93	117.20
1	C	125	LEU	CA-CB-CG	12.39	143.81	115.30
1	C	133	SER	O-C-N	12.39	142.53	122.70
2	B	129	PHE	CD1-CE1-CZ	-12.39	105.23	120.10
2	B	100	GLN	CB-CG-CD	12.39	143.80	111.60
1	C	95	PRO	C-N-CA	12.38	152.66	121.70
1	C	1	VAL	CA-CB-CG2	12.38	129.47	110.90
1	A	12	ALA	CA-C-O	12.37	146.07	120.10
2	B	41	PHE	CA-C-N	-12.37	89.99	117.20
2	D	132	VAL	CA-CB-CG2	12.37	129.45	110.90
2	D	21	VAL	CA-C-O	-12.35	94.17	120.10
1	C	11	LYS	CA-CB-CG	-12.33	86.27	113.40
1	C	8	SER	N-CA-CB	12.32	128.99	110.50
1	C	132	ASP	CB-CA-C	12.32	135.05	110.40
1	C	10	VAL	O-C-N	-12.30	103.02	122.70
1	C	40	LYS	CB-CG-CD	12.30	143.58	111.60
2	B	59	VAL	CB-CA-C	-12.29	88.05	111.40
1	A	138	SER	CB-CA-C	12.28	133.43	110.10
2	B	49	SER	CA-C-O	-12.28	94.31	120.10
1	A	87	HIS	CB-CA-C	-12.26	85.88	110.40
1	C	87	HIS	C-N-CA	12.26	152.34	121.70
2	B	58	LYS	O-C-N	-12.25	103.10	122.70
1	C	20	ASN	O-C-N	-12.25	103.10	122.70
1	C	133	SER	N-CA-CB	12.25	128.88	110.50
1	A	54	GLN	CG-CD-OE1	12.24	146.09	121.60
1	C	110	ALA	O-C-N	12.24	142.29	122.70
2	D	135	GLY	CA-C-N	12.24	144.13	117.20
2	B	123	PRO	CA-C-N	12.24	144.12	117.20
1	C	41	THR	CA-CB-CG2	12.23	129.53	112.40
2	B	67	LEU	O-C-N	12.23	142.27	122.70
1	C	121	VAL	CA-C-O	-12.23	94.42	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	93	ASN	CA-C-O	-12.22	94.43	120.10
1	A	51	GLY	C-N-CA	12.22	152.26	121.70
1	C	78	GLY	O-C-N	12.21	142.24	122.70
1	A	87	HIS	N-CA-CB	12.20	132.57	110.60
2	B	75	LYS	CA-CB-CG	-12.20	86.56	113.40
2	D	59	VAL	CA-C-O	-12.20	94.48	120.10
1	C	45	HIS	N-CA-C	12.19	143.92	111.00
1	C	3	SER	O-C-N	-12.19	103.19	122.70
2	D	71	THR	N-CA-CB	-12.19	87.14	110.30
1	A	10	VAL	CA-CB-CG1	12.19	129.18	110.90
2	B	33	VAL	CA-C-N	12.18	143.99	117.20
1	A	74	ASN	CA-C-N	12.15	143.94	117.20
1	C	128	PHE	CD1-CG-CD2	-12.15	102.50	118.30
2	D	44	PHE	CZ-CE2-CD2	-12.15	105.52	120.10
2	B	5	GLU	N-CA-CB	-12.15	88.73	110.60
2	B	30	LEU	CA-C-O	12.15	145.61	120.10
2	D	65	ARG	CA-C-O	-12.14	94.60	120.10
2	B	41	PHE	O-C-N	12.14	142.12	122.70
1	C	47	ASP	OD1-CG-OD2	12.14	146.36	123.30
1	A	80	LEU	C-N-CA	12.13	152.03	121.70
2	B	12	GLY	O-C-N	-12.13	103.28	122.70
2	D	34	TYR	CA-CB-CG	12.13	136.45	113.40
1	C	3	SER	C-N-CA	-12.13	91.37	121.70
2	B	113	VAL	CG1-CB-CG2	-12.11	91.52	110.90
2	B	34	TYR	CD1-CG-CD2	-12.11	104.58	117.90
1	C	134	THR	CA-C-N	12.10	143.81	117.20
1	A	119	PRO	CA-C-O	-12.09	91.18	120.20
2	D	57	PRO	C-N-CA	12.09	151.92	121.70
1	A	12	ALA	CA-C-N	-12.09	90.61	117.20
1	A	129	LEU	O-C-N	12.09	142.04	122.70
2	D	40	PHE	CD1-CE1-CZ	12.08	134.59	120.10
1	A	67	THR	CA-CB-OG1	-12.07	83.66	109.00
2	D	22	VAL	CA-CB-CG2	12.07	129.00	110.90
2	B	83	ALA	N-CA-CB	-12.05	93.23	110.10
1	A	103	HIS	ND1-CG-CD2	-12.04	89.14	106.00
2	D	136	VAL	C-N-CA	-12.04	91.59	121.70
2	B	99	PRO	N-CA-CB	-12.03	88.86	103.30
2	B	67	LEU	CA-C-N	12.03	143.66	117.20
2	D	122	THR	CA-CB-OG1	-12.03	83.74	109.00
1	C	3	SER	CA-C-O	12.02	145.35	120.10
1	C	17	VAL	CG1-CB-CG2	-12.02	91.67	110.90
2	B	22	VAL	N-CA-C	-12.01	78.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	LEU	C-N-CA	12.00	151.70	121.70
1	C	17	VAL	CA-CB-CG2	12.00	128.90	110.90
2	D	82	GLY	C-N-CA	11.99	151.68	121.70
1	A	100	LEU	CB-CG-CD1	-11.98	90.64	111.00
1	A	110	ALA	CA-C-O	-11.97	94.96	120.10
2	B	50	ALA	C-N-CA	11.97	147.44	122.30
1	C	32	MET	CA-C-O	-11.97	94.97	120.10
2	B	59	VAL	O-C-N	11.96	141.84	122.70
1	A	39	THR	CA-C-N	11.96	143.51	117.20
1	C	105	LEU	CB-CG-CD1	11.95	131.32	111.00
1	C	107	VAL	CA-C-O	-11.95	95.00	120.10
1	C	24	TYR	O-C-N	-11.95	102.89	123.20
2	D	14	TRP	O-C-N	11.94	143.50	123.20
1	A	119	PRO	O-C-N	11.94	141.80	122.70
2	B	84	PHE	CB-CG-CD2	11.93	129.15	120.80
1	A	98	PHE	CG-CD2-CE2	11.93	133.92	120.80
1	A	101	LEU	CB-CG-CD1	11.93	131.28	111.00
2	D	112	VAL	O-C-N	11.92	141.78	122.70
2	B	80	LEU	CA-CB-CG	11.92	142.71	115.30
2	B	83	ALA	O-C-N	-11.91	103.64	122.70
2	B	77	LEU	CB-CA-C	-11.89	87.61	110.20
2	D	87	LEU	CB-CG-CD1	11.88	131.19	111.00
1	C	96	VAL	CA-CB-CG1	11.87	128.71	110.90
2	D	19	VAL	CA-C-N	11.87	143.32	117.20
2	D	97	VAL	CA-C-N	11.87	143.31	117.20
2	B	72	GLN	CB-CG-CD	11.87	142.46	111.60
1	A	34	LEU	N-CA-CB	11.86	134.13	110.40
1	A	47	ASP	O-C-N	-11.86	103.72	122.70
2	B	64	LYS	CA-C-O	11.86	145.01	120.10
2	D	115	ARG	CA-C-O	11.85	144.99	120.10
1	C	43	PHE	O-C-N	11.85	143.61	121.10
2	D	26	ALA	N-CA-CB	11.85	126.69	110.10
1	A	60	GLN	CA-C-N	-11.84	91.16	117.20
1	C	11	LYS	CA-C-N	11.84	143.24	117.20
2	B	125	VAL	C-N-CA	11.83	151.27	121.70
1	C	88	ALA	CA-C-N	11.82	143.20	117.20
2	B	36	TRP	CD1-CG-CD2	-11.82	96.85	106.30
1	C	61	LYS	CA-C-N	11.81	143.18	117.20
2	D	2	LEU	CB-CA-C	-11.80	87.79	110.20
1	C	139	LYS	C-N-CA	11.79	151.17	121.70
1	C	106	LEU	CB-CG-CD1	11.76	131.00	111.00
2	D	53	VAL	N-CA-C	-11.76	79.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	TYR	CB-CG-CD1	11.75	128.05	121.00
1	A	130	ALA	CA-C-O	11.75	144.77	120.10
2	B	100	GLN	OE1-CD-NE2	-11.75	94.89	121.90
1	A	93	VAL	N-CA-CB	11.73	137.30	111.50
1	A	114	PRO	CA-C-N	11.71	142.96	117.20
2	B	81	LYS	CA-C-N	11.71	139.62	116.20
1	C	28	ALA	N-CA-CB	-11.70	93.72	110.10
2	D	129	PHE	CA-C-O	11.69	144.66	120.10
2	B	47	LEU	N-CA-CB	-11.69	87.02	110.40
2	B	78	ASP	CA-C-O	11.69	144.65	120.10
2	B	4	ALA	CB-CA-C	11.69	127.63	110.10
2	B	76	HIS	CB-CG-ND1	-11.69	93.98	123.20
2	B	143	LYS	CA-C-N	11.68	142.90	117.20
1	C	127	LYS	CG-CD-CE	11.68	146.94	111.90
2	D	36	TRP	CB-CG-CD2	11.66	141.76	126.60
2	D	18	ASP	CB-CG-OD1	11.66	128.79	118.30
1	A	40	LYS	CA-C-N	11.66	142.85	117.20
2	D	2	LEU	N-CA-CB	-11.65	87.09	110.40
2	D	125	VAL	O-C-N	-11.65	104.06	122.70
1	A	22	PRO	O-C-N	-11.65	104.07	122.70
2	B	133	VAL	CB-CA-C	11.65	133.53	111.40
2	D	57	PRO	N-CA-CB	-11.64	89.33	103.30
2	D	114	ALA	CA-C-N	11.64	142.81	117.20
2	D	107	ASN	CB-CG-OD1	11.64	144.88	121.60
2	D	109	LEU	CA-C-O	-11.63	95.67	120.10
1	C	56	LYS	CA-C-N	11.62	142.77	117.20
2	B	38	GLN	CG-CD-OE1	-11.62	98.36	121.60
1	C	36	PHE	CA-C-O	11.62	144.51	120.10
2	D	67	LEU	CB-CG-CD2	-11.62	91.25	111.00
2	D	68	ASP	CA-CB-CG	-11.62	87.85	113.40
2	D	115	ARG	CB-CA-C	11.61	133.61	110.40
1	A	65	ALA	C-N-CA	11.60	150.70	121.70
2	D	79	ASP	CB-CG-OD1	-11.60	107.86	118.30
1	A	38	THR	O-C-N	11.59	141.25	122.70
2	D	25	GLN	OE1-CD-NE2	11.59	148.55	121.90
1	A	28	ALA	CA-C-N	11.58	142.68	117.20
2	B	78	ASP	C-N-CA	11.57	150.62	121.70
1	A	32	MET	CB-CG-SD	11.57	147.10	112.40
2	D	76	HIS	CG-CD2-NE2	-11.56	87.23	109.20
1	C	48	LEU	CA-C-O	11.56	144.37	120.10
2	B	94	LYS	N-CA-CB	11.54	131.37	110.60
2	D	119	GLY	CA-C-O	11.53	141.36	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	GLY	C-N-CA	11.52	146.49	122.30
2	B	76	HIS	CG-ND1-CE1	-11.49	90.76	105.70
2	B	103	ARG	CB-CG-CD	-11.49	81.73	111.60
2	D	76	HIS	N-CA-CB	-11.49	89.92	110.60
1	A	74	ASN	O-C-N	-11.47	104.35	122.70
2	B	116	ASN	CB-CG-OD1	11.46	144.52	121.60
1	A	137	THR	C-N-CA	11.46	150.34	121.70
2	B	57	PRO	O-C-N	11.46	141.03	122.70
1	A	62	VAL	O-C-N	-11.45	104.38	122.70
2	B	69	ALA	O-C-N	-11.45	104.38	122.70
2	D	79	ASP	CB-CG-OD2	-11.45	107.99	118.30
1	C	29	LEU	CD1-CG-CD2	-11.45	76.16	110.50
1	A	33	PHE	CD1-CG-CD2	-11.45	103.42	118.30
1	C	55	GLN	CB-CG-CD	-11.45	81.84	111.60
1	C	39	THR	O-C-N	11.44	141.00	122.70
2	B	84	PHE	CE1-CZ-CE2	-11.43	99.42	120.00
1	C	27	GLN	O-C-N	11.43	140.99	122.70
2	D	43	HIS	C-N-CA	11.43	150.26	121.70
1	C	70	GLN	CG-CD-NE2	-11.42	89.29	116.70
1	A	91	LEU	CB-CA-C	11.41	131.88	110.20
1	A	43	PHE	CA-C-N	-11.41	85.15	117.10
1	A	134	THR	CA-C-N	11.41	142.29	117.20
2	B	30	LEU	CA-CB-CG	11.41	141.54	115.30
2	B	34	TYR	CE1-CZ-CE2	11.41	138.05	119.80
2	D	31	LEU	CA-C-O	-11.41	96.15	120.10
2	B	113	VAL	CA-C-O	-11.40	96.16	120.10
1	A	111	SER	N-CA-CB	11.40	127.60	110.50
1	A	80	LEU	CB-CG-CD2	11.39	130.37	111.00
2	B	40	PHE	CB-CA-C	11.39	133.18	110.40
2	B	68	ASP	CA-C-N	11.39	142.25	117.20
1	C	44	PRO	CA-C-O	-11.38	92.88	120.20
1	C	101	LEU	C-N-CA	11.38	150.16	121.70
1	A	91	LEU	CD1-CG-CD2	-11.38	76.35	110.50
1	C	62	VAL	O-C-N	-11.38	104.50	122.70
2	D	140	LEU	CA-CB-CG	11.37	141.46	115.30
1	A	27	GLN	CB-CA-C	11.35	133.11	110.40
1	C	89	HIS	CG-CD2-NE2	-11.35	87.63	109.20
1	A	65	ALA	CA-C-N	11.34	142.15	117.20
2	D	1	MET	CA-CB-CG	11.33	132.56	113.30
1	A	8	SER	C-N-CA	11.33	150.02	121.70
1	A	34	LEU	O-C-N	11.32	140.82	122.70
1	A	124	ASN	CA-CB-CG	11.32	138.31	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	SER	CB-CA-C	11.32	131.60	110.10
1	C	44	PRO	C-N-CA	-11.31	93.42	121.70
2	B	31	LEU	O-C-N	11.31	140.80	122.70
2	D	68	ASP	CB-CA-C	-11.31	87.78	110.40
2	B	116	ASN	N-CA-CB	11.30	130.94	110.60
1	C	134	THR	CA-CB-CG2	-11.29	96.59	112.40
2	B	73	GLY	CA-C-O	-11.28	100.30	120.60
1	C	126	ASN	O-C-N	-11.28	104.66	122.70
1	C	32	MET	CA-C-N	11.27	141.99	117.20
2	B	96	HIS	CA-CB-CG	11.26	132.75	113.60
2	B	93	ASN	C-N-CA	-11.26	93.56	121.70
1	C	33	PHE	CA-C-O	11.26	143.74	120.10
2	D	70	PHE	CA-CB-CG	11.25	140.89	113.90
2	B	42	GLN	CA-C-O	11.24	143.71	120.10
2	B	44	PHE	C-N-CA	-11.24	98.69	122.30
1	A	43	PHE	C-N-CD	11.23	151.99	128.40
2	B	75	LYS	O-C-N	11.22	140.65	122.70
1	C	110	ALA	N-CA-C	-11.19	80.80	111.00
2	D	71	THR	CA-CB-OG1	11.17	132.45	109.00
1	A	15	GLY	O-C-N	-11.17	104.83	122.70
2	B	13	PHE	CE1-CZ-CE2	11.16	140.09	120.00
1	C	86	LEU	CB-CA-C	-11.16	89.00	110.20
1	C	112	HIS	CB-CG-CD2	11.16	165.39	130.80
2	B	87	LEU	CB-CG-CD2	11.15	129.96	111.00
2	D	143	LYS	N-CA-C	11.15	141.11	111.00
2	D	69	ALA	N-CA-CB	11.14	125.69	110.10
2	D	22	VAL	CG1-CB-CG2	-11.14	93.08	110.90
1	C	88	ALA	N-CA-CB	11.13	125.68	110.10
1	C	37	PRO	CA-CB-CG	11.12	125.94	104.80
1	A	90	LYS	C-N-CA	11.12	149.50	121.70
2	B	140	LEU	C-N-CA	-11.10	93.94	121.70
1	A	123	ALA	N-CA-CB	-11.10	94.56	110.10
2	B	104	LEU	CB-CA-C	11.09	131.27	110.20
2	B	98	ASN	CB-CG-OD1	-11.08	99.44	121.60
2	D	133	VAL	C-N-CA	11.07	149.37	121.70
1	A	77	PRO	CA-C-O	-11.07	93.64	120.20
1	C	50	HIS	ND1-CE1-NE2	-11.07	85.56	109.90
2	D	86	GLN	CG-CD-NE2	11.05	143.23	116.70
2	B	64	LYS	CB-CA-C	11.05	132.50	110.40
1	C	110	ALA	CA-C-O	-11.05	96.90	120.10
1	A	140	TYR	CB-CG-CD2	11.04	127.62	121.00
1	C	48	LEU	CD1-CG-CD2	11.04	143.61	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	95	LEU	CB-CA-C	-11.03	89.25	110.20
1	A	38	THR	N-CA-CB	-11.02	89.36	110.30
2	D	142	HIS	ND1-CG-CD2	-11.02	90.57	106.00
1	C	70	GLN	N-CA-C	11.02	140.75	111.00
1	A	98	PHE	CA-CB-CG	11.01	140.33	113.90
1	A	33	PHE	CB-CG-CD1	-11.01	113.09	120.80
2	B	53	VAL	C-N-CA	-11.00	94.19	121.70
1	C	97	ASN	CA-C-N	-11.00	92.99	117.20
1	C	117	PHE	CD1-CE1-CZ	11.00	133.30	120.10
2	D	56	ASN	CA-C-O	-11.00	97.00	120.10
2	B	90	LEU	CB-CA-C	10.99	131.09	110.20
1	C	54	GLN	CA-C-O	-10.98	97.04	120.10
1	C	125	LEU	CA-C-N	10.98	141.36	117.20
1	C	95	PRO	CA-N-CD	-10.97	96.14	111.50
2	B	38	GLN	CA-CB-CG	10.97	137.53	113.40
1	C	44	PRO	CA-C-N	10.96	141.32	117.20
2	D	26	ALA	O-C-N	10.96	140.23	122.70
1	C	108	THR	C-N-CA	10.96	149.09	121.70
2	B	1	MET	CA-C-N	10.95	141.30	117.20
2	B	53	VAL	O-C-N	10.95	140.22	122.70
2	B	36	TRP	CZ3-CH2-CZ2	10.95	134.74	121.60
2	D	14	TRP	CZ3-CH2-CZ2	10.95	134.74	121.60
2	B	74	LEU	CB-CA-C	-10.94	89.41	110.20
2	D	14	TRP	CH2-CZ2-CE2	-10.94	106.46	117.40
2	D	50	ALA	N-CA-CB	10.93	125.40	110.10
2	B	27	LEU	CA-CB-CG	10.93	140.43	115.30
1	C	135	VAL	CA-C-N	10.92	141.23	117.20
2	D	89	GLY	N-CA-C	-10.92	85.81	113.10
1	A	11	LYS	O-C-N	10.91	140.16	122.70
2	D	117	PHE	CA-C-O	-10.91	97.19	120.10
2	B	21	VAL	O-C-N	-10.91	105.25	122.70
2	D	136	VAL	CA-C-N	10.91	141.19	117.20
2	B	80	LEU	N-CA-CB	-10.90	88.60	110.40
1	C	2	LEU	C-N-CA	10.90	148.94	121.70
2	B	13	PHE	CA-C-O	-10.89	97.22	120.10
1	C	10	VAL	CA-CB-CG2	10.89	127.24	110.90
1	C	63	ALA	CA-C-N	10.89	141.15	117.20
2	D	14	TRP	CD1-NE1-CE2	-10.88	99.20	109.00
1	A	20	ASN	O-C-N	10.88	140.10	122.70
1	A	128	PHE	CD1-CE1-CZ	-10.87	107.05	120.10
1	C	19	GLY	CA-C-O	10.87	140.17	120.60
1	C	77	PRO	N-CD-CG	-10.86	86.91	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	57	PRO	O-C-N	-10.86	105.33	122.70
2	D	79	ASP	CA-CB-CG	10.86	137.29	113.40
2	D	128	LEU	CD1-CG-CD2	-10.86	77.92	110.50
2	B	30	LEU	CB-CG-CD1	10.85	129.45	111.00
2	B	57	PRO	CA-C-O	-10.85	94.17	120.20
1	C	61	LYS	CA-C-O	-10.84	97.33	120.10
2	D	92	CYS	CA-CB-SG	-10.84	94.48	114.00
1	A	10	VAL	N-CA-CB	10.84	135.35	111.50
1	A	36	PHE	CD1-CG-CD2	-10.84	104.21	118.30
2	D	55	ASN	N-CA-CB	10.83	130.10	110.60
1	C	32	MET	CG-SD-CE	10.83	117.52	100.20
1	C	52	SER	CA-C-O	-10.83	97.36	120.10
1	A	77	PRO	N-CD-CG	-10.82	86.97	103.20
1	C	61	LYS	CG-CD-CE	10.82	144.36	111.90
1	C	52	SER	CA-CB-OG	10.82	140.41	111.20
1	A	11	LYS	C-N-CA	-10.81	94.67	121.70
2	B	78	ASP	N-CA-CB	-10.81	91.15	110.60
2	D	60	LYS	CB-CG-CD	10.81	139.69	111.60
2	B	123	PRO	C-N-CA	10.79	148.69	121.70
2	B	108	VAL	CA-CB-CG2	-10.79	94.72	110.90
1	C	87	HIS	CA-CB-CG	10.79	131.93	113.60
2	D	112	VAL	CA-C-O	-10.79	97.45	120.10
1	C	59	GLY	CA-C-O	-10.78	101.19	120.60
1	A	114	PRO	CB-CG-CD	-10.78	64.45	106.50
1	C	96	VAL	N-CA-CB	-10.78	87.78	111.50
2	D	7	LYS	CA-C-N	10.78	140.91	117.20
1	A	17	VAL	O-C-N	-10.77	104.89	123.20
2	D	73	GLY	CA-C-N	10.77	140.89	117.20
2	D	15	GLY	CA-C-N	-10.77	93.52	117.20
1	A	74	ASN	CB-CG-ND2	-10.76	90.89	116.70
1	C	5	ALA	O-C-N	10.75	139.91	122.70
1	C	70	GLN	CG-CD-OE1	10.74	143.08	121.60
1	C	94	ASN	C-N-CD	10.74	150.95	128.40
1	A	136	LEU	CB-CA-C	-10.73	89.81	110.20
1	C	130	ALA	O-C-N	-10.73	105.53	122.70
2	B	79	ASP	CB-CG-OD1	10.73	127.95	118.30
1	C	82	ASN	CA-C-O	-10.70	97.62	120.10
1	A	27	GLN	N-CA-CB	10.70	129.87	110.60
2	B	52	ALA	CA-C-N	-10.70	93.66	117.20
1	C	80	LEU	CA-C-N	10.68	140.71	117.20
2	B	88	SER	C-N-CA	10.68	144.73	122.30
2	B	21	VAL	CA-C-N	10.68	140.69	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	68	ASP	N-CA-CB	10.68	129.82	110.60
1	C	24	TYR	CA-C-N	10.67	137.53	116.20
2	B	80	LEU	CB-CG-CD2	-10.66	92.87	111.00
1	C	122	HIS	CB-CG-CD2	10.66	163.86	130.80
1	A	24	TYR	O-C-N	-10.66	105.08	123.20
1	C	80	LEU	CB-CG-CD1	-10.66	92.88	111.00
1	C	130	ALA	N-CA-CB	-10.66	95.18	110.10
1	C	137	THR	CA-CB-CG2	10.65	127.31	112.40
1	C	74	ASN	O-C-N	-10.64	105.67	122.70
1	A	50	HIS	CB-CG-ND1	-10.64	96.60	123.20
1	A	111	SER	O-C-N	-10.63	105.69	122.70
1	A	25	GLY	CA-C-N	-10.63	93.81	117.20
2	B	42	GLN	CA-CB-CG	10.62	136.76	113.40
2	D	90	LEU	CD1-CG-CD2	10.62	142.36	110.50
1	C	88	ALA	CA-C-O	-10.61	97.81	120.10
2	D	74	LEU	CA-CB-CG	10.61	139.71	115.30
1	C	105	LEU	CA-C-O	-10.61	97.81	120.10
2	D	28	GLY	C-N-CA	10.61	148.22	121.70
1	A	9	ASN	N-CA-CB	-10.61	91.51	110.60
2	B	133	VAL	CA-CB-CG2	10.60	126.81	110.90
1	C	1	VAL	CA-C-N	10.60	140.52	117.20
2	D	13	PHE	CB-CG-CD2	10.60	128.22	120.80
1	C	7	LYS	O-C-N	10.60	139.65	122.70
1	A	110	ALA	N-CA-C	-10.59	82.40	111.00
2	D	78	ASP	CA-C-N	-10.58	93.92	117.20
1	A	33	PHE	CZ-CE2-CD2	10.58	132.79	120.10
1	A	96	VAL	CA-CB-CG1	-10.57	95.04	110.90
1	C	73	LEU	CB-CG-CD1	10.57	128.97	111.00
2	D	68	ASP	OD1-CG-OD2	-10.57	103.22	123.30
2	D	129	PHE	CA-CB-CG	-10.56	88.55	113.90
1	A	120	ALA	O-C-N	-10.56	105.80	122.70
1	A	79	THR	O-C-N	-10.56	105.80	122.70
2	B	140	LEU	CA-C-O	10.55	142.25	120.10
1	C	87	HIS	CG-ND1-CE1	-10.55	91.99	105.70
2	B	34	TYR	CB-CG-CD2	10.54	127.33	121.00
2	D	13	PHE	CA-C-N	10.54	140.40	117.20
2	B	133	VAL	CA-C-O	-10.54	97.96	120.10
2	D	107	ASN	OD1-CG-ND2	-10.54	97.66	121.90
1	A	24	TYR	C-N-CA	10.53	144.40	122.30
2	B	133	VAL	CG1-CB-CG2	-10.53	94.06	110.90
1	C	132	ASP	CA-CB-CG	-10.53	90.25	113.40
2	D	78	ASP	CB-CG-OD2	-10.52	108.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	130	GLN	O-C-N	-10.52	105.86	122.70
2	D	96	HIS	CB-CG-ND1	10.52	149.49	123.20
2	D	137	ALA	N-CA-C	-10.52	82.61	111.00
1	A	73	LEU	C-N-CA	10.51	147.98	121.70
1	A	94	ASN	CB-CA-C	10.49	131.37	110.40
1	A	128	PHE	CZ-CE2-CD2	-10.48	107.53	120.10
1	A	33	PHE	CA-CB-CG	10.48	139.05	113.90
1	C	56	LYS	N-CA-C	-10.47	82.72	111.00
2	D	124	ASN	CA-C-O	-10.47	98.11	120.10
2	B	67	LEU	CB-CG-CD1	-10.47	93.20	111.00
1	C	137	THR	OG1-CB-CG2	10.47	134.07	110.00
1	A	93	VAL	CA-CB-CG2	10.45	126.57	110.90
1	C	29	LEU	CB-CG-CD1	10.44	128.75	111.00
2	D	107	ASN	CA-C-O	-10.44	98.17	120.10
1	C	45	HIS	C-N-CA	10.44	147.80	121.70
2	D	51	GLY	C-N-CA	-10.44	95.60	121.70
2	B	44	PHE	CZ-CE2-CD2	10.44	132.62	120.10
1	A	38	THR	CA-C-O	-10.43	98.21	120.10
2	D	104	LEU	CB-CG-CD1	-10.43	93.28	111.00
1	C	35	SER	C-N-CA	10.42	147.76	121.70
1	A	47	ASP	OD1-CG-OD2	-10.42	103.50	123.30
2	B	38	GLN	CB-CG-CD	10.41	138.67	111.60
2	B	67	LEU	N-CA-CB	10.41	131.22	110.40
1	C	85	ASN	C-N-CA	10.41	147.71	121.70
2	B	70	PHE	C-N-CA	10.40	147.71	121.70
2	B	73	GLY	CA-C-N	-10.40	94.32	117.20
2	D	39	ARG	NE-CZ-NH1	10.40	125.50	120.30
2	D	102	PHE	CD1-CE1-CZ	-10.40	107.62	120.10
2	D	20	ASP	N-CA-C	-10.40	82.92	111.00
1	A	14	TRP	NE1-CE2-CZ2	10.38	141.82	130.40
2	B	104	LEU	C-N-CA	10.37	147.62	121.70
1	C	70	GLN	CB-CG-CD	-10.36	84.66	111.60
1	C	128	PHE	CG-CD1-CE1	10.36	132.20	120.80
2	D	13	PHE	C-N-CA	10.36	147.61	121.70
2	B	87	LEU	O-C-N	-10.36	106.13	122.70
2	B	11	THR	CA-CB-OG1	-10.35	87.27	109.00
2	B	133	VAL	CA-CB-CG1	10.34	126.41	110.90
1	A	9	ASN	CB-CG-OD1	-10.33	100.94	121.60
2	B	102	PHE	CG-CD1-CE1	10.33	132.16	120.80
1	C	76	LEU	CD1-CG-CD2	10.32	141.47	110.50
2	D	117	PHE	CD1-CG-CD2	10.32	131.72	118.30
1	A	94	ASN	CB-CG-OD1	-10.32	100.96	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	PHE	CE1-CZ-CE2	-10.32	101.43	120.00
1	A	8	SER	N-CA-CB	-10.31	95.03	110.50
2	B	39	ARG	CA-C-O	10.31	141.75	120.10
1	A	19	GLY	C-N-CA	10.30	147.46	121.70
2	B	132	VAL	CA-CB-CG1	10.30	126.36	110.90
2	D	112	VAL	CA-CB-CG2	10.30	126.35	110.90
2	B	37	THR	C-N-CA	10.29	147.43	121.70
1	C	48	LEU	O-C-N	-10.29	106.23	122.70
2	D	39	ARG	NE-CZ-NH2	10.29	125.45	120.30
1	C	8	SER	CA-C-N	-10.29	94.56	117.20
1	C	25	GLY	CA-C-N	10.29	139.84	117.20
1	C	141	ARG	N-CA-CB	10.28	129.10	110.60
2	D	77	LEU	CB-CG-CD2	10.28	128.48	111.00
1	C	92	ARG	CA-C-N	-10.27	94.61	117.20
1	C	114	PRO	CB-CA-C	10.27	137.66	112.00
1	A	50	HIS	CB-CA-C	10.26	130.93	110.40
1	C	109	LEU	CA-CB-CG	10.26	138.90	115.30
2	B	87	LEU	N-CA-C	-10.26	83.30	111.00
1	C	47	ASP	CA-C-O	10.26	141.64	120.10
1	A	66	LEU	O-C-N	-10.25	106.30	122.70
2	B	79	ASP	N-CA-C	-10.25	83.32	111.00
1	C	49	SER	CA-CB-OG	10.25	138.86	111.20
1	C	5	ALA	N-CA-C	-10.24	83.34	111.00
1	A	115	THR	C-N-CA	10.24	147.29	121.70
1	A	67	THR	OG1-CB-CG2	10.23	133.54	110.00
1	C	103	HIS	C-N-CA	10.23	147.28	121.70
2	D	14	TRP	CA-C-O	-10.23	98.61	120.10
2	D	121	PHE	N-CA-C	10.23	138.63	111.00
2	B	29	ARG	C-N-CA	10.23	147.28	121.70
1	A	118	THR	OG1-CB-CG2	-10.23	86.48	110.00
2	B	44	PHE	CE1-CZ-CE2	-10.22	101.61	120.00
1	A	29	LEU	CA-C-O	-10.21	98.66	120.10
2	D	13	PHE	O-C-N	-10.21	106.37	122.70
1	C	90	LYS	CA-C-O	-10.20	98.67	120.10
1	C	80	LEU	CB-CA-C	10.20	129.58	110.20
1	C	103	HIS	CE1-NE2-CD2	-10.20	81.10	106.60
2	D	69	ALA	CA-C-N	-10.20	94.76	117.20
1	A	39	THR	CB-CA-C	10.20	139.13	111.60
2	D	131	LYS	O-C-N	10.19	139.01	122.70
2	D	60	LYS	CA-C-N	10.19	139.62	117.20
1	C	98	PHE	CB-CA-C	10.18	130.76	110.40
2	D	14	TRP	CB-CG-CD1	-10.18	113.76	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	85	ALA	CB-CA-C	10.18	125.38	110.10
1	C	136	LEU	CB-CG-CD1	10.18	128.31	111.00
2	B	46	ASN	CB-CG-ND2	10.18	141.12	116.70
1	C	14	TRP	CB-CA-C	-10.18	90.05	110.40
1	A	138	SER	CA-C-N	10.17	139.57	117.20
2	D	134	ALA	N-CA-C	-10.17	83.55	111.00
2	B	45	GLY	N-CA-C	-10.16	87.71	113.10
1	A	135	VAL	CG1-CB-CG2	-10.15	94.65	110.90
2	B	32	VAL	N-CA-CB	-10.15	89.17	111.50
1	C	113	LEU	CB-CA-C	10.15	129.48	110.20
1	A	104	SER	N-CA-CB	10.13	125.70	110.50
2	D	20	ASP	CA-CB-CG	10.13	135.68	113.40
2	D	59	VAL	N-CA-CB	10.13	133.78	111.50
2	B	93	ASN	CB-CG-ND2	10.12	141.00	116.70
2	D	145	HIS	N-CA-CB	10.12	128.82	110.60
2	D	134	ALA	CA-C-N	10.12	136.44	116.20
1	A	94	ASN	O-C-N	10.11	140.31	121.10
1	C	92	ARG	N-CA-CB	10.10	128.79	110.60
2	D	14	TRP	CE2-CD2-CG	10.10	115.38	107.30
2	D	104	LEU	CB-CG-CD2	10.10	128.16	111.00
1	C	26	ALA	CA-C-O	10.09	141.28	120.10
1	A	107	VAL	CA-CB-CG2	10.08	126.02	110.90
2	B	120	GLN	O-C-N	-10.08	106.58	122.70
2	B	126	GLN	N-CA-C	-10.08	83.79	111.00
2	D	77	LEU	CA-C-N	10.07	139.36	117.20
2	B	101	ASN	CA-C-O	-10.06	98.97	120.10
2	D	44	PHE	CE1-CZ-CE2	10.06	138.10	120.00
1	A	3	SER	N-CA-CB	-10.05	95.42	110.50
2	B	39	ARG	CA-C-N	-10.05	95.10	117.20
2	D	101	ASN	CA-C-N	-10.05	95.09	117.20
1	A	99	LYS	C-N-CA	10.04	146.81	121.70
2	B	17	VAL	CA-CB-CG2	-10.04	95.83	110.90
2	D	111	LEU	CA-CB-CG	10.04	138.40	115.30
2	B	89	GLY	C-N-CA	10.03	146.78	121.70
2	D	102	PHE	N-CA-C	-10.03	83.92	111.00
1	A	11	LYS	CA-C-N	-10.02	95.15	117.20
1	C	2	LEU	CD1-CG-CD2	10.02	140.55	110.50
2	D	100	GLN	O-C-N	10.02	138.73	122.70
1	A	23	ALA	CA-C-O	-10.01	99.08	120.10
1	C	14	TRP	O-C-N	10.00	140.21	123.20
1	C	98	PHE	N-CA-CB	-10.00	92.60	110.60
2	D	144	TYR	CZ-CE2-CD2	-10.00	110.80	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	134	THR	CB-CA-C	9.99	138.58	111.60
2	B	80	LEU	C-N-CA	9.99	146.68	121.70
2	D	76	HIS	CB-CG-CD2	-9.99	99.82	130.80
2	B	125	VAL	CA-CB-CG2	9.98	125.87	110.90
1	A	117	PHE	CA-C-O	9.97	141.05	120.10
2	D	19	VAL	CG1-CB-CG2	-9.97	94.94	110.90
2	D	54	MET	CA-C-N	9.97	139.13	117.20
2	B	42	GLN	N-CA-CB	9.96	128.53	110.60
1	A	74	ASN	CA-CB-CG	9.95	135.30	113.40
2	B	43	HIS	N-CA-C	-9.96	84.12	111.00
1	C	68	LYS	CA-C-N	9.95	139.09	117.20
1	A	133	SER	CA-CB-OG	9.95	138.06	111.20
1	C	128	PHE	CA-CB-CG	9.95	137.77	113.90
1	C	74	ASN	CB-CA-C	-9.94	90.52	110.40
1	C	31	ARG	O-C-N	9.94	138.60	122.70
1	A	24	TYR	CA-C-O	-9.94	99.23	120.10
1	A	88	ALA	O-C-N	-9.93	106.81	122.70
2	D	29	ARG	CA-CB-CG	9.93	135.24	113.40
2	B	91	HIS	CG-CD2-NE2	9.92	128.06	109.20
2	D	123	PRO	CB-CA-C	9.91	136.78	112.00
1	C	60	GLN	CG-CD-NE2	9.91	140.48	116.70
2	D	118	GLY	C-N-CA	9.91	143.10	122.30
2	D	88	SER	C-N-CA	9.90	143.10	122.30
1	C	125	LEU	CA-C-O	-9.90	99.30	120.10
2	D	143	LYS	CB-CG-CD	9.90	137.34	111.60
1	A	44	PRO	CA-CB-CG	9.89	123.59	104.80
2	B	34	TYR	CA-C-N	9.88	144.78	117.10
1	A	66	LEU	C-N-CA	9.88	146.40	121.70
1	A	136	LEU	O-C-N	-9.88	106.90	122.70
2	B	29	ARG	CA-C-N	9.87	138.91	117.20
1	C	54	GLN	C-N-CA	9.86	146.35	121.70
2	D	144	TYR	OH-CZ-CE2	-9.86	93.48	120.10
2	B	91	HIS	CG-ND1-CE1	9.86	122.00	108.20
2	B	41	PHE	CB-CG-CD2	9.85	127.69	120.80
1	C	19	GLY	C-N-CA	9.85	146.31	121.70
1	A	20	ASN	CB-CA-C	9.84	130.09	110.40
1	C	33	PHE	CB-CA-C	9.84	130.08	110.40
2	D	62	HIS	CA-CB-CG	-9.84	96.88	113.60
1	C	102	SER	C-N-CA	-9.84	97.11	121.70
1	A	8	SER	CB-CA-C	9.82	128.76	110.10
1	C	93	VAL	O-C-N	-9.82	106.98	122.70
1	A	120	ALA	C-N-CA	9.82	146.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	74	LEU	N-CA-C	-9.82	84.49	111.00
1	A	122	HIS	ND1-CE1-NE2	-9.81	88.31	109.90
2	D	76	HIS	CA-CB-CG	-9.81	96.92	113.60
2	B	48	SER	CB-CA-C	9.80	128.71	110.10
1	A	4	ALA	C-N-CA	-9.79	97.22	121.70
1	C	16	LYS	CG-CD-CE	9.79	141.28	111.90
1	C	75	ASP	CB-CA-C	-9.79	90.82	110.40
2	D	53	VAL	N-CA-CB	9.79	133.03	111.50
2	B	142	HIS	CA-C-O	9.78	140.63	120.10
2	B	75	LYS	CA-C-N	-9.78	95.69	117.20
1	A	29	LEU	N-CA-C	-9.77	84.62	111.00
1	C	120	ALA	CA-C-N	9.77	138.68	117.20
1	C	6	ASN	CB-CG-ND2	9.76	140.12	116.70
1	A	23	ALA	O-C-N	9.76	138.31	122.70
1	A	107	VAL	CG1-CB-CG2	-9.76	95.29	110.90
2	B	8	ALA	CA-C-O	-9.76	99.61	120.10
2	B	27	LEU	CB-CG-CD1	9.76	127.58	111.00
2	B	84	PHE	CG-CD1-CE1	-9.76	110.07	120.80
1	C	33	PHE	N-CA-CB	-9.75	93.05	110.60
2	D	54	MET	O-C-N	-9.75	107.10	122.70
1	A	80	LEU	N-CA-CB	-9.73	90.94	110.40
1	A	113	LEU	O-C-N	-9.73	102.62	121.10
2	D	37	THR	CA-C-O	9.72	140.52	120.10
2	B	63	GLY	O-C-N	-9.72	107.15	122.70
2	B	117	PHE	CE1-CZ-CE2	-9.71	102.51	120.00
2	D	72	GLN	CB-CG-CD	9.71	136.86	111.60
2	D	131	LYS	N-CA-CB	-9.71	93.12	110.60
2	B	76	HIS	CB-CG-CD2	9.70	160.88	130.80
1	A	96	VAL	O-C-N	9.70	138.22	122.70
2	B	103	ARG	CB-CA-C	-9.70	91.00	110.40
1	C	4	ALA	O-C-N	-9.70	107.19	122.70
1	C	116	ASN	CA-C-O	-9.70	99.74	120.10
2	D	113	VAL	N-CA-C	-9.70	84.82	111.00
1	A	101	LEU	C-N-CA	9.69	145.93	121.70
2	D	141	ALA	C-N-CA	-9.69	97.47	121.70
1	C	79	THR	CA-CB-OG1	-9.69	88.66	109.00
2	D	10	VAL	N-CA-C	9.67	137.12	111.00
1	A	59	GLY	N-CA-C	-9.66	88.94	113.10
2	B	1	MET	CG-SD-CE	-9.65	84.77	100.20
1	C	93	VAL	CA-CB-CG1	-9.63	96.45	110.90
1	C	109	LEU	CB-CG-CD2	9.63	127.37	111.00
2	D	26	ALA	CA-C-O	-9.63	99.89	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	ASN	O-C-N	9.62	138.10	122.70
2	D	3	THR	CA-CB-CG2	-9.62	98.93	112.40
1	C	129	LEU	O-C-N	-9.62	107.31	122.70
1	C	67	THR	CA-C-O	-9.61	99.91	120.10
1	C	70	GLN	C-N-CA	9.62	142.49	122.30
1	C	16	LYS	CD-CE-NZ	-9.61	89.59	111.70
1	C	75	ASP	CA-C-O	9.61	140.28	120.10
1	C	141	ARG	NE-CZ-NH2	9.61	125.11	120.30
2	D	128	LEU	C-N-CA	-9.60	97.70	121.70
2	B	107	ASN	CA-C-O	-9.60	99.95	120.10
1	A	7	LYS	O-C-N	9.59	138.05	122.70
1	A	36	PHE	CE1-CZ-CE2	-9.59	102.73	120.00
2	B	49	SER	N-CA-CB	9.59	124.88	110.50
1	C	131	ASN	O-C-N	-9.59	107.36	122.70
1	A	6	ASN	CB-CA-C	9.57	129.55	110.40
1	C	12	ALA	CA-C-O	-9.57	100.00	120.10
1	C	119	PRO	C-N-CA	9.57	145.64	121.70
1	A	16	LYS	C-N-CA	9.57	145.62	121.70
1	C	9	ASN	C-N-CA	9.57	145.61	121.70
2	B	38	GLN	N-CA-CB	9.56	127.82	110.60
2	D	140	LEU	CA-C-O	-9.56	100.02	120.10
1	C	33	PHE	CZ-CE2-CD2	9.56	131.57	120.10
1	C	75	ASP	CB-CG-OD2	9.56	126.90	118.30
1	A	2	LEU	C-N-CA	-9.56	97.81	121.70
2	B	119	GLY	C-N-CA	9.55	145.58	121.70
2	D	60	LYS	O-C-N	-9.55	107.41	122.70
2	B	33	VAL	CA-C-O	-9.55	100.04	120.10
2	B	126	GLN	CG-CD-OE1	9.55	140.70	121.60
2	D	18	ASP	CB-CG-OD2	-9.55	109.71	118.30
1	A	23	ALA	N-CA-CB	9.54	123.46	110.10
2	B	62	HIS	CA-C-N	9.54	135.27	116.20
1	C	31	ARG	CB-CA-C	9.54	129.47	110.40
1	C	140	TYR	CA-C-N	-9.54	96.22	117.20
2	D	57	PRO	CA-CB-CG	-9.54	85.88	104.00
1	C	69	ALA	N-CA-CB	9.53	123.45	110.10
1	A	34	LEU	CB-CG-CD2	-9.53	94.80	111.00
2	D	136	VAL	CG1-CB-CG2	-9.53	95.65	110.90
1	C	94	ASN	O-C-N	-9.52	103.00	121.10
2	B	24	ALA	CA-C-N	-9.52	96.27	117.20
1	C	118	THR	N-CA-CB	9.52	128.38	110.30
1	A	45	HIS	O-C-N	9.51	137.92	122.70
1	A	137	THR	N-CA-CB	-9.51	92.23	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ASN	CB-CG-OD1	-9.51	102.58	121.60
2	D	75	LYS	CD-CE-NZ	-9.49	89.87	111.70
1	C	47	ASP	N-CA-C	-9.48	85.42	111.00
2	D	13	PHE	CB-CG-CD1	-9.47	114.17	120.80
1	A	48	LEU	N-CA-C	-9.46	85.46	111.00
1	A	77	PRO	CA-C-N	-9.46	97.28	116.20
1	C	33	PHE	O-C-N	-9.46	107.57	122.70
2	D	34	TYR	CA-C-O	-9.45	100.25	120.10
2	D	75	LYS	CB-CA-C	-9.45	91.51	110.40
2	D	44	PHE	O-C-N	-9.44	107.14	123.20
1	C	132	ASP	CA-C-O	9.44	139.93	120.10
2	B	30	LEU	CB-CG-CD2	9.44	127.04	111.00
1	A	44	PRO	N-CA-CB	-9.43	91.98	103.30
2	D	58	LYS	CB-CA-C	9.43	129.26	110.40
1	A	42	TYR	C-N-CA	-9.43	98.14	121.70
1	C	117	PHE	CG-CD2-CE2	-9.43	110.43	120.80
2	D	79	ASP	OD1-CG-OD2	9.43	141.21	123.30
2	B	122	THR	OG1-CB-CG2	9.42	131.66	110.00
2	D	134	ALA	O-C-N	-9.41	107.20	123.20
2	D	41	PHE	CD1-CE1-CZ	-9.40	108.81	120.10
2	B	114	ALA	C-N-CA	9.40	145.21	121.70
1	A	113	LEU	CB-CG-CD2	9.40	126.98	111.00
2	B	121	PHE	CA-C-N	9.39	137.87	117.20
2	B	56	ASN	CB-CG-ND2	9.39	139.23	116.70
2	D	115	ARG	N-CA-CB	-9.39	93.70	110.60
1	A	50	HIS	CA-C-O	-9.39	100.39	120.10
1	A	115	THR	N-CA-CB	9.39	128.14	110.30
2	B	118	GLY	CA-C-N	9.38	134.97	116.20
1	A	95	PRO	N-CD-CG	-9.38	89.13	103.20
2	D	29	ARG	CD-NE-CZ	-9.37	110.48	123.60
2	D	47	LEU	CA-C-N	-9.37	96.59	117.20
2	D	117	PHE	CG-CD2-CE2	9.36	131.10	120.80
1	A	87	HIS	CA-C-N	-9.35	96.63	117.20
1	C	83	LEU	CB-CG-CD2	-9.35	95.11	111.00
1	C	37	PRO	N-CA-CB	-9.35	92.08	103.30
1	A	34	LEU	CA-C-O	-9.34	100.48	120.10
2	B	98	ASN	CB-CG-ND2	9.34	139.12	116.70
2	B	34	TYR	CB-CG-CD1	9.33	126.60	121.00
1	C	101	LEU	CB-CA-C	9.33	127.92	110.20
1	A	32	MET	O-C-N	9.32	137.62	122.70
1	C	140	TYR	CD1-CE1-CZ	9.32	128.19	119.80
2	D	134	ALA	CB-CA-C	9.32	124.08	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	LEU	CA-C-O	-9.32	100.53	120.10
2	B	116	ASN	C-N-CA	9.32	144.99	121.70
1	A	64	ASN	O-C-N	-9.31	107.80	122.70
1	C	21	ALA	O-C-N	-9.31	103.41	121.10
2	D	109	LEU	CA-CB-CG	9.31	136.72	115.30
1	A	128	PHE	CA-C-O	9.30	139.64	120.10
2	D	46	ASN	CB-CA-C	9.30	129.01	110.40
1	C	28	ALA	CA-C-N	-9.29	96.76	117.20
1	C	50	HIS	O-C-N	9.29	138.99	123.20
1	C	7	LYS	CA-C-N	-9.28	96.78	117.20
2	D	93	ASN	CB-CA-C	-9.28	91.84	110.40
2	D	125	VAL	CA-C-N	9.27	137.60	117.20
2	D	93	ASN	CA-CB-CG	9.27	133.79	113.40
1	A	38	THR	CA-CB-OG1	-9.24	89.59	109.00
2	D	37	THR	C-N-CA	9.24	144.81	121.70
2	B	47	LEU	CB-CG-CD2	9.24	126.71	111.00
1	A	30	GLN	CB-CA-C	9.23	128.87	110.40
2	B	124	ASN	CB-CA-C	-9.23	91.94	110.40
2	D	42	GLN	CG-CD-NE2	-9.23	94.55	116.70
2	D	143	LYS	N-CA-CB	-9.23	93.99	110.60
2	B	143	LYS	N-CA-C	-9.22	86.09	111.00
1	C	14	TRP	CE2-CD2-CG	9.22	114.68	107.30
1	C	27	GLN	CG-CD-NE2	9.22	138.84	116.70
1	A	24	TYR	CG-CD2-CE2	9.22	128.68	121.30
1	C	93	VAL	CA-CB-CG2	9.22	124.73	110.90
2	D	121	PHE	CB-CG-CD2	-9.21	114.35	120.80
2	B	2	LEU	N-CA-CB	9.21	128.82	110.40
1	C	138	SER	CA-CB-OG	-9.21	86.34	111.20
1	C	140	TYR	CG-CD2-CE2	9.19	128.65	121.30
1	A	109	LEU	N-CA-CB	9.18	128.76	110.40
1	C	78	GLY	N-CA-C	-9.18	90.15	113.10
1	A	140	TYR	CD1-CG-CD2	9.18	127.99	117.90
2	B	120	GLN	CA-C-N	9.17	137.38	117.20
2	B	100	GLN	O-C-N	9.17	137.37	122.70
1	A	50	HIS	ND1-CE1-NE2	-9.17	89.73	109.90
1	C	83	LEU	O-C-N	9.16	137.36	122.70
1	A	111	SER	CA-C-O	-9.16	100.86	120.10
2	B	54	MET	N-CA-CB	-9.16	94.12	110.60
2	D	71	THR	N-CA-C	9.16	135.72	111.00
2	D	116	ASN	OD1-CG-ND2	9.15	142.95	121.90
1	C	129	LEU	CD1-CG-CD2	-9.15	83.06	110.50
1	A	50	HIS	CA-CB-CG	-9.15	98.05	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	MET	CG-SD-CE	-9.15	85.57	100.20
2	D	56	ASN	CA-C-N	9.15	142.71	117.10
1	A	40	LYS	CB-CA-C	-9.14	92.11	110.40
1	A	126	ASN	CA-C-N	-9.14	97.10	117.20
1	C	30	GLN	CB-CG-CD	-9.14	87.84	111.60
1	A	25	GLY	CA-C-O	9.13	137.04	120.60
2	D	29	ARG	CB-CG-CD	9.13	135.35	111.60
2	B	16	LYS	CA-C-N	9.13	137.28	117.20
1	A	49	SER	CA-CB-OG	9.13	135.84	111.20
2	D	132	VAL	O-C-N	9.13	137.30	122.70
2	B	50	ALA	N-CA-CB	9.13	122.88	110.10
1	C	65	ALA	CA-C-O	-9.12	100.94	120.10
2	D	97	VAL	CA-CB-CG1	9.12	124.58	110.90
1	A	87	HIS	CB-CG-CD2	-9.12	102.54	130.80
1	A	92	ARG	CG-CD-NE	-9.12	92.66	111.80
2	B	7	LYS	CA-C-N	-9.12	97.15	117.20
2	B	108	VAL	N-CA-CB	9.11	131.55	111.50
2	D	44	PHE	N-CA-C	9.11	135.59	111.00
2	D	108	VAL	C-N-CA	9.10	144.45	121.70
2	D	41	PHE	CD1-CG-CD2	9.10	130.13	118.30
1	A	87	HIS	CA-CB-CG	-9.10	98.14	113.60
2	B	5	GLU	OE1-CD-OE2	9.09	134.21	123.30
2	B	128	LEU	CB-CG-CD2	9.09	126.45	111.00
2	B	121	PHE	N-CA-C	-9.09	86.47	111.00
2	D	96	HIS	O-C-N	9.09	137.24	122.70
2	B	138	ASN	O-C-N	-9.08	108.17	122.70
2	B	24	ALA	CB-CA-C	9.07	123.71	110.10
1	C	80	LEU	N-CA-C	9.07	135.50	111.00
2	D	10	VAL	N-CA-CB	9.07	131.46	111.50
1	A	107	VAL	O-C-N	-9.07	108.19	122.70
2	D	114	ALA	CA-C-O	-9.07	101.06	120.10
1	A	94	ASN	CA-CB-CG	-9.07	93.45	113.40
2	B	41	PHE	CE1-CZ-CE2	-9.06	103.69	120.00
1	C	62	VAL	CB-CA-C	9.05	128.59	111.40
1	C	100	LEU	C-N-CA	-9.05	99.08	121.70
2	B	72	GLN	N-CA-CB	9.05	126.88	110.60
2	D	56	ASN	N-CA-CB	9.04	126.88	110.60
1	C	85	ASN	CB-CG-OD1	-9.04	103.52	121.60
1	C	20	ASN	CA-C-N	9.03	137.07	117.20
2	D	14	TRP	CA-CB-CG	-9.03	96.54	113.70
1	A	72	HIS	CG-CD2-NE2	-9.03	92.04	109.20
2	D	20	ASP	N-CA-CB	9.03	126.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	THR	N-CA-C	-9.03	86.63	111.00
2	B	34	TYR	CG-CD1-CE1	9.01	128.51	121.30
1	C	68	LYS	CB-CA-C	-9.01	92.38	110.40
2	D	85	ALA	N-CA-CB	-9.01	97.49	110.10
2	D	123	PRO	CA-C-N	-9.01	97.38	117.20
1	A	136	LEU	N-CA-C	9.00	135.31	111.00
1	C	116	ASN	O-C-N	9.00	137.10	122.70
2	D	134	ALA	N-CA-CB	9.00	122.70	110.10
2	D	58	LYS	C-N-CA	9.00	144.20	121.70
1	A	59	GLY	C-N-CA	9.00	144.19	121.70
1	C	140	TYR	CZ-CE2-CD2	8.99	127.89	119.80
2	D	36	TRP	N-CA-C	-8.99	86.72	111.00
1	C	107	VAL	N-CA-C	-8.99	86.72	111.00
1	C	28	ALA	CA-C-O	8.99	138.98	120.10
1	A	43	PHE	O-C-N	8.99	138.18	121.10
1	C	20	ASN	N-CA-C	-8.99	86.73	111.00
2	B	91	HIS	CA-CB-CG	-8.98	98.34	113.60
2	B	3	THR	O-C-N	-8.97	108.34	122.70
2	D	84	PHE	CD1-CG-CD2	8.97	129.97	118.30
2	D	82	GLY	CA-C-N	-8.97	97.46	117.20
2	B	140	LEU	CA-C-N	-8.97	97.47	117.20
2	D	131	LYS	CB-CA-C	-8.97	92.47	110.40
1	A	63	ALA	CA-C-N	8.96	136.92	117.20
2	B	43	HIS	CA-CB-CG	-8.96	98.36	113.60
2	B	139	ALA	O-C-N	-8.96	108.36	122.70
2	B	70	PHE	CB-CG-CD1	-8.96	114.53	120.80
1	C	128	PHE	CA-C-N	8.95	136.90	117.20
2	B	64	LYS	N-CA-C	-8.95	86.83	111.00
2	D	1	MET	C-N-CA	8.95	144.07	121.70
2	D	71	THR	OG1-CB-CG2	-8.94	89.43	110.00
1	C	108	THR	N-CA-C	-8.94	86.87	111.00
2	D	46	ASN	CA-CB-CG	8.93	133.05	113.40
2	D	77	LEU	CB-CA-C	8.93	127.17	110.20
1	A	116	ASN	CB-CA-C	8.93	128.26	110.40
1	A	27	GLN	OE1-CD-NE2	-8.93	101.36	121.90
1	A	66	LEU	CD1-CG-CD2	8.93	137.28	110.50
2	D	13	PHE	CA-CB-CG	8.93	135.32	113.90
1	C	108	THR	CA-C-O	-8.92	101.36	120.10
2	D	31	LEU	CB-CG-CD2	-8.92	95.83	111.00
1	C	117	PHE	O-C-N	8.92	136.97	122.70
1	C	140	TYR	N-CA-C	8.92	135.07	111.00
1	C	30	GLN	OE1-CD-NE2	8.91	142.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	28	GLY	CA-C-O	-8.90	104.57	120.60
1	A	99	LYS	CA-CB-CG	-8.90	93.82	113.40
1	A	72	HIS	C-N-CA	8.89	143.93	121.70
1	C	91	LEU	CB-CG-CD1	-8.89	95.89	111.00
1	C	11	LYS	CA-C-O	-8.89	101.44	120.10
2	B	5	GLU	O-C-N	-8.87	108.51	122.70
2	B	112	VAL	CG1-CB-CG2	8.86	125.08	110.90
1	C	100	LEU	N-CA-CB	8.86	128.12	110.40
1	A	97	ASN	CA-C-N	8.86	136.68	117.20
2	B	93	ASN	N-CA-C	8.85	134.89	111.00
2	D	38	GLN	CA-C-N	-8.84	97.75	117.20
1	C	140	TYR	CB-CG-CD2	-8.83	115.70	121.00
1	A	133	SER	CA-C-O	8.83	138.64	120.10
1	A	1	VAL	CA-C-N	8.83	136.62	117.20
2	D	110	ALA	CB-CA-C	-8.83	96.86	110.10
1	C	128	PHE	C-N-CA	8.82	143.76	121.70
1	A	57	ALA	N-CA-C	-8.82	87.18	111.00
1	A	113	LEU	CA-CB-CG	8.82	135.58	115.30
2	D	28	GLY	CA-C-N	8.82	136.60	117.20
2	D	110	ALA	C-N-CA	8.82	143.74	121.70
1	A	17	VAL	CA-CB-CG1	8.81	124.11	110.90
2	D	15	GLY	N-CA-C	-8.81	91.08	113.10
1	A	92	ARG	O-C-N	-8.80	108.61	122.70
1	C	42	TYR	N-CA-C	-8.80	87.23	111.00
2	D	101	ASN	O-C-N	8.80	136.78	122.70
1	C	103	HIS	CB-CG-ND1	-8.80	101.21	123.20
2	D	22	VAL	N-CA-CB	-8.80	92.14	111.50
1	C	90	LYS	O-C-N	8.79	136.77	122.70
2	D	85	ALA	C-N-CA	8.79	143.67	121.70
1	A	68	LYS	CA-C-O	8.78	138.55	120.10
2	B	26	ALA	CA-C-O	-8.78	101.66	120.10
2	B	50	ALA	CB-CA-C	8.78	123.27	110.10
2	B	29	ARG	CD-NE-CZ	-8.78	111.31	123.60
2	B	94	LYS	CB-CG-CD	-8.78	88.78	111.60
1	C	51	GLY	N-CA-C	-8.77	91.17	113.10
1	C	51	GLY	C-N-CA	-8.77	99.78	121.70
1	C	52	SER	N-CA-CB	8.77	123.65	110.50
2	D	80	LEU	CD1-CG-CD2	8.76	136.78	110.50
2	B	62	HIS	C-N-CA	8.75	140.67	122.30
1	A	58	HIS	C-N-CA	8.74	140.66	122.30
1	C	58	HIS	CA-C-N	8.74	133.68	116.20
2	D	34	TYR	N-CA-C	-8.73	87.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	74	LEU	C-N-CA	8.73	143.53	121.70
1	A	111	SER	CB-CA-C	-8.73	93.52	110.10
2	D	55	ASN	OD1-CG-ND2	-8.73	101.82	121.90
1	A	85	ASN	CB-CA-C	-8.71	92.97	110.40
1	A	6	ASN	O-C-N	8.71	136.64	122.70
1	A	77	PRO	CB-CA-C	8.71	133.78	112.00
1	A	99	LYS	O-C-N	-8.71	108.77	122.70
2	D	25	GLN	CA-CB-CG	-8.71	94.25	113.40
2	B	95	LEU	CD1-CG-CD2	-8.70	84.40	110.50
1	C	37	PRO	CA-N-CD	-8.70	99.32	111.50
2	D	47	LEU	CA-C-O	8.70	138.36	120.10
2	B	30	LEU	CA-C-N	-8.69	98.08	117.20
2	D	43	HIS	ND1-CE1-NE2	-8.69	90.78	109.90
1	A	14	TRP	CA-C-N	8.69	133.58	116.20
1	A	24	TYR	CD1-CE1-CZ	8.69	127.62	119.80
2	D	67	LEU	O-C-N	8.68	136.59	122.70
2	D	123	PRO	C-N-CA	8.68	143.40	121.70
2	B	111	LEU	C-N-CA	8.67	143.38	121.70
1	C	106	LEU	CA-C-N	8.67	136.28	117.20
2	D	77	LEU	CB-CG-CD1	-8.67	96.27	111.00
1	C	76	LEU	CA-C-O	-8.66	101.90	120.10
1	A	131	ASN	C-N-CA	8.66	143.35	121.70
2	B	144	TYR	CA-CB-CG	-8.66	96.94	113.40
2	D	1	MET	CB-CG-SD	-8.66	86.42	112.40
2	D	24	ALA	CA-C-N	8.66	136.25	117.20
2	D	41	PHE	CG-CD1-CE1	8.66	130.33	120.80
2	D	42	GLN	CB-CG-CD	-8.66	89.09	111.60
1	A	39	THR	CA-CB-CG2	8.65	124.51	112.40
1	C	137	THR	CA-C-O	-8.65	101.93	120.10
1	A	61	LYS	CD-CE-NZ	-8.64	91.82	111.70
2	B	83	ALA	CB-CA-C	8.64	123.07	110.10
2	B	7	LYS	O-C-N	8.64	136.53	122.70
1	C	67	THR	OG1-CB-CG2	-8.64	90.13	110.00
1	C	117	PHE	N-CA-CB	8.64	126.15	110.60
2	D	103	ARG	NH1-CZ-NH2	-8.64	109.90	119.40
1	A	112	HIS	ND1-CE1-NE2	-8.63	90.91	109.90
2	B	119	GLY	N-CA-C	8.62	134.65	113.10
2	B	81	LYS	C-N-CA	8.62	140.40	122.30
1	A	49	SER	CA-C-O	8.62	138.19	120.10
1	C	65	ALA	CA-C-N	8.61	136.15	117.20
2	D	124	ASN	CA-CB-CG	-8.61	94.46	113.40
2	B	72	GLN	CG-CD-OE1	-8.61	104.39	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	29	ARG	NH1-CZ-NH2	-8.60	109.94	119.40
2	D	100	GLN	CG-CD-OE1	-8.59	104.42	121.60
1	A	118	THR	N-CA-C	8.59	134.19	111.00
1	C	21	ALA	C-N-CD	8.59	146.44	128.40
2	D	34	TYR	N-CA-CB	-8.58	95.15	110.60
2	D	59	VAL	CB-CA-C	-8.58	95.09	111.40
2	D	14	TRP	CE3-CZ3-CH2	-8.58	111.76	121.20
1	A	107	VAL	N-CA-CB	8.57	130.35	111.50
1	A	76	LEU	N-CA-CB	-8.56	93.27	110.40
1	A	43	PHE	CZ-CE2-CD2	-8.56	109.83	120.10
1	C	40	LYS	N-CA-CB	8.56	126.01	110.60
2	B	35	PRO	CA-C-O	8.56	140.74	120.20
2	D	144	TYR	CB-CG-CD2	-8.56	115.86	121.00
2	B	138	ASN	CA-C-N	8.56	136.02	117.20
2	D	102	PHE	CA-C-N	8.55	136.01	117.20
1	A	70	GLN	CG-CD-NE2	8.55	137.22	116.70
1	A	80	LEU	CA-C-N	8.54	135.99	117.20
1	C	51	GLY	CA-C-N	-8.54	98.41	117.20
1	C	31	ARG	CD-NE-CZ	8.54	135.55	123.60
2	B	109	LEU	O-C-N	8.53	136.34	122.70
2	D	107	ASN	CB-CA-C	8.53	127.45	110.40
2	D	44	PHE	CB-CA-C	-8.52	93.35	110.40
1	C	37	PRO	CA-C-O	8.52	140.64	120.20
1	C	76	LEU	CB-CA-C	-8.51	94.03	110.20
1	A	47	ASP	CB-CA-C	-8.51	93.38	110.40
2	D	35	PRO	CA-CB-CG	-8.50	87.84	104.00
1	C	66	LEU	CB-CG-CD1	-8.50	96.55	111.00
2	D	142	HIS	CE1-NE2-CD2	8.50	127.84	106.60
2	B	36	TRP	CE3-CZ3-CH2	-8.49	111.86	121.20
1	A	1	VAL	CA-CB-CG2	-8.49	98.16	110.90
2	D	79	ASP	CB-CA-C	-8.49	93.42	110.40
2	B	98	ASN	C-N-CD	-8.48	101.93	120.60
2	B	13	PHE	CA-C-N	8.48	135.86	117.20
1	A	88	ALA	C-N-CA	8.48	142.90	121.70
2	B	115	ARG	C-N-CA	8.47	142.88	121.70
2	B	19	VAL	CA-CB-CG2	-8.47	98.19	110.90
2	B	107	ASN	CB-CG-ND2	-8.47	96.37	116.70
1	C	9	ASN	OD1-CG-ND2	-8.46	102.43	121.90
1	A	81	SER	N-CA-C	-8.46	88.15	111.00
1	C	3	SER	CA-CB-OG	-8.46	88.37	111.20
2	B	109	LEU	CB-CG-CD1	-8.45	96.63	111.00
2	D	40	PHE	O-C-N	8.45	136.22	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	LEU	CA-C-O	8.45	137.84	120.10
1	C	21	ALA	CB-CA-C	8.45	122.77	110.10
2	D	69	ALA	CB-CA-C	-8.44	97.44	110.10
1	C	9	ASN	CA-CB-CG	-8.44	94.84	113.40
2	B	25	GLN	C-N-CA	8.43	142.78	121.70
2	D	139	ALA	C-N-CA	8.43	142.76	121.70
2	B	81	LYS	N-CA-C	-8.42	88.26	111.00
1	C	71	GLY	N-CA-C	-8.42	92.05	113.10
2	B	22	VAL	CA-CB-CG1	8.42	123.53	110.90
1	C	121	VAL	CA-CB-CG2	-8.41	98.29	110.90
1	A	84	SER	CB-CA-C	-8.40	94.13	110.10
1	C	86	LEU	CD1-CG-CD2	-8.40	85.29	110.50
1	A	82	ASN	CB-CG-ND2	8.40	136.86	116.70
1	C	140	TYR	N-CA-CB	-8.40	95.48	110.60
2	B	48	SER	N-CA-CB	8.39	123.09	110.50
2	B	80	LEU	CD1-CG-CD2	-8.39	85.34	110.50
2	D	17	VAL	CG1-CB-CG2	8.38	124.31	110.90
1	C	138	SER	N-CA-CB	-8.38	97.93	110.50
2	D	102	PHE	CE1-CZ-CE2	8.38	135.07	120.00
2	B	93	ASN	CA-C-O	-8.37	102.52	120.10
1	C	134	THR	C-N-CA	8.37	142.62	121.70
2	D	85	ALA	O-C-N	-8.37	109.31	122.70
2	B	62	HIS	CE1-NE2-CD2	8.36	127.51	106.60
1	A	3	SER	C-N-CA	-8.36	100.81	121.70
1	C	98	PHE	CG-CD2-CE2	-8.36	111.61	120.80
1	C	139	LYS	CD-CE-NZ	-8.35	92.50	111.70
2	B	87	LEU	CA-CB-CG	8.35	134.49	115.30
2	B	96	HIS	CB-CG-ND1	-8.34	102.36	123.20
2	D	94	LYS	N-CA-C	8.34	133.51	111.00
1	A	97	ASN	N-CA-CB	8.34	125.60	110.60
2	B	140	LEU	CA-CB-CG	8.33	134.46	115.30
2	D	39	ARG	CA-C-N	-8.31	98.91	117.20
1	A	62	VAL	CA-C-O	-8.30	102.66	120.10
2	B	79	ASP	CB-CA-C	8.30	127.00	110.40
1	A	109	LEU	CB-CG-CD1	-8.30	96.89	111.00
2	B	56	ASN	CB-CG-OD1	-8.29	105.01	121.60
1	A	104	SER	CA-C-O	-8.29	102.69	120.10
2	D	96	HIS	CG-CD2-NE2	8.29	124.96	109.20
2	D	13	PHE	CG-CD1-CE1	8.29	129.91	120.80
1	A	20	ASN	CA-C-O	-8.28	102.71	120.10
2	D	42	GLN	CG-CD-OE1	8.28	138.16	121.60
2	B	1	MET	N-CA-C	-8.27	88.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ASN	OD1-CG-ND2	-8.27	102.88	121.90
2	B	77	LEU	N-CA-CB	-8.27	93.87	110.40
1	C	32	MET	CB-CG-SD	8.27	137.19	112.40
1	C	38	THR	CA-CB-CG2	8.26	123.97	112.40
1	C	42	TYR	CB-CG-CD2	8.26	125.95	121.00
2	B	96	HIS	CE1-NE2-CD2	-8.25	85.98	106.60
2	B	40	PHE	CG-CD1-CE1	8.25	129.87	120.80
2	B	106	GLY	N-CA-C	8.24	133.71	113.10
1	C	54	GLN	O-C-N	8.24	135.88	122.70
1	A	105	LEU	CD1-CG-CD2	-8.23	85.80	110.50
1	A	105	LEU	CB-CG-CD1	-8.23	97.01	111.00
2	B	145	HIS	CG-ND1-CE1	-8.23	95.00	105.70
2	D	97	VAL	CG1-CB-CG2	-8.22	97.75	110.90
2	B	36	TRP	O-C-N	8.21	135.84	122.70
2	D	98	ASN	CA-C-O	-8.21	102.85	120.10
2	B	139	ALA	CA-C-O	8.21	137.34	120.10
1	C	71	GLY	CA-C-O	8.21	135.37	120.60
2	D	98	ASN	C-N-CD	8.20	145.62	128.40
2	B	81	LYS	CA-C-O	-8.20	102.88	120.10
1	A	61	LYS	CA-C-O	-8.20	102.89	120.10
1	A	67	THR	N-CA-CB	8.20	125.87	110.30
2	B	122	THR	CA-CB-CG2	-8.20	100.93	112.40
1	A	126	ASN	CB-CG-ND2	8.19	136.36	116.70
1	C	56	LYS	N-CA-CB	8.19	125.34	110.60
2	D	81	LYS	CB-CA-C	8.18	126.76	110.40
1	A	64	ASN	N-CA-CB	8.18	125.31	110.60
1	C	95	PRO	CA-CB-CG	8.18	120.33	104.80
1	A	74	ASN	CB-CA-C	8.17	126.75	110.40
2	B	113	VAL	CA-C-N	8.17	135.17	117.20
1	C	65	ALA	CB-CA-C	8.17	122.35	110.10
2	B	129	PHE	CG-CD2-CE2	8.17	129.78	120.80
2	B	43	HIS	O-C-N	8.16	135.76	122.70
1	C	117	PHE	CB-CA-C	8.16	126.72	110.40
2	B	77	LEU	CA-C-N	-8.16	99.25	117.20
2	B	130	GLN	CB-CA-C	8.16	126.72	110.40
1	A	25	GLY	C-N-CA	-8.15	101.31	121.70
1	A	75	ASP	CB-CG-OD1	-8.15	110.96	118.30
2	B	144	TYR	OH-CZ-CE2	-8.14	98.12	120.10
1	C	97	ASN	CB-CA-C	-8.14	94.12	110.40
1	A	47	ASP	N-CA-C	-8.13	89.05	111.00
1	A	81	SER	N-CA-CB	8.12	122.68	110.50
1	C	46	PHE	O-C-N	-8.12	109.71	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	80	LEU	CA-CB-CG	8.12	133.97	115.30
2	D	103	ARG	CA-C-N	-8.12	99.35	117.20
1	A	60	GLN	CB-CA-C	8.10	126.61	110.40
1	A	76	LEU	CA-C-O	8.10	137.11	120.10
1	C	48	LEU	N-CA-C	-8.09	89.15	111.00
1	A	67	THR	O-C-N	8.09	135.64	122.70
2	B	43	HIS	CG-ND1-CE1	8.08	119.52	108.20
1	C	121	VAL	CA-C-N	8.08	134.97	117.20
2	D	85	ALA	CA-C-O	8.08	137.06	120.10
1	A	45	HIS	C-N-CA	8.07	141.88	121.70
1	A	117	PHE	CZ-CE2-CD2	8.07	129.78	120.10
1	C	68	LYS	CD-CE-NZ	-8.07	93.14	111.70
2	D	31	LEU	CA-C-N	8.06	134.93	117.20
2	B	52	ALA	N-CA-CB	-8.05	98.82	110.10
1	C	49	SER	C-N-CA	8.05	141.83	121.70
1	C	139	LYS	CG-CD-CE	8.05	136.05	111.90
2	D	63	GLY	N-CA-C	-8.05	92.98	113.10
1	C	17	VAL	N-CA-CB	8.05	129.20	111.50
1	C	61	LYS	C-N-CA	8.05	141.82	121.70
1	C	83	LEU	N-CA-C	8.03	132.69	111.00
2	D	41	PHE	CG-CD2-CE2	-8.03	111.97	120.80
2	B	96	HIS	C-N-CA	8.03	141.77	121.70
1	C	45	HIS	CA-C-O	8.02	136.95	120.10
1	A	5	ALA	N-CA-CB	-8.02	98.87	110.10
2	D	84	PHE	CE1-CZ-CE2	8.02	134.44	120.00
2	D	136	VAL	CA-CB-CG2	-8.02	98.87	110.90
1	C	53	ALA	N-CA-C	8.01	132.63	111.00
1	A	43	PHE	CG-CD2-CE2	-8.01	111.99	120.80
1	A	90	LYS	CA-C-O	-8.01	103.28	120.10
1	C	30	GLN	O-C-N	-8.01	109.89	122.70
1	C	40	LYS	CB-CA-C	-8.01	94.39	110.40
1	C	105	LEU	CB-CG-CD2	-8.01	97.39	111.00
1	C	86	LEU	CA-C-O	8.00	136.90	120.10
1	C	131	ASN	CA-CB-CG	-8.00	95.80	113.40
2	B	2	LEU	CB-CA-C	-8.00	95.01	110.20
1	A	17	VAL	N-CA-CB	7.99	129.09	111.50
1	A	103	HIS	ND1-CE1-NE2	-7.99	92.31	109.90
1	A	103	HIS	CB-CG-CD2	7.99	155.57	130.80
1	C	83	LEU	CA-C-O	-7.99	103.32	120.10
2	B	78	ASP	OD1-CG-OD2	-7.99	108.12	123.30
2	D	3	THR	CA-C-O	7.99	136.88	120.10
1	A	117	PHE	N-CA-C	7.99	132.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	LEU	O-C-N	-7.99	105.93	121.10
2	B	134	ALA	N-CA-CB	7.98	121.28	110.10
1	C	43	PHE	N-CA-C	7.98	132.56	111.00
1	C	47	ASP	CA-CB-CG	7.98	130.96	113.40
2	D	126	GLN	CG-CD-OE1	7.98	137.55	121.60
2	D	4	ALA	CB-CA-C	-7.97	98.14	110.10
2	D	117	PHE	CB-CG-CD1	-7.97	115.22	120.80
1	A	98	PHE	CB-CA-C	7.97	126.35	110.40
2	B	64	LYS	C-N-CA	7.96	141.60	121.70
1	C	107	VAL	CG1-CB-CG2	7.96	123.64	110.90
2	D	17	VAL	O-C-N	-7.96	109.96	122.70
1	C	126	ASN	CB-CG-OD1	7.96	137.51	121.60
2	B	43	HIS	ND1-CE1-NE2	-7.95	92.40	109.90
1	A	59	GLY	O-C-N	-7.95	109.98	122.70
1	C	124	ASN	CB-CA-C	7.95	126.30	110.40
2	B	34	TYR	C-N-CD	-7.95	103.12	120.60
2	D	78	ASP	N-CA-C	-7.95	89.55	111.00
1	A	5	ALA	C-N-CA	7.94	141.55	121.70
1	A	42	TYR	CB-CG-CD1	7.94	125.76	121.00
1	C	122	HIS	C-N-CA	7.94	141.55	121.70
1	A	124	ASN	CA-C-N	7.94	134.66	117.20
2	B	91	HIS	N-CA-CB	7.93	124.88	110.60
2	B	126	GLN	CA-CB-CG	7.93	130.85	113.40
1	A	117	PHE	CD1-CE1-CZ	-7.93	110.58	120.10
1	C	103	HIS	CA-C-N	7.93	134.64	117.20
2	D	47	LEU	CB-CA-C	7.92	125.26	110.20
2	D	74	LEU	CB-CA-C	7.92	125.25	110.20
2	B	51	GLY	N-CA-C	-7.92	93.30	113.10
2	B	40	PHE	C-N-CA	-7.91	101.91	121.70
2	D	142	HIS	CB-CG-ND1	7.91	142.98	123.20
1	A	140	TYR	CB-CA-C	7.91	126.22	110.40
1	A	37	PRO	CA-N-CD	-7.91	100.43	111.50
2	D	83	ALA	C-N-CA	-7.90	101.95	121.70
1	A	113	LEU	N-CA-CB	-7.89	94.61	110.40
1	A	56	LYS	C-N-CA	7.89	141.43	121.70
1	C	68	LYS	CA-CB-CG	-7.89	96.04	113.40
1	C	138	SER	C-N-CA	7.89	141.43	121.70
2	D	75	LYS	CA-C-N	7.89	134.55	117.20
1	C	128	PHE	N-CA-C	-7.89	89.71	111.00
2	D	60	LYS	C-N-CA	7.88	141.40	121.70
2	D	138	ASN	CA-CB-CG	7.88	130.73	113.40
2	B	16	LYS	CA-CB-CG	7.88	130.73	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	GLY	O-C-N	7.87	135.30	122.70
2	B	129	PHE	CA-C-O	7.87	136.63	120.10
2	B	62	HIS	O-C-N	-7.86	109.83	123.20
2	B	80	LEU	CA-C-O	7.86	136.61	120.10
2	B	86	GLN	CA-CB-CG	-7.86	96.10	113.40
1	C	84	SER	CA-CB-OG	-7.86	89.98	111.20
1	A	85	ASN	CB-CG-ND2	-7.86	97.84	116.70
1	A	95	PRO	CA-N-CD	-7.86	100.50	111.50
1	A	123	ALA	O-C-N	-7.86	110.13	122.70
1	A	76	LEU	CB-CA-C	7.85	125.12	110.20
1	C	77	PRO	C-N-CA	-7.85	105.81	122.30
1	A	65	ALA	CB-CA-C	-7.85	98.33	110.10
2	B	11	THR	OG1-CB-CG2	-7.84	91.96	110.00
2	B	29	ARG	CB-CG-CD	7.84	132.00	111.60
2	D	111	LEU	CB-CG-CD2	-7.84	97.66	111.00
1	C	67	THR	CA-CB-OG1	-7.84	92.54	109.00
1	A	124	ASN	OD1-CG-ND2	7.84	139.92	121.90
1	C	80	LEU	C-N-CA	7.84	141.29	121.70
2	D	116	ASN	CB-CG-OD1	-7.84	105.93	121.60
2	D	37	THR	N-CA-CB	-7.83	95.42	110.30
2	D	129	PHE	C-N-CA	7.81	141.23	121.70
2	B	120	GLN	N-CA-CB	7.81	124.66	110.60
2	B	108	VAL	CB-CA-C	-7.81	96.56	111.40
1	C	87	HIS	N-CA-C	-7.81	89.92	111.00
2	B	102	PHE	CA-C-O	7.80	136.48	120.10
2	D	78	ASP	O-C-N	7.80	135.18	122.70
2	D	144	TYR	CA-C-N	7.79	134.35	117.20
2	B	31	LEU	CB-CG-CD2	-7.79	97.76	111.00
2	B	138	ASN	CB-CG-OD1	-7.79	106.03	121.60
2	D	29	ARG	N-CA-CB	-7.78	96.59	110.60
1	C	121	VAL	N-CA-C	-7.78	90.00	111.00
2	D	125	VAL	N-CA-CB	-7.78	94.39	111.50
1	A	68	LYS	CD-CE-NZ	7.78	129.58	111.70
1	C	58	HIS	CG-CD2-NE2	-7.77	94.43	109.20
2	B	68	ASP	N-CA-CB	7.77	124.58	110.60
2	B	138	ASN	OD1-CG-ND2	7.77	139.76	121.90
2	D	112	VAL	N-CA-CB	7.76	128.58	111.50
1	A	109	LEU	CA-C-N	-7.76	100.12	117.20
1	C	59	GLY	N-CA-C	-7.76	93.70	113.10
2	D	80	LEU	CA-C-O	-7.76	103.80	120.10
2	D	119	GLY	C-N-CA	7.76	141.10	121.70
1	A	9	ASN	CB-CG-ND2	7.75	135.31	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ALA	O-C-N	7.75	135.10	122.70
1	C	101	LEU	CA-CB-CG	7.75	133.13	115.30
1	A	27	GLN	CA-C-O	-7.75	103.83	120.10
1	A	2	LEU	CA-C-N	-7.74	100.16	117.20
1	C	33	PHE	CG-CD2-CE2	-7.74	112.28	120.80
1	A	73	LEU	O-C-N	-7.74	110.31	122.70
1	A	134	THR	N-CA-C	-7.73	90.12	111.00
1	C	68	LYS	N-CA-CB	7.73	124.52	110.60
1	C	50	HIS	ND1-CG-CD2	-7.73	95.18	106.00
2	B	10	VAL	CA-CB-CG1	-7.73	99.31	110.90
2	B	87	LEU	C-N-CA	7.73	141.02	121.70
2	D	74	LEU	CB-CG-CD1	7.73	124.14	111.00
1	C	132	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	86	LEU	CB-CG-CD1	7.72	124.13	111.00
1	C	65	ALA	N-CA-CB	7.72	120.91	110.10
1	C	90	LYS	CB-CG-CD	7.72	131.67	111.60
2	D	114	ALA	O-C-N	-7.72	110.35	122.70
1	C	108	THR	CA-C-N	7.72	134.18	117.20
2	D	66	VAL	CA-C-N	-7.72	100.22	117.20
1	C	12	ALA	N-CA-CB	-7.71	99.30	110.10
1	A	61	LYS	N-CA-C	7.71	131.82	111.00
1	C	129	LEU	CB-CA-C	7.71	124.85	110.20
1	A	2	LEU	CD1-CG-CD2	-7.71	87.37	110.50
2	B	85	ALA	CA-C-N	7.71	134.16	117.20
2	B	77	LEU	CD1-CG-CD2	7.71	133.61	110.50
1	C	31	ARG	CB-CG-CD	-7.71	91.57	111.60
2	B	14	TRP	CB-CG-CD2	-7.70	116.59	126.60
1	C	43	PHE	CG-CD1-CE1	-7.70	112.33	120.80
1	C	86	LEU	CB-CG-CD2	7.70	124.09	111.00
1	A	138	SER	N-CA-C	-7.70	90.22	111.00
2	D	94	LYS	C-N-CA	-7.69	102.47	121.70
2	B	17	VAL	CB-CA-C	-7.69	96.79	111.40
2	B	87	LEU	CD1-CG-CD2	-7.69	87.43	110.50
2	B	117	PHE	CZ-CE2-CD2	7.69	129.33	120.10
2	D	46	ASN	CA-C-O	-7.69	103.95	120.10
2	D	141	ALA	CA-C-N	-7.69	100.28	117.20
1	A	118	THR	O-C-N	7.69	135.71	121.10
1	A	96	VAL	CB-CA-C	-7.69	96.80	111.40
1	C	114	PRO	O-C-N	7.68	134.99	122.70
2	D	101	ASN	N-CA-C	7.68	131.74	111.00
1	A	27	GLN	C-N-CA	7.67	140.88	121.70
1	C	85	ASN	CB-CA-C	-7.67	95.06	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASN	O-C-N	-7.67	110.43	122.70
2	B	121	PHE	CG-CD1-CE1	7.67	129.24	120.80
1	C	122	HIS	CG-CD2-NE2	7.67	123.77	109.20
2	B	96	HIS	ND1-CG-CD2	7.67	119.53	108.80
2	D	127	ALA	N-CA-C	-7.66	90.31	111.00
2	D	62	HIS	CG-ND1-CE1	-7.66	95.74	105.70
1	C	92	ARG	CG-CD-NE	-7.66	95.72	111.80
1	C	33	PHE	CB-CG-CD2	-7.65	115.44	120.80
1	C	61	LYS	N-CA-C	-7.65	90.34	111.00
2	D	114	ALA	C-N-CA	7.64	140.81	121.70
2	D	99	PRO	N-CD-CG	-7.64	91.74	103.20
2	D	20	ASP	OD1-CG-OD2	7.63	137.80	123.30
2	D	145	HIS	ND1-CE1-NE2	7.63	126.69	109.90
2	B	82	GLY	N-CA-C	-7.63	94.03	113.10
1	C	127	LYS	CD-CE-NZ	7.63	129.25	111.70
1	A	21	ALA	N-CA-C	-7.63	90.41	111.00
1	A	50	HIS	CG-CD2-NE2	-7.63	94.71	109.20
2	D	10	VAL	CG1-CB-CG2	7.63	123.10	110.90
2	D	73	GLY	CA-C-O	-7.62	106.87	120.60
2	B	30	LEU	N-CA-CB	7.62	125.65	110.40
1	A	121	VAL	CA-CB-CG1	7.62	122.33	110.90
1	C	128	PHE	CA-C-O	-7.62	104.09	120.10
2	B	19	VAL	CA-C-N	7.62	133.96	117.20
1	C	125	LEU	N-CA-CB	7.62	125.63	110.40
1	C	24	TYR	CE1-CZ-OH	7.61	140.66	120.10
2	B	75	LYS	CG-CD-CE	-7.61	89.07	111.90
1	C	23	ALA	N-CA-C	7.61	131.54	111.00
2	D	24	ALA	CA-C-O	-7.61	104.12	120.10
2	B	4	ALA	N-CA-CB	7.60	120.75	110.10
2	B	33	VAL	N-CA-CB	7.60	128.22	111.50
2	D	57	PRO	CA-C-N	7.60	133.92	117.20
2	D	55	ASN	CA-C-N	7.60	133.91	117.20
2	B	3	THR	N-CA-CB	-7.59	95.87	110.30
2	B	48	SER	CA-CB-OG	-7.59	90.70	111.20
2	B	84	PHE	CA-C-N	7.59	133.90	117.20
1	A	68	LYS	CA-C-N	-7.59	100.51	117.20
2	D	37	THR	CB-CA-C	7.59	132.08	111.60
2	B	44	PHE	CG-CD1-CE1	-7.58	112.46	120.80
2	B	33	VAL	N-CA-C	-7.58	90.53	111.00
2	D	53	VAL	O-C-N	-7.58	110.57	122.70
1	A	99	LYS	CA-C-N	7.58	133.87	117.20
2	B	8	ALA	CB-CA-C	7.58	121.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LEU	O-C-N	-7.58	110.58	122.70
1	A	95	PRO	CA-CB-CG	-7.57	89.62	104.00
1	A	20	ASN	OD1-CG-ND2	-7.56	104.50	121.90
2	B	2	LEU	CB-CG-CD2	7.56	123.86	111.00
2	D	29	ARG	C-N-CA	7.56	140.61	121.70
2	D	103	ARG	N-CA-C	7.56	131.41	111.00
2	B	77	LEU	CB-CG-CD2	7.56	123.85	111.00
2	D	124	ASN	O-C-N	7.56	134.80	122.70
1	C	82	ASN	CA-CB-CG	-7.56	96.78	113.40
2	D	42	GLN	CB-CA-C	-7.56	95.28	110.40
1	A	3	SER	O-C-N	-7.55	110.61	122.70
2	B	104	LEU	CA-C-O	-7.55	104.25	120.10
1	A	45	HIS	CB-CA-C	-7.55	95.30	110.40
1	A	127	LYS	CA-C-N	7.55	133.81	117.20
1	C	22	PRO	CB-CG-CD	-7.55	77.06	106.50
2	D	10	VAL	CA-CB-CG1	7.54	122.22	110.90
1	A	86	LEU	O-C-N	7.54	134.77	122.70
2	B	125	VAL	CA-C-O	-7.54	104.26	120.10
2	B	25	GLN	CG-CD-OE1	7.54	136.68	121.60
1	A	8	SER	N-CA-C	-7.53	90.66	111.00
2	D	9	ALA	C-N-CA	7.53	140.53	121.70
1	C	31	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	C	53	ALA	O-C-N	-7.53	110.66	122.70
1	C	45	HIS	CG-CD2-NE2	-7.53	94.90	109.20
1	C	17	VAL	CA-CB-CG1	7.52	122.18	110.90
2	B	102	PHE	CA-C-N	7.52	133.74	117.20
1	A	52	SER	CA-CB-OG	-7.52	90.91	111.20
1	A	11	LYS	CA-CB-CG	-7.51	96.88	113.40
1	C	11	LYS	CG-CD-CE	7.51	134.43	111.90
2	D	22	VAL	CA-CB-CG1	7.50	122.15	110.90
2	D	90	LEU	CA-C-O	-7.50	104.35	120.10
1	A	62	VAL	C-N-CA	7.50	140.44	121.70
2	B	126	GLN	C-N-CA	7.50	140.45	121.70
2	D	96	HIS	CE1-NE2-CD2	-7.50	87.86	106.60
2	B	67	LEU	CB-CA-C	-7.49	95.97	110.20
1	C	115	THR	CA-C-O	-7.49	104.38	120.10
1	C	135	VAL	C-N-CA	7.48	140.41	121.70
1	A	128	PHE	CA-CB-CG	7.48	131.86	113.90
2	D	104	LEU	CA-C-N	7.48	133.66	117.20
2	D	124	ASN	CB-CA-C	-7.48	95.44	110.40
1	C	48	LEU	CA-CB-CG	7.48	132.50	115.30
1	A	3	SER	CA-C-O	7.47	135.80	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	VAL	CB-CA-C	-7.47	97.20	111.40
2	D	100	GLN	N-CA-C	-7.47	90.82	111.00
2	D	107	ASN	N-CA-C	-7.47	90.82	111.00
2	D	123	PRO	CB-CG-CD	7.47	135.65	106.50
1	A	52	SER	N-CA-C	7.47	131.17	111.00
1	A	125	LEU	N-CA-C	7.47	131.17	111.00
1	C	99	LYS	CD-CE-NZ	7.47	128.88	111.70
1	A	124	ASN	CB-CA-C	7.47	125.33	110.40
2	D	110	ALA	N-CA-C	-7.47	90.84	111.00
2	D	126	GLN	CG-CD-NE2	7.47	134.62	116.70
2	B	76	HIS	CA-C-O	-7.46	104.43	120.10
2	D	35	PRO	CB-CA-C	7.46	130.65	112.00
2	D	58	LYS	CD-CE-NZ	7.46	128.86	111.70
2	D	100	GLN	CA-C-N	-7.46	100.78	117.20
1	C	72	HIS	ND1-CE1-NE2	7.46	126.31	109.90
1	C	122	HIS	CA-C-N	7.45	133.60	117.20
2	B	128	LEU	C-N-CA	7.45	140.32	121.70
1	C	97	ASN	N-CA-CB	7.45	124.01	110.60
1	A	84	SER	CA-C-O	7.45	135.74	120.10
2	B	17	VAL	N-CA-CB	7.45	127.88	111.50
2	D	30	LEU	CD1-CG-CD2	7.44	132.83	110.50
2	B	72	GLN	OE1-CD-NE2	7.44	139.02	121.90
2	B	121	PHE	CD1-CE1-CZ	7.44	129.02	120.10
1	C	23	ALA	CA-C-O	-7.44	104.48	120.10
1	A	44	PRO	CB-CA-C	7.44	130.59	112.00
2	D	83	ALA	CB-CA-C	-7.44	98.94	110.10
1	C	73	LEU	O-C-N	-7.43	110.80	122.70
1	C	130	ALA	C-N-CA	7.43	140.28	121.70
2	D	46	ASN	CA-C-N	7.43	133.55	117.20
1	A	57	ALA	CA-C-O	-7.42	104.51	120.10
1	A	138	SER	O-C-N	7.42	134.57	122.70
2	D	62	HIS	C-N-CA	7.42	137.88	122.30
2	D	112	VAL	C-N-CA	7.42	140.25	121.70
2	D	95	LEU	CB-CG-CD2	-7.42	98.39	111.00
1	A	45	HIS	CA-C-O	-7.42	104.53	120.10
2	B	93	ASN	CB-CG-OD1	7.42	136.43	121.60
2	D	63	GLY	C-N-CA	7.42	140.24	121.70
1	C	43	PHE	CD1-CE1-CZ	-7.42	111.20	120.10
1	A	42	TYR	CE1-CZ-OH	7.41	140.11	120.10
2	B	66	VAL	N-CA-CB	7.41	127.80	111.50
2	D	4	ALA	CA-C-N	-7.41	100.90	117.20
2	D	75	LYS	CA-C-O	-7.41	104.55	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ALA	N-CA-C	7.40	130.98	111.00
1	A	92	ARG	CA-C-O	7.40	135.64	120.10
1	A	69	ALA	N-CA-CB	7.40	120.45	110.10
2	B	117	PHE	CG-CD2-CE2	-7.40	112.66	120.80
2	D	39	ARG	O-C-N	7.39	134.52	122.70
2	B	25	GLN	CA-C-O	-7.39	104.59	120.10
2	D	98	ASN	N-CA-C	7.39	130.95	111.00
1	C	69	ALA	O-C-N	-7.39	110.88	122.70
1	A	46	PHE	CA-CB-CG	7.38	131.62	113.90
1	A	24	TYR	N-CA-C	-7.38	91.07	111.00
2	D	75	LYS	CA-CB-CG	7.38	129.64	113.40
1	C	64	ASN	CB-CG-ND2	-7.38	98.98	116.70
2	D	16	LYS	CA-C-O	-7.38	104.60	120.10
1	A	122	HIS	CG-ND1-CE1	7.38	118.53	108.20
2	B	67	LEU	CA-CB-CG	7.38	132.27	115.30
1	C	27	GLN	C-N-CA	-7.38	103.26	121.70
1	C	65	ALA	N-CA-C	-7.38	91.08	111.00
1	A	86	LEU	CA-CB-CG	7.38	132.26	115.30
2	D	137	ALA	CA-C-O	7.38	135.59	120.10
2	B	54	MET	N-CA-C	7.37	130.91	111.00
2	D	38	GLN	C-N-CA	-7.37	103.27	121.70
2	B	77	LEU	N-CA-C	7.37	130.90	111.00
1	A	54	GLN	CA-C-O	7.36	135.56	120.10
2	D	105	LEU	N-CA-C	-7.36	91.12	111.00
1	A	68	LYS	N-CA-CB	-7.36	97.35	110.60
2	B	93	ASN	CA-C-N	7.36	133.40	117.20
1	A	43	PHE	N-CA-C	7.36	130.88	111.00
2	D	46	ASN	CB-CG-ND2	7.36	134.37	116.70
2	B	64	LYS	CG-CD-CE	-7.36	89.82	111.90
1	C	44	PRO	N-CD-CG	7.36	114.24	103.20
1	C	41	THR	C-N-CA	7.36	140.09	121.70
1	A	9	ASN	CA-C-O	-7.35	104.67	120.10
1	C	74	ASN	C-N-CA	7.35	140.07	121.70
2	D	87	LEU	O-C-N	-7.35	110.94	122.70
1	A	80	LEU	CA-CB-CG	-7.34	98.41	115.30
2	B	6	GLU	CB-CG-CD	7.34	134.02	114.20
1	A	77	PRO	N-CA-C	-7.34	93.02	112.10
2	B	128	LEU	O-C-N	7.34	134.44	122.70
1	C	116	ASN	C-N-CA	7.34	140.05	121.70
2	D	86	GLN	CA-C-O	-7.34	104.69	120.10
1	A	40	LYS	C-N-CA	7.34	140.04	121.70
2	D	41	PHE	CA-C-N	7.34	133.34	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	LEU	CA-C-O	7.34	135.51	120.10
1	C	76	LEU	C-N-CD	7.34	143.81	128.40
1	A	85	ASN	OD1-CG-ND2	7.33	138.76	121.90
2	B	16	LYS	CD-CE-NZ	7.33	128.56	111.70
2	D	47	LEU	CB-CG-CD1	-7.33	98.55	111.00
2	D	18	ASP	N-CA-C	7.32	130.78	111.00
1	A	109	LEU	CB-CG-CD2	7.32	123.44	111.00
1	C	96	VAL	CB-CA-C	7.32	125.31	111.40
2	B	24	ALA	CA-C-O	7.32	135.47	120.10
2	D	84	PHE	CB-CA-C	-7.31	95.77	110.40
2	B	122	THR	CA-C-N	7.31	137.57	117.10
1	C	131	ASN	CA-C-N	7.31	133.28	117.20
1	A	56	LYS	CA-CB-CG	7.31	129.48	113.40
2	B	25	GLN	CG-CD-NE2	-7.30	99.18	116.70
1	C	13	ALA	C-N-CA	7.30	139.95	121.70
1	A	112	HIS	CB-CG-ND1	-7.30	104.95	123.20
2	D	36	TRP	CG-CD2-CE3	-7.30	127.33	133.90
1	A	33	PHE	CB-CA-C	7.29	124.99	110.40
2	B	36	TRP	CG-CD1-NE1	7.29	117.39	110.10
2	D	73	GLY	N-CA-C	-7.29	94.88	113.10
2	B	43	HIS	CA-C-O	-7.28	104.81	120.10
2	D	3	THR	O-C-N	7.28	134.35	122.70
2	B	65	ARG	CD-NE-CZ	-7.28	113.41	123.60
1	A	89	HIS	CB-CG-ND1	-7.28	105.00	123.20
2	B	118	GLY	O-C-N	7.28	135.57	123.20
1	A	36	PHE	CA-C-O	7.28	135.38	120.10
1	A	42	TYR	N-CA-CB	7.28	123.70	110.60
1	A	103	HIS	O-C-N	-7.27	111.06	122.70
2	B	85	ALA	O-C-N	-7.27	111.06	122.70
2	B	50	ALA	CA-C-N	7.27	130.74	116.20
1	A	2	LEU	CA-CB-CG	-7.27	98.58	115.30
2	D	122	THR	N-CA-C	7.27	130.62	111.00
2	B	58	LYS	CD-CE-NZ	-7.26	95.00	111.70
1	C	52	SER	O-C-N	7.26	134.32	122.70
2	B	36	TRP	CE2-CD2-CE3	7.26	127.41	118.70
2	D	141	ALA	CB-CA-C	7.26	120.98	110.10
2	B	143	LYS	O-C-N	-7.25	111.09	122.70
1	C	38	THR	OG1-CB-CG2	-7.25	93.32	110.00
1	C	97	ASN	CB-CG-OD1	-7.25	107.09	121.60
2	B	141	ALA	O-C-N	-7.24	111.12	122.70
1	C	11	LYS	CB-CA-C	7.24	124.88	110.40
2	D	119	GLY	N-CA-C	-7.24	95.00	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	SER	C-N-CA	7.24	139.79	121.70
2	B	83	ALA	N-CA-C	-7.23	91.47	111.00
1	C	41	THR	CB-CA-C	7.23	131.12	111.60
2	D	22	VAL	C-N-CA	7.23	137.48	122.30
1	C	75	ASP	CA-C-N	-7.23	101.30	117.20
2	D	84	PHE	CD1-CE1-CZ	-7.23	111.43	120.10
1	C	103	HIS	O-C-N	-7.23	111.14	122.70
2	D	74	LEU	CB-CG-CD2	-7.22	98.72	111.00
2	B	34	TYR	OH-CZ-CE2	-7.22	100.61	120.10
2	B	118	GLY	N-CA-C	7.21	131.14	113.10
1	C	85	ASN	CB-CG-ND2	7.21	134.01	116.70
2	D	5	GLU	CA-CB-CG	7.21	129.27	113.40
1	C	54	GLN	CG-CD-OE1	-7.21	107.18	121.60
1	C	18	GLY	C-N-CA	7.21	137.44	122.30
2	D	112	VAL	CG1-CB-CG2	7.20	122.41	110.90
1	A	114	PRO	N-CA-CB	-7.19	94.67	103.30
1	C	44	PRO	N-CA-CB	7.19	111.92	103.30
2	D	94	LYS	CA-C-N	7.19	133.01	117.20
2	D	101	ASN	N-CA-CB	7.18	123.53	110.60
1	C	115	THR	N-CA-C	-7.18	91.61	111.00
2	B	20	ASP	OD1-CG-OD2	7.18	136.94	123.30
2	D	94	LYS	O-C-N	7.18	134.19	122.70
1	C	36	PHE	CA-C-N	-7.18	97.00	117.10
1	A	31	ARG	O-C-N	-7.17	111.22	122.70
2	B	50	ALA	N-CA-C	-7.17	91.64	111.00
2	B	71	THR	CA-CB-CG2	-7.17	102.36	112.40
2	B	60	LYS	C-N-CA	7.17	139.62	121.70
1	A	71	GLY	O-C-N	-7.15	111.26	122.70
2	B	143	LYS	CA-C-O	-7.15	105.08	120.10
2	B	69	ALA	CA-C-N	-7.15	101.48	117.20
1	A	62	VAL	N-CA-CB	7.14	127.21	111.50
1	A	6	ASN	C-N-CA	7.14	139.54	121.70
2	B	110	ALA	CA-C-O	7.13	135.08	120.10
1	C	6	ASN	CB-CG-OD1	7.13	135.86	121.60
1	C	8	SER	CA-C-O	7.13	135.07	120.10
2	D	7	LYS	CG-CD-CE	7.13	133.28	111.90
2	B	47	LEU	CB-CG-CD1	-7.12	98.89	111.00
2	D	82	GLY	N-CA-C	-7.12	95.29	113.10
1	A	119	PRO	CB-CG-CD	7.12	134.27	106.50
1	A	18	GLY	O-C-N	-7.12	111.10	123.20
2	B	34	TYR	CA-C-O	-7.12	105.16	120.10
2	D	105	LEU	CA-CB-CG	-7.11	98.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	THR	CB-CA-C	7.11	130.78	111.60
2	B	113	VAL	C-N-CA	7.10	139.45	121.70
2	D	105	LEU	CA-C-O	-7.10	105.19	120.10
1	A	66	LEU	CA-C-O	7.10	135.00	120.10
2	B	31	LEU	CB-CA-C	7.10	123.69	110.20
2	D	117	PHE	O-C-N	-7.10	111.13	123.20
1	A	83	LEU	CB-CG-CD1	-7.09	98.94	111.00
1	A	27	GLN	N-CA-C	-7.09	91.85	111.00
1	A	35	SER	O-C-N	-7.09	111.35	122.70
2	B	27	LEU	C-N-CA	7.09	137.18	122.30
1	A	89	HIS	N-CA-C	-7.08	91.89	111.00
1	C	20	ASN	N-CA-CB	7.08	123.34	110.60
1	A	60	GLN	OE1-CD-NE2	-7.08	105.62	121.90
2	B	114	ALA	CA-C-O	7.07	134.95	120.10
1	C	131	ASN	OD1-CG-ND2	7.07	138.15	121.90
1	A	90	LYS	CA-C-N	7.06	132.73	117.20
1	A	33	PHE	CA-C-O	7.06	134.92	120.10
2	D	103	ARG	CG-CD-NE	-7.06	96.98	111.80
1	A	29	LEU	N-CA-CB	-7.05	96.29	110.40
1	C	76	LEU	O-C-N	7.05	134.50	121.10
1	A	87	HIS	N-CA-C	7.05	130.04	111.00
2	D	30	LEU	CA-C-O	7.04	134.89	120.10
2	D	102	PHE	O-C-N	7.04	133.97	122.70
2	B	103	ARG	NH1-CZ-NH2	7.04	127.14	119.40
1	C	63	ALA	CB-CA-C	-7.04	99.55	110.10
2	B	127	ALA	O-C-N	7.03	133.94	122.70
2	B	95	LEU	O-C-N	-7.02	111.46	122.70
2	D	6	GLU	CG-CD-OE2	-7.01	104.27	118.30
1	C	64	ASN	N-CA-C	7.01	129.92	111.00
1	C	124	ASN	C-N-CA	7.01	139.22	121.70
1	A	63	ALA	N-CA-CB	7.01	119.91	110.10
2	D	70	PHE	N-CA-CB	-7.01	97.99	110.60
2	D	38	GLN	CG-CD-OE1	-7.00	107.59	121.60
2	B	116	ASN	CB-CG-ND2	7.00	133.49	116.70
1	C	9	ASN	CB-CG-ND2	6.99	133.48	116.70
1	C	102	SER	CA-CB-OG	-6.99	92.32	111.20
1	C	125	LEU	C-N-CA	6.99	139.18	121.70
2	B	60	LYS	O-C-N	-6.99	111.52	122.70
1	C	29	LEU	CA-C-N	6.99	132.57	117.20
1	A	14	TRP	CD1-CG-CD2	-6.98	100.71	106.30
1	A	123	ALA	CA-C-O	6.98	134.77	120.10
2	B	6	GLU	C-N-CA	6.98	139.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	PHE	CD1-CG-CD2	-6.98	109.22	118.30
2	D	117	PHE	CB-CA-C	6.98	124.36	110.40
1	A	107	VAL	CB-CA-C	6.98	124.66	111.40
1	C	112	HIS	CA-C-N	6.98	132.56	117.20
2	D	78	ASP	CB-CA-C	6.98	124.36	110.40
1	A	48	LEU	C-N-CA	6.98	139.14	121.70
2	B	128	LEU	N-CA-CB	-6.97	96.45	110.40
1	C	112	HIS	CB-CA-C	6.97	124.35	110.40
1	A	41	THR	CB-CA-C	-6.97	92.78	111.60
1	C	43	PHE	CG-CD2-CE2	-6.96	113.14	120.80
1	C	106	LEU	O-C-N	-6.96	111.56	122.70
2	D	32	VAL	CA-CB-CG2	6.96	121.33	110.90
2	D	80	LEU	C-N-CA	-6.96	104.31	121.70
1	A	75	ASP	O-C-N	6.95	133.82	122.70
2	B	6	GLU	CG-CD-OE2	-6.95	104.39	118.30
2	D	109	LEU	C-N-CA	6.95	139.08	121.70
1	A	76	LEU	CB-CG-CD2	-6.95	99.19	111.00
2	B	142	HIS	CE1-NE2-CD2	6.95	123.96	106.60
2	D	19	VAL	N-CA-CB	6.94	126.77	111.50
1	C	93	VAL	C-N-CA	6.94	139.05	121.70
2	B	26	ALA	CB-CA-C	6.94	120.51	110.10
1	C	43	PHE	CA-C-N	-6.93	97.69	117.10
2	B	132	VAL	CA-C-N	6.93	132.45	117.20
1	A	45	HIS	ND1-CG-CD2	-6.93	96.30	106.00
2	B	129	PHE	O-C-N	-6.93	111.61	122.70
2	D	131	LYS	CG-CD-CE	-6.93	91.11	111.90
1	C	74	ASN	OD1-CG-ND2	-6.93	105.97	121.90
2	D	25	GLN	CB-CA-C	-6.93	96.54	110.40
1	C	41	THR	CA-C-N	6.92	132.43	117.20
2	D	30	LEU	CB-CG-CD2	-6.92	99.24	111.00
2	B	78	ASP	O-C-N	-6.91	111.64	122.70
2	D	140	LEU	CA-C-N	6.91	132.40	117.20
1	C	16	LYS	CB-CA-C	6.91	124.21	110.40
1	C	48	LEU	N-CA-CB	6.90	124.20	110.40
1	A	84	SER	N-CA-CB	6.90	120.85	110.50
2	B	74	LEU	N-CA-C	6.90	129.63	111.00
1	C	10	VAL	CA-C-N	-6.90	102.02	117.20
2	B	95	LEU	N-CA-C	-6.90	92.37	111.00
1	C	103	HIS	N-CA-CB	-6.90	98.18	110.60
2	D	16	LYS	CA-CB-CG	-6.89	98.24	113.40
2	B	109	LEU	C-N-CA	-6.89	104.48	121.70
1	A	48	LEU	N-CA-CB	6.89	124.18	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	LEU	C-N-CA	-6.88	104.50	121.70
2	B	99	PRO	CA-C-N	-6.88	102.06	117.20
2	D	133	VAL	CB-CA-C	6.88	124.47	111.40
2	D	58	LYS	CG-CD-CE	6.88	132.53	111.90
2	B	22	VAL	N-CA-CB	6.88	126.63	111.50
1	C	53	ALA	CA-C-O	6.88	134.54	120.10
1	C	127	LYS	N-CA-CB	6.87	122.97	110.60
2	B	78	ASP	CA-C-N	-6.86	102.10	117.20
1	C	76	LEU	N-CA-CB	6.86	124.12	110.40
1	A	6	ASN	N-CA-CB	6.86	122.94	110.60
2	B	104	LEU	O-C-N	6.86	133.67	122.70
1	C	7	LYS	CB-CG-CD	6.85	129.41	111.60
2	D	36	TRP	CD1-NE1-CE2	-6.85	102.83	109.00
2	B	136	VAL	C-N-CA	6.85	138.83	121.70
2	D	95	LEU	C-N-CA	6.85	138.82	121.70
2	B	83	ALA	CA-C-N	6.85	132.26	117.20
1	C	50	HIS	C-N-CA	-6.84	107.93	122.30
1	A	127	LYS	CA-CB-CG	6.84	128.45	113.40
1	C	129	LEU	CB-CG-CD2	-6.84	99.37	111.00
2	D	14	TRP	NE1-CE2-CZ2	-6.84	122.88	130.40
2	D	36	TRP	CE3-CZ3-CH2	6.84	128.72	121.20
1	C	31	ARG	CA-C-O	-6.83	105.75	120.10
1	C	67	THR	C-N-CA	6.83	138.78	121.70
2	D	145	HIS	CG-ND1-CE1	-6.83	96.82	105.70
1	C	38	THR	C-N-CA	6.83	138.77	121.70
2	B	71	THR	OG1-CB-CG2	6.83	125.70	110.00
1	C	111	SER	CA-C-O	6.82	134.43	120.10
2	D	104	LEU	CA-CB-CG	-6.82	99.61	115.30
1	C	103	HIS	ND1-CG-CD2	6.82	118.34	108.80
2	B	124	ASN	C-N-CA	-6.81	104.67	121.70
1	C	31	ARG	CG-CD-NE	6.81	126.10	111.80
2	B	22	VAL	CA-CB-CG2	6.81	121.11	110.90
1	C	39	THR	CA-C-N	-6.81	102.22	117.20
2	D	50	ALA	N-CA-C	-6.81	92.62	111.00
1	C	51	GLY	CA-C-O	6.81	132.85	120.60
1	C	14	TRP	NE1-CE2-CZ2	6.81	137.89	130.40
2	D	72	GLN	CA-CB-CG	6.80	128.36	113.40
1	C	56	LYS	C-N-CA	6.80	138.70	121.70
1	C	54	GLN	CB-CG-CD	6.80	129.27	111.60
2	B	59	VAL	N-CA-C	-6.79	92.66	111.00
1	A	30	GLN	CA-C-O	6.79	134.36	120.10
1	A	5	ALA	CB-CA-C	6.79	120.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	LEU	N-CA-CB	6.78	123.96	110.40
2	B	33	VAL	C-N-CA	6.77	138.63	121.70
1	C	73	LEU	N-CA-CB	6.77	123.95	110.40
1	C	81	SER	N-CA-CB	-6.77	100.34	110.50
1	C	137	THR	C-N-CA	6.77	138.63	121.70
2	B	57	PRO	CB-CG-CD	-6.77	80.10	106.50
2	B	71	THR	N-CA-CB	-6.77	97.44	110.30
2	B	31	LEU	N-CA-CB	6.76	123.93	110.40
1	A	3	SER	CB-CA-C	-6.76	97.25	110.10
1	A	12	ALA	CB-CA-C	-6.76	99.96	110.10
1	A	14	TRP	NE1-CE2-CD2	6.76	114.06	107.30
1	C	97	ASN	CA-C-O	6.76	134.30	120.10
1	C	105	LEU	N-CA-CB	-6.76	96.88	110.40
2	B	7	LYS	CD-CE-NZ	-6.76	96.15	111.70
1	A	122	HIS	CG-CD2-NE2	-6.76	96.36	109.20
1	A	43	PHE	CA-C-O	6.75	134.28	120.10
2	B	72	GLN	CA-C-N	6.75	129.70	116.20
1	A	79	THR	CA-C-O	6.75	134.28	120.10
1	A	4	ALA	N-CA-CB	-6.75	100.66	110.10
1	A	36	PHE	O-C-N	-6.75	108.28	121.10
1	C	121	VAL	C-N-CA	-6.74	104.84	121.70
1	A	4	ALA	CB-CA-C	6.74	120.21	110.10
2	B	128	LEU	CA-C-N	6.74	132.03	117.20
1	A	70	GLN	CG-CD-OE1	6.74	135.07	121.60
2	B	127	ALA	CB-CA-C	-6.74	99.99	110.10
2	D	6	GLU	CA-C-O	-6.73	105.96	120.10
1	C	141	ARG	CA-C-O	-6.73	105.96	120.10
2	B	72	GLN	C-N-CA	6.73	136.43	122.30
1	A	110	ALA	C-N-CA	6.72	138.50	121.70
1	C	27	GLN	OE1-CD-NE2	-6.72	106.45	121.90
2	B	16	LYS	CB-CG-CD	6.71	129.06	111.60
2	B	55	ASN	CB-CG-OD1	-6.71	108.17	121.60
1	C	27	GLN	CA-C-N	-6.71	102.43	117.20
1	C	35	SER	CB-CA-C	6.71	122.86	110.10
1	A	88	ALA	CB-CA-C	6.71	120.16	110.10
1	A	126	ASN	CB-CA-C	-6.71	96.99	110.40
2	B	126	GLN	CB-CG-CD	-6.71	94.17	111.60
1	A	125	LEU	CA-CB-CG	6.70	130.72	115.30
2	D	31	LEU	CA-CB-CG	-6.70	99.88	115.30
1	C	105	LEU	CA-C-N	6.70	131.94	117.20
2	D	36	TRP	CD2-CE2-CZ2	-6.70	114.26	122.30
2	B	42	GLN	CG-CD-OE1	-6.69	108.21	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	SER	CA-C-N	-6.68	102.50	117.20
1	A	78	GLY	CA-C-N	6.68	131.89	117.20
2	D	73	GLY	O-C-N	-6.67	112.02	122.70
1	A	113	LEU	C-N-CD	6.67	142.41	128.40
1	C	118	THR	CA-CB-OG1	6.67	123.01	109.00
2	B	102	PHE	CB-CA-C	6.67	123.74	110.40
2	D	10	VAL	CA-C-N	-6.67	102.52	117.20
2	B	144	TYR	CE1-CZ-OH	6.66	138.08	120.10
1	A	82	ASN	O-C-N	6.66	133.35	122.70
2	B	2	LEU	O-C-N	6.66	133.35	122.70
1	C	13	ALA	CA-C-O	-6.66	106.12	120.10
1	C	75	ASP	N-CA-C	6.66	128.97	111.00
2	D	99	PRO	N-CA-CB	-6.66	95.28	102.60
1	A	74	ASN	N-CA-C	-6.65	93.04	111.00
2	D	144	TYR	CB-CA-C	-6.65	97.10	110.40
1	C	36	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	C	104	SER	CA-C-O	6.63	134.03	120.10
1	A	80	LEU	CB-CA-C	6.63	122.80	110.20
2	D	81	LYS	CD-CE-NZ	-6.63	96.45	111.70
2	B	38	GLN	OE1-CD-NE2	-6.63	106.65	121.90
2	B	70	PHE	CA-CB-CG	6.63	129.81	113.90
1	C	17	VAL	C-N-CA	-6.63	108.38	122.30
1	C	81	SER	CA-C-N	-6.62	102.63	117.20
2	B	87	LEU	N-CA-CB	6.62	123.64	110.40
2	D	40	PHE	CA-C-O	-6.62	106.20	120.10
2	B	16	LYS	N-CA-CB	-6.62	98.69	110.60
2	D	62	HIS	CG-CD2-NE2	-6.62	96.63	109.20
2	D	134	ALA	C-N-CA	6.62	136.19	122.30
1	A	27	GLN	CG-CD-NE2	6.61	132.57	116.70
1	C	112	HIS	C-N-CA	-6.61	105.17	121.70
1	A	62	VAL	N-CA-C	-6.61	93.15	111.00
2	D	122	THR	N-CA-CB	-6.61	97.75	110.30
1	A	11	LYS	CG-CD-CE	6.60	131.71	111.90
1	C	5	ALA	CB-CA-C	6.60	120.00	110.10
2	B	2	LEU	C-N-CA	-6.60	105.21	121.70
2	B	92	CYS	CA-CB-SG	6.59	125.86	114.00
2	D	104	LEU	C-N-CA	6.59	138.16	121.70
2	B	22	VAL	CB-CA-C	6.58	123.91	111.40
1	A	81	SER	CB-CA-C	6.58	122.61	110.10
2	D	76	HIS	C-N-CA	6.58	138.16	121.70
2	D	76	HIS	O-C-N	-6.58	112.17	122.70
2	B	94	LYS	CA-C-O	6.58	133.92	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	ALA	C-N-CA	6.57	138.13	121.70
1	C	87	HIS	CG-CD2-NE2	6.57	121.68	109.20
2	D	60	LYS	CD-CE-NZ	-6.57	96.59	111.70
2	D	108	VAL	O-C-N	-6.56	112.20	122.70
1	A	72	HIS	N-CA-CB	6.56	122.41	110.60
1	C	115	THR	O-C-N	6.56	133.20	122.70
1	C	137	THR	N-CA-C	-6.56	93.29	111.00
2	D	136	VAL	CA-C-O	-6.56	106.33	120.10
2	B	121	PHE	O-C-N	-6.55	112.22	122.70
1	A	48	LEU	CA-CB-CG	-6.54	100.25	115.30
2	B	42	GLN	CB-CA-C	-6.54	97.31	110.40
1	A	69	ALA	O-C-N	-6.54	112.23	122.70
1	C	6	ASN	N-CA-CB	6.54	122.37	110.60
2	D	81	LYS	N-CA-C	6.53	128.64	111.00
1	A	93	VAL	CA-C-O	6.52	133.79	120.10
2	D	67	LEU	CD1-CG-CD2	-6.52	90.94	110.50
2	B	71	THR	CA-C-O	6.52	133.79	120.10
2	D	34	TYR	CZ-CE2-CD2	6.52	125.67	119.80
1	C	42	TYR	N-CA-CB	-6.52	98.87	110.60
1	C	28	ALA	N-CA-C	6.51	128.59	111.00
1	C	55	GLN	CB-CA-C	6.51	123.42	110.40
1	A	85	ASN	CA-CB-CG	-6.50	99.09	113.40
1	A	128	PHE	CG-CD2-CE2	6.50	127.95	120.80
2	B	56	ASN	CA-C-N	6.50	135.29	117.10
2	D	63	GLY	CA-C-O	-6.50	108.91	120.60
2	B	89	GLY	O-C-N	6.49	133.09	122.70
1	C	38	THR	CA-C-N	6.49	131.47	117.20
1	C	109	LEU	CA-C-O	6.48	133.71	120.10
2	D	70	PHE	CB-CG-CD1	-6.48	116.26	120.80
2	B	21	VAL	CA-CB-CG1	6.48	120.61	110.90
2	D	9	ALA	O-C-N	-6.48	112.34	122.70
1	C	50	HIS	CA-C-N	6.47	129.14	116.20
1	C	131	ASN	CB-CA-C	-6.47	97.45	110.40
2	D	100	GLN	C-N-CA	-6.47	105.53	121.70
2	B	43	HIS	C-N-CA	-6.47	105.53	121.70
1	C	77	PRO	N-CA-C	6.47	128.91	112.10
2	B	40	PHE	CA-CB-CG	-6.46	98.39	113.90
1	A	122	HIS	O-C-N	6.46	133.04	122.70
2	D	59	VAL	N-CA-C	-6.46	93.55	111.00
1	A	16	LYS	CA-C-N	-6.46	102.99	117.20
2	B	131	LYS	CA-C-N	-6.46	102.99	117.20
1	C	123	ALA	CA-C-N	-6.46	102.99	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	VAL	CA-C-O	6.46	133.66	120.10
1	A	102	SER	CA-C-O	-6.46	106.54	120.10
1	C	58	HIS	N-CA-CB	6.46	122.22	110.60
1	A	35	SER	C-N-CA	6.46	137.84	121.70
2	B	64	LYS	CA-CB-CG	-6.46	99.19	113.40
2	B	52	ALA	O-C-N	6.45	133.02	122.70
1	C	11	LYS	O-C-N	-6.45	112.39	122.70
2	D	95	LEU	CA-C-N	6.45	131.38	117.20
1	C	129	LEU	N-CA-C	-6.44	93.60	111.00
2	D	20	ASP	CA-C-O	-6.44	106.57	120.10
2	D	80	LEU	CA-C-N	-6.44	103.02	117.20
1	C	72	HIS	CG-CD2-NE2	-6.44	96.97	109.20
1	A	94	ASN	N-CA-CB	-6.43	99.02	110.60
1	C	36	PHE	CD1-CE1-CZ	-6.43	112.38	120.10
1	C	103	HIS	CG-CD2-NE2	6.43	121.42	109.20
2	D	108	VAL	CA-C-N	6.42	131.33	117.20
2	D	57	PRO	CA-N-CD	-6.42	102.51	111.50
1	A	112	HIS	N-CA-CB	-6.42	99.05	110.60
1	C	66	LEU	CB-CG-CD2	6.41	121.90	111.00
2	B	91	HIS	CE1-NE2-CD2	-6.41	90.57	106.60
1	A	139	LYS	CG-CD-CE	6.41	131.13	111.90
1	C	36	PHE	N-CA-C	6.41	128.30	111.00
2	D	136	VAL	O-C-N	-6.41	112.45	122.70
1	A	51	GLY	N-CA-C	-6.40	97.09	113.10
1	A	63	ALA	CA-C-O	-6.40	106.66	120.10
1	C	96	VAL	C-N-CA	6.40	137.71	121.70
2	B	42	GLN	CG-CD-NE2	6.40	132.06	116.70
2	B	69	ALA	N-CA-C	6.39	128.26	111.00
2	D	129	PHE	N-CA-C	6.39	128.26	111.00
1	C	125	LEU	O-C-N	-6.39	112.47	122.70
1	A	16	LYS	CB-CA-C	6.38	123.16	110.40
2	B	9	ALA	CB-CA-C	6.38	119.67	110.10
1	A	115	THR	CA-C-N	-6.38	103.17	117.20
1	A	11	LYS	CB-CA-C	6.37	123.15	110.40
2	B	132	VAL	O-C-N	-6.37	112.50	122.70
2	D	12	GLY	CA-C-N	-6.37	103.18	117.20
1	C	42	TYR	CA-CB-CG	-6.36	101.31	113.40
2	B	109	LEU	CA-C-O	-6.36	106.74	120.10
1	C	17	VAL	O-C-N	6.36	134.02	123.20
1	C	95	PRO	CB-CA-C	-6.36	96.10	112.00
2	D	56	ASN	CB-CG-OD1	-6.36	108.88	121.60
2	D	40	PHE	N-CA-CB	6.36	122.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	84	PHE	C-N-CA	-6.36	105.81	121.70
1	C	130	ALA	CA-C-O	-6.35	106.76	120.10
2	B	120	GLN	CA-CB-CG	-6.35	99.43	113.40
2	B	46	ASN	N-CA-C	6.35	128.13	111.00
2	D	68	ASP	CA-C-O	6.33	133.40	120.10
2	B	86	GLN	N-CA-CB	6.32	121.98	110.60
2	D	76	HIS	CA-C-N	6.32	131.11	117.20
1	A	99	LYS	CB-CG-CD	-6.32	95.16	111.60
1	A	132	ASP	CA-C-N	-6.32	103.29	117.20
1	A	141	ARG	N-CA-C	6.32	128.06	111.00
1	C	101	LEU	N-CA-CB	-6.32	97.77	110.40
1	A	30	GLN	CB-CG-CD	6.31	128.01	111.60
1	C	58	HIS	CE1-NE2-CD2	6.31	122.38	106.60
2	D	36	TRP	CD2-CE3-CZ3	-6.31	110.60	118.80
1	C	104	SER	CA-CB-OG	-6.30	94.19	111.20
2	D	62	HIS	O-C-N	-6.30	112.49	123.20
2	B	109	LEU	CD1-CG-CD2	6.30	129.39	110.50
1	C	34	LEU	O-C-N	-6.30	112.63	122.70
2	D	25	GLN	C-N-CA	6.30	137.44	121.70
1	A	135	VAL	O-C-N	6.29	132.77	122.70
1	C	42	TYR	CA-C-O	-6.29	106.89	120.10
2	D	3	THR	N-CA-C	-6.29	94.01	111.00
2	B	100	GLN	C-N-CA	-6.29	105.98	121.70
1	A	125	LEU	CB-CG-CD2	6.29	121.69	111.00
1	A	117	PHE	CA-CB-CG	6.28	128.98	113.90
1	C	131	ASN	C-N-CA	6.28	137.41	121.70
2	D	64	LYS	CA-C-O	6.28	133.29	120.10
2	D	67	LEU	N-CA-CB	6.28	122.96	110.40
2	B	76	HIS	CE1-NE2-CD2	6.27	122.28	106.60
2	D	54	MET	CG-SD-CE	-6.27	90.16	100.20
1	C	122	HIS	ND1-CE1-NE2	-6.27	96.10	109.90
2	D	144	TYR	CG-CD1-CE1	-6.27	116.28	121.30
1	C	100	LEU	N-CA-C	-6.27	94.07	111.00
1	A	129	LEU	CA-C-O	-6.27	106.93	120.10
2	B	117	PHE	CD1-CE1-CZ	6.27	127.62	120.10
2	D	55	ASN	CB-CA-C	-6.27	97.87	110.40
1	A	69	ALA	CB-CA-C	6.27	119.50	110.10
2	B	35	PRO	N-CA-CB	6.27	110.82	103.30
1	C	18	GLY	CA-C-O	-6.26	109.33	120.60
1	A	44	PRO	CA-N-CD	-6.26	102.74	111.50
2	B	8	ALA	CA-C-N	6.25	130.96	117.20
2	D	53	VAL	CB-CA-C	-6.25	99.52	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	VAL	O-C-N	6.25	132.70	122.70
2	B	25	GLN	CA-C-N	6.25	130.95	117.20
1	C	126	ASN	CA-C-N	6.24	130.93	117.20
2	B	42	GLN	CB-CG-CD	6.24	127.83	111.60
1	C	60	GLN	CA-CB-CG	-6.24	99.67	113.40
2	B	51	GLY	O-C-N	-6.24	112.72	122.70
2	D	116	ASN	C-N-CA	6.24	137.29	121.70
1	A	45	HIS	N-CA-CB	6.23	121.82	110.60
1	A	108	THR	CA-CB-CG2	6.23	121.12	112.40
2	D	86	GLN	CB-CA-C	6.23	122.86	110.40
1	A	46	PHE	CD1-CG-CD2	-6.23	110.20	118.30
1	A	141	ARG	CA-CB-CG	-6.23	99.70	113.40
1	A	44	PRO	N-CA-C	6.23	128.29	112.10
2	B	29	ARG	O-C-N	-6.23	112.74	122.70
2	B	52	ALA	CA-C-O	6.22	133.16	120.10
2	B	18	ASP	CA-C-O	-6.21	107.05	120.10
2	D	142	HIS	N-CA-C	-6.21	94.22	111.00
1	A	14	TRP	CD2-CE3-CZ3	6.21	126.87	118.80
2	D	106	GLY	C-N-CA	6.21	137.22	121.70
1	A	10	VAL	CA-CB-CG2	-6.20	101.59	110.90
1	C	32	MET	N-CA-CB	-6.20	99.44	110.60
1	C	31	ARG	C-N-CA	-6.20	106.19	121.70
1	C	4	ALA	CA-C-O	6.20	133.12	120.10
1	C	109	LEU	N-CA-CB	6.20	122.80	110.40
2	B	84	PHE	N-CA-CB	-6.20	99.45	110.60
1	C	102	SER	CB-CA-C	6.20	121.87	110.10
2	B	117	PHE	CB-CG-CD2	-6.19	116.46	120.80
2	B	136	VAL	N-CA-C	-6.19	94.28	111.00
1	C	126	ASN	CB-CG-ND2	6.19	131.55	116.70
1	C	126	ASN	C-N-CA	6.18	137.16	121.70
2	D	45	GLY	CA-C-N	-6.18	103.60	117.20
1	A	7	LYS	CA-CB-CG	6.18	127.00	113.40
2	D	138	ASN	C-N-CA	6.18	137.15	121.70
2	D	145	HIS	CG-CD2-NE2	-6.17	97.47	109.20
2	D	27	LEU	CA-CB-CG	6.17	129.50	115.30
1	A	20	ASN	CA-CB-CG	-6.17	99.82	113.40
2	D	6	GLU	CG-CD-OE1	6.17	130.64	118.30
2	B	18	ASP	N-CA-CB	-6.17	99.50	110.60
1	A	93	VAL	CA-C-N	-6.17	103.64	117.20
1	C	141	ARG	CD-NE-CZ	6.17	132.23	123.60
1	A	134	THR	OG1-CB-CG2	-6.16	95.83	110.00
1	C	38	THR	O-C-N	-6.16	112.85	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	LYS	CB-CA-C	6.16	122.71	110.40
1	A	133	SER	CA-C-N	6.15	130.74	117.20
1	A	24	TYR	CE1-CZ-CE2	-6.15	109.96	119.80
1	C	133	SER	N-CA-C	-6.15	94.39	111.00
2	D	34	TYR	CE1-CZ-OH	-6.15	103.50	120.10
2	D	53	VAL	CA-CB-CG2	6.14	120.12	110.90
1	A	14	TRP	CZ3-CH2-CZ2	6.14	128.97	121.60
2	B	40	PHE	N-CA-C	-6.14	94.42	111.00
2	B	103	ARG	CA-C-N	6.14	130.71	117.20
2	D	65	ARG	CA-CB-CG	6.14	126.90	113.40
2	B	39	ARG	CD-NE-CZ	-6.12	115.03	123.60
1	C	100	LEU	CB-CA-C	6.12	121.82	110.20
1	C	105	LEU	CB-CA-C	6.12	121.82	110.20
2	D	121	PHE	CA-C-O	6.11	132.94	120.10
1	C	127	LYS	CB-CA-C	-6.11	98.18	110.40
1	A	41	THR	CA-C-N	6.11	130.63	117.20
1	A	125	LEU	C-N-CA	6.11	136.96	121.70
2	B	94	LYS	CB-CA-C	-6.11	98.19	110.40
1	A	87	HIS	CA-C-O	6.10	132.91	120.10
2	B	103	ARG	O-C-N	-6.10	112.94	122.70
1	A	23	ALA	CB-CA-C	6.10	119.25	110.10
1	A	105	LEU	C-N-CA	-6.10	106.46	121.70
1	C	82	ASN	CB-CG-ND2	6.09	131.33	116.70
1	A	2	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	A	18	GLY	CA-C-O	6.09	131.56	120.60
1	A	84	SER	CA-C-N	6.08	130.58	117.20
1	A	42	TYR	CZ-CE2-CD2	6.08	125.27	119.80
1	A	74	ASN	C-N-CA	-6.08	106.50	121.70
2	D	12	GLY	N-CA-C	-6.08	97.90	113.10
2	D	107	ASN	CA-C-N	6.08	130.57	117.20
2	D	121	PHE	CB-CA-C	-6.08	98.25	110.40
2	B	142	HIS	CG-CD2-NE2	-6.08	97.66	109.20
1	C	98	PHE	CA-CB-CG	-6.07	99.33	113.90
2	B	65	ARG	CB-CA-C	-6.07	98.26	110.40
1	C	141	ARG	CB-CG-CD	-6.07	95.82	111.60
2	B	81	LYS	CB-CG-CD	6.07	127.37	111.60
1	C	62	VAL	CG1-CB-CG2	-6.07	101.19	110.90
1	C	40	LYS	C-N-CA	6.06	136.86	121.70
2	D	99	PRO	CA-CB-CG	-6.06	92.49	104.00
1	C	92	ARG	CB-CA-C	-6.05	98.29	110.40
2	B	99	PRO	CA-CB-CG	6.05	116.30	104.80
1	C	137	THR	CA-CB-OG1	-6.05	96.29	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	31	LEU	CB-CA-C	6.05	121.70	110.20
2	D	69	ALA	C-N-CA	-6.05	106.58	121.70
2	D	128	LEU	N-CA-CB	-6.05	98.30	110.40
1	C	4	ALA	N-CA-C	-6.04	94.69	111.00
2	D	101	ASN	CA-CB-CG	-6.04	100.11	113.40
2	B	102	PHE	CZ-CE2-CD2	-6.04	112.86	120.10
1	C	22	PRO	CA-C-N	6.04	130.48	117.20
1	A	107	VAL	CA-C-N	6.03	130.47	117.20
2	B	126	GLN	CB-CA-C	6.03	122.46	110.40
1	C	85	ASN	CA-CB-CG	6.03	126.67	113.40
2	B	18	ASP	CB-CA-C	6.03	122.46	110.40
1	C	134	THR	N-CA-CB	-6.03	98.85	110.30
1	C	37	PRO	CB-CG-CD	-6.03	83.00	106.50
2	D	126	GLN	CA-C-N	6.02	130.45	117.20
2	D	42	GLN	N-CA-C	6.02	127.26	111.00
2	B	20	ASP	CB-CG-OD2	6.02	123.72	118.30
2	B	23	GLY	CA-C-O	-6.02	109.77	120.60
2	B	27	LEU	N-CA-CB	6.01	122.43	110.40
2	B	34	TYR	O-C-N	-6.01	109.67	121.10
1	C	47	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	71	GLY	O-C-N	-6.01	113.08	122.70
1	A	30	GLN	O-C-N	-6.01	113.09	122.70
2	D	41	PHE	CB-CA-C	6.01	122.41	110.40
1	A	73	LEU	CA-C-N	6.00	130.41	117.20
1	C	55	GLN	C-N-CA	6.00	136.71	121.70
2	B	66	VAL	CA-C-N	6.00	130.40	117.20
2	D	81	LYS	CA-CB-CG	6.00	126.61	113.40
1	C	117	PHE	CA-CB-CG	6.00	128.30	113.90
1	A	73	LEU	CD1-CG-CD2	-6.00	92.52	110.50
1	C	55	GLN	CG-CD-OE1	-5.99	109.61	121.60
2	D	62	HIS	CA-C-N	5.99	128.17	116.20
2	D	144	TYR	CA-CB-CG	5.99	124.78	113.40
1	C	56	LYS	CB-CG-CD	-5.98	96.05	111.60
2	D	105	LEU	N-CA-CB	5.98	122.36	110.40
2	D	18	ASP	C-N-CA	-5.98	106.76	121.70
1	C	114	PRO	CA-C-O	-5.97	105.86	120.20
2	B	35	PRO	C-N-CA	5.97	136.63	121.70
2	B	19	VAL	CA-C-O	-5.97	107.57	120.10
2	B	138	ASN	N-CA-C	5.97	127.11	111.00
1	C	40	LYS	CA-CB-CG	5.96	126.52	113.40
1	C	97	ASN	O-C-N	5.96	132.24	122.70
2	B	36	TRP	NE1-CE2-CD2	-5.96	101.34	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	LYS	N-CA-C	5.95	127.07	111.00
2	B	36	TRP	CD2-CE2-CZ2	5.95	129.44	122.30
1	C	46	PHE	CA-CB-CG	-5.95	99.62	113.90
2	B	34	TYR	C-N-CA	5.95	146.97	122.00
2	B	143	LYS	CD-CE-NZ	-5.94	98.03	111.70
1	C	101	LEU	CB-CG-CD2	5.94	121.11	111.00
1	A	60	GLN	CG-CD-OE1	5.94	133.48	121.60
2	B	24	ALA	N-CA-CB	5.94	118.41	110.10
2	B	3	THR	CA-CB-CG2	5.94	120.71	112.40
1	A	120	ALA	CB-CA-C	5.93	119.00	110.10
1	A	60	GLN	CA-C-O	5.93	132.56	120.10
1	C	109	LEU	CA-C-N	5.93	130.25	117.20
2	D	89	GLY	CA-C-N	5.93	130.25	117.20
1	A	129	LEU	C-N-CA	5.92	136.51	121.70
2	D	100	GLN	CB-CG-CD	5.92	127.00	111.60
2	B	40	PHE	CE1-CZ-CE2	-5.92	109.34	120.00
1	A	83	LEU	CA-C-N	5.92	130.22	117.20
1	A	131	ASN	N-CA-C	-5.92	95.02	111.00
2	B	48	SER	N-CA-C	-5.92	95.02	111.00
2	B	57	PRO	N-CA-CB	5.91	110.40	103.30
2	B	136	VAL	CA-CB-CG2	5.91	119.77	110.90
1	C	90	LYS	C-N-CA	-5.91	106.93	121.70
1	A	58	HIS	CB-CA-C	5.91	122.21	110.40
2	D	79	ASP	O-C-N	5.90	132.15	122.70
2	B	107	ASN	CA-C-N	5.90	130.18	117.20
1	C	94	ASN	CA-C-N	5.90	133.62	117.10
1	A	98	PHE	CG-CD1-CE1	5.90	127.29	120.80
1	A	51	GLY	CA-C-O	-5.89	109.99	120.60
1	C	67	THR	CA-C-N	5.89	130.17	117.20
1	A	6	ASN	N-CA-C	-5.89	95.09	111.00
2	B	36	TRP	CB-CG-CD2	5.89	134.26	126.60
2	B	134	ALA	O-C-N	-5.89	113.18	123.20
2	B	94	LYS	CA-C-N	-5.89	104.24	117.20
1	C	53	ALA	CB-CA-C	-5.89	101.27	110.10
2	D	46	ASN	OD1-CG-ND2	-5.89	108.36	121.90
1	A	87	HIS	CB-CG-ND1	-5.88	108.49	123.20
2	B	40	PHE	CD1-CE1-CZ	5.88	127.16	120.10
1	A	79	THR	OG1-CB-CG2	5.88	123.52	110.00
1	A	96	VAL	CA-CB-CG2	5.88	119.72	110.90
1	C	36	PHE	CG-CD1-CE1	5.88	127.26	120.80
2	B	122	THR	O-C-N	-5.87	109.94	121.10
1	C	103	HIS	N-CA-C	5.87	126.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	120	GLN	N-CA-CB	5.87	121.17	110.60
2	B	117	PHE	C-N-CA	5.87	134.63	122.30
2	D	56	ASN	CB-CG-ND2	5.87	130.79	116.70
1	C	122	HIS	CB-CG-ND1	-5.87	108.53	123.20
1	C	17	VAL	CB-CA-C	5.86	122.54	111.40
1	C	90	LYS	N-CA-CB	-5.86	100.05	110.60
1	C	116	ASN	OD1-CG-ND2	-5.86	108.42	121.90
1	C	135	VAL	N-CA-C	-5.86	95.17	111.00
1	C	70	GLN	CA-CB-CG	5.86	126.28	113.40
2	B	141	ALA	CB-CA-C	5.85	118.88	110.10
2	B	94	LYS	CG-CD-CE	-5.85	94.35	111.90
2	D	123	PRO	CA-CB-CG	5.85	115.91	104.80
1	C	23	ALA	C-N-CA	5.85	136.31	121.70
2	B	130	GLN	O-C-N	5.84	132.05	122.70
2	B	133	VAL	N-CA-CB	-5.84	98.65	111.50
2	B	59	VAL	CG1-CB-CG2	5.84	120.24	110.90
1	C	52	SER	C-N-CA	-5.84	107.10	121.70
2	D	41	PHE	CB-CG-CD1	5.83	124.88	120.80
1	C	30	GLN	CG-CD-NE2	5.83	130.69	116.70
1	C	117	PHE	CA-C-N	5.83	130.02	117.20
1	A	78	GLY	CA-C-O	-5.82	110.12	120.60
2	B	99	PRO	CB-CA-C	-5.82	97.45	112.00
1	C	18	GLY	O-C-N	5.82	133.10	123.20
2	D	117	PHE	CA-CB-CG	5.82	127.87	113.90
2	B	126	GLN	CG-CD-NE2	5.82	130.67	116.70
1	A	116	ASN	CA-C-O	-5.81	107.89	120.10
2	B	56	ASN	CA-C-O	-5.81	107.89	120.10
1	C	41	THR	O-C-N	-5.81	113.40	122.70
2	D	98	ASN	CB-CA-C	-5.81	98.78	110.40
1	C	136	LEU	C-N-CA	5.81	136.23	121.70
1	A	54	GLN	N-CA-C	-5.80	95.33	111.00
1	C	61	LYS	CA-CB-CG	-5.80	100.63	113.40
2	D	129	PHE	CZ-CE2-CD2	-5.80	113.14	120.10
1	A	52	SER	C-N-CA	-5.80	107.21	121.70
2	D	67	LEU	CB-CA-C	5.79	121.21	110.20
2	B	85	ALA	N-CA-CB	-5.79	101.99	110.10
1	A	29	LEU	CD1-CG-CD2	-5.79	93.14	110.50
1	A	64	ASN	CA-C-O	5.79	132.25	120.10
2	B	111	LEU	CA-CB-CG	5.78	128.60	115.30
2	D	129	PHE	CD1-CE1-CZ	-5.77	113.17	120.10
2	D	49	SER	C-N-CA	5.77	136.13	121.70
2	B	11	THR	CA-CB-CG2	5.76	120.47	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	VAL	CA-C-O	-5.76	107.99	120.10
2	B	84	PHE	CB-CA-C	5.76	121.92	110.40
2	B	2	LEU	CA-CB-CG	-5.76	102.06	115.30
2	B	100	GLN	CG-CD-NE2	5.76	130.52	116.70
2	B	106	GLY	CA-C-O	5.76	130.97	120.60
2	B	89	GLY	N-CA-C	-5.76	98.71	113.10
1	C	118	THR	OG1-CB-CG2	-5.76	96.76	110.00
2	B	82	GLY	CA-C-O	-5.75	110.25	120.60
2	B	145	HIS	CB-CG-CD2	-5.75	112.98	130.80
1	A	52	SER	CB-CA-C	5.74	121.01	110.10
2	D	29	ARG	CB-CA-C	5.74	121.89	110.40
2	D	12	GLY	O-C-N	5.74	131.88	122.70
1	A	100	LEU	CA-C-N	-5.73	104.59	117.20
1	C	113	LEU	CA-CB-CG	-5.73	102.12	115.30
1	C	12	ALA	O-C-N	-5.73	113.53	122.70
2	B	75	LYS	CD-CE-NZ	5.73	124.88	111.70
2	B	112	VAL	CA-CB-CG1	-5.73	102.31	110.90
2	B	84	PHE	CA-CB-CG	-5.72	100.16	113.90
2	D	93	ASN	CB-CG-OD1	5.72	133.05	121.60
2	D	122	THR	CA-CB-CG2	5.72	120.41	112.40
2	B	124	ASN	N-CA-CB	5.72	120.89	110.60
1	A	109	LEU	CA-C-O	5.71	132.10	120.10
1	A	119	PRO	CA-CB-CG	-5.71	93.15	104.00
2	B	68	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	C	72	HIS	CB-CG-ND1	5.71	137.47	123.20
2	D	46	ASN	C-N-CA	-5.71	107.42	121.70
2	B	29	ARG	N-CA-CB	-5.71	100.33	110.60
2	D	44	PHE	CA-CB-CG	-5.71	100.20	113.90
2	B	101	ASN	OD1-CG-ND2	5.70	135.02	121.90
2	B	131	LYS	CA-C-O	5.70	132.07	120.10
1	C	130	ALA	CB-CA-C	5.70	118.65	110.10
1	C	17	VAL	N-CA-C	-5.70	95.62	111.00
1	A	68	LYS	CG-CD-CE	-5.69	94.82	111.90
2	B	14	TRP	C-N-CA	5.68	134.24	122.30
2	B	110	ALA	O-C-N	-5.68	113.60	122.70
1	C	35	SER	N-CA-CB	5.68	119.03	110.50
1	C	38	THR	N-CA-C	-5.68	95.66	111.00
2	D	83	ALA	O-C-N	5.68	131.79	122.70
2	B	134	ALA	C-N-CA	5.68	134.23	122.30
1	C	104	SER	CB-CA-C	-5.68	99.31	110.10
1	C	13	ALA	CA-C-N	5.68	129.69	117.20
1	A	117	PHE	CA-C-N	-5.67	104.72	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	90	LEU	O-C-N	5.67	131.78	122.70
2	D	12	GLY	C-N-CA	-5.66	107.54	121.70
2	D	68	ASP	CA-C-N	5.66	129.65	117.20
1	C	42	TYR	OH-CZ-CE2	5.66	135.38	120.10
1	A	98	PHE	C-N-CA	5.66	135.84	121.70
2	D	53	VAL	CA-C-N	5.66	129.64	117.20
1	C	14	TRP	C-N-CA	-5.65	110.43	122.30
1	A	83	LEU	O-C-N	-5.65	113.66	122.70
2	D	104	LEU	CB-CA-C	5.65	120.94	110.20
1	C	10	VAL	C-N-CA	5.64	135.81	121.70
2	B	111	LEU	CA-C-O	-5.64	108.25	120.10
1	C	64	ASN	O-C-N	5.64	131.72	122.70
2	B	55	ASN	CB-CA-C	5.64	121.67	110.40
2	B	74	LEU	O-C-N	-5.63	113.69	122.70
2	B	29	ARG	N-CA-C	5.63	126.21	111.00
1	A	36	PHE	CG-CD2-CE2	-5.63	114.61	120.80
2	D	93	ASN	C-N-CA	-5.63	107.62	121.70
1	A	10	VAL	CB-CA-C	-5.63	100.71	111.40
2	D	14	TRP	C-N-CA	5.62	134.11	122.30
2	B	139	ALA	N-CA-C	5.62	126.18	111.00
1	A	66	LEU	CB-CA-C	5.62	120.87	110.20
1	A	136	LEU	CB-CG-CD2	5.62	120.55	111.00
2	B	29	ARG	CA-C-O	-5.61	108.31	120.10
1	C	45	HIS	CA-C-N	5.61	129.54	117.20
2	B	35	PRO	CA-CB-CG	-5.61	93.35	104.00
2	B	2	LEU	CA-C-O	-5.60	108.33	120.10
1	C	124	ASN	CA-C-N	5.60	129.52	117.20
2	D	139	ALA	CA-C-O	-5.59	108.36	120.10
2	D	30	LEU	CA-C-N	-5.59	104.90	117.20
1	A	107	VAL	N-CA-C	-5.58	95.93	111.00
2	B	31	LEU	CA-C-N	-5.58	104.92	117.20
1	A	122	HIS	CE1-NE2-CD2	5.58	120.55	106.60
1	A	90	LYS	N-CA-CB	5.58	120.64	110.60
2	B	124	ASN	CB-CG-ND2	5.58	130.09	116.70
2	B	3	THR	CA-C-O	5.58	131.81	120.10
1	C	122	HIS	CG-ND1-CE1	5.57	116.00	108.20
2	D	60	LYS	CG-CD-CE	5.57	128.62	111.90
1	C	7	LYS	N-CA-C	5.57	126.04	111.00
1	C	29	LEU	CB-CA-C	5.57	120.79	110.20
2	D	130	GLN	N-CA-C	-5.57	95.95	111.00
1	A	33	PHE	C-N-CA	5.57	135.63	121.70
2	B	59	VAL	CA-CB-CG2	5.57	119.26	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	VAL	C-N-CA	5.56	135.61	121.70
2	B	99	PRO	CB-CG-CD	-5.56	84.81	106.50
2	B	5	GLU	N-CA-C	-5.56	95.99	111.00
1	C	89	HIS	ND1-CE1-NE2	5.55	122.12	109.90
2	D	31	LEU	N-CA-C	-5.55	96.02	111.00
1	C	36	PHE	CA-CB-CG	5.55	127.21	113.90
1	A	41	THR	CA-C-O	5.54	131.75	120.10
1	A	70	GLN	N-CA-C	-5.54	96.03	111.00
1	A	133	SER	CB-CA-C	5.54	120.63	110.10
1	C	133	SER	CA-C-O	-5.54	108.46	120.10
1	A	128	PHE	CG-CD1-CE1	-5.54	114.70	120.80
1	A	35	SER	CA-CB-OG	-5.54	96.24	111.20
2	D	25	GLN	CB-CG-CD	-5.54	97.20	111.60
2	B	3	THR	C-N-CA	-5.53	107.86	121.70
2	D	38	GLN	N-CA-C	5.53	125.94	111.00
1	C	67	THR	CB-CA-C	5.53	126.53	111.60
1	A	23	ALA	C-N-CA	5.52	135.51	121.70
1	A	61	LYS	CG-CD-CE	5.52	128.46	111.90
2	B	99	PRO	CA-N-CD	5.52	119.43	111.70
2	B	99	PRO	N-CD-CG	-5.52	94.92	103.20
2	D	67	LEU	CA-C-N	5.52	129.34	117.20
1	A	40	LYS	N-CA-CB	5.52	120.53	110.60
1	C	34	LEU	CA-C-N	5.52	129.33	117.20
2	B	26	ALA	N-CA-CB	5.51	117.82	110.10
2	B	37	THR	OG1-CB-CG2	-5.51	97.32	110.00
1	C	50	HIS	CG-CD2-NE2	5.51	119.68	109.20
1	A	54	GLN	CA-C-N	-5.51	105.07	117.20
2	B	33	VAL	CB-CA-C	5.51	121.87	111.40
1	C	98	PHE	CB-CG-CD2	5.51	124.66	120.80
2	D	40	PHE	CA-CB-CG	5.51	127.12	113.90
1	A	17	VAL	CB-CA-C	5.50	121.85	111.40
1	A	97	ASN	CB-CA-C	5.50	121.40	110.40
1	A	37	PRO	CA-C-O	-5.50	107.00	120.20
1	C	73	LEU	N-CA-C	-5.50	96.15	111.00
2	B	123	PRO	N-CA-CB	5.49	109.89	103.30
2	D	48	SER	CA-CB-OG	5.49	126.02	111.20
1	C	140	TYR	OH-CZ-CE2	5.48	134.91	120.10
1	A	136	LEU	CB-CG-CD1	-5.48	101.68	111.00
2	B	36	TRP	CG-CD2-CE3	-5.48	128.97	133.90
1	A	140	TYR	CA-C-O	5.48	131.61	120.10
1	C	59	GLY	CA-C-N	5.48	129.26	117.20
2	B	32	VAL	N-CA-C	-5.48	96.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	THR	O-C-N	-5.47	113.95	122.70
1	C	79	THR	CB-CA-C	-5.47	96.83	111.60
2	D	45	GLY	O-C-N	5.47	131.45	122.70
1	A	51	GLY	CA-C-N	5.47	129.23	117.20
2	B	99	PRO	C-N-CA	5.46	135.36	121.70
1	C	87	HIS	N-CA-CB	5.46	120.44	110.60
1	A	1	VAL	CA-CB-CG1	-5.46	102.71	110.90
2	B	137	ALA	CB-CA-C	-5.46	101.91	110.10
2	B	107	ASN	CB-CG-OD1	5.46	132.52	121.60
1	C	22	PRO	N-CD-CG	5.46	111.39	103.20
2	B	35	PRO	CB-CA-C	-5.46	98.36	112.00
1	C	62	VAL	CA-CB-CG2	5.46	119.08	110.90
1	C	111	SER	N-CA-CB	-5.46	102.31	110.50
2	B	121	PHE	CG-CD2-CE2	-5.46	114.80	120.80
1	C	100	LEU	CB-CG-CD2	-5.46	101.73	111.00
1	A	26	ALA	N-CA-CB	-5.45	102.47	110.10
1	A	118	THR	N-CA-CB	-5.45	99.95	110.30
1	C	32	MET	C-N-CA	5.45	135.32	121.70
1	C	29	LEU	N-CA-C	-5.45	96.29	111.00
1	C	20	ASN	C-N-CA	5.44	135.31	121.70
1	A	104	SER	CA-CB-OG	-5.44	96.51	111.20
1	C	98	PHE	CE1-CZ-CE2	-5.44	110.21	120.00
1	C	29	LEU	CA-C-O	-5.44	108.68	120.10
1	A	105	LEU	N-CA-CB	-5.43	99.53	110.40
2	D	61	ALA	CA-C-N	-5.43	105.24	117.20
2	D	37	THR	N-CA-C	5.43	125.67	111.00
1	A	14	TRP	CA-C-O	5.43	131.50	120.10
1	C	77	PRO	CA-C-N	-5.43	105.34	116.20
2	D	102	PHE	CA-CB-CG	5.43	126.92	113.90
1	C	74	ASN	CA-C-O	5.42	131.49	120.10
1	A	92	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	36	PHE	CZ-CE2-CD2	5.42	126.60	120.10
1	A	44	PRO	CB-CG-CD	-5.42	85.38	106.50
1	C	124	ASN	CA-CB-CG	-5.42	101.48	113.40
2	D	144	TYR	CE1-CZ-OH	-5.41	105.49	120.10
2	B	60	LYS	CB-CG-CD	-5.41	97.53	111.60
1	C	94	ASN	N-CA-C	-5.41	96.40	111.00
1	C	69	ALA	CA-C-O	5.41	131.46	120.10
1	A	136	LEU	CA-C-N	-5.40	105.31	117.20
2	D	90	LEU	CB-CG-CD2	5.40	120.19	111.00
2	B	113	VAL	CB-CA-C	5.40	121.66	111.40
1	C	101	LEU	N-CA-C	5.40	125.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	62	HIS	CB-CG-ND1	-5.40	109.71	123.20
1	C	72	HIS	CB-CG-CD2	-5.39	114.08	130.80
1	C	7	LYS	CA-CB-CG	5.39	125.27	113.40
2	D	96	HIS	N-CA-C	-5.39	96.44	111.00
2	D	126	GLN	CA-C-O	5.39	131.42	120.10
2	D	44	PHE	N-CA-CB	5.38	120.29	110.60
2	D	112	VAL	CA-CB-CG1	-5.37	102.84	110.90
2	D	66	VAL	CA-CB-CG1	5.37	118.96	110.90
1	C	120	ALA	CB-CA-C	-5.37	102.05	110.10
2	D	49	SER	N-CA-C	-5.37	96.51	111.00
1	C	124	ASN	O-C-N	-5.36	114.12	122.70
1	A	48	LEU	CA-C-N	5.36	128.99	117.20
1	A	128	PHE	CA-C-N	-5.36	105.41	117.20
2	B	65	ARG	CG-CD-NE	-5.36	100.54	111.80
2	D	65	ARG	CA-C-N	-5.36	105.41	117.20
2	B	39	ARG	CB-CG-CD	-5.36	97.67	111.60
2	B	65	ARG	O-C-N	-5.35	114.14	122.70
2	B	38	GLN	N-CA-C	-5.35	96.56	111.00
1	A	22	PRO	N-CA-C	5.34	125.98	112.10
2	B	89	GLY	CA-C-N	-5.34	105.45	117.20
2	B	101	ASN	CB-CG-ND2	-5.34	103.88	116.70
1	C	33	PHE	C-N-CA	5.34	135.05	121.70
1	C	12	ALA	N-CA-C	-5.33	96.60	111.00
2	D	11	THR	CA-C-O	5.33	131.29	120.10
1	A	53	ALA	CA-C-N	5.33	128.93	117.20
2	B	36	TRP	CA-CB-CG	5.33	123.83	113.70
2	B	127	ALA	CA-C-O	-5.33	108.91	120.10
1	C	104	SER	CA-C-N	-5.33	105.47	117.20
2	B	22	VAL	O-C-N	5.33	132.25	123.20
2	B	128	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	A	117	PHE	O-C-N	-5.33	114.18	122.70
1	A	58	HIS	ND1-CE1-NE2	-5.32	98.19	109.90
2	D	141	ALA	O-C-N	5.32	131.22	122.70
2	D	93	ASN	OD1-CG-ND2	-5.32	109.67	121.90
1	A	128	PHE	O-C-N	-5.31	114.20	122.70
1	C	57	ALA	CA-C-N	5.31	128.89	117.20
2	D	135	GLY	C-N-CA	5.31	134.98	121.70
1	A	14	TRP	CE3-CZ3-CH2	-5.31	115.36	121.20
2	D	5	GLU	CG-CD-OE2	-5.31	107.68	118.30
1	A	112	HIS	CE1-NE2-CD2	5.31	119.87	106.60
1	C	132	ASP	N-CA-CB	-5.31	101.05	110.60
2	B	115	ARG	CB-CA-C	-5.30	99.80	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	121	PHE	CA-C-O	-5.30	108.97	120.10
2	B	128	LEU	CA-CB-CG	-5.30	103.12	115.30
2	B	32	VAL	CB-CA-C	5.29	121.46	111.40
2	B	34	TYR	N-CA-C	-5.29	96.72	111.00
2	D	57	PRO	CB-CG-CD	-5.29	85.88	106.50
2	B	120	GLN	CG-CD-OE1	-5.29	111.03	121.60
2	D	27	LEU	CD1-CG-CD2	-5.29	94.64	110.50
1	C	5	ALA	C-N-CA	5.28	134.90	121.70
1	C	133	SER	CB-CA-C	5.28	120.13	110.10
2	D	130	GLN	CA-CB-CG	5.28	125.01	113.40
2	B	123	PRO	N-CA-C	-5.27	98.39	112.10
1	A	112	HIS	CG-ND1-CE1	5.27	115.58	108.20
1	A	121	VAL	C-N-CA	5.27	134.87	121.70
2	D	43	HIS	N-CA-CB	-5.27	101.12	110.60
2	D	120	GLN	CA-CB-CG	-5.27	101.81	113.40
1	C	132	ASP	OD1-CG-OD2	-5.26	113.30	123.30
1	A	103	HIS	CE1-NE2-CD2	5.25	119.73	106.60
2	B	92	CYS	N-CA-CB	-5.25	101.14	110.60
2	B	86	GLN	CG-CD-NE2	-5.25	104.09	116.70
1	A	71	GLY	CA-C-O	5.25	130.05	120.60
2	D	89	GLY	O-C-N	-5.25	114.30	122.70
1	A	57	ALA	CA-C-N	5.24	128.73	117.20
2	B	122	THR	CB-CA-C	-5.24	97.45	111.60
1	C	101	LEU	O-C-N	-5.24	114.31	122.70
2	B	23	GLY	CA-C-N	5.24	128.72	117.20
2	B	93	ASN	CB-CA-C	-5.24	99.92	110.40
1	A	92	ARG	N-CA-C	5.24	125.14	111.00
2	D	30	LEU	CB-CG-CD1	5.24	119.90	111.00
1	C	34	LEU	CB-CG-CD2	5.23	119.90	111.00
1	A	72	HIS	CE1-NE2-CD2	5.23	119.68	106.60
1	A	125	LEU	CD1-CG-CD2	-5.23	94.81	110.50
1	C	100	LEU	CA-CB-CG	5.22	127.32	115.30
2	B	97	VAL	C-N-CA	5.22	134.76	121.70
2	D	96	HIS	CA-C-O	-5.22	109.13	120.10
2	B	5	GLU	C-N-CA	5.22	134.75	121.70
2	B	136	VAL	O-C-N	-5.22	114.35	122.70
2	B	118	GLY	C-N-CA	-5.22	111.34	122.30
2	D	128	LEU	N-CA-C	-5.22	96.91	111.00
1	A	4	ALA	CA-C-O	-5.22	109.14	120.10
1	A	119	PRO	CA-N-CD	5.22	119.00	111.70
2	D	43	HIS	CB-CA-C	5.22	120.83	110.40
1	C	75	ASP	N-CA-CB	-5.21	101.22	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	LEU	N-CA-CB	-5.21	99.99	110.40
1	C	55	GLN	O-C-N	-5.21	114.37	122.70
2	B	22	VAL	CA-C-O	-5.20	109.17	120.10
2	B	41	PHE	CD1-CG-CD2	-5.20	111.53	118.30
1	A	45	HIS	CA-CB-CG	-5.20	104.76	113.60
2	B	122	THR	N-CA-C	-5.20	96.96	111.00
1	C	1	VAL	N-CA-C	-5.19	96.99	111.00
2	B	25	GLN	CB-CA-C	-5.19	100.03	110.40
2	D	96	HIS	N-CA-CB	5.19	119.94	110.60
2	D	84	PHE	N-CA-C	5.19	125.00	111.00
2	B	72	GLN	CA-CB-CG	5.18	124.81	113.40
2	D	55	ASN	CB-CG-ND2	5.18	129.14	116.70
2	B	136	VAL	N-CA-CB	5.18	122.90	111.50
1	C	64	ASN	C-N-CA	5.18	134.66	121.70
1	A	124	ASN	CA-C-O	-5.18	109.22	120.10
1	A	135	VAL	CA-CB-CG1	5.18	118.67	110.90
2	B	131	LYS	N-CA-CB	5.18	119.92	110.60
2	D	91	HIS	N-CA-C	-5.18	97.02	111.00
2	B	27	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	C	101	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	A	22	PRO	N-CA-CB	-5.17	96.91	102.60
2	B	41	PHE	N-CA-C	5.17	124.97	111.00
2	D	66	VAL	O-C-N	5.17	130.98	122.70
2	D	102	PHE	N-CA-CB	-5.17	101.29	110.60
2	D	92	CYS	N-CA-CB	5.17	119.91	110.60
2	D	84	PHE	CG-CD2-CE2	-5.17	115.12	120.80
2	D	121	PHE	O-C-N	-5.16	114.45	122.70
1	A	7	LYS	N-CA-C	-5.15	97.09	111.00
1	A	45	HIS	N-CA-C	5.15	124.91	111.00
2	B	125	VAL	O-C-N	5.15	130.94	122.70
1	A	33	PHE	CA-C-N	-5.15	105.87	117.20
1	C	102	SER	N-CA-C	-5.14	97.13	111.00
2	B	29	ARG	CB-CA-C	-5.14	100.12	110.40
1	A	75	ASP	N-CA-CB	-5.13	101.36	110.60
2	B	21	VAL	N-CA-C	-5.13	97.15	111.00
2	B	36	TRP	CA-C-N	-5.13	105.91	117.20
1	A	76	LEU	O-C-N	-5.13	111.36	121.10
2	D	91	HIS	CA-CB-CG	-5.13	104.88	113.60
1	A	122	HIS	ND1-CG-CD2	5.12	115.97	108.80
2	B	134	ALA	CA-C-O	5.12	130.86	120.10
2	D	26	ALA	N-CA-C	-5.12	97.17	111.00
2	B	19	VAL	CB-CA-C	-5.12	101.67	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	THR	CA-C-O	-5.12	109.36	120.10
1	C	140	TYR	C-N-CA	5.12	134.49	121.70
1	A	90	LYS	CA-CB-CG	5.11	124.64	113.40
1	A	85	ASN	O-C-N	5.11	130.87	122.70
1	C	127	LYS	CB-CG-CD	5.10	124.86	111.60
1	A	50	HIS	O-C-N	5.10	131.87	123.20
1	A	45	HIS	CE1-NE2-CD2	-5.09	93.87	106.60
1	C	42	TYR	C-N-CA	5.09	134.43	121.70
2	D	45	GLY	C-N-CA	-5.09	108.97	121.70
2	D	108	VAL	CB-CA-C	5.09	121.08	111.40
2	D	124	ASN	N-CA-C	-5.09	97.26	111.00
1	A	98	PHE	CA-C-O	-5.09	109.42	120.10
2	B	124	ASN	CA-CB-CG	5.09	124.59	113.40
2	B	1	MET	O-C-N	5.08	130.84	122.70
2	B	14	TRP	CB-CA-C	-5.08	100.23	110.40
1	C	14	TRP	CZ3-CH2-CZ2	5.08	127.70	121.60
1	C	110	ALA	CB-CA-C	-5.08	102.47	110.10
2	D	96	HIS	CA-CB-CG	-5.08	104.96	113.60
1	A	32	MET	CA-C-O	-5.08	109.43	120.10
1	A	46	PHE	O-C-N	-5.08	114.57	122.70
1	A	140	TYR	CE1-CZ-OH	-5.08	106.39	120.10
2	B	41	PHE	CA-CB-CG	5.07	126.08	113.90
2	B	100	GLN	N-CA-C	-5.07	97.30	111.00
1	C	33	PHE	CA-CB-CG	5.07	126.07	113.90
1	A	108	THR	CB-CA-C	5.07	125.29	111.60
1	C	14	TRP	CA-CB-CG	-5.06	104.09	113.70
2	B	61	ALA	CA-C-N	-5.05	106.08	117.20
1	A	115	THR	CA-C-O	5.05	130.71	120.10
1	C	99	LYS	CA-C-O	-5.05	109.50	120.10
1	A	54	GLN	CA-CB-CG	-5.05	102.30	113.40
2	D	91	HIS	CB-CA-C	5.05	120.49	110.40
1	C	112	HIS	N-CA-C	-5.04	97.39	111.00
2	B	31	LEU	CA-CB-CG	-5.04	103.71	115.30
2	B	140	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	C	2	LEU	CA-C-N	5.03	128.28	117.20
2	B	126	GLN	O-C-N	5.03	130.74	122.70
1	C	1	VAL	C-N-CA	-5.03	109.13	121.70
1	A	127	LYS	CB-CA-C	-5.02	100.35	110.40
2	B	84	PHE	O-C-N	-5.02	114.67	122.70
1	C	52	SER	CA-C-N	5.02	128.24	117.20
1	A	135	VAL	N-CA-CB	5.02	122.54	111.50
2	B	115	ARG	CG-CD-NE	-5.02	101.27	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PHE	CB-CA-C	-5.01	100.37	110.40
1	C	112	HIS	ND1-CE1-NE2	5.01	120.93	109.90
1	A	93	VAL	CG1-CB-CG2	5.01	118.92	110.90
1	A	97	ASN	CA-CB-CG	-5.00	102.39	113.40
1	A	101	LEU	CD1-CG-CD2	-5.00	95.49	110.50

All (19) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2	LEU	CA
1	A	31	ARG	CA
1	A	33	PHE	CA
1	A	93	VAL	CA
1	A	100	LEU	CA
1	A	108	THR	CB
1	A	122	HIS	CA
1	A	132	ASP	CA
1	A	139	LYS	CA
2	B	24	ALA	CA
2	B	112	VAL	CA
1	C	1	VAL	CA
1	C	108	THR	CB
2	D	11	THR	CA
2	D	56	ASN	CA
2	D	101	ASN	CA
2	D	103	ARG	CA
2	D	116	ASN	CA
2	D	145	HIS	CA

All (184) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Mainchain,Peptide
1	A	100	LEU	Mainchain
1	A	102	SER	Mainchain
1	A	103	HIS	Mainchain
1	A	104	SER	Mainchain
1	A	106	LEU	Mainchain
1	A	107	VAL	Peptide
1	A	111	SER	Mainchain
1	A	117	PHE	Sidechain
1	A	127	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	131	ASN	Mainchain
1	A	132	ASP	Sidechain
1	A	138	SER	Mainchain
1	A	15	GLY	Peptide
1	A	22	PRO	Mainchain
1	A	24	TYR	Sidechain
1	A	26	ALA	Mainchain
1	A	28	ALA	Mainchain,Peptide
1	A	29	LEU	Mainchain
1	A	3	SER	Mainchain
1	A	30	GLN	Peptide
1	A	31	ARG	Sidechain
1	A	33	PHE	Sidechain
1	A	37	PRO	Mainchain
1	A	40	LYS	Mainchain
1	A	41	THR	Peptide
1	A	42	TYR	Sidechain
1	A	45	HIS	Peptide
1	A	46	PHE	Mainchain,Peptide
1	A	49	SER	Mainchain,Peptide
1	A	50	HIS	Mainchain
1	A	51	GLY	Mainchain
1	A	55	GLN	Mainchain
1	A	70	GLN	Mainchain
1	A	74	ASN	Mainchain
1	A	8	SER	Mainchain,Peptide
1	A	80	LEU	Peptide
1	A	85	ASN	Sidechain,Mainchain
1	A	89	HIS	Sidechain,Mainchain
1	A	92	ARG	Sidechain,Peptide
1	A	97	ASN	Mainchain
1	A	98	PHE	Sidechain,Mainchain
1	A	99	LYS	Mainchain
2	B	1	MET	Mainchain
2	B	10	VAL	Mainchain
2	B	100	GLN	Sidechain
2	B	101	ASN	Mainchain
2	B	102	PHE	Sidechain
2	B	103	ARG	Sidechain,Mainchain
2	B	115	ARG	Sidechain
2	B	118	GLY	Mainchain
2	B	121	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	B	129	PHE	Sidechain
2	B	13	PHE	Mainchain
2	B	136	VAL	Mainchain
2	B	137	ALA	Mainchain
2	B	144	TYR	Sidechain
2	B	16	LYS	Mainchain
2	B	18	ASP	Sidechain
2	B	21	VAL	Mainchain
2	B	29	ARG	Sidechain
2	B	32	VAL	Mainchain
2	B	39	ARG	Sidechain
2	B	43	HIS	Sidechain
2	B	44	PHE	Sidechain
2	B	46	ASN	Mainchain
2	B	5	GLU	Mainchain
2	B	55	ASN	Sidechain
2	B	59	VAL	Mainchain
2	B	6	GLU	Mainchain
2	B	65	ARG	Sidechain
2	B	67	LEU	Mainchain
2	B	68	ASP	Peptide
2	B	71	THR	Mainchain
2	B	72	GLN	Mainchain
2	B	74	LEU	Mainchain
2	B	76	HIS	Sidechain
2	B	82	GLY	Peptide
2	B	84	PHE	Mainchain
2	B	87	LEU	Mainchain
2	B	95	LEU	Mainchain
2	B	96	HIS	Sidechain
1	C	1	VAL	Mainchain
1	C	103	HIS	Mainchain
1	C	11	LYS	Mainchain
1	C	111	SER	Mainchain
1	C	115	THR	Mainchain
1	C	117	PHE	Peptide
1	C	12	ALA	Mainchain
1	C	120	ALA	Mainchain
1	C	125	LEU	Mainchain
1	C	126	ASN	Sidechain
1	C	131	ASN	Mainchain
1	C	135	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	C	137	THR	Mainchain
1	C	139	LYS	Peptide
1	C	140	TYR	Mainchain
1	C	16	LYS	Mainchain
1	C	2	LEU	Mainchain
1	C	24	TYR	Sidechain
1	C	35	SER	Mainchain
1	C	38	THR	Mainchain
1	C	42	TYR	Sidechain,Mainchain
1	C	47	ASP	Peptide
1	C	49	SER	Mainchain
1	C	50	HIS	Sidechain
1	C	54	GLN	Mainchain
1	C	55	GLN	Mainchain
1	C	57	ALA	Mainchain
1	C	58	HIS	Sidechain
1	C	62	VAL	Peptide
1	C	72	HIS	Sidechain
1	C	79	THR	Mainchain
1	C	80	LEU	Mainchain
1	C	82	ASN	Sidechain
1	C	83	LEU	Peptide
1	C	84	SER	Mainchain,Peptide
1	C	85	ASN	Mainchain
1	C	91	LEU	Mainchain
1	C	92	ARG	Sidechain
1	C	93	VAL	Mainchain
2	D	10	VAL	Mainchain
2	D	102	PHE	Sidechain
2	D	103	ARG	Sidechain
2	D	105	LEU	Mainchain
2	D	114	ALA	Mainchain
2	D	115	ARG	Sidechain
2	D	116	ASN	Sidechain
2	D	117	PHE	Sidechain,Mainchain,Peptide
2	D	12	GLY	Mainchain
2	D	124	ASN	Mainchain
2	D	126	GLN	Sidechain
2	D	127	ALA	Mainchain
2	D	129	PHE	Sidechain
2	D	133	VAL	Mainchain
2	D	135	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	D	137	ALA	Peptide
2	D	138	ASN	Mainchain,Peptide
2	D	142	HIS	Sidechain,Peptide
2	D	143	LYS	Mainchain
2	D	144	TYR	Sidechain
2	D	17	VAL	Mainchain
2	D	18	ASP	Sidechain
2	D	2	LEU	Mainchain
2	D	28	GLY	Mainchain
2	D	29	ARG	Mainchain
2	D	34	TYR	Sidechain
2	D	39	ARG	Sidechain
2	D	42	GLN	Peptide
2	D	44	PHE	Sidechain
2	D	5	GLU	Mainchain,Peptide
2	D	53	VAL	Mainchain
2	D	55	ASN	Sidechain
2	D	65	ARG	Sidechain
2	D	67	LEU	Mainchain
2	D	69	ALA	Mainchain
2	D	71	THR	Peptide
2	D	72	GLN	Mainchain
2	D	73	GLY	Peptide
2	D	76	HIS	Sidechain,Mainchain
2	D	77	LEU	Mainchain
2	D	8	ALA	Peptide
2	D	88	SER	Mainchain
2	D	89	GLY	Peptide
2	D	9	ALA	Mainchain
2	D	99	PRO	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	1076	0	1032	834	80
1	C	1076	0	1034	805	3
2	B	1116	0	1070	1126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1116	0	1068	917	77
3	A	43	0	30	49	0
3	B	43	0	30	56	0
3	C	43	0	30	42	0
3	D	43	0	30	29	0
All	All	4556	0	4324	3698	80

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 416.

All (3698) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:TYR:CZ	2:B:34:TYR:CE2	1.79	1.70
2:B:144:TYR:CG	2:B:144:TYR:CD2	1.76	1.69
3:A:142:HEM:CMA	3:A:142:HEM:C3A	1.75	1.67
1:C:140:TYR:CB	1:C:140:TYR:CG	1.77	1.67
2:D:14:TRP:CZ3	2:D:14:TRP:CE3	1.76	1.66
1:C:103:HIS:CB	1:C:103:HIS:CG	1.78	1.66
2:D:22:VAL:CB	2:D:22:VAL:CG1	1.74	1.65
2:B:84:PHE:CB	2:B:84:PHE:CG	1.76	1.65
1:A:14:TRP:CZ2	1:A:14:TRP:CH2	1.79	1.65
3:C:142:HEM:CAB	3:C:142:HEM:C3B	1.80	1.65
1:C:91:LEU:CG	1:C:91:LEU:CB	1.75	1.65
1:C:86:LEU:CG	1:C:86:LEU:CD1	1.75	1.64
1:A:36:PHE:CB	1:A:36:PHE:CG	1.78	1.64
2:B:70:PHE:CE2	2:B:70:PHE:CZ	1.84	1.64
2:D:123:PRO:CG	2:D:123:PRO:CD	1.74	1.64
1:A:2:LEU:CB	1:A:2:LEU:CA	1.76	1.64
2:B:70:PHE:CZ	2:B:70:PHE:CE1	1.76	1.64
1:A:140:TYR:CB	1:A:140:TYR:CG	1.79	1.64
1:C:7:LYS:CB	1:C:7:LYS:CG	1.75	1.63
2:D:41:PHE:CE2	2:D:41:PHE:CD2	1.75	1.63
1:A:63:ALA:CA	1:A:63:ALA:CB	1.75	1.63
1:A:81:SER:CB	1:A:81:SER:CA	1.76	1.63
3:A:142:HEM:CBA	3:A:142:HEM:CAA	1.75	1.62
3:A:142:HEM:CAD	3:A:142:HEM:CBD	1.74	1.62
2:B:41:PHE:CE1	2:B:41:PHE:CZ	1.78	1.62
1:C:24:TYR:CG	1:C:24:TYR:CB	1.83	1.62
2:B:64:LYS:CD	2:B:64:LYS:CG	1.75	1.62
1:C:23:ALA:CA	1:C:23:ALA:CB	1.75	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:LEU:CB	2:D:2:LEU:CG	1.76	1.62
2:D:60:LYS:CD	2:D:60:LYS:CE	1.78	1.62
3:D:146:HEM:CAA	3:D:146:HEM:CBA	1.77	1.61
3:B:146:HEM:CAD	3:B:146:HEM:C3D	1.77	1.61
1:C:92:ARG:CD	1:C:92:ARG:CG	1.78	1.61
3:A:142:HEM:C1D	3:A:142:HEM:C2D	1.78	1.61
2:D:81:LYS:CB	2:D:81:LYS:CA	1.76	1.61
2:B:102:PHE:CG	2:B:102:PHE:CD1	1.89	1.61
2:B:36:TRP:CD2	2:B:36:TRP:CG	1.85	1.61
2:D:120:GLN:CG	2:D:120:GLN:CB	1.78	1.61
1:C:117:PHE:CE2	1:C:117:PHE:CD2	1.82	1.61
1:C:136:LEU:CB	1:C:136:LEU:CA	1.78	1.60
2:B:11:THR:CA	2:B:11:THR:CB	1.79	1.60
1:C:54:GLN:CG	1:C:54:GLN:CB	1.75	1.60
2:D:59:VAL:CG2	2:D:59:VAL:CB	1.77	1.60
2:D:84:PHE:CD1	2:D:84:PHE:CG	1.84	1.60
1:A:22:PRO:CG	1:A:22:PRO:CB	1.77	1.60
1:A:93:VAL:CG1	1:A:93:VAL:CB	1.79	1.60
2:B:10:VAL:CB	2:B:10:VAL:CG1	1.79	1.60
1:A:137:THR:CA	1:A:137:THR:CB	1.79	1.60
1:C:24:TYR:CD2	1:C:24:TYR:CE2	1.89	1.60
2:D:22:VAL:CG2	2:D:22:VAL:CB	1.74	1.60
2:B:117:PHE:CD1	2:B:117:PHE:CG	1.81	1.60
1:C:68:LYS:CG	1:C:68:LYS:CB	1.75	1.60
2:B:21:VAL:CB	2:B:21:VAL:CA	1.77	1.59
2:B:16:LYS:CE	2:B:16:LYS:CD	1.80	1.59
2:B:77:LEU:CB	2:B:77:LEU:CA	1.79	1.59
1:C:128:PHE:CE1	1:C:128:PHE:CZ	1.84	1.59
3:D:146:HEM:CMB	3:D:146:HEM:C2B	1.80	1.59
1:A:16:LYS:CD	1:A:16:LYS:CE	1.77	1.59
1:A:2:LEU:CB	1:A:2:LEU:CG	1.74	1.59
1:A:79:THR:CB	1:A:79:THR:CA	1.76	1.59
1:A:41:THR:CB	1:A:41:THR:CA	1.80	1.59
1:C:60:GLN:CG	1:C:60:GLN:CB	1.76	1.59
1:C:61:LYS:CD	1:C:61:LYS:CG	1.76	1.59
2:D:86:GLN:CB	2:D:86:GLN:CA	1.76	1.59
2:B:103:ARG:CB	2:B:103:ARG:CG	1.78	1.59
1:A:127:LYS:CD	1:A:127:LYS:CE	1.77	1.59
1:A:91:LEU:CD2	1:A:91:LEU:CG	1.78	1.59
2:B:10:VAL:HG11	2:B:128:LEU:CD2	1.17	1.59
1:A:12:ALA:CA	1:A:12:ALA:CB	1.81	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:VAL:CB	1:A:1:VAL:CG1	1.75	1.59
1:C:17:VAL:CG1	1:C:17:VAL:CB	1.78	1.58
1:C:32:MET:CA	1:C:32:MET:CB	1.76	1.58
1:C:75:ASP:CB	1:C:75:ASP:CA	1.77	1.58
1:C:91:LEU:CG	1:C:91:LEU:CD1	1.79	1.58
2:D:6:GLU:CA	2:D:6:GLU:CB	1.79	1.58
2:D:75:LYS:CD	2:D:75:LYS:CG	1.76	1.58
1:C:76:LEU:CG	1:C:76:LEU:CD1	1.78	1.58
2:D:47:LEU:CB	2:D:47:LEU:CA	1.77	1.58
1:A:73:LEU:CG	1:A:73:LEU:CD2	1.81	1.58
2:B:31:LEU:CD1	2:B:31:LEU:CG	1.77	1.58
2:D:76:HIS:CB	2:D:76:HIS:CG	1.86	1.58
1:A:3:SER:CA	1:A:3:SER:CB	1.75	1.58
1:A:65:ALA:CB	1:A:65:ALA:CA	1.76	1.58
3:B:146:HEM:CMB	3:B:146:HEM:C2B	1.84	1.58
1:A:93:VAL:CG2	1:A:93:VAL:CB	1.74	1.58
2:B:97:VAL:CB	2:B:97:VAL:CA	1.75	1.58
1:A:55:GLN:CA	1:A:55:GLN:CB	1.81	1.58
1:A:128:PHE:CE1	1:A:128:PHE:CD1	1.83	1.58
1:A:31:ARG:CD	1:A:31:ARG:CG	1.74	1.58
1:A:41:THR:CB	1:A:41:THR:CG2	1.77	1.58
2:B:68:ASP:CA	2:B:71:THR:CG2	1.75	1.58
1:C:138:SER:CA	1:C:138:SER:CB	1.82	1.58
1:C:83:LEU:CD2	1:C:83:LEU:CG	1.78	1.57
2:B:16:LYS:CE	2:B:16:LYS:NZ	1.67	1.57
1:A:127:LYS:CB	1:A:127:LYS:CG	1.78	1.57
1:C:66:LEU:CG	1:C:66:LEU:CD2	1.81	1.57
1:A:139:LYS:CD	1:A:139:LYS:CE	1.77	1.57
1:A:104:SER:CB	1:A:104:SER:CA	1.78	1.57
2:B:128:LEU:CG	2:B:128:LEU:CD1	1.74	1.57
2:B:1:MET:HG2	2:B:77:LEU:CD1	1.29	1.57
1:A:43:PHE:CB	1:A:43:PHE:CA	1.77	1.57
1:A:7:LYS:CE	1:A:7:LYS:CD	1.79	1.57
2:B:86:GLN:CB	2:B:86:GLN:CG	1.75	1.57
2:D:64:LYS:CG	2:D:64:LYS:CD	1.74	1.57
1:C:108:THR:CB	1:C:108:THR:CG2	1.78	1.56
1:C:22:PRO:CD	1:C:22:PRO:CG	1.82	1.56
2:D:121:PHE:CA	2:D:121:PHE:CB	1.83	1.56
2:B:94:LYS:CD	2:B:94:LYS:CG	1.75	1.56
1:A:136:LEU:CG	1:A:136:LEU:CD1	1.79	1.56
3:A:142:HEM:C4B	3:A:142:HEM:NB	1.67	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:N	1:A:97:ASN:CA	1.69	1.56
2:D:31:LEU:CB	2:D:31:LEU:CA	1.81	1.56
2:D:43:HIS:CB	2:D:43:HIS:CA	1.84	1.56
1:A:43:PHE:CD2	1:A:43:PHE:CG	1.86	1.56
1:A:57:ALA:CB	1:A:57:ALA:CA	1.74	1.56
1:C:80:LEU:CD1	1:C:80:LEU:CG	1.83	1.56
2:D:103:ARG:CD	2:D:103:ARG:CG	1.75	1.56
2:B:3:THR:HG23	2:B:5:GLU:CB	1.12	1.56
2:B:64:LYS:CE	2:B:64:LYS:NZ	1.68	1.56
2:B:116:ASN:CA	2:B:116:ASN:CB	1.77	1.56
1:A:50:HIS:CG	1:A:50:HIS:CB	1.87	1.56
1:C:28:ALA:N	1:C:28:ALA:CA	1.69	1.56
1:C:76:LEU:CG	1:C:76:LEU:CD2	1.76	1.56
2:B:140:LEU:CG	2:B:140:LEU:CD1	1.75	1.56
1:C:133:SER:CB	1:C:133:SER:CA	1.74	1.56
2:D:12:GLY:N	2:D:12:GLY:CA	1.68	1.56
2:D:144:TYR:CZ	2:D:144:TYR:CE1	1.94	1.56
1:A:62:VAL:CB	1:A:62:VAL:CG1	1.83	1.55
1:C:3:SER:C	1:C:3:SER:CA	1.74	1.55
2:D:81:LYS:CE	2:D:81:LYS:CD	1.75	1.55
1:A:105:LEU:CD1	1:A:105:LEU:CG	1.76	1.55
2:B:45:GLY:CA	2:B:45:GLY:N	1.67	1.55
1:C:101:LEU:CA	1:C:101:LEU:CB	1.77	1.55
1:C:29:LEU:CA	1:C:29:LEU:CB	1.77	1.55
1:C:36:PHE:CA	1:C:36:PHE:CB	1.84	1.55
2:B:128:LEU:CA	2:B:128:LEU:CB	1.82	1.55
2:D:105:LEU:CG	2:D:105:LEU:CD1	1.76	1.55
2:B:16:LYS:CA	2:B:16:LYS:N	1.68	1.55
2:D:62:HIS:ND1	2:D:62:HIS:CG	1.70	1.55
2:D:62:HIS:NE2	2:D:62:HIS:CE1	1.68	1.55
2:B:37:THR:CA	2:B:37:THR:N	1.69	1.55
2:D:65:ARG:C	2:D:65:ARG:CA	1.75	1.55
1:A:119:PRO:CB	1:A:119:PRO:CA	1.81	1.55
2:B:68:ASP:CB	2:B:68:ASP:CG	1.74	1.55
1:C:53:ALA:N	1:C:53:ALA:CA	1.70	1.55
1:C:72:HIS:CG	1:C:72:HIS:CD2	1.85	1.55
1:C:86:LEU:CD2	1:C:86:LEU:CG	1.75	1.55
1:A:35:SER:CA	1:A:35:SER:CB	1.79	1.55
1:A:58:HIS:CB	1:A:58:HIS:CA	1.85	1.55
1:C:15:GLY:CA	1:C:15:GLY:N	1.69	1.55
1:C:80:LEU:C	1:C:80:LEU:CA	1.75	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:PHE:CE2	2:D:40:PHE:CZ	1.90	1.55
2:D:2:LEU:CB	2:D:2:LEU:CA	1.81	1.54
3:A:142:HEM:CHA	3:A:142:HEM:C4D	1.89	1.54
1:A:91:LEU:CG	1:A:91:LEU:CD1	1.79	1.54
2:B:128:LEU:C	2:B:128:LEU:CA	1.75	1.54
2:B:143:LYS:CD	2:B:143:LYS:CE	1.84	1.54
1:C:55:GLN:CB	1:C:55:GLN:CA	1.84	1.54
2:D:90:LEU:CG	2:D:90:LEU:CB	1.84	1.54
1:A:139:LYS:CE	1:A:139:LYS:NZ	1.69	1.54
2:B:141:ALA:CA	2:B:141:ALA:N	1.69	1.54
2:D:18:ASP:CA	2:D:18:ASP:CB	1.81	1.54
2:B:64:LYS:CA	2:B:64:LYS:N	1.67	1.54
2:B:19:VAL:CB	2:B:19:VAL:CA	1.81	1.54
1:A:108:THR:CB	1:A:108:THR:CA	1.82	1.54
2:B:130:GLN:CB	2:B:130:GLN:CG	1.77	1.54
1:C:114:PRO:N	1:C:114:PRO:CA	1.67	1.54
2:D:131:LYS:CB	2:D:131:LYS:CG	1.78	1.54
3:B:146:HEM:NA	3:B:146:HEM:C4A	1.68	1.54
2:D:110:ALA:N	2:D:110:ALA:CA	1.69	1.54
1:A:86:LEU:CD2	1:A:86:LEU:CG	1.84	1.54
2:B:71:THR:CB	2:B:71:THR:CG2	1.78	1.54
1:C:141:ARG:CD	1:C:141:ARG:NE	1.71	1.54
1:C:39:THR:CA	1:C:39:THR:CB	1.76	1.54
1:C:43:PHE:CB	1:C:43:PHE:CA	1.83	1.54
1:C:64:ASN:CA	1:C:64:ASN:CB	1.82	1.54
1:A:137:THR:CB	1:A:137:THR:CG2	1.86	1.53
2:B:26:ALA:C	2:B:26:ALA:CA	1.74	1.53
2:B:94:LYS:CA	2:B:94:LYS:C	1.74	1.53
2:B:123:PRO:CG	2:B:123:PRO:CB	1.79	1.53
1:C:113:LEU:CG	1:C:113:LEU:CD2	1.84	1.53
1:C:115:THR:CG2	1:C:115:THR:CB	1.77	1.53
1:A:45:HIS:CB	1:A:45:HIS:CA	1.85	1.53
1:C:45:HIS:CB	1:C:45:HIS:CA	1.81	1.53
2:B:4:ALA:N	2:B:4:ALA:CA	1.69	1.53
2:B:66:VAL:CB	2:B:66:VAL:CG1	1.84	1.53
1:C:116:ASN:C	1:C:116:ASN:CA	1.77	1.53
1:C:83:LEU:CA	1:C:83:LEU:CB	1.79	1.53
2:D:17:VAL:CA	2:D:17:VAL:C	1.75	1.53
1:A:114:PRO:CG	1:A:114:PRO:CD	1.81	1.53
2:B:87:LEU:CA	2:B:87:LEU:C	1.76	1.53
2:D:16:LYS:CB	2:D:16:LYS:CD	1.85	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:GLY:C	2:D:73:GLY:CA	1.75	1.53
1:A:106:LEU:CG	1:A:106:LEU:CD2	1.85	1.53
1:C:43:PHE:CG	1:C:43:PHE:CD1	1.96	1.53
2:D:101:ASN:CA	2:D:101:ASN:N	1.68	1.53
1:C:99:LYS:CG	1:C:99:LYS:CD	1.82	1.53
2:D:14:TRP:C	2:D:14:TRP:CA	1.77	1.53
1:A:56:LYS:CE	1:A:56:LYS:NZ	1.71	1.53
2:D:127:ALA:CB	2:D:127:ALA:CA	1.81	1.53
2:D:61:ALA:CA	2:D:61:ALA:CB	1.84	1.53
1:A:116:ASN:N	1:A:116:ASN:CA	1.69	1.53
1:C:114:PRO:N	1:C:114:PRO:CD	1.71	1.53
2:D:107:ASN:CA	2:D:107:ASN:N	1.69	1.52
2:D:112:VAL:CG1	2:D:112:VAL:CB	1.79	1.52
2:D:119:GLY:N	2:D:119:GLY:CA	1.72	1.52
1:A:11:LYS:NZ	1:A:11:LYS:CE	1.72	1.52
1:C:134:THR:CA	1:C:134:THR:N	1.70	1.52
1:C:137:THR:CA	1:C:137:THR:N	1.71	1.52
1:A:88:ALA:CA	1:A:88:ALA:C	1.76	1.52
2:B:131:LYS:CG	2:B:131:LYS:CD	1.82	1.52
1:C:71:GLY:CA	1:C:71:GLY:C	1.76	1.52
1:A:85:ASN:C	1:A:85:ASN:CA	1.76	1.52
2:B:59:VAL:CG1	2:B:59:VAL:CB	1.82	1.52
2:D:69:ALA:C	2:D:69:ALA:CA	1.74	1.52
1:A:10:VAL:C	1:A:10:VAL:CA	1.76	1.52
2:B:43:HIS:C	2:B:43:HIS:CA	1.78	1.52
2:B:58:LYS:CG	2:B:58:LYS:CB	1.86	1.52
2:B:65:ARG:N	2:B:65:ARG:CA	1.72	1.52
2:D:100:GLN:CG	2:D:100:GLN:CB	1.83	1.52
2:B:24:ALA:CA	2:B:24:ALA:N	1.68	1.52
2:B:80:LEU:CG	2:B:80:LEU:CD2	1.81	1.52
1:C:17:VAL:CG2	1:C:17:VAL:CB	1.87	1.52
1:C:90:LYS:CE	1:C:90:LYS:NZ	1.70	1.52
2:D:93:ASN:CB	2:D:93:ASN:CG	1.76	1.52
2:D:27:LEU:CD1	2:D:27:LEU:CG	1.84	1.52
2:D:43:HIS:NE2	2:D:43:HIS:CD2	1.75	1.52
2:B:4:ALA:CA	2:B:4:ALA:C	1.75	1.52
1:C:131:ASN:CA	1:C:131:ASN:CB	1.81	1.51
2:D:140:LEU:CD1	2:D:140:LEU:CG	1.85	1.51
2:D:16:LYS:CB	2:D:16:LYS:HD3	1.38	1.51
2:D:34:TYR:N	2:D:34:TYR:CA	1.73	1.51
2:B:130:GLN:CB	2:B:130:GLN:CA	1.84	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:GLN:N	2:B:25:GLN:CA	1.68	1.51
1:C:81:SER:CA	1:C:81:SER:CB	1.88	1.51
2:B:17:VAL:C	2:B:17:VAL:CA	1.76	1.51
1:A:100:LEU:CB	1:A:100:LEU:CG	1.86	1.51
2:B:8:ALA:CA	2:B:8:ALA:CB	1.82	1.51
2:D:68:ASP:CG	2:D:68:ASP:CB	1.78	1.51
2:B:119:GLY:CA	2:B:119:GLY:N	1.67	1.51
2:B:43:HIS:CG	2:B:43:HIS:ND1	1.75	1.51
2:D:75:LYS:CA	2:D:75:LYS:CB	1.85	1.51
1:A:73:LEU:CD1	1:A:73:LEU:CG	1.86	1.51
2:B:22:VAL:CB	2:B:22:VAL:CG2	1.86	1.51
2:D:52:ALA:CB	2:D:52:ALA:CA	1.83	1.51
1:C:16:LYS:CD	1:C:16:LYS:CG	1.88	1.51
1:A:60:GLN:CA	1:A:60:GLN:C	1.77	1.51
2:B:49:SER:C	2:B:49:SER:CA	1.75	1.51
1:C:79:THR:N	1:C:79:THR:CA	1.69	1.51
2:B:2:LEU:CB	2:B:2:LEU:CA	1.88	1.51
2:B:125:VAL:CG1	2:B:125:VAL:CB	1.89	1.50
2:B:74:LEU:CB	2:B:74:LEU:CG	1.83	1.50
1:C:126:ASN:CA	1:C:126:ASN:C	1.76	1.50
1:C:20:ASN:N	1:C:20:ASN:CA	1.71	1.50
2:D:120:GLN:CD	2:D:120:GLN:CG	1.78	1.50
2:B:2:LEU:CG	2:B:2:LEU:CD2	1.89	1.50
2:D:100:GLN:CB	2:D:100:GLN:CA	1.82	1.50
2:B:104:LEU:N	2:B:104:LEU:CA	1.74	1.50
2:B:13:PHE:CA	2:B:13:PHE:C	1.79	1.50
2:B:40:PHE:C	2:B:40:PHE:CA	1.79	1.50
1:C:54:GLN:C	1:C:54:GLN:CA	1.76	1.50
1:A:122:HIS:CA	1:A:122:HIS:C	1.74	1.50
3:A:142:HEM:C4D	3:A:142:HEM:C2D	1.98	1.50
1:A:2:LEU:CD1	1:A:2:LEU:CG	1.87	1.50
1:C:105:LEU:CD1	1:C:105:LEU:CG	1.89	1.50
2:D:38:GLN:CG	2:D:38:GLN:CD	1.75	1.50
2:B:57:PRO:N	2:B:57:PRO:CD	1.74	1.50
2:D:39:ARG:CD	2:D:39:ARG:NE	1.70	1.50
1:A:48:LEU:CB	1:A:48:LEU:CA	1.86	1.50
1:A:80:LEU:CG	1:A:80:LEU:CD2	1.85	1.50
2:B:137:ALA:N	2:B:137:ALA:CA	1.71	1.50
2:D:109:LEU:CG	2:D:109:LEU:CD2	1.89	1.50
2:D:46:ASN:N	2:D:46:ASN:CA	1.68	1.50
2:D:44:PHE:CA	2:D:44:PHE:CB	1.86	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:THR:CG2	2:B:5:GLU:HB3	1.39	1.50
2:B:83:ALA:CA	2:B:83:ALA:CB	1.86	1.50
2:B:143:LYS:CG	2:B:143:LYS:CD	1.88	1.50
1:C:47:ASP:CG	1:C:47:ASP:CB	1.76	1.50
2:B:24:ALA:CB	2:B:24:ALA:CA	1.85	1.50
1:C:129:LEU:CB	1:C:129:LEU:CG	1.87	1.50
2:D:75:LYS:CE	2:D:75:LYS:NZ	1.71	1.50
2:B:43:HIS:NE2	2:B:43:HIS:CD2	1.79	1.49
2:D:11:THR:C	2:D:11:THR:CA	1.79	1.49
1:A:48:LEU:CD2	1:A:48:LEU:CG	1.90	1.49
2:B:110:ALA:CB	2:B:110:ALA:CA	1.90	1.49
1:C:67:THR:CB	1:C:67:THR:CG2	1.87	1.49
1:A:114:PRO:CB	1:A:114:PRO:CD	1.89	1.49
1:A:135:VAL:CA	1:A:135:VAL:C	1.77	1.49
2:B:75:LYS:CG	2:B:75:LYS:CD	1.87	1.49
1:C:133:SER:C	1:C:133:SER:CA	1.77	1.49
1:C:44:PRO:CG	1:C:44:PRO:CB	1.91	1.49
2:D:129:PHE:CA	2:D:129:PHE:N	1.76	1.49
1:A:19:GLY:C	1:A:19:GLY:CA	1.79	1.49
1:C:11:LYS:CA	1:C:11:LYS:N	1.73	1.49
1:C:19:GLY:C	1:C:19:GLY:CA	1.79	1.49
1:C:91:LEU:N	1:C:91:LEU:CA	1.69	1.49
2:D:10:VAL:CA	2:D:10:VAL:C	1.77	1.49
2:D:142:HIS:CB	2:D:142:HIS:CA	1.87	1.49
1:A:105:LEU:CA	1:A:105:LEU:N	1.73	1.49
2:B:6:GLU:CB	2:B:6:GLU:CA	1.87	1.49
2:D:88:SER:CB	2:D:88:SER:CA	1.85	1.49
2:D:36:TRP:CA	2:D:36:TRP:C	1.79	1.49
2:B:62:HIS:CG	2:B:62:HIS:ND1	1.68	1.49
1:C:135:VAL:CB	1:C:135:VAL:CG2	1.90	1.49
2:B:128:LEU:CG	2:B:128:LEU:CD2	1.89	1.49
2:D:67:LEU:CA	2:D:67:LEU:CB	1.84	1.49
2:D:76:HIS:CA	2:D:76:HIS:N	1.72	1.49
1:A:61:LYS:CB	1:A:61:LYS:CA	1.88	1.48
2:B:62:HIS:N	2:B:62:HIS:CA	1.74	1.48
2:B:72:GLN:N	2:B:72:GLN:CA	1.70	1.48
1:A:103:HIS:CA	1:A:103:HIS:CB	1.88	1.48
2:D:132:VAL:N	2:D:132:VAL:CA	1.72	1.48
2:B:54:MET:CA	2:B:54:MET:N	1.72	1.48
1:A:136:LEU:CA	1:A:136:LEU:C	1.80	1.48
2:B:57:PRO:CG	2:B:57:PRO:CD	1.87	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:LEU:C	2:D:31:LEU:CA	1.81	1.48
1:A:29:LEU:CG	1:A:29:LEU:CD2	1.91	1.48
2:B:106:GLY:C	2:B:106:GLY:CA	1.80	1.48
2:D:93:ASN:CA	2:D:93:ASN:C	1.80	1.48
2:B:52:ALA:N	2:B:52:ALA:CA	1.75	1.48
2:D:128:LEU:N	2:D:128:LEU:CA	1.72	1.48
1:C:104:SER:CA	1:C:104:SER:C	1.77	1.48
1:C:10:VAL:CG2	1:C:10:VAL:CB	1.90	1.48
2:B:141:ALA:C	2:B:142:HIS:N	1.68	1.47
3:B:146:HEM:CMA	3:B:146:HEM:C3A	1.95	1.47
3:D:146:HEM:C1A	3:D:146:HEM:CHA	1.94	1.47
1:A:94:ASN:N	1:A:94:ASN:CA	1.75	1.47
1:A:126:ASN:C	1:A:126:ASN:CA	1.79	1.47
2:B:76:HIS:N	2:B:76:HIS:CA	1.74	1.47
1:C:25:GLY:N	1:C:25:GLY:CA	1.75	1.47
1:A:141:ARG:NH2	1:A:141:ARG:CZ	1.76	1.47
1:C:90:LYS:CE	1:C:90:LYS:CD	1.90	1.47
1:C:46:PHE:CE2	1:C:46:PHE:CZ	2.01	1.47
1:C:97:ASN:CA	1:C:97:ASN:C	1.76	1.47
2:D:143:LYS:CE	2:D:143:LYS:CD	1.90	1.47
2:D:78:ASP:CG	2:D:78:ASP:CB	1.83	1.47
1:A:29:LEU:CA	1:A:29:LEU:CB	1.92	1.47
1:A:67:THR:CA	1:A:67:THR:C	1.82	1.47
2:D:104:LEU:CG	2:D:104:LEU:CB	1.91	1.47
2:D:108:VAL:O	2:D:108:VAL:CA	1.63	1.47
2:D:68:ASP:CA	2:D:68:ASP:C	1.82	1.47
2:B:1:MET:CG	2:B:77:LEU:CD1	1.91	1.47
1:C:30:GLN:CD	1:C:30:GLN:CG	1.82	1.47
2:B:93:ASN:CG	2:B:93:ASN:CB	1.79	1.46
2:B:95:LEU:CA	2:B:95:LEU:CB	1.90	1.46
1:C:85:ASN:CB	1:C:85:ASN:CG	1.79	1.46
1:A:64:ASN:CA	1:A:64:ASN:C	1.81	1.46
2:D:115:ARG:CB	2:D:115:ARG:CA	1.93	1.46
2:B:140:LEU:CD2	2:B:140:LEU:CG	1.93	1.46
2:D:105:LEU:CB	2:D:105:LEU:CD1	1.90	1.46
2:D:142:HIS:ND1	2:D:142:HIS:CE1	1.68	1.46
2:B:18:ASP:CG	2:B:18:ASP:CB	1.83	1.46
2:B:70:PHE:CZ	2:B:70:PHE:CD2	2.04	1.46
1:C:139:LYS:CB	1:C:139:LYS:CG	1.91	1.46
2:B:34:TYR:CA	2:B:34:TYR:N	1.77	1.46
2:D:145:HIS:C	2:D:145:HIS:CA	1.83	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:VAL:CA	2:D:59:VAL:C	1.84	1.46
1:A:17:VAL:CB	1:A:17:VAL:CG2	1.89	1.46
2:B:138:ASN:ND2	2:B:138:ASN:CG	1.70	1.46
2:D:124:ASN:CG	2:D:124:ASN:CB	1.84	1.46
2:D:94:LYS:CE	2:D:94:LYS:CD	1.93	1.46
1:A:78:GLY:CA	1:A:78:GLY:C	1.81	1.46
1:C:118:THR:OG1	1:C:118:THR:CB	1.63	1.46
2:B:95:LEU:N	2:B:95:LEU:CB	1.77	1.45
2:D:86:GLN:C	2:D:86:GLN:CA	1.84	1.45
1:C:61:LYS:CD	1:C:61:LYS:CE	1.92	1.45
1:A:69:ALA:CA	1:A:69:ALA:N	1.76	1.45
1:C:108:THR:C	1:C:108:THR:CA	1.85	1.45
1:A:119:PRO:C	1:A:120:ALA:N	1.69	1.45
2:B:42:GLN:CD	2:B:42:GLN:NE2	1.69	1.45
2:D:78:ASP:CA	2:D:78:ASP:C	1.85	1.45
2:B:124:ASN:C	2:B:125:VAL:N	1.68	1.45
2:D:71:THR:CB	2:D:71:THR:CG2	1.92	1.45
1:A:16:LYS:CD	1:A:16:LYS:NZ	1.74	1.45
2:B:113:VAL:CB	2:B:113:VAL:CG1	1.92	1.45
2:B:74:LEU:CG	2:B:74:LEU:CD1	1.93	1.45
2:D:1:MET:N	2:D:1:MET:CA	1.80	1.45
2:B:101:ASN:CA	2:B:101:ASN:C	1.85	1.45
1:C:3:SER:CB	1:C:3:SER:CA	1.94	1.45
2:D:87:LEU:CB	2:D:87:LEU:CA	1.92	1.45
1:A:44:PRO:CA	1:A:44:PRO:CB	1.76	1.45
2:D:131:LYS:CA	2:D:131:LYS:CB	1.94	1.45
3:D:146:HEM:C3C	3:D:146:HEM:C4C	1.83	1.45
1:A:11:LYS:C	1:A:12:ALA:N	1.69	1.45
1:A:86:LEU:C	1:A:87:HIS:N	1.68	1.45
1:A:91:LEU:CA	1:A:91:LEU:N	1.78	1.45
2:D:124:ASN:CA	2:D:124:ASN:C	1.83	1.45
2:D:42:GLN:CA	2:D:42:GLN:CG	1.93	1.45
2:B:86:GLN:CD	2:B:86:GLN:NE2	1.70	1.44
1:C:85:ASN:CA	1:C:85:ASN:C	1.83	1.44
2:D:96:HIS:C	2:D:96:HIS:CA	1.84	1.44
2:B:96:HIS:NE2	2:B:96:HIS:CE1	1.68	1.44
2:D:141:ALA:C	2:D:142:HIS:N	1.71	1.44
1:C:68:LYS:CE	1:C:68:LYS:NZ	1.78	1.44
1:C:69:ALA:CA	1:C:69:ALA:C	1.83	1.44
1:A:32:MET:CE	1:A:32:MET:SD	2.04	1.44
2:B:133:VAL:CB	2:B:133:VAL:CG2	1.96	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:LEU:C	2:D:67:LEU:CA	1.86	1.44
2:B:136:VAL:C	2:B:136:VAL:CA	1.81	1.44
2:B:6:GLU:N	2:B:6:GLU:CA	1.79	1.44
1:C:18:GLY:N	1:C:18:GLY:CA	1.77	1.44
2:D:36:TRP:CA	2:D:36:TRP:N	1.80	1.44
2:B:54:MET:CG	2:B:54:MET:CB	1.95	1.44
2:D:77:LEU:CG	2:D:77:LEU:CB	1.93	1.44
2:B:95:LEU:CA	2:B:95:LEU:N	1.81	1.44
2:D:99:PRO:CB	2:D:99:PRO:CG	1.76	1.43
1:A:9:ASN:CA	1:A:9:ASN:N	1.82	1.43
2:B:41:PHE:CA	2:B:41:PHE:C	1.85	1.43
2:B:43:HIS:NE2	2:B:43:HIS:CE1	1.84	1.43
1:C:96:VAL:CG2	1:C:96:VAL:CB	1.97	1.43
1:A:62:VAL:CG2	1:A:62:VAL:CG1	1.93	1.43
1:C:84:SER:CA	1:C:84:SER:C	1.87	1.43
2:D:3:THR:N	2:D:3:THR:CA	1.81	1.43
1:C:79:THR:CA	1:C:79:THR:CB	1.94	1.43
1:A:20:ASN:CG	1:A:20:ASN:CB	1.87	1.43
2:B:144:TYR:CZ	2:B:144:TYR:OH	1.70	1.43
2:D:96:HIS:N	2:D:96:HIS:CA	1.80	1.43
2:B:46:ASN:CB	2:B:46:ASN:CA	1.97	1.43
2:B:87:LEU:CG	2:B:87:LEU:CD1	1.94	1.43
1:C:126:ASN:CG	1:C:126:ASN:ND2	1.70	1.43
2:D:57:PRO:CA	2:D:57:PRO:CB	1.97	1.42
2:B:69:ALA:CB	2:B:69:ALA:N	1.68	1.42
2:B:97:VAL:CG2	2:B:97:VAL:CB	1.95	1.42
2:D:138:ASN:CA	2:D:138:ASN:N	1.82	1.42
1:A:34:LEU:CB	1:A:34:LEU:CA	1.94	1.42
2:B:98:ASN:CG	2:B:98:ASN:ND2	1.73	1.42
2:D:120:GLN:NE2	2:D:120:GLN:CD	1.72	1.42
1:A:138:SER:CB	1:A:138:SER:OG	1.67	1.42
1:C:4:ALA:CA	1:C:4:ALA:CB	1.94	1.42
1:A:99:LYS:NZ	1:A:99:LYS:CE	1.79	1.42
2:B:57:PRO:CA	2:B:57:PRO:CD	1.97	1.42
1:C:17:VAL:C	1:C:17:VAL:CA	1.86	1.42
3:D:146:HEM:CBA	3:D:146:HEM:CGA	1.98	1.42
1:A:25:GLY:C	1:A:25:GLY:CA	1.87	1.42
2:D:16:LYS:CB	2:D:16:LYS:CG	1.95	1.42
1:C:20:ASN:C	1:C:21:ALA:N	1.71	1.42
2:B:10:VAL:CG1	2:B:128:LEU:CD2	1.76	1.41
2:B:58:LYS:C	2:B:59:VAL:N	1.71	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:SER:C	1:C:111:SER:CA	1.86	1.41
2:B:131:LYS:CE	2:B:131:LYS:CD	1.97	1.41
2:B:80:LEU:C	2:B:81:LYS:N	1.71	1.41
1:C:55:GLN:CD	1:C:55:GLN:CG	1.86	1.41
2:B:110:ALA:C	2:B:111:LEU:N	1.74	1.41
3:A:142:HEM:CAD	3:A:142:HEM:C2D	2.02	1.41
1:A:32:MET:C	1:A:33:PHE:N	1.69	1.41
2:B:103:ARG:CZ	2:B:103:ARG:NH2	1.83	1.41
1:C:100:LEU:N	1:C:100:LEU:CA	1.82	1.41
1:C:45:HIS:CA	1:C:45:HIS:N	1.81	1.41
2:D:20:ASP:C	2:D:21:VAL:N	1.70	1.41
2:D:92:CYS:CA	2:D:92:CYS:C	1.88	1.41
1:A:1:VAL:CA	1:A:1:VAL:C	1.87	1.41
1:A:55:GLN:NE2	1:A:55:GLN:CD	1.73	1.41
1:A:77:PRO:C	1:A:78:GLY:N	1.68	1.41
2:B:10:VAL:N	2:B:10:VAL:CA	1.83	1.41
2:D:103:ARG:CB	2:D:103:ARG:CA	1.96	1.41
2:D:79:ASP:CB	2:D:79:ASP:CA	1.97	1.41
2:B:11:THR:CB	2:B:11:THR:CG2	1.99	1.41
1:A:115:THR:CB	1:A:115:THR:OG1	1.66	1.41
1:C:22:PRO:N	1:C:22:PRO:CA	1.81	1.41
2:D:141:ALA:C	2:D:141:ALA:CA	1.86	1.41
1:A:124:ASN:CG	1:A:124:ASN:CB	1.87	1.41
2:B:126:GLN:CA	2:B:126:GLN:C	1.89	1.41
2:B:145:HIS:CE1	2:B:145:HIS:NE2	1.79	1.40
1:C:115:THR:C	1:C:115:THR:CA	1.90	1.40
2:D:53:VAL:CG2	2:D:53:VAL:CB	1.99	1.40
2:B:11:THR:CB	2:B:11:THR:OG1	1.68	1.40
2:B:10:VAL:CG1	2:B:128:LEU:HD21	0.93	1.40
3:B:146:HEM:C4D	3:B:146:HEM:C3D	1.96	1.40
2:B:36:TRP:CH2	2:B:36:TRP:CE2	1.89	1.40
2:B:3:THR:HG22	2:B:6:GLU:N	1.24	1.40
2:D:14:TRP:CG	2:D:14:TRP:CD1	1.81	1.40
1:C:46:PHE:CB	1:C:46:PHE:CG	2.04	1.40
1:A:58:HIS:C	1:A:59:GLY:N	1.71	1.40
1:C:49:SER:OG	1:C:49:SER:CB	1.65	1.40
2:D:123:PRO:C	2:D:123:PRO:CA	1.89	1.40
2:D:26:ALA:C	2:D:26:ALA:CA	1.90	1.40
2:D:2:LEU:CB	2:D:2:LEU:CD1	1.98	1.40
1:A:106:LEU:CA	1:A:106:LEU:N	1.83	1.40
1:C:16:LYS:CA	1:C:16:LYS:N	1.83	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:CG	1:A:80:LEU:CB	1.98	1.40
2:B:105:LEU:CA	2:B:105:LEU:C	1.87	1.40
2:B:68:ASP:HA	2:B:71:THR:CG2	0.92	1.40
1:C:70:GLN:CA	1:C:70:GLN:CB	2.00	1.40
1:A:12:ALA:CA	1:A:12:ALA:C	1.89	1.39
2:D:101:ASN:HA	2:D:101:ASN:N	1.26	1.39
1:A:7:LYS:CA	1:A:7:LYS:C	1.90	1.39
2:B:60:LYS:CE	2:B:60:LYS:NZ	1.83	1.39
2:D:116:ASN:C	2:D:117:PHE:N	1.71	1.39
2:B:145:HIS:CB	2:B:145:HIS:CA	2.00	1.39
1:A:94:ASN:CA	1:A:94:ASN:CB	2.00	1.39
1:A:20:ASN:CG	1:A:20:ASN:ND2	1.75	1.39
2:D:143:LYS:CB	2:D:143:LYS:CA	1.99	1.39
1:C:100:LEU:CB	1:C:100:LEU:CG	1.98	1.39
2:D:35:PRO:N	2:D:35:PRO:CD	1.80	1.39
2:D:81:LYS:CG	2:D:81:LYS:CD	2.00	1.39
1:A:16:LYS:C	1:A:17:VAL:N	1.76	1.39
1:A:82:ASN:N	1:A:82:ASN:CA	1.86	1.39
2:B:109:LEU:CB	2:B:109:LEU:CG	1.97	1.39
1:C:53:ALA:CA	1:C:53:ALA:CB	1.99	1.39
2:B:65:ARG:CZ	2:B:65:ARG:NH2	1.84	1.39
2:D:11:THR:CA	2:D:11:THR:N	1.83	1.39
2:D:84:PHE:CA	2:D:84:PHE:CB	1.99	1.38
1:A:135:VAL:CG2	1:A:135:VAL:CB	2.00	1.38
2:B:107:ASN:ND2	2:B:107:ASN:CG	1.72	1.38
1:C:117:PHE:CA	1:C:117:PHE:C	1.88	1.38
1:C:44:PRO:N	1:C:44:PRO:CD	1.85	1.38
1:C:98:PHE:CG	1:C:98:PHE:CD1	1.79	1.38
1:C:85:ASN:CG	1:C:85:ASN:ND2	1.75	1.38
1:C:6:ASN:C	1:C:7:LYS:N	1.75	1.38
2:D:58:LYS:CE	2:D:58:LYS:NZ	1.86	1.38
2:B:143:LYS:CG	2:B:143:LYS:CB	2.00	1.38
2:B:21:VAL:CB	2:B:21:VAL:C	1.90	1.38
2:B:57:PRO:CB	2:B:57:PRO:CD	1.98	1.38
2:B:125:VAL:C	2:B:125:VAL:CA	1.89	1.38
1:C:121:VAL:C	1:C:122:HIS:N	1.74	1.38
1:A:32:MET:N	1:A:32:MET:CA	1.86	1.38
2:B:144:TYR:CZ	2:B:144:TYR:CE2	2.11	1.38
1:C:122:HIS:CG	1:C:122:HIS:ND1	1.70	1.38
1:C:93:VAL:CA	1:C:93:VAL:CB	2.00	1.38
2:B:23:GLY:CA	2:B:23:GLY:N	1.84	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:CA	1:C:61:LYS:CB	2.00	1.38
2:D:104:LEU:CG	2:D:104:LEU:CD1	2.01	1.38
2:D:65:ARG:CB	2:D:65:ARG:CG	2.00	1.38
1:A:42:TYR:C	1:A:43:PHE:N	1.73	1.38
1:C:37:PRO:CG	1:C:37:PRO:CD	1.99	1.38
2:B:113:VAL:CB	2:B:113:VAL:CG2	2.01	1.38
2:D:54:MET:SD	2:D:54:MET:CG	2.12	1.38
1:A:70:GLN:NE2	1:A:70:GLN:CD	1.75	1.37
1:C:134:THR:CA	1:C:134:THR:CB	1.99	1.37
2:B:43:HIS:ND1	2:B:43:HIS:CE1	1.92	1.37
1:C:74:ASN:CA	1:C:74:ASN:N	1.86	1.37
1:A:29:LEU:CG	1:A:29:LEU:CB	2.03	1.37
1:C:44:PRO:N	1:C:44:PRO:CA	1.86	1.37
1:C:59:GLY:CA	1:C:59:GLY:C	1.92	1.37
2:D:131:LYS:NZ	2:D:131:LYS:CE	1.84	1.37
2:D:50:ALA:C	2:D:50:ALA:CA	1.91	1.37
1:A:43:PHE:C	1:A:44:PRO:N	1.78	1.37
1:A:126:ASN:ND2	1:A:126:ASN:CG	1.77	1.36
2:D:83:ALA:C	2:D:83:ALA:CA	1.90	1.36
1:A:118:THR:CG2	1:A:118:THR:CB	2.01	1.36
1:A:70:GLN:CD	1:A:70:GLN:CG	1.92	1.36
1:C:119:PRO:CA	1:C:119:PRO:C	1.93	1.36
2:D:130:GLN:CA	2:D:130:GLN:CG	2.02	1.36
2:D:6:GLU:O	2:D:6:GLU:C	1.63	1.36
1:A:31:ARG:O	1:A:31:ARG:C	1.64	1.36
2:B:117:PHE:C	2:B:118:GLY:CA	1.90	1.36
2:D:108:VAL:N	2:D:108:VAL:CA	1.86	1.36
1:C:36:PHE:C	1:C:37:PRO:N	1.76	1.36
1:C:41:THR:CG2	1:C:41:THR:CB	2.03	1.36
2:D:109:LEU:C	2:D:109:LEU:CA	1.91	1.36
1:A:54:GLN:O	1:A:54:GLN:C	1.65	1.36
1:C:7:LYS:NZ	1:C:7:LYS:CE	1.89	1.36
2:D:57:PRO:N	2:D:57:PRO:CG	1.89	1.36
2:B:32:VAL:CA	2:B:32:VAL:N	1.89	1.35
2:D:42:GLN:CG	2:D:42:GLN:CB	2.04	1.35
1:A:127:LYS:C	1:A:128:PHE:CA	1.95	1.35
2:B:103:ARG:CD	2:B:103:ARG:CG	2.01	1.35
2:D:65:ARG:CZ	2:D:65:ARG:NH1	1.90	1.35
2:B:110:ALA:N	2:B:110:ALA:CA	1.87	1.35
2:B:39:ARG:CG	2:B:39:ARG:CB	2.04	1.35
2:B:109:LEU:CB	2:B:109:LEU:CD2	2.02	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:SER:C	1:C:103:HIS:N	1.78	1.35
2:D:100:GLN:C	2:D:101:ASN:HA	1.43	1.35
1:A:22:PRO:N	1:A:22:PRO:CD	1.87	1.35
1:A:84:SER:N	1:A:84:SER:CA	1.86	1.35
1:C:131:ASN:OD1	1:C:131:ASN:CG	1.65	1.35
1:C:1:VAL:CA	1:C:1:VAL:C	1.94	1.35
1:A:50:HIS:CE1	1:A:50:HIS:NE2	1.89	1.35
2:D:102:PHE:CA	2:D:102:PHE:N	1.90	1.35
1:A:127:LYS:O	1:A:127:LYS:C	1.63	1.34
1:C:35:SER:OG	1:C:35:SER:CB	1.75	1.34
2:D:138:ASN:CG	2:D:138:ASN:OD1	1.66	1.34
1:C:130:ALA:N	1:C:130:ALA:CA	1.91	1.34
2:D:16:LYS:CB	2:D:16:LYS:CA	2.05	1.34
2:B:68:ASP:CA	2:B:71:THR:HG22	1.37	1.34
2:B:99:PRO:CD	2:B:99:PRO:CG	1.96	1.34
1:A:8:SER:C	1:A:8:SER:O	1.64	1.34
2:D:92:CYS:CB	2:D:92:CYS:SG	2.16	1.34
1:A:37:PRO:CD	1:A:37:PRO:N	1.77	1.34
2:B:55:ASN:O	2:B:60:LYS:NZ	1.60	1.34
2:D:30:LEU:CA	2:D:30:LEU:C	1.94	1.34
2:B:139:ALA:O	2:B:139:ALA:C	1.66	1.34
1:C:116:ASN:ND2	1:C:116:ASN:CG	1.82	1.33
1:A:141:ARG:C	1:A:141:ARG:CA	1.95	1.33
1:A:74:ASN:CG	1:A:74:ASN:CB	1.95	1.33
2:B:78:ASP:OD2	2:B:78:ASP:CG	1.65	1.33
1:A:56:LYS:C	1:A:56:LYS:O	1.63	1.33
2:B:65:ARG:NH1	3:B:146:HEM:O2D	1.61	1.33
2:D:59:VAL:HA	2:D:59:VAL:CG2	1.57	1.33
1:A:45:HIS:CD2	1:A:45:HIS:NE2	1.84	1.33
2:B:71:THR:CB	2:B:71:THR:CA	2.06	1.33
2:B:22:VAL:C	2:B:22:VAL:CA	1.93	1.33
1:C:124:ASN:ND2	1:C:124:ASN:CG	1.79	1.33
2:B:46:ASN:CG	2:B:46:ASN:CB	1.96	1.33
1:C:135:VAL:O	1:C:135:VAL:C	1.65	1.33
2:B:55:ASN:C	2:B:56:ASN:N	1.78	1.33
2:B:94:LYS:NZ	2:B:94:LYS:CE	1.90	1.33
1:C:119:PRO:CG	1:C:119:PRO:CB	1.85	1.33
2:D:56:ASN:O	2:D:56:ASN:C	1.66	1.33
2:D:2:LEU:HD22	2:D:3:THR:O	1.23	1.33
1:C:130:ALA:O	1:C:130:ALA:C	1.64	1.33
2:B:115:ARG:CA	2:B:115:ARG:CB	2.08	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:PHE:C	2:D:44:PHE:CA	1.97	1.32
1:A:124:ASN:N	1:A:124:ASN:CB	1.92	1.32
2:B:39:ARG:NH1	2:B:40:PHE:CZ	1.97	1.32
2:B:69:ALA:C	2:B:69:ALA:CB	1.93	1.32
1:C:11:LYS:CE	1:C:11:LYS:CD	2.07	1.32
1:C:90:LYS:N	1:C:90:LYS:CA	1.90	1.32
1:C:30:GLN:NE2	1:C:30:GLN:CD	1.83	1.32
1:A:31:ARG:C	1:A:32:MET:N	1.81	1.32
1:A:53:ALA:O	1:A:53:ALA:C	1.68	1.32
2:D:70:PHE:HA	2:D:70:PHE:O	1.26	1.32
1:A:114:PRO:N	1:A:114:PRO:CD	1.90	1.32
1:A:78:GLY:CA	1:A:78:GLY:N	1.91	1.32
1:C:115:THR:O	1:C:115:THR:C	1.66	1.31
1:A:26:ALA:CB	1:A:26:ALA:CA	2.07	1.31
2:B:126:GLN:CG	2:B:126:GLN:CD	1.99	1.31
2:B:4:ALA:N	2:B:5:GLU:H	1.26	1.31
2:D:41:PHE:C	2:D:42:GLN:N	1.83	1.31
2:B:68:ASP:CG	2:B:71:THR:HG23	1.47	1.31
2:D:42:GLN:CG	2:D:42:GLN:HA	1.57	1.31
2:D:95:LEU:CG	2:D:95:LEU:CB	2.07	1.31
2:D:6:GLU:CD	2:D:6:GLU:OE2	1.67	1.31
1:C:31:ARG:CA	1:C:31:ARG:C	1.99	1.31
2:D:144:TYR:OH	2:D:144:TYR:CZ	1.82	1.31
3:C:142:HEM:C3C	3:C:142:HEM:CHD	2.13	1.30
1:C:22:PRO:CB	1:C:22:PRO:CD	2.09	1.30
1:C:12:ALA:O	1:C:12:ALA:C	1.66	1.30
2:D:57:PRO:N	2:D:57:PRO:CD	1.93	1.30
2:B:108:VAL:CG2	2:B:108:VAL:CB	2.07	1.30
2:D:59:VAL:CA	2:D:59:VAL:CG2	2.09	1.30
2:D:11:THR:CB	2:D:11:THR:OG1	1.78	1.30
1:A:3:SER:O	1:A:3:SER:C	1.67	1.30
1:C:33:PHE:C	1:C:33:PHE:O	1.68	1.30
1:C:38:THR:CG2	1:C:38:THR:CB	2.09	1.30
1:C:86:LEU:CB	1:C:86:LEU:CA	2.10	1.30
2:B:5:GLU:N	2:B:5:GLU:CA	1.93	1.30
2:D:19:VAL:CG2	2:D:19:VAL:CB	2.10	1.30
2:B:98:ASN:OD1	2:B:98:ASN:CG	1.67	1.29
1:C:74:ASN:C	1:C:75:ASP:N	1.84	1.29
2:D:105:LEU:CD2	2:D:105:LEU:CD1	2.10	1.29
2:D:124:ASN:CG	2:D:124:ASN:OD1	1.70	1.29
1:C:94:ASN:OD1	1:C:94:ASN:CG	1.69	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:146:HEM:CGD	3:D:146:HEM:CBD	2.10	1.29
2:B:7:LYS:CA	2:B:7:LYS:C	2.01	1.29
2:B:1:MET:CG	2:B:77:LEU:HD13	1.57	1.29
2:B:95:LEU:H	2:B:95:LEU:CB	1.35	1.29
1:C:84:SER:C	1:C:84:SER:CB	2.00	1.29
2:D:25:GLN:CD	2:D:25:GLN:CG	1.99	1.29
2:B:38:GLN:C	2:B:38:GLN:CA	2.00	1.29
2:B:64:LYS:CD	2:B:64:LYS:CE	2.09	1.29
2:B:68:ASP:CB	2:B:71:THR:HG23	1.60	1.29
1:C:141:ARG:CG	1:C:141:ARG:CD	2.10	1.29
1:A:74:ASN:CG	1:A:74:ASN:ND2	1.86	1.29
3:C:142:HEM:C4C	3:C:142:HEM:C1D	2.18	1.29
3:C:142:HEM:CGD	3:C:142:HEM:O1D	1.80	1.29
3:A:142:HEM:CBD	3:A:142:HEM:CGD	2.12	1.28
2:B:59:VAL:O	2:B:59:VAL:C	1.70	1.28
1:A:127:LYS:CD	1:A:127:LYS:NZ	1.94	1.28
2:D:130:GLN:CG	2:D:130:GLN:CD	2.01	1.28
2:D:71:THR:CB	2:D:71:THR:OG1	1.78	1.28
1:A:40:LYS:CG	1:A:40:LYS:CB	2.10	1.28
2:B:45:GLY:C	2:B:45:GLY:O	1.69	1.28
2:B:39:ARG:NH1	2:B:40:PHE:HZ	1.27	1.28
1:C:56:LYS:CE	1:C:56:LYS:NZ	1.96	1.28
1:A:4:ALA:N	1:A:4:ALA:CA	1.97	1.27
2:B:34:TYR:CZ	2:B:34:TYR:CD2	2.22	1.27
2:B:81:LYS:HZ2	2:B:142:HIS:CG	1.51	1.27
1:A:87:HIS:CG	1:A:87:HIS:CB	2.16	1.27
2:D:14:TRP:CZ3	2:D:14:TRP:CD2	2.16	1.27
2:D:1:MET:SD	2:D:1:MET:CE	2.22	1.27
2:D:110:ALA:CA	2:D:110:ALA:C	2.02	1.27
2:B:20:ASP:OD1	2:B:20:ASP:CG	1.72	1.27
2:B:68:ASP:N	2:B:71:THR:CG2	1.94	1.27
2:D:7:LYS:O	2:D:8:ALA:CA	1.80	1.27
1:C:77:PRO:CG	1:C:77:PRO:CB	1.95	1.27
2:D:54:MET:O	2:D:54:MET:C	1.73	1.27
2:D:111:LEU:C	2:D:112:VAL:CA	2.01	1.27
1:A:52:SER:OG	1:A:52:SER:CB	1.82	1.27
2:B:133:VAL:O	2:B:134:ALA:N	1.68	1.26
2:B:36:TRP:CZ2	2:B:36:TRP:NE1	2.03	1.26
1:C:137:THR:O	1:C:137:THR:C	1.71	1.26
1:A:85:ASN:C	1:A:85:ASN:O	1.69	1.26
2:D:51:GLY:C	2:D:52:ALA:N	1.87	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:SER:C	1:C:8:SER:O	1.72	1.26
2:D:55:ASN:CG	2:D:55:ASN:OD1	1.73	1.26
2:D:84:PHE:CD1	2:D:84:PHE:CB	2.16	1.26
2:B:41:PHE:C	2:B:42:GLN:N	1.85	1.26
2:B:54:MET:HB3	2:B:55:ASN:OD1	1.32	1.26
1:C:75:ASP:CA	1:C:75:ASP:C	2.04	1.26
2:B:84:PHE:CB	2:B:84:PHE:CD1	2.18	1.26
2:D:34:TYR:CE1	2:D:34:TYR:CE2	2.09	1.26
1:C:9:ASN:CG	1:C:9:ASN:CB	2.03	1.26
2:D:145:HIS:C	2:D:145:HIS:O	1.75	1.26
2:D:3:THR:CB	2:D:3:THR:OG1	1.83	1.26
1:C:114:PRO:CG	1:C:114:PRO:CB	2.13	1.25
2:D:48:SER:CB	2:D:48:SER:OG	1.81	1.25
1:A:3:SER:OG	1:A:3:SER:CB	1.83	1.25
2:B:84:PHE:CE2	2:B:84:PHE:CG	1.77	1.25
1:C:45:HIS:CD2	1:C:45:HIS:NE2	1.78	1.25
1:A:9:ASN:OD1	1:A:9:ASN:CG	1.71	1.25
2:D:2:LEU:HD23	2:D:7:LYS:CG	1.66	1.25
2:D:4:ALA:C	2:D:4:ALA:CA	2.04	1.25
2:D:5:GLU:CD	2:D:5:GLU:CG	2.04	1.25
2:B:74:LEU:HD13	2:B:77:LEU:CB	1.65	1.25
2:B:79:ASP:C	2:B:79:ASP:O	1.76	1.24
1:A:2:LEU:C	1:A:2:LEU:CA	2.05	1.24
2:B:49:SER:O	2:B:49:SER:C	1.75	1.24
1:A:103:HIS:ND1	1:A:103:HIS:CG	1.71	1.24
2:B:145:HIS:O	2:D:1:MET:SD	1.95	1.24
1:A:124:ASN:O	1:A:124:ASN:C	1.76	1.24
1:C:85:ASN:CA	1:C:85:ASN:O	1.83	1.24
2:D:145:HIS:CG	2:D:145:HIS:ND1	2.06	1.24
1:A:79:THR:CB	1:A:80:LEU:HD23	1.67	1.24
2:B:95:LEU:CA	2:B:95:LEU:CG	2.14	1.24
1:A:18:GLY:O	1:A:19:GLY:N	1.69	1.23
2:D:95:LEU:CD1	2:D:95:LEU:CG	2.14	1.23
1:A:89:HIS:CE1	1:A:89:HIS:NE2	1.68	1.23
2:D:55:ASN:CB	2:D:55:ASN:CA	2.17	1.23
3:D:146:HEM:NB	3:D:146:HEM:C1B	1.85	1.23
2:B:41:PHE:CD2	2:B:44:PHE:CE1	2.24	1.23
1:C:80:LEU:C	1:C:80:LEU:O	1.73	1.23
2:D:51:GLY:O	2:D:52:ALA:HA	1.34	1.22
2:B:75:LYS:HG3	2:B:76:HIS:CE1	1.72	1.22
1:A:112:HIS:CG	1:A:112:HIS:ND1	1.71	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:PRO:CG	1:C:114:PRO:N	2.00	1.22
1:C:29:LEU:CG	1:C:29:LEU:CD2	2.16	1.22
1:A:72:HIS:NE2	1:A:72:HIS:CE1	1.94	1.22
2:B:92:CYS:CB	2:B:92:CYS:SG	2.27	1.22
2:B:55:ASN:CA	2:B:55:ASN:C	2.07	1.22
1:A:49:SER:CB	1:A:52:SER:HB3	1.68	1.22
2:B:42:GLN:C	2:B:43:HIS:N	1.93	1.22
2:D:10:VAL:CB	2:D:10:VAL:C	2.07	1.22
1:C:110:ALA:C	1:C:110:ALA:CA	2.08	1.21
2:B:53:VAL:C	2:B:54:MET:CA	2.08	1.21
2:D:90:LEU:CB	2:D:90:LEU:CD1	2.19	1.21
1:A:8:SER:CA	1:A:8:SER:O	1.87	1.21
2:B:7:LYS:CE	2:B:7:LYS:NZ	2.04	1.21
1:C:61:LYS:CE	1:C:61:LYS:NZ	2.03	1.21
2:D:72:GLN:HE21	2:D:73:GLY:N	1.39	1.21
2:D:7:LYS:O	2:D:7:LYS:CA	1.89	1.20
1:A:85:ASN:CB	1:A:85:ASN:CG	2.10	1.20
2:B:117:PHE:CZ	2:B:117:PHE:CD1	2.30	1.20
2:B:38:GLN:O	2:B:39:ARG:N	1.72	1.20
2:B:41:PHE:CD2	2:B:44:PHE:CZ	2.30	1.20
2:B:1:MET:CG	2:B:1:MET:SD	2.30	1.19
1:A:131:ASN:N	1:A:131:ASN:CA	2.05	1.19
1:C:89:HIS:HB2	1:C:139:LYS:NZ	1.53	1.19
1:A:124:ASN:C	1:A:124:ASN:CB	2.10	1.19
1:C:56:LYS:HA	1:C:56:LYS:CG	1.72	1.19
2:B:68:ASP:N	2:B:71:THR:HG21	1.57	1.19
1:A:119:PRO:CG	1:A:119:PRO:CA	2.20	1.19
2:B:41:PHE:HD2	2:B:44:PHE:CZ	1.60	1.19
2:B:130:GLN:NE2	2:B:130:GLN:CG	2.06	1.19
1:A:108:THR:HB	1:A:108:THR:CA	1.51	1.19
1:A:94:ASN:CA	1:A:94:ASN:O	1.88	1.19
1:C:135:VAL:CG2	1:C:135:VAL:CG1	2.20	1.18
1:A:77:PRO:C	1:A:77:PRO:CA	2.12	1.18
1:A:91:LEU:CD2	1:A:91:LEU:CD1	2.21	1.18
2:D:7:LYS:CB	2:D:7:LYS:CA	2.20	1.18
1:A:79:THR:CA	1:A:79:THR:CG2	2.21	1.18
1:A:91:LEU:HD23	3:A:142:HEM:C4D	1.79	1.18
1:A:100:LEU:CB	1:A:100:LEU:CD1	2.21	1.18
1:A:31:ARG:CG	2:B:126:GLN:HE21	1.57	1.17
1:A:36:PHE:O	1:A:39:THR:HG22	1.40	1.17
2:B:75:LYS:CA	2:B:75:LYS:N	2.07	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:LEU:HD23	2:D:7:LYS:HG2	1.22	1.17
2:D:70:PHE:HD1	2:D:71:THR:OG1	1.22	1.17
2:B:95:LEU:CA	2:B:95:LEU:HG	1.73	1.17
1:A:70:GLN:OE1	1:A:70:GLN:CD	1.80	1.17
1:A:105:LEU:CD1	1:A:105:LEU:CD2	2.23	1.17
2:B:62:HIS:CB	2:B:62:HIS:CG	2.28	1.17
1:C:52:SER:HB3	1:C:55:GLN:HE21	1.08	1.16
2:D:2:LEU:CD1	2:D:2:LEU:HB3	1.65	1.16
1:A:49:SER:CB	1:A:49:SER:OG	1.93	1.16
1:A:60:GLN:CA	1:A:61:LYS:N	2.09	1.16
1:C:74:ASN:CB	1:C:74:ASN:CG	2.13	1.16
1:C:87:HIS:HA	1:C:91:LEU:HD12	1.17	1.16
2:D:75:LYS:CD	2:D:75:LYS:CE	2.24	1.16
1:C:98:PHE:C	1:C:99:LYS:N	1.99	1.16
1:A:85:ASN:CB	1:A:85:ASN:C	2.13	1.16
2:D:81:LYS:CB	2:D:81:LYS:N	2.06	1.16
1:A:99:LYS:CD	1:A:99:LYS:CG	2.24	1.16
2:B:102:PHE:CD1	2:B:102:PHE:CD2	2.10	1.16
1:C:72:HIS:HB2	1:C:74:ASN:HD21	0.99	1.16
2:B:3:THR:CG2	2:B:6:GLU:N	2.09	1.15
1:C:46:PHE:CD2	1:C:46:PHE:CZ	2.18	1.15
2:D:85:ALA:N	2:D:85:ALA:CA	2.08	1.15
2:D:94:LYS:HG3	2:D:95:LEU:HD23	1.29	1.15
2:B:133:VAL:O	2:B:133:VAL:CA	1.93	1.15
2:D:10:VAL:CG1	2:D:128:LEU:HD22	1.76	1.15
2:D:6:GLU:HB2	2:D:128:LEU:HD23	1.22	1.15
1:A:42:TYR:O	1:A:42:TYR:CA	1.95	1.15
2:B:1:MET:N	2:B:1:MET:CA	2.10	1.15
2:D:59:VAL:CG1	2:D:59:VAL:CG2	2.25	1.14
3:A:142:HEM:C3D	3:A:142:HEM:CMD	2.30	1.14
2:B:71:THR:HA	2:B:71:THR:N	1.55	1.14
1:C:141:ARG:O	1:C:141:ARG:C	1.84	1.14
2:D:105:LEU:HD22	2:D:105:LEU:CD1	1.72	1.14
2:D:105:LEU:HB2	2:D:105:LEU:CD1	1.65	1.14
2:D:62:HIS:CG	2:D:62:HIS:CE1	2.33	1.14
2:D:10:VAL:HG11	2:D:128:LEU:HD22	1.29	1.14
1:C:26:ALA:H	1:C:56:LYS:HE2	1.12	1.14
1:A:137:THR:OG1	1:A:137:THR:CA	1.95	1.14
2:D:11:THR:CB	2:D:11:THR:N	2.08	1.14
2:B:93:ASN:CG	2:B:93:ASN:CA	2.16	1.13
2:B:3:THR:CG2	2:B:5:GLU:C	2.17	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LEU:CB	2:B:80:LEU:CD2	2.25	1.13
2:D:14:TRP:NE1	2:D:71:THR:HG23	1.62	1.13
2:B:68:ASP:OD2	2:B:71:THR:HG21	1.48	1.13
1:C:56:LYS:CB	1:C:56:LYS:CG	2.26	1.13
1:A:62:VAL:HG21	1:A:62:VAL:CG1	1.64	1.13
1:C:20:ASN:C	1:C:20:ASN:N	2.02	1.12
2:D:11:THR:CA	2:D:11:THR:OG1	1.95	1.12
2:D:126:GLN:CD	2:D:126:GLN:OE1	1.87	1.12
2:D:111:LEU:O	2:D:112:VAL:N	1.82	1.12
1:A:49:SER:HB2	1:A:52:SER:CB	1.80	1.12
2:B:1:MET:N	2:B:2:LEU:HD23	1.63	1.12
2:B:68:ASP:HB3	2:B:71:THR:O	1.46	1.12
1:A:114:PRO:HB2	1:A:114:PRO:CD	1.62	1.12
1:C:138:SER:OG	1:C:138:SER:CB	1.96	1.12
2:D:51:GLY:O	2:D:52:ALA:CA	1.97	1.12
1:A:31:ARG:NE	1:A:31:ARG:CG	2.11	1.12
2:B:77:LEU:C	2:B:77:LEU:CB	2.16	1.12
2:B:3:THR:HG22	2:B:5:GLU:C	1.68	1.12
2:B:1:MET:CE	2:B:1:MET:SD	2.37	1.12
1:A:119:PRO:CD	1:A:119:PRO:CG	2.27	1.11
2:B:64:LYS:C	2:B:64:LYS:N	2.03	1.11
2:D:39:ARG:CG	2:D:39:ARG:NE	2.10	1.11
2:B:56:ASN:O	2:B:56:ASN:CA	1.97	1.11
2:B:80:LEU:HB3	2:B:80:LEU:CD2	1.75	1.11
1:A:74:ASN:C	1:A:74:ASN:O	1.87	1.11
1:A:108:THR:HA	1:A:108:THR:CB	1.70	1.11
2:D:10:VAL:HB	2:D:10:VAL:C	1.71	1.11
2:D:19:VAL:CG2	2:D:19:VAL:HA	1.81	1.11
2:B:81:LYS:NZ	2:B:142:HIS:CG	2.18	1.11
2:B:64:LYS:HB3	2:B:64:LYS:NZ	1.66	1.11
2:B:11:THR:O	2:B:12:GLY:N	1.84	1.11
2:B:95:LEU:HB2	2:B:95:LEU:H	1.07	1.11
2:D:14:TRP:HE1	2:D:71:THR:HG23	1.09	1.11
2:D:34:TYR:CD2	2:D:34:TYR:CZ	2.21	1.11
2:D:7:LYS:CE	2:D:7:LYS:NZ	2.14	1.10
1:A:137:THR:OG1	1:A:137:THR:CG2	1.98	1.10
2:B:15:GLY:C	2:B:15:GLY:O	1.89	1.10
2:D:84:PHE:CD1	2:D:84:PHE:HB2	1.79	1.10
1:A:41:THR:CA	1:A:41:THR:CG2	2.29	1.10
2:B:47:LEU:HD12	2:B:53:VAL:HG23	1.32	1.10
2:B:3:THR:CG2	2:B:5:GLU:CB	2.09	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:PRO:N	1:C:114:PRO:CB	2.13	1.10
2:D:53:VAL:HG22	2:D:54:MET:CE	1.81	1.10
1:A:140:TYR:CB	1:A:140:TYR:CD1	2.33	1.10
2:B:4:ALA:CA	2:B:5:GLU:N	2.15	1.10
2:B:113:VAL:HA	2:B:113:VAL:CG1	1.77	1.10
1:A:132:ASP:OD2	1:A:132:ASP:CG	1.88	1.10
1:A:26:ALA:HA	1:A:29:LEU:CD2	1.81	1.10
2:B:71:THR:C	2:B:71:THR:N	2.03	1.10
2:B:10:VAL:HG11	2:B:128:LEU:HD22	1.31	1.10
1:A:126:ASN:CA	1:A:127:LYS:N	2.15	1.10
1:A:127:LYS:O	1:A:127:LYS:CA	1.99	1.10
1:C:44:PRO:CD	1:C:44:PRO:CB	2.29	1.10
1:C:75:ASP:CB	1:C:75:ASP:N	2.15	1.09
2:D:70:PHE:O	2:D:70:PHE:CA	2.00	1.09
2:D:18:ASP:N	2:D:18:ASP:CB	2.12	1.09
2:D:100:GLN:CG	2:D:100:GLN:HA	1.83	1.09
2:D:131:LYS:NZ	2:D:131:LYS:CD	2.13	1.09
1:A:91:LEU:HD21	3:A:142:HEM:HAD1	1.29	1.09
2:D:75:LYS:C	2:D:75:LYS:O	1.90	1.09
1:A:109:LEU:CA	1:A:109:LEU:C	2.19	1.09
1:A:74:ASN:O	1:A:75:ASP:HA	1.53	1.09
1:A:118:THR:CG2	1:A:118:THR:CA	2.30	1.09
1:C:45:HIS:HE1	3:C:142:HEM:HBD1	0.99	1.09
2:B:87:LEU:CD2	2:B:87:LEU:CD1	2.29	1.09
2:B:68:ASP:CG	2:B:71:THR:CG2	2.20	1.09
1:C:108:THR:HB	1:C:108:THR:CG2	1.61	1.09
1:C:69:ALA:CB	1:C:69:ALA:C	2.21	1.09
2:D:100:GLN:CG	2:D:100:GLN:CA	2.31	1.09
1:C:7:LYS:HG2	1:C:73:LEU:HB2	1.34	1.08
1:A:137:THR:N	1:A:137:THR:CB	2.15	1.08
2:D:2:LEU:HD22	2:D:4:ALA:HA	1.18	1.08
1:C:4:ALA:N	1:C:4:ALA:CB	2.13	1.08
2:B:68:ASP:OD2	2:B:71:THR:CG2	1.99	1.08
2:B:69:ALA:CB	2:B:69:ALA:HA	1.63	1.08
1:C:89:HIS:HB2	1:C:139:LYS:HZ3	0.95	1.08
2:B:55:ASN:C	2:B:60:LYS:NZ	2.05	1.08
2:D:99:PRO:HD2	2:D:144:TYR:OH	1.51	1.08
1:A:105:LEU:CB	1:A:105:LEU:CD1	2.31	1.08
2:D:42:GLN:HG2	2:D:42:GLN:HA	1.29	1.08
1:A:77:PRO:N	1:A:77:PRO:CA	1.75	1.08
1:A:30:GLN:NE2	1:A:30:GLN:CD	2.08	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PRO:HB2	1:A:114:PRO:HD2	1.08	1.07
1:A:26:ALA:HA	1:A:29:LEU:HD22	1.29	1.07
2:D:1:MET:N	2:D:1:MET:C	2.06	1.07
2:D:103:ARG:C	2:D:103:ARG:CB	2.21	1.07
1:A:100:LEU:CB	1:A:100:LEU:CD2	2.33	1.07
1:A:56:LYS:HE3	1:A:56:LYS:HA	1.33	1.07
2:B:118:GLY:C	2:B:118:GLY:N	2.07	1.06
1:A:10:VAL:O	1:A:13:ALA:HB3	1.55	1.06
2:B:43:HIS:CD2	3:B:146:HEM:O2A	2.07	1.06
2:D:140:LEU:CD1	2:D:140:LEU:CD2	2.33	1.06
2:B:101:ASN:O	3:B:146:HEM:HBB1	1.54	1.06
2:B:3:THR:H	2:B:6:GLU:HB2	1.19	1.06
1:C:87:HIS:CG	1:C:87:HIS:ND1	1.69	1.06
1:A:26:ALA:HB1	1:A:56:LYS:CE	1.86	1.06
1:A:93:VAL:HB	1:A:93:VAL:CG2	1.79	1.06
1:A:65:ALA:CB	1:A:65:ALA:C	2.23	1.06
2:B:41:PHE:CG	2:B:44:PHE:CE1	2.42	1.06
2:B:54:MET:CA	2:B:54:MET:CG	2.33	1.06
1:C:29:LEU:CD1	1:C:29:LEU:CD2	2.34	1.06
1:C:38:THR:C	1:C:38:THR:O	1.92	1.06
2:B:140:LEU:CB	2:B:140:LEU:CD1	2.32	1.06
2:D:93:ASN:CB	2:D:93:ASN:C	2.23	1.06
1:A:79:THR:HB	1:A:80:LEU:CD2	1.86	1.06
2:D:57:PRO:N	2:D:57:PRO:HG2	1.62	1.05
2:D:7:LYS:C	2:D:7:LYS:CB	2.23	1.05
1:A:105:LEU:HA	1:A:108:THR:HG22	1.37	1.05
2:D:44:PHE:CA	2:D:44:PHE:CG	2.39	1.05
2:D:53:VAL:HG22	2:D:54:MET:HE2	1.08	1.05
3:D:146:HEM:CBA	3:D:146:HEM:C2A	2.39	1.05
1:A:34:LEU:HD11	2:B:123:PRO:HB2	1.38	1.05
2:B:1:MET:HG3	2:B:77:LEU:O	1.55	1.05
2:B:34:TYR:CE2	2:B:34:TYR:CG	2.43	1.05
2:B:81:LYS:CG	2:B:81:LYS:CD	2.35	1.05
1:C:80:LEU:C	1:C:80:LEU:HA	1.63	1.05
1:A:136:LEU:CB	1:A:136:LEU:CD1	2.34	1.05
1:A:91:LEU:CD2	3:A:142:HEM:HAD1	1.85	1.05
1:A:91:LEU:HD23	3:A:142:HEM:C3D	1.92	1.05
1:C:55:GLN:CD	1:C:55:GLN:CB	2.23	1.05
2:B:21:VAL:HB	2:B:21:VAL:C	1.75	1.05
2:B:74:LEU:CD1	2:B:77:LEU:HB2	1.86	1.05
2:B:113:VAL:CA	2:B:113:VAL:CG1	2.34	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:GLY:HA2	2:B:66:VAL:HG13	1.36	1.04
2:B:75:LYS:CG	2:B:76:HIS:ND1	2.20	1.04
1:C:133:SER:HA	1:C:133:SER:CB	1.84	1.04
2:D:2:LEU:CB	2:D:2:LEU:N	2.20	1.04
2:B:87:LEU:N	2:B:87:LEU:C	2.11	1.04
1:C:140:TYR:O	1:C:141:ARG:HD3	1.58	1.04
1:C:45:HIS:CE1	3:C:142:HEM:HBD1	1.91	1.04
1:A:57:ALA:CB	1:A:57:ALA:N	2.19	1.04
2:B:69:ALA:HB1	2:B:69:ALA:CA	1.52	1.04
2:D:65:ARG:CA	2:D:66:VAL:N	2.19	1.04
1:A:20:ASN:HA	1:A:20:ASN:CG	1.72	1.04
1:C:24:TYR:CD2	1:C:24:TYR:CB	2.40	1.04
2:D:68:ASP:CA	2:D:68:ASP:CG	2.27	1.04
2:B:43:HIS:N	2:B:43:HIS:C	2.09	1.04
1:C:135:VAL:HG11	1:C:135:VAL:CG2	1.85	1.04
2:B:88:SER:OG	2:B:143:LYS:HB3	1.55	1.03
2:B:94:LYS:CD	2:B:94:LYS:CB	2.37	1.03
1:C:72:HIS:HB2	1:C:74:ASN:ND2	1.73	1.03
2:B:103:ARG:NE	2:B:103:ARG:NH1	2.04	1.03
2:D:16:LYS:HB2	2:D:16:LYS:HD3	1.09	1.03
1:A:16:LYS:NZ	1:A:16:LYS:HD3	1.71	1.03
1:C:22:PRO:CD	1:C:22:PRO:CA	2.35	1.03
2:D:145:HIS:CD2	2:D:145:HIS:NE2	2.27	1.03
1:A:41:THR:C	1:A:41:THR:CB	2.27	1.03
1:C:56:LYS:NZ	1:C:59:GLY:HA3	1.74	1.03
2:D:123:PRO:N	2:D:123:PRO:CD	2.22	1.03
2:B:139:ALA:O	2:B:143:LYS:HB2	1.57	1.03
2:B:76:HIS:CB	2:B:76:HIS:N	2.22	1.03
2:D:84:PHE:N	2:D:84:PHE:CB	2.21	1.03
2:B:3:THR:N	2:B:6:GLU:HB2	1.72	1.03
2:B:84:PHE:CD2	2:B:84:PHE:CD1	2.43	1.03
2:D:5:GLU:HB3	2:D:9:ALA:HB3	1.41	1.03
2:B:69:ALA:CA	2:B:69:ALA:HB2	1.52	1.02
2:B:144:TYR:CE2	2:B:144:TYR:CG	2.46	1.02
2:D:19:VAL:CG2	2:D:19:VAL:CA	2.38	1.02
2:B:144:TYR:CD2	2:B:144:TYR:CB	2.42	1.02
2:B:1:MET:HG2	2:B:77:LEU:HD11	1.04	1.02
1:A:48:LEU:CA	1:A:48:LEU:CG	2.38	1.02
2:B:30:LEU:HD23	2:B:105:LEU:HA	1.35	1.02
2:D:107:ASN:CB	2:D:107:ASN:N	2.23	1.02
2:B:4:ALA:N	2:B:5:GLU:N	2.08	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:TRP:HE1	2:B:68:ASP:CG	1.62	1.02
2:B:124:ASN:C	2:B:125:VAL:CA	2.27	1.02
2:B:38:GLN:C	2:B:38:GLN:O	0.82	1.02
1:C:70:GLN:N	1:C:70:GLN:CB	2.21	1.02
2:D:34:TYR:CE2	2:D:34:TYR:OH	2.10	1.02
1:A:18:GLY:O	1:A:18:GLY:C	0.82	1.02
1:A:56:LYS:HE3	1:A:56:LYS:CA	1.83	1.02
1:A:85:ASN:CA	1:A:85:ASN:O	2.08	1.02
2:B:4:ALA:C	2:B:4:ALA:O	0.82	1.02
2:D:105:LEU:HD12	2:D:105:LEU:HB2	1.37	1.02
3:D:146:HEM:NA	3:D:146:HEM:C4A	1.73	1.02
1:C:86:LEU:CD2	1:C:86:LEU:CD1	2.37	1.01
1:A:89:HIS:CD2	1:A:139:LYS:HD2	1.94	1.01
1:C:84:SER:OG	1:C:84:SER:CB	2.06	1.01
2:B:118:GLY:HA2	2:B:118:GLY:N	1.35	1.01
1:C:140:TYR:HD1	1:C:140:TYR:O	1.42	1.01
1:C:70:GLN:C	1:C:70:GLN:CB	2.28	1.01
2:B:22:VAL:C	2:B:23:GLY:CA	2.28	1.01
2:B:69:ALA:HB3	2:B:69:ALA:CA	1.52	1.01
2:B:1:MET:HG3	2:B:77:LEU:HD13	1.02	1.01
2:B:103:ARG:CZ	2:B:103:ARG:NH1	0.86	1.01
1:C:83:LEU:CD2	1:C:83:LEU:CB	2.38	1.01
2:D:130:GLN:CG	2:D:130:GLN:HA	1.86	1.01
1:A:85:ASN:HD21	1:A:90:LYS:HE3	1.25	1.01
2:D:70:PHE:C	2:D:70:PHE:O	1.98	1.01
1:A:39:THR:CB	1:A:40:LYS:HZ3	1.74	1.00
2:B:80:LEU:HB3	2:B:81:LYS:O	1.60	1.00
3:C:142:HEM:C4C	3:C:142:HEM:HHD	1.60	1.00
2:D:72:GLN:NE2	2:D:73:GLY:N	2.08	1.00
2:B:128:LEU:CD2	2:B:128:LEU:HG	1.88	1.00
1:A:108:THR:C	1:A:108:THR:O	0.81	1.00
1:A:91:LEU:CD2	3:A:142:HEM:C3D	2.43	1.00
2:D:41:PHE:CE2	2:D:41:PHE:CG	2.48	1.00
2:D:81:LYS:H	2:D:81:LYS:HB3	1.26	1.00
1:C:124:ASN:ND2	1:C:124:ASN:OD1	1.94	1.00
2:D:140:LEU:CB	2:D:140:LEU:CD1	2.38	1.00
1:A:2:LEU:HG	1:A:73:LEU:HD23	1.44	1.00
2:B:109:LEU:CB	2:B:109:LEU:CD1	2.40	1.00
2:B:11:THR:C	2:B:11:THR:O	0.80	1.00
2:B:19:VAL:HG23	2:B:68:ASP:OD2	1.62	1.00
2:B:84:PHE:CB	2:B:84:PHE:CD2	2.45	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:PRO:C	2:D:123:PRO:HA	1.78	1.00
1:C:10:VAL:CG1	1:C:10:VAL:CG2	2.40	1.00
1:A:12:ALA:O	1:A:12:ALA:C	0.80	1.00
2:B:65:ARG:NH1	2:B:65:ARG:NH2	2.08	1.00
2:D:2:LEU:HG	2:D:7:LYS:HE3	1.42	1.00
2:D:68:ASP:C	2:D:68:ASP:CB	2.30	1.00
2:B:98:ASN:HB3	2:B:100:GLN:H	1.28	0.99
1:A:3:SER:CB	1:A:3:SER:C	2.30	0.99
2:B:98:ASN:OD1	1:C:96:VAL:HG11	1.59	0.99
1:A:108:THR:O	1:A:109:LEU:N	1.95	0.99
2:B:133:VAL:C	2:B:133:VAL:O	0.80	0.99
2:B:2:LEU:CG	2:B:6:GLU:HB3	1.92	0.99
2:B:80:LEU:CD1	2:B:80:LEU:CD2	2.40	0.99
1:C:135:VAL:HG21	1:C:135:VAL:HG11	1.40	0.99
2:D:140:LEU:CD1	2:D:140:LEU:HB2	1.92	0.99
2:B:118:GLY:C	2:B:119:GLY:CA	2.30	0.99
2:B:118:GLY:HA3	2:B:118:GLY:N	1.35	0.99
1:C:17:VAL:C	1:C:18:GLY:CA	2.30	0.99
1:C:55:GLN:CD	1:C:55:GLN:HB2	1.83	0.99
2:D:22:VAL:HG12	2:D:67:LEU:HD13	1.45	0.99
1:A:26:ALA:HB1	1:A:56:LYS:NZ	1.78	0.99
2:B:2:LEU:HB3	2:B:131:LYS:NZ	1.76	0.99
2:B:71:THR:CA	2:B:71:THR:N	0.85	0.99
1:A:62:VAL:HG11	1:A:62:VAL:HG21	1.03	0.99
1:C:44:PRO:CG	1:C:44:PRO:CA	2.40	0.99
2:D:101:ASN:O	3:D:146:HEM:HBB1	1.62	0.99
2:B:141:ALA:CB	2:B:141:ALA:N	2.24	0.99
2:B:41:PHE:CB	2:B:44:PHE:CE1	2.45	0.99
1:C:23:ALA:C	1:C:23:ALA:CB	2.31	0.99
2:D:74:LEU:O	2:D:77:LEU:HD11	1.61	0.99
1:A:36:PHE:CB	1:A:36:PHE:CD2	2.43	0.99
2:D:73:GLY:C	2:D:73:GLY:N	2.15	0.99
1:A:76:LEU:O	1:A:77:PRO:C	2.01	0.99
2:B:142:HIS:O	2:B:144:TYR:N	1.95	0.99
1:A:74:ASN:O	1:A:75:ASP:CA	2.11	0.98
2:B:75:LYS:CG	2:B:75:LYS:CE	2.40	0.98
3:C:142:HEM:C4C	3:C:142:HEM:CHD	0.94	0.98
2:D:108:VAL:O	2:D:109:LEU:N	1.94	0.98
2:D:81:LYS:N	2:D:81:LYS:HB3	1.77	0.98
1:A:136:LEU:HD23	1:A:136:LEU:H	1.24	0.98
1:C:61:LYS:CB	1:C:61:LYS:HA	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:VAL:HB	2:B:32:VAL:N	1.79	0.98
2:B:20:ASP:HB2	2:B:64:LYS:HD2	1.46	0.98
1:C:95:PRO:HG3	1:C:141:ARG:CZ	1.92	0.98
2:B:109:LEU:C	2:B:110:ALA:CA	2.31	0.98
2:B:56:ASN:C	2:B:56:ASN:O	0.78	0.98
2:B:77:LEU:HD13	2:B:77:LEU:O	1.64	0.98
1:A:8:SER:HA	1:A:8:SER:O	1.62	0.98
2:B:1:MET:H2	2:B:2:LEU:CD2	1.76	0.98
1:C:98:PHE:O	1:C:98:PHE:C	0.78	0.98
1:A:9:ASN:N	1:A:9:ASN:CB	2.26	0.97
2:D:103:ARG:C	2:D:103:ARG:HB3	1.84	0.97
2:D:59:VAL:CB	2:D:59:VAL:C	2.33	0.97
1:A:1:VAL:CG2	1:A:1:VAL:CG1	2.42	0.97
2:D:130:GLN:CB	2:D:130:GLN:HG2	1.48	0.97
1:C:61:LYS:CA	1:C:61:LYS:CG	2.43	0.97
1:C:9:ASN:OD1	1:C:9:ASN:ND2	1.97	0.97
1:A:91:LEU:HD21	3:A:142:HEM:CAD	1.95	0.97
2:D:52:ALA:N	2:D:52:ALA:CB	2.28	0.97
2:B:66:VAL:CG2	2:B:66:VAL:CG1	2.41	0.97
1:A:31:ARG:HG2	2:B:126:GLN:HE21	1.27	0.97
2:D:137:ALA:HB1	2:D:140:LEU:HD13	1.47	0.97
2:D:2:LEU:HG	2:D:7:LYS:CE	1.95	0.97
1:A:42:TYR:C	1:A:42:TYR:O	0.77	0.97
1:A:43:PHE:CA	1:A:44:PRO:N	2.27	0.97
2:B:109:LEU:CB	2:B:109:LEU:HD22	1.95	0.97
2:B:94:LYS:CE	2:B:94:LYS:CG	2.42	0.97
2:D:72:GLN:NE2	2:D:73:GLY:CA	2.28	0.97
2:B:117:PHE:O	2:B:120:GLN:OE1	1.81	0.97
2:B:36:TRP:CD2	2:B:36:TRP:CZ2	2.36	0.96
1:C:102:SER:C	1:C:103:HIS:CA	2.34	0.96
2:D:130:GLN:CB	2:D:130:GLN:HG3	1.48	0.96
2:B:87:LEU:HD21	2:B:87:LEU:CD1	1.94	0.96
2:D:72:GLN:HE21	2:D:73:GLY:CA	1.77	0.96
2:B:103:ARG:HB3	2:B:103:ARG:CD	1.95	0.96
2:B:3:THR:HG23	2:B:5:GLU:CA	1.94	0.96
2:D:25:GLN:HB3	2:D:112:VAL:HG21	1.45	0.96
1:C:133:SER:N	1:C:133:SER:C	2.16	0.96
1:A:106:LEU:CD1	1:A:106:LEU:CD2	2.42	0.96
2:B:16:LYS:HD3	2:B:117:PHE:HE1	1.28	0.96
1:A:110:ALA:O	1:A:114:PRO:HG3	1.64	0.96
2:B:1:MET:HG2	2:B:77:LEU:HD12	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ALA:O	1:C:57:ALA:HB3	1.66	0.96
2:D:42:GLN:OE1	2:D:42:GLN:CD	2.04	0.96
2:D:53:VAL:CG2	2:D:54:MET:HE2	1.94	0.96
2:D:128:LEU:C	2:D:129:PHE:CA	2.32	0.96
2:D:145:HIS:C	2:D:145:HIS:CB	2.34	0.96
2:B:71:THR:H	2:B:71:THR:CB	1.78	0.96
2:B:77:LEU:N	2:B:77:LEU:CB	2.29	0.96
1:C:76:LEU:HG	1:C:76:LEU:CD2	1.91	0.96
2:D:22:VAL:HG12	2:D:67:LEU:CD1	1.95	0.96
2:D:59:VAL:HG13	2:D:59:VAL:CG2	1.94	0.96
2:D:130:GLN:CG	2:D:130:GLN:HB2	1.45	0.96
2:B:60:LYS:NZ	2:B:60:LYS:CD	2.28	0.95
2:B:76:HIS:ND1	2:B:76:HIS:CG	1.81	0.95
2:B:80:LEU:HD22	2:B:82:GLY:HA2	1.48	0.95
1:A:81:SER:HA	1:A:81:SER:CB	1.93	0.95
2:B:81:LYS:NZ	2:B:142:HIS:ND1	2.15	0.95
2:D:130:GLN:CG	2:D:130:GLN:HB3	1.45	0.95
1:C:30:GLN:CD	1:C:30:GLN:CB	2.35	0.95
1:A:2:LEU:CD1	1:A:2:LEU:CD2	2.44	0.95
1:A:57:ALA:HA	1:A:60:GLN:CD	1.87	0.95
2:B:70:PHE:C	2:B:71:THR:CA	2.34	0.95
1:C:9:ASN:OD1	1:C:9:ASN:CG	0.76	0.95
2:D:131:LYS:HZ2	2:D:131:LYS:HD3	1.30	0.95
2:D:94:LYS:CG	2:D:95:LEU:HD23	1.97	0.95
2:B:34:TYR:CD2	2:B:34:TYR:HE2	1.65	0.95
1:C:56:LYS:HZ1	1:C:59:GLY:HA3	1.28	0.95
1:C:28:ALA:N	1:C:28:ALA:CB	2.29	0.95
1:A:87:HIS:CD2	1:A:87:HIS:NE2	1.70	0.95
1:A:108:THR:HA	1:A:108:THR:HB	1.36	0.95
1:A:124:ASN:CA	1:A:124:ASN:HB2	1.45	0.95
2:D:131:LYS:NZ	2:D:131:LYS:HD3	1.79	0.95
2:D:93:ASN:C	2:D:93:ASN:HB3	1.85	0.95
2:B:57:PRO:O	2:B:60:LYS:HB3	1.66	0.95
2:D:144:TYR:CZ	2:D:144:TYR:CD1	2.38	0.95
2:D:2:LEU:HD23	2:D:7:LYS:HB3	1.48	0.95
2:D:2:LEU:CD2	2:D:7:LYS:HG2	1.97	0.95
2:B:128:LEU:N	2:B:128:LEU:CB	2.29	0.94
1:C:48:LEU:HD12	1:C:49:SER:HB2	1.49	0.94
3:D:146:HEM:CMB	3:D:146:HEM:C1B	2.50	0.94
2:D:2:LEU:CB	2:D:2:LEU:C	2.34	0.94
2:D:69:ALA:CB	2:D:69:ALA:C	2.35	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:GLN:NE2	2:D:73:GLY:HA2	1.82	0.94
2:B:17:VAL:C	2:B:17:VAL:HG12	1.85	0.94
2:B:41:PHE:O	2:B:41:PHE:C	0.74	0.94
2:B:2:LEU:HB2	2:B:6:GLU:CB	1.96	0.94
2:D:126:GLN:HE22	2:D:130:GLN:HB2	1.29	0.94
2:B:20:ASP:CB	2:B:64:LYS:HD2	1.97	0.94
2:D:111:LEU:CA	2:D:112:VAL:N	2.29	0.94
2:D:2:LEU:HD12	2:D:2:LEU:HB3	1.47	0.94
3:A:142:HEM:C1D	3:A:142:HEM:CMD	2.50	0.94
1:A:1:VAL:HG12	1:C:141:ARG:O	1.68	0.94
1:A:91:LEU:HD11	1:A:91:LEU:HD21	1.49	0.94
2:B:1:MET:N	2:B:2:LEU:CD2	2.29	0.94
2:B:70:PHE:O	2:B:71:THR:CA	2.16	0.94
2:B:68:ASP:N	2:B:71:THR:HG22	1.70	0.94
1:A:16:LYS:CD	1:A:16:LYS:HZ2	1.55	0.94
1:A:17:VAL:CG2	1:A:17:VAL:CG1	2.44	0.94
1:A:79:THR:HB	1:A:80:LEU:HD23	0.95	0.94
1:A:94:ASN:C	1:A:94:ASN:O	0.74	0.94
2:B:64:LYS:HZ2	2:B:64:LYS:HB3	1.18	0.94
2:B:84:PHE:HB2	2:B:84:PHE:CD1	2.03	0.94
2:D:69:ALA:CA	2:D:70:PHE:N	2.30	0.94
1:A:124:ASN:CA	1:A:124:ASN:HB3	1.45	0.94
2:B:1:MET:CG	2:B:77:LEU:HD11	1.76	0.94
2:D:75:LYS:C	2:D:75:LYS:CB	2.36	0.94
3:A:142:HEM:CHC	3:A:142:HEM:NB	2.28	0.94
1:A:43:PHE:HA	1:A:44:PRO:N	1.82	0.94
2:B:124:ASN:C	2:B:125:VAL:HA	1.85	0.94
1:C:52:SER:HB3	1:C:55:GLN:NE2	1.82	0.94
2:B:81:LYS:HZ2	2:B:142:HIS:CE1	1.85	0.93
1:C:91:LEU:N	1:C:91:LEU:CB	2.30	0.93
1:A:136:LEU:HD23	1:A:136:LEU:N	1.81	0.93
2:B:107:ASN:ND2	2:B:107:ASN:CB	2.30	0.93
2:B:22:VAL:C	2:B:22:VAL:N	2.20	0.93
2:D:108:VAL:HA	2:D:108:VAL:O	1.66	0.93
2:D:142:HIS:CB	2:D:142:HIS:HA	1.94	0.93
2:D:27:LEU:CD1	2:D:27:LEU:CD2	2.44	0.93
2:D:75:LYS:CA	2:D:75:LYS:CG	2.46	0.93
2:B:24:ALA:CB	2:B:24:ALA:HA	1.93	0.93
2:B:22:VAL:HG12	2:B:67:LEU:HD21	1.49	0.93
1:C:67:THR:OG1	1:C:67:THR:CG2	2.16	0.93
1:C:68:LYS:CG	1:C:68:LYS:CA	2.45	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:LEU:HD23	2:B:109:LEU:CB	1.95	0.93
2:B:59:VAL:CG1	2:B:59:VAL:CA	2.45	0.93
2:D:108:VAL:C	2:D:108:VAL:O	0.73	0.93
2:D:34:TYR:CE2	2:D:34:TYR:CZ	0.93	0.93
1:A:11:LYS:C	1:A:11:LYS:O	0.73	0.93
1:A:10:VAL:C	1:A:10:VAL:CB	2.37	0.93
3:A:142:HEM:C3D	3:A:142:HEM:C2D	0.93	0.93
1:A:77:PRO:C	1:A:78:GLY:CA	2.37	0.93
1:C:44:PRO:C	1:C:45:HIS:CA	2.37	0.93
2:D:100:GLN:HG3	2:D:100:GLN:CA	1.98	0.93
2:D:2:LEU:HD23	2:D:7:LYS:CB	1.99	0.93
2:B:140:LEU:C	2:B:141:ALA:CA	2.37	0.93
1:C:135:VAL:O	1:C:138:SER:HB2	1.68	0.93
1:A:43:PHE:CD2	1:A:43:PHE:CB	2.52	0.93
1:C:115:THR:HB	1:C:115:THR:CG2	1.97	0.93
1:C:91:LEU:CG	1:C:91:LEU:CA	2.47	0.93
2:D:59:VAL:HA	2:D:59:VAL:HG22	1.51	0.93
2:D:75:LYS:CG	2:D:75:LYS:HB3	1.42	0.93
1:A:106:LEU:N	1:A:106:LEU:CB	2.32	0.92
1:A:13:ALA:HB1	1:A:125:LEU:HD21	1.50	0.92
1:A:127:LYS:CA	1:A:128:PHE:N	2.32	0.92
1:A:25:GLY:CA	1:A:26:ALA:N	2.32	0.92
2:B:84:PHE:CD2	2:B:84:PHE:CG	0.92	0.92
1:A:126:ASN:C	1:A:126:ASN:CB	2.36	0.92
1:C:36:PHE:CA	1:C:37:PRO:N	2.30	0.92
2:D:144:TYR:HD1	2:D:145:HIS:H	1.10	0.92
2:B:75:LYS:HG3	2:B:76:HIS:ND1	1.80	0.92
1:C:119:PRO:CB	1:C:119:PRO:C	2.36	0.92
1:C:140:TYR:CB	1:C:140:TYR:CD2	2.51	0.92
2:D:75:LYS:HB2	2:D:75:LYS:CG	1.42	0.92
1:A:62:VAL:CG2	1:A:62:VAL:HG11	1.76	0.92
2:B:16:LYS:HD3	2:B:117:PHE:CE1	2.02	0.92
2:B:84:PHE:CG	2:B:84:PHE:HD2	1.70	0.92
2:B:31:LEU:CD1	2:B:31:LEU:HG	1.94	0.92
1:C:108:THR:N	1:C:108:THR:C	2.23	0.92
1:C:60:GLN:CG	1:C:60:GLN:CA	2.47	0.92
1:A:36:PHE:O	1:A:39:THR:CG2	2.17	0.92
2:B:103:ARG:NE	2:B:103:ARG:CG	2.31	0.92
2:B:75:LYS:N	2:B:75:LYS:C	2.23	0.92
1:A:39:THR:HG23	1:A:40:LYS:HZ1	1.34	0.92
2:B:95:LEU:HD11	3:B:146:HEM:C3A	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:HIS:CG	2:B:62:HIS:CA	2.53	0.92
1:C:92:ARG:CB	1:C:92:ARG:CD	2.47	0.92
2:D:28:GLY:C	2:D:54:MET:HE3	1.90	0.92
2:D:8:ALA:O	2:D:8:ALA:C	2.08	0.92
2:B:68:ASP:HA	2:B:71:THR:HG23	1.07	0.92
2:D:67:LEU:CB	2:D:67:LEU:HA	2.00	0.92
1:A:57:ALA:HA	1:A:60:GLN:NE2	1.84	0.92
2:D:2:LEU:CD2	2:D:4:ALA:HA	2.00	0.92
2:D:42:GLN:CB	2:D:42:GLN:CD	2.37	0.92
2:B:106:GLY:HA3	2:B:133:VAL:HG22	1.51	0.91
1:C:45:HIS:HE1	3:C:142:HEM: CBD	1.82	0.91
2:B:31:LEU:C	2:B:32:VAL:CA	2.38	0.91
1:C:71:GLY:C	1:C:71:GLY:N	2.22	0.91
2:B:117:PHE:CG	2:B:117:PHE:CE1	2.41	0.91
2:B:34:TYR:CD2	2:B:34:TYR:CE2	0.91	0.91
1:C:89:HIS:CB	1:C:139:LYS:HZ3	1.83	0.91
1:A:85:ASN:ND2	1:A:90:LYS:HE3	1.84	0.91
2:B:13:PHE:CA	2:B:13:PHE:O	2.18	0.91
2:B:32:VAL:CB	2:B:32:VAL:N	2.32	0.91
2:D:67:LEU:CA	2:D:67:LEU:CG	2.48	0.91
2:B:103:ARG:CB	2:B:103:ARG:CD	2.49	0.91
2:B:113:VAL:HG12	2:B:117:PHE:CD2	2.04	0.91
1:C:80:LEU:HD23	1:C:135:VAL:CG2	2.00	0.91
1:C:78:GLY:C	1:C:79:THR:CA	2.37	0.91
2:D:131:LYS:C	2:D:132:VAL:CA	2.38	0.91
2:B:75:LYS:CG	2:B:76:HIS:CE1	2.53	0.91
1:C:126:ASN:OD1	1:C:126:ASN:ND2	2.03	0.91
1:C:113:LEU:HD23	1:C:113:LEU:H	1.36	0.91
2:B:128:LEU:O	2:B:128:LEU:CA	2.17	0.91
2:D:2:LEU:CD2	2:D:3:THR:O	2.15	0.91
1:A:47:ASP:OD2	1:A:49:SER:HA	1.70	0.91
1:A:80:LEU:HG	1:A:80:LEU:CB	2.00	0.91
2:B:10:VAL:HG13	2:B:128:LEU:HD21	0.91	0.91
2:D:100:GLN:HA	2:D:100:GLN:CB	1.99	0.91
3:B:146:HEM:C3D	3:B:146:HEM: CBD	2.54	0.91
2:B:71:THR:CB	2:B:71:THR:N	2.33	0.90
2:B:74:LEU:HD13	2:B:77:LEU:HB2	0.91	0.90
1:C:44:PRO:CD	1:C:44:PRO:CA	2.49	0.90
2:B:126:GLN:N	2:B:126:GLN:C	2.24	0.90
1:C:76:LEU:HG	1:C:76:LEU:CD1	2.01	0.90
1:A:141:ARG:HB3	1:C:1:VAL:HG23	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LEU:HD22	2:B:77:LEU:HD23	1.53	0.90
1:C:54:GLN:CG	1:C:54:GLN:CA	2.50	0.90
2:B:116:ASN:HA	2:B:116:ASN:CB	2.00	0.90
2:B:128:LEU:C	2:B:128:LEU:HA	1.90	0.90
2:B:145:HIS:CB	2:B:145:HIS:N	2.34	0.90
2:B:25:GLN:OE1	2:B:112:VAL:CG1	2.19	0.90
2:B:33:VAL:HG12	2:B:34:TYR:CE1	2.06	0.90
2:D:75:LYS:CD	2:D:75:LYS:CB	2.49	0.90
2:B:86:GLN:CA	2:B:86:GLN:CG	2.50	0.90
1:C:87:HIS:CB	1:C:87:HIS:ND1	2.33	0.90
2:D:57:PRO:CA	2:D:57:PRO:CG	2.37	0.90
2:B:41:PHE:CD2	2:B:44:PHE:HE1	1.85	0.90
1:C:93:VAL:HG13	3:C:142:HEM:HAC	1.54	0.90
2:B:44:PHE:C	2:B:45:GLY:CA	2.40	0.90
1:C:52:SER:CB	1:C:55:GLN:HE21	1.84	0.90
2:D:107:ASN:H	2:D:107:ASN:HB2	1.35	0.90
2:B:20:ASP:HB3	2:B:64:LYS:CE	2.02	0.90
2:D:107:ASN:C	2:D:107:ASN:N	2.24	0.90
2:D:34:TYR:C	2:D:34:TYR:N	2.25	0.90
1:C:39:THR:CA	1:C:39:THR:HB	2.01	0.89
3:A:142:HEM:CBA	3:A:142:HEM:C2A	2.54	0.89
1:C:89:HIS:HE1	1:C:90:LYS:HG2	1.36	0.89
2:D:57:PRO:CA	2:D:57:PRO:CD	2.46	0.89
1:A:124:ASN:CA	1:A:124:ASN:CB	0.90	0.89
2:B:36:TRP:CZ2	2:B:36:TRP:CE2	0.90	0.89
2:B:45:GLY:C	2:B:45:GLY:N	2.26	0.89
2:D:100:GLN:O	2:D:101:ASN:HA	1.72	0.89
2:B:69:ALA:CA	2:B:69:ALA:CB	0.89	0.89
2:D:111:LEU:C	2:D:112:VAL:N	0.84	0.89
1:A:132:ASP:CB	1:A:132:ASP:OD2	2.20	0.89
1:A:39:THR:HG23	1:A:40:LYS:NZ	1.88	0.89
2:B:141:ALA:C	2:B:142:HIS:CA	2.38	0.89
1:C:45:HIS:CE1	3:C:142:HEM:CGD	2.56	0.89
2:D:2:LEU:HD13	2:D:2:LEU:HB3	1.52	0.89
1:A:135:VAL:CG2	1:A:135:VAL:CG1	2.51	0.89
1:C:85:ASN:CB	1:C:85:ASN:C	2.40	0.89
2:D:14:TRP:O	2:D:14:TRP:CA	2.19	0.89
2:D:2:LEU:HD22	2:D:4:ALA:CA	2.03	0.89
2:D:75:LYS:CB	2:D:75:LYS:HG3	1.37	0.89
1:A:127:LYS:CD	1:A:127:LYS:HZ2	1.85	0.89
2:B:36:TRP:HZ2	2:B:36:TRP:CE2	1.65	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:LEU:HG	2:D:7:LYS:CD	2.02	0.89
2:D:71:THR:CG2	2:D:71:THR:CA	2.51	0.89
2:B:54:MET:CB	2:B:55:ASN:OD1	2.20	0.89
1:C:61:LYS:CB	1:C:61:LYS:CD	2.45	0.89
1:A:11:LYS:C	1:A:12:ALA:CA	2.42	0.88
1:A:3:SER:O	1:A:4:ALA:CA	2.20	0.88
2:B:16:LYS:N	2:B:16:LYS:CB	2.36	0.88
1:C:113:LEU:CD2	1:C:113:LEU:H	1.86	0.88
2:D:7:LYS:O	2:D:8:ALA:N	0.75	0.88
1:A:45:HIS:C	1:A:45:HIS:CB	2.41	0.88
2:B:22:VAL:HA	2:B:22:VAL:CG2	2.01	0.88
2:B:60:LYS:HZ2	2:B:60:LYS:HD2	1.35	0.88
1:A:115:THR:CA	1:A:115:THR:OG1	2.20	0.88
1:A:20:ASN:CA	1:A:20:ASN:CG	2.41	0.88
2:D:30:LEU:CB	2:D:30:LEU:C	2.41	0.88
2:B:117:PHE:CD1	2:B:117:PHE:CE1	0.88	0.88
2:B:2:LEU:HB2	2:B:3:THR:H	1.37	0.88
2:B:3:THR:CB	2:B:5:GLU:HB3	2.03	0.88
2:B:46:ASN:CG	2:B:46:ASN:CA	2.41	0.88
2:D:25:GLN:HE22	2:D:115:ARG:HH22	1.22	0.88
3:A:142:HEM:HAD2	3:A:142:HEM:C2D	2.07	0.88
1:A:52:SER:C	1:A:56:LYS:HG2	1.93	0.88
2:B:41:PHE:CG	2:B:44:PHE:HE1	1.88	0.88
1:C:89:HIS:CE1	1:C:90:LYS:HG2	2.08	0.88
2:D:11:THR:C	2:D:11:THR:HA	1.91	0.88
1:C:56:LYS:NZ	1:C:59:GLY:CA	2.36	0.88
1:C:97:ASN:CA	1:C:98:PHE:N	2.36	0.88
1:A:2:LEU:CB	1:A:2:LEU:HA	2.00	0.88
2:B:118:GLY:N	2:B:118:GLY:CA	0.73	0.88
2:B:40:PHE:HB3	3:B:146:HEM:CMA	2.03	0.88
2:B:87:LEU:HD11	2:B:87:LEU:HD21	1.56	0.88
1:C:52:SER:C	1:C:53:ALA:CA	2.40	0.88
1:C:95:PRO:HG3	1:C:141:ARG:NH1	1.89	0.88
2:D:100:GLN:HG3	2:D:100:GLN:HA	1.52	0.88
2:D:131:LYS:CA	2:D:131:LYS:CG	2.52	0.88
2:B:2:LEU:CD1	2:B:6:GLU:HB3	2.04	0.88
2:B:17:VAL:CG1	2:B:17:VAL:C	2.42	0.88
1:C:85:ASN:CG	1:C:89:HIS:HB3	1.93	0.88
2:B:11:THR:CA	2:B:11:THR:O	2.21	0.87
1:A:119:PRO:C	1:A:120:ALA:CA	2.41	0.87
1:A:49:SER:HB2	1:A:52:SER:HB3	0.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:GLN:NE2	2:B:47:LEU:O	2.07	0.87
2:B:131:LYS:NZ	2:B:131:LYS:CD	2.37	0.87
1:C:140:TYR:CD1	1:C:140:TYR:O	2.28	0.87
1:C:68:LYS:CD	1:C:68:LYS:NZ	2.37	0.87
2:D:102:PHE:N	2:D:102:PHE:C	2.27	0.87
2:D:55:ASN:O	2:D:60:LYS:HD3	1.74	0.87
1:A:16:LYS:HD2	1:A:16:LYS:HZ2	1.37	0.87
1:A:85:ASN:HD22	1:A:86:LEU:N	1.72	0.87
1:C:93:VAL:HG13	3:C:142:HEM:CAC	2.05	0.87
1:A:25:GLY:O	1:A:29:LEU:HD22	1.75	0.87
1:A:67:THR:CA	1:A:68:LYS:N	2.35	0.87
2:B:10:VAL:HG13	2:B:128:LEU:CD2	1.72	0.87
2:B:75:LYS:HE3	2:B:75:LYS:CG	2.05	0.87
1:A:108:THR:O	1:A:108:THR:CA	2.22	0.86
1:A:127:LYS:C	1:A:128:PHE:N	0.82	0.86
1:A:11:LYS:O	1:A:11:LYS:CA	2.22	0.86
2:B:79:ASP:O	2:B:80:LEU:N	2.06	0.86
1:C:29:LEU:HB3	1:C:29:LEU:CA	2.06	0.86
2:D:107:ASN:N	2:D:107:ASN:HB2	1.88	0.86
2:D:14:TRP:HE1	2:D:71:THR:CG2	1.87	0.86
2:B:55:ASN:C	2:B:60:LYS:HZ1	1.77	0.86
2:B:68:ASP:CB	2:B:71:THR:O	2.22	0.86
2:B:2:LEU:HD12	2:B:6:GLU:HB3	1.55	0.86
1:A:124:ASN:HA	1:A:124:ASN:CB	1.35	0.86
2:D:22:VAL:CG2	2:D:22:VAL:CG1	2.53	0.86
1:C:14:TRP:HB2	1:C:70:GLN:HE22	1.40	0.86
2:D:127:ALA:CB	2:D:127:ALA:C	2.44	0.86
2:D:34:TYR:HE2	2:D:34:TYR:CZ	1.59	0.86
2:D:34:TYR:HB3	2:D:36:TRP:CZ2	2.10	0.86
1:A:114:PRO:CA	1:A:114:PRO:CD	2.54	0.86
1:A:33:PHE:HB3	1:A:40:LYS:HG3	1.57	0.86
1:A:42:TYR:C	1:A:43:PHE:CA	2.44	0.86
2:B:128:LEU:O	2:B:128:LEU:HA	1.76	0.86
2:B:130:GLN:CD	2:B:130:GLN:HE21	1.42	0.86
2:B:67:LEU:C	2:B:71:THR:HG22	1.96	0.86
1:C:55:GLN:CB	1:C:55:GLN:HA	2.04	0.86
2:D:126:GLN:NE2	2:D:130:GLN:HB2	1.91	0.86
2:B:144:TYR:O	2:D:1:MET:SD	2.33	0.86
2:B:87:LEU:O	2:B:87:LEU:CA	2.23	0.86
1:C:89:HIS:N	1:C:139:LYS:HG3	1.91	0.86
2:D:75:LYS:HG2	2:D:75:LYS:CB	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASN:OD1	1:A:126:ASN:ND2	2.08	0.86
2:B:57:PRO:HB3	2:B:57:PRO:CD	2.02	0.86
2:B:55:ASN:C	2:B:60:LYS:HZ3	1.70	0.86
1:C:115:THR:C	1:C:115:THR:N	2.29	0.86
2:B:144:TYR:O	2:D:1:MET:CE	2.23	0.86
1:A:46:PHE:HB2	1:A:48:LEU:HD23	1.55	0.86
2:B:130:GLN:HE22	2:B:130:GLN:CD	1.43	0.86
1:C:137:THR:O	1:C:138:SER:N	2.07	0.86
1:C:48:LEU:CD1	1:C:49:SER:HB2	2.05	0.86
2:D:68:ASP:N	2:D:68:ASP:C	2.26	0.86
3:A:142:HEM:CGA	3:A:142:HEM:CAA	2.54	0.85
1:A:22:PRO:CD	1:A:22:PRO:CB	2.54	0.85
2:D:34:TYR:N	2:D:34:TYR:CB	2.37	0.85
2:D:17:VAL:N	2:D:17:VAL:C	2.28	0.85
1:A:16:LYS:HZ3	1:A:16:LYS:HD3	1.38	0.85
2:B:133:VAL:CG2	2:B:133:VAL:CG1	2.53	0.85
1:A:9:ASN:N	1:A:9:ASN:HB2	1.89	0.85
2:B:3:THR:HG23	2:B:5:GLU:CG	2.06	0.85
2:B:19:VAL:CG2	2:B:68:ASP:H	1.90	0.85
1:C:17:VAL:C	1:C:17:VAL:N	2.30	0.85
2:B:116:ASN:CA	2:B:116:ASN:CG	2.45	0.85
2:B:17:VAL:CB	2:B:17:VAL:C	2.44	0.85
2:D:1:MET:HG3	2:D:131:LYS:HZ1	1.42	0.85
2:D:75:LYS:HB3	2:D:76:HIS:H	1.42	0.85
2:B:25:GLN:OE1	2:B:112:VAL:HG12	1.74	0.85
2:D:11:THR:HA	2:D:14:TRP:H	1.40	0.85
2:D:67:LEU:HD23	2:D:71:THR:HG21	1.59	0.85
2:D:90:LEU:HB3	2:D:90:LEU:CD1	2.04	0.85
1:C:133:SER:C	1:C:134:THR:CA	2.45	0.85
1:A:96:VAL:HG11	2:D:100:GLN:HG2	1.58	0.85
2:D:31:LEU:CA	2:D:31:LEU:CG	2.54	0.85
1:A:89:HIS:HD2	1:A:139:LYS:HD2	1.38	0.85
3:A:142:HEM:CBD	3:A:142:HEM:HAD2	2.07	0.85
2:B:14:TRP:NE1	2:B:68:ASP:OD1	2.10	0.85
2:B:70:PHE:CD1	2:B:70:PHE:CZ	2.59	0.85
2:D:78:ASP:CA	2:D:79:ASP:N	2.38	0.85
1:C:80:LEU:CD1	1:C:80:LEU:CB	2.55	0.84
1:A:39:THR:CA	1:A:40:LYS:HZ3	1.90	0.84
1:C:30:GLN:OE1	1:C:30:GLN:CG	2.24	0.84
2:D:95:LEU:HD23	2:D:95:LEU:N	1.91	0.84
1:A:16:LYS:H	1:A:17:VAL:N	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PHE:C	1:C:36:PHE:CB	2.46	0.84
1:A:105:LEU:HD22	1:A:105:LEU:CD1	2.05	0.84
2:B:80:LEU:HD23	2:B:81:LYS:O	1.77	0.84
2:D:144:TYR:CD1	2:D:145:HIS:N	2.45	0.84
2:D:14:TRP:CA	2:D:15:GLY:N	2.38	0.84
2:D:73:GLY:CA	2:D:73:GLY:O	2.24	0.84
1:A:35:SER:HA	1:A:35:SER:CB	2.05	0.84
2:B:20:ASP:O	2:B:21:VAL:CG2	2.25	0.84
2:D:75:LYS:HB3	2:D:76:HIS:N	1.93	0.84
2:D:76:HIS:CG	2:D:76:HIS:H	1.96	0.84
1:A:31:ARG:HD3	2:B:126:GLN:HG3	1.59	0.84
2:B:106:GLY:CA	2:B:133:VAL:HG22	2.07	0.84
2:B:23:GLY:C	2:B:24:ALA:CA	2.46	0.84
2:D:109:LEU:C	2:D:109:LEU:N	2.30	0.84
1:A:128:PHE:CZ	1:A:128:PHE:CD1	2.58	0.84
1:A:1:VAL:CA	1:A:1:VAL:CG1	2.56	0.84
1:A:46:PHE:CB	1:A:48:LEU:HD23	2.07	0.84
2:B:75:LYS:HG3	2:B:76:HIS:HE1	1.40	0.84
2:B:95:LEU:HB2	2:B:95:LEU:N	1.74	0.84
1:C:72:HIS:CB	1:C:74:ASN:HD21	1.89	0.84
1:A:31:ARG:HH21	2:B:126:GLN:CB	1.88	0.84
2:B:130:GLN:CD	2:B:130:GLN:NE2	0.78	0.84
2:B:19:VAL:CB	2:B:19:VAL:C	2.46	0.84
1:C:43:PHE:HB3	1:C:46:PHE:HD1	1.43	0.84
2:D:2:LEU:CB	2:D:2:LEU:HD13	2.01	0.84
1:A:104:SER:OG	1:A:104:SER:CB	2.26	0.84
2:B:34:TYR:HD2	2:B:34:TYR:CE2	1.54	0.84
2:B:56:ASN:O	2:B:57:PRO:N	2.09	0.84
2:B:2:LEU:HD12	2:B:6:GLU:CB	2.06	0.84
2:B:74:LEU:HD13	2:B:77:LEU:CG	2.06	0.84
1:A:69:ALA:C	1:A:69:ALA:N	2.31	0.83
3:C:142:HEM:NC	3:C:142:HEM:CHD	2.41	0.83
2:D:16:LYS:CD	2:D:16:LYS:HB3	2.07	0.83
1:A:136:LEU:CB	1:A:136:LEU:C	2.47	0.83
2:B:2:LEU:HD12	2:B:6:GLU:CG	2.08	0.83
1:C:29:LEU:HD13	1:C:29:LEU:CD2	2.06	0.83
1:C:92:ARG:NE	1:C:92:ARG:CG	2.41	0.83
2:D:130:GLN:CB	2:D:130:GLN:CG	0.84	0.83
2:B:117:PHE:HE1	2:B:117:PHE:CD1	1.54	0.83
1:C:7:LYS:HG2	1:C:73:LEU:CB	2.08	0.83
1:C:87:HIS:CA	1:C:91:LEU:HD12	2.04	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:GLY:N	2:D:119:GLY:C	2.31	0.83
2:D:130:GLN:CB	2:D:130:GLN:CD	2.46	0.83
2:D:2:LEU:CB	2:D:2:LEU:HD12	2.01	0.83
2:D:67:LEU:CD2	2:D:71:THR:HG21	2.09	0.83
2:D:105:LEU:HD13	2:D:105:LEU:CB	2.06	0.83
1:A:88:ALA:O	1:A:92:ARG:HA	1.77	0.83
2:B:74:LEU:HD22	2:B:77:LEU:CD2	2.09	0.83
2:D:25:GLN:CG	2:D:25:GLN:OE1	2.27	0.83
2:D:95:LEU:HD12	2:D:97:VAL:CG2	2.08	0.83
1:A:3:SER:HB3	1:A:6:ASN:HD22	1.42	0.83
2:B:103:ARG:CZ	2:B:103:ARG:HH11	1.49	0.83
2:B:4:ALA:CA	2:B:4:ALA:O	2.27	0.83
2:B:60:LYS:NZ	2:B:60:LYS:HD2	1.91	0.83
2:D:44:PHE:CD2	2:D:58:LYS:HB3	2.13	0.83
2:D:53:VAL:CG2	2:D:54:MET:CE	2.53	0.83
2:D:99:PRO:CD	2:D:144:TYR:OH	2.27	0.83
1:A:33:PHE:HD1	1:A:40:LYS:HE3	1.42	0.83
2:B:103:ARG:HH12	2:B:103:ARG:CZ	1.49	0.83
1:C:110:ALA:N	1:C:110:ALA:C	2.32	0.83
1:C:45:HIS:CD2	1:C:46:PHE:CE1	2.67	0.83
1:A:18:GLY:O	1:A:18:GLY:CA	2.26	0.83
1:C:103:HIS:O	1:C:107:VAL:HG12	1.78	0.83
1:C:131:ASN:C	1:C:131:ASN:CB	2.47	0.83
1:A:55:GLN:CA	1:A:55:GLN:CG	2.54	0.83
1:A:85:ASN:C	1:A:85:ASN:HD22	1.81	0.82
2:B:113:VAL:HG12	2:B:117:PHE:HD2	1.43	0.82
2:B:68:ASP:CA	2:B:71:THR:HG23	1.68	0.82
2:B:88:SER:CB	2:B:143:LYS:HB3	2.08	0.82
1:C:122:HIS:ND1	1:C:122:HIS:HB2	1.91	0.82
2:B:3:THR:HB	2:B:6:GLU:HB2	1.61	0.82
1:C:122:HIS:ND1	1:C:122:HIS:CB	2.36	0.82
1:C:3:SER:CA	1:C:4:ALA:N	2.42	0.82
1:A:86:LEU:CD2	1:A:86:LEU:CB	2.58	0.82
2:D:62:HIS:CE1	2:D:62:HIS:CD2	2.67	0.82
1:A:48:LEU:CB	1:A:48:LEU:HA	2.08	0.82
2:B:2:LEU:CB	2:B:6:GLU:HB3	2.08	0.82
1:C:104:SER:C	1:C:104:SER:CB	2.48	0.82
1:A:31:ARG:NE	1:A:31:ARG:HG2	1.94	0.82
2:B:14:TRP:NE1	2:B:68:ASP:CG	2.32	0.82
2:B:52:ALA:N	2:B:52:ALA:CB	2.43	0.82
2:B:53:VAL:O	2:B:59:VAL:HG21	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:SER:O	1:C:114:PRO:HG3	1.80	0.82
1:C:48:LEU:HA	1:C:55:GLN:OE1	1.80	0.82
2:D:75:LYS:CB	2:D:75:LYS:CG	0.82	0.82
1:A:112:HIS:CB	1:A:112:HIS:ND1	2.40	0.82
1:C:45:HIS:CD2	1:C:46:PHE:CD1	2.68	0.82
1:C:88:ALA:CB	1:C:139:LYS:HB2	2.09	0.82
1:A:7:LYS:CA	1:A:8:SER:N	2.40	0.82
1:C:29:LEU:CA	1:C:29:LEU:HB2	2.06	0.82
2:D:20:ASP:C	2:D:21:VAL:CA	2.44	0.82
1:A:53:ALA:CA	1:A:56:LYS:HG2	2.10	0.82
2:B:31:LEU:CD1	2:B:31:LEU:CD2	2.58	0.82
2:B:70:PHE:CG	2:B:70:PHE:CZ	2.67	0.81
1:C:88:ALA:HB1	1:C:139:LYS:HB2	1.61	0.81
2:D:14:TRP:N	2:D:14:TRP:C	2.32	0.81
2:D:49:SER:O	2:D:53:VAL:CG1	2.27	0.81
2:D:68:ASP:HA	2:D:68:ASP:CG	1.98	0.81
1:A:3:SER:C	1:A:4:ALA:CA	2.49	0.81
1:C:83:LEU:HD11	3:C:142:HEM:HMA1	1.62	0.81
1:A:137:THR:OG1	1:A:137:THR:HG23	1.80	0.81
1:A:137:THR:OG1	1:A:137:THR:HA	1.79	0.81
1:C:130:ALA:N	1:C:130:ALA:CB	2.43	0.81
2:D:45:GLY:C	2:D:46:ASN:CA	2.48	0.81
2:B:4:ALA:CA	2:B:5:GLU:H	1.89	0.81
1:C:101:LEU:O	1:C:105:LEU:HB3	1.78	0.81
1:C:129:LEU:CB	1:C:129:LEU:CD2	2.57	0.81
2:D:103:ARG:CB	2:D:103:ARG:CD	2.58	0.81
1:A:20:ASN:O	1:A:23:ALA:HB3	1.80	0.81
1:A:50:HIS:CG	1:A:50:HIS:CA	2.62	0.81
1:C:135:VAL:O	1:C:138:SER:CB	2.29	0.81
2:D:110:ALA:CB	2:D:110:ALA:C	2.48	0.81
2:B:128:LEU:CD1	2:B:128:LEU:CB	2.58	0.81
2:B:3:THR:HG22	2:B:6:GLU:CA	2.11	0.81
1:C:138:SER:CB	1:C:138:SER:N	2.44	0.81
2:D:137:ALA:HB1	2:D:140:LEU:CD1	2.09	0.81
1:A:29:LEU:CD1	1:A:29:LEU:CD2	2.58	0.81
2:B:1:MET:H2	2:B:2:LEU:HD23	1.30	0.81
2:B:94:LYS:C	2:B:94:LYS:CB	2.49	0.81
1:C:100:LEU:N	1:C:100:LEU:C	2.34	0.81
1:C:22:PRO:CB	1:C:22:PRO:HD2	2.11	0.81
2:B:19:VAL:CG2	2:B:19:VAL:CA	2.59	0.81
2:B:1:MET:HE1	2:B:78:ASP:OD2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:VAL:O	2:B:59:VAL:CA	2.28	0.81
1:C:41:THR:HB	1:C:41:THR:CG2	2.10	0.81
2:D:76:HIS:CB	2:D:76:HIS:N	2.44	0.81
1:A:57:ALA:H	1:A:57:ALA:CB	1.92	0.81
3:B:146:HEM:C3D	3:B:146:HEM:CHA	2.64	0.81
1:C:43:PHE:CB	1:C:43:PHE:N	2.44	0.81
2:D:11:THR:CG2	2:D:11:THR:N	2.42	0.81
2:D:67:LEU:O	2:D:67:LEU:CA	2.29	0.81
1:A:2:LEU:CB	1:A:2:LEU:HG	2.08	0.81
2:B:32:VAL:CB	2:B:32:VAL:CG2	2.59	0.81
1:C:39:THR:N	1:C:39:THR:CB	2.40	0.81
1:A:89:HIS:HD2	1:A:139:LYS:HG2	1.46	0.80
2:B:98:ASN:HB3	2:B:100:GLN:N	1.95	0.80
2:B:106:GLY:CA	2:B:133:VAL:CG2	2.59	0.80
2:B:65:ARG:NH1	3:B:146:HEM:CGD	2.44	0.80
1:C:14:TRP:C	1:C:15:GLY:CA	2.49	0.80
2:D:51:GLY:C	2:D:52:ALA:CA	2.42	0.80
2:B:39:ARG:NH1	2:B:40:PHE:CE1	2.48	0.80
1:A:109:LEU:HD12	1:A:117:PHE:HE1	1.46	0.80
3:A:142:HEM:CBD	3:A:142:HEM:HAD1	2.07	0.80
1:A:104:SER:C	1:A:104:SER:CB	2.49	0.80
2:B:65:ARG:HD3	3:B:146:HEM:HBD1	1.64	0.80
2:B:1:MET:CE	2:B:78:ASP:OD2	2.29	0.80
2:B:2:LEU:HB2	2:B:6:GLU:HB3	1.64	0.80
1:C:14:TRP:HB2	1:C:70:GLN:NE2	1.96	0.80
1:C:79:THR:CA	1:C:79:THR:OG1	2.28	0.80
1:C:84:SER:HB2	1:C:84:SER:C	1.98	0.80
1:A:110:ALA:HB1	2:B:115:ARG:HB2	1.63	0.80
2:B:2:LEU:HB3	2:B:131:LYS:HZ1	1.46	0.80
1:C:84:SER:OG	1:C:136:LEU:HD22	1.82	0.80
2:D:121:PHE:C	2:D:121:PHE:CB	2.49	0.80
2:D:7:LYS:C	2:D:7:LYS:O	0.70	0.80
1:C:93:VAL:HG11	3:C:142:HEM:C3C	2.16	0.80
2:D:112:VAL:CG1	2:D:112:VAL:CA	2.59	0.80
2:B:41:PHE:HB3	2:B:44:PHE:CE1	2.16	0.80
1:C:22:PRO:HB2	1:C:22:PRO:CD	2.10	0.80
2:D:50:ALA:O	2:D:53:VAL:HG13	1.82	0.80
1:C:3:SER:C	1:C:3:SER:CB	2.51	0.80
1:C:99:LYS:CE	1:C:99:LYS:CG	2.59	0.80
2:D:115:ARG:CB	2:D:115:ARG:N	2.44	0.80
2:B:117:PHE:HD1	2:B:117:PHE:CE1	1.56	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASN:C	1:C:85:ASN:N	2.33	0.80
2:D:99:PRO:HD2	2:D:144:TYR:CZ	2.17	0.80
1:A:31:ARG:HE	1:A:31:ARG:CG	1.95	0.80
1:C:121:VAL:C	1:C:122:HIS:CA	2.50	0.80
1:C:133:SER:CA	1:C:134:THR:N	2.43	0.80
1:C:45:HIS:NE2	1:C:46:PHE:CE1	2.50	0.80
1:C:49:SER:HA	1:C:55:GLN:OE1	1.82	0.80
1:A:26:ALA:HB2	1:A:59:GLY:HA3	1.63	0.79
1:A:58:HIS:CB	1:A:58:HIS:HA	2.10	0.79
1:A:83:LEU:C	1:A:84:SER:CA	2.49	0.79
1:C:110:ALA:O	1:C:114:PRO:HB3	1.82	0.79
1:C:56:LYS:CG	1:C:56:LYS:CA	2.56	0.79
1:C:22:PRO:O	1:C:56:LYS:CE	2.30	0.79
1:C:89:HIS:ND1	1:C:89:HIS:C	2.34	0.79
2:D:16:LYS:HD3	2:D:16:LYS:HB3	1.57	0.79
1:A:119:PRO:N	1:A:119:PRO:CG	2.46	0.79
2:B:3:THR:C	2:B:4:ALA:CA	2.50	0.79
2:D:28:GLY:O	2:D:54:MET:HE3	1.82	0.79
1:A:122:HIS:CA	1:A:123:ALA:N	2.42	0.79
1:A:39:THR:OG1	1:A:40:LYS:NZ	2.16	0.79
2:B:2:LEU:HB2	2:B:6:GLU:OE2	1.83	0.79
1:C:24:TYR:CG	1:C:24:TYR:HA	2.17	0.79
1:C:70:GLN:OE1	1:C:70:GLN:O	2.00	0.79
2:D:47:LEU:HB3	2:D:47:LEU:CA	2.09	0.79
2:B:122:THR:OG1	2:B:125:VAL:N	2.15	0.79
2:B:2:LEU:HB2	2:B:3:THR:N	1.96	0.79
1:C:84:SER:OG	1:C:136:LEU:HD13	1.82	0.79
2:D:131:LYS:CB	2:D:131:LYS:CD	2.56	0.79
1:C:86:LEU:CB	1:C:86:LEU:C	2.50	0.79
1:C:97:ASN:CB	1:C:97:ASN:C	2.50	0.79
1:C:116:ASN:O	1:C:116:ASN:CA	2.31	0.79
1:C:117:PHE:CA	1:C:117:PHE:O	2.30	0.79
2:D:121:PHE:CA	2:D:121:PHE:CG	2.60	0.79
2:D:31:LEU:HD11	2:D:41:PHE:CE1	2.17	0.79
1:A:91:LEU:CD2	1:A:91:LEU:HD11	2.07	0.79
1:A:8:SER:O	1:A:9:ASN:N	2.16	0.79
2:B:101:ASN:C	3:B:146:HEM:HBB1	2.04	0.79
2:D:14:TRP:CB	2:D:14:TRP:CD1	2.64	0.79
1:A:124:ASN:HA	1:A:124:ASN:HB3	1.17	0.79
1:A:2:LEU:HD13	1:A:3:SER:N	1.98	0.79
1:A:3:SER:CB	1:A:6:ASN:HD22	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:HIS:HA	2:B:95:LEU:HD23	1.65	0.78
1:C:69:ALA:N	1:C:69:ALA:C	2.36	0.78
2:D:47:LEU:HA	2:D:47:LEU:CB	2.10	0.78
2:D:86:GLN:O	2:D:86:GLN:CA	2.29	0.78
2:D:94:LYS:HG3	2:D:95:LEU:CD2	2.10	0.78
1:A:34:LEU:CG	1:A:34:LEU:CA	2.61	0.78
1:A:76:LEU:C	1:A:77:PRO:CA	2.51	0.78
2:B:25:GLN:CD	2:B:112:VAL:HG11	2.04	0.78
2:B:1:MET:HG3	2:B:77:LEU:CD1	1.81	0.78
2:B:88:SER:OG	2:B:143:LYS:CB	2.31	0.78
1:C:83:LEU:CA	1:C:83:LEU:CG	2.61	0.78
1:A:91:LEU:HD21	3:A:142:HEM:C3D	2.15	0.78
2:B:5:GLU:O	2:B:8:ALA:HB3	1.83	0.78
2:B:65:ARG:HH12	2:B:65:ARG:NH2	1.81	0.78
1:C:29:LEU:HA	1:C:29:LEU:CB	2.07	0.78
2:B:54:MET:HG3	2:B:54:MET:CA	2.14	0.78
2:B:67:LEU:C	2:B:71:THR:CG2	2.50	0.78
1:C:26:ALA:H	1:C:56:LYS:CE	1.92	0.78
2:B:1:MET:N	2:B:77:LEU:HD11	1.99	0.78
2:B:95:LEU:HA	2:B:95:LEU:HG	1.65	0.78
1:A:31:ARG:CD	1:A:31:ARG:HG3	2.12	0.78
1:A:2:LEU:HD13	1:A:3:SER:H	1.46	0.78
2:B:7:LYS:CA	2:B:8:ALA:N	2.46	0.78
2:B:62:HIS:CG	2:B:62:HIS:HA	2.18	0.78
1:A:103:HIS:CA	1:A:103:HIS:CG	2.64	0.78
1:C:3:SER:C	1:C:3:SER:N	2.29	0.78
1:C:54:GLN:C	1:C:54:GLN:CB	2.49	0.78
2:B:15:GLY:C	2:B:16:LYS:CA	2.51	0.78
2:D:6:GLU:CB	2:D:128:LEU:HD23	2.09	0.78
2:B:117:PHE:CE2	2:B:117:PHE:CD1	2.72	0.78
2:B:34:TYR:N	2:B:35:PRO:CD	2.47	0.78
2:B:98:ASN:OD1	2:B:98:ASN:CB	2.32	0.78
1:C:67:THR:CA	1:C:67:THR:CG2	2.62	0.78
1:A:31:ARG:HG2	1:A:31:ARG:CD	2.12	0.77
1:A:39:THR:CB	1:A:40:LYS:NZ	2.45	0.77
1:A:31:ARG:CB	2:B:126:GLN:HE21	1.93	0.77
2:B:3:THR:H	2:B:6:GLU:CB	1.97	0.77
2:B:3:THR:HG21	2:B:5:GLU:CD	2.04	0.77
1:C:45:HIS:CE1	1:C:46:PHE:HE1	2.03	0.77
2:D:4:ALA:CA	2:D:5:GLU:N	2.44	0.77
1:A:31:ARG:CG	2:B:126:GLN:NE2	2.42	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LYS:HZ1	1:C:59:GLY:CA	1.95	0.77
2:B:20:ASP:HB3	2:B:64:LYS:CD	2.15	0.77
2:B:65:ARG:N	2:B:65:ARG:C	2.34	0.77
2:B:95:LEU:C	2:B:95:LEU:N	2.37	0.77
1:C:21:ALA:O	1:C:22:PRO:CA	2.30	0.77
1:C:68:LYS:CD	1:C:68:LYS:CB	2.63	0.77
1:A:43:PHE:C	1:A:44:PRO:CA	2.52	0.77
2:B:62:HIS:CD2	2:B:66:VAL:CB	2.67	0.77
2:B:74:LEU:CB	2:B:74:LEU:CD2	2.63	0.77
2:B:80:LEU:HB2	2:B:82:GLY:HA3	1.66	0.77
2:B:98:ASN:HB3	2:B:101:ASN:H	1.50	0.77
1:C:91:LEU:CD1	1:C:91:LEU:CB	2.63	0.77
1:A:33:PHE:CD1	1:A:40:LYS:HE3	2.19	0.77
1:A:91:LEU:CD2	3:A:142:HEM:CAD	2.60	0.77
2:D:65:ARG:O	2:D:65:ARG:CA	2.31	0.77
2:D:2:LEU:CD2	2:D:7:LYS:CG	2.57	0.77
2:B:76:HIS:O	2:B:78:ASP:HB3	1.84	0.77
1:C:27:GLN:C	1:C:28:ALA:CA	2.52	0.77
2:D:141:ALA:C	2:D:142:HIS:CA	2.53	0.77
2:B:1:MET:O	2:B:2:LEU:HD23	1.84	0.77
1:C:68:LYS:HD3	1:C:79:THR:HG22	1.66	0.77
2:D:34:TYR:O	2:D:37:THR:HB	1.85	0.77
1:A:46:PHE:CD1	1:A:55:GLN:NE2	2.52	0.77
1:A:57:ALA:O	1:A:60:GLN:HB3	1.85	0.77
1:A:86:LEU:C	1:A:87:HIS:HA	2.02	0.77
2:B:108:VAL:CG2	2:B:108:VAL:CA	2.62	0.77
2:B:49:SER:HB3	2:B:52:ALA:CB	2.15	0.77
1:C:90:LYS:C	1:C:91:LEU:CA	2.52	0.77
2:D:41:PHE:O	2:D:42:GLN:N	2.18	0.77
1:A:48:LEU:CD2	1:A:48:LEU:CD1	2.62	0.77
3:B:146:HEM:HMA2	3:B:146:HEM:HHB	1.67	0.77
2:B:84:PHE:CG	2:B:84:PHE:CA	2.67	0.77
2:B:64:LYS:CB	2:B:64:LYS:N	2.43	0.77
1:C:17:VAL:CG2	1:C:17:VAL:CG1	2.62	0.77
1:C:69:ALA:C	1:C:69:ALA:HB3	2.03	0.77
2:D:78:ASP:C	2:D:78:ASP:N	2.37	0.77
2:B:123:PRO:HB3	2:B:126:GLN:NE2	2.00	0.76
1:C:45:HIS:CB	1:C:45:HIS:N	2.48	0.76
2:D:31:LEU:C	2:D:31:LEU:N	2.38	0.76
2:B:34:TYR:C	2:B:34:TYR:N	2.38	0.76
2:B:76:HIS:N	2:B:76:HIS:ND1	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:ALA:CB	2:D:61:ALA:C	2.52	0.76
1:A:16:LYS:CD	1:A:16:LYS:HZ3	1.86	0.76
2:B:20:ASP:CB	2:B:64:LYS:CD	2.63	0.76
2:B:69:ALA:CB	2:B:70:PHE:N	2.49	0.76
2:B:2:LEU:HD12	2:B:6:GLU:HG2	1.66	0.76
1:C:22:PRO:HB2	1:C:22:PRO:HD2	1.67	0.76
1:C:26:ALA:N	1:C:56:LYS:HE2	1.96	0.76
2:B:33:VAL:O	2:B:35:PRO:HD2	1.85	0.76
2:D:26:ALA:C	2:D:26:ALA:CB	2.53	0.76
1:A:41:THR:N	1:A:41:THR:CB	2.38	0.76
2:B:20:ASP:O	2:B:21:VAL:HG23	1.85	0.76
1:C:108:THR:CB	1:C:108:THR:C	2.54	0.76
2:B:25:GLN:CG	2:B:112:VAL:HG11	2.16	0.76
2:B:130:GLN:OE1	2:B:130:GLN:NE2	2.17	0.76
2:B:47:LEU:HD12	2:B:53:VAL:CG2	2.13	0.76
1:A:1:VAL:CG1	1:C:141:ARG:O	2.33	0.76
1:A:94:ASN:OD1	1:A:96:VAL:HG22	1.86	0.76
2:B:32:VAL:C	2:B:32:VAL:N	2.37	0.76
1:C:3:SER:OG	1:C:3:SER:CA	2.34	0.76
1:C:87:HIS:HB3	1:C:93:VAL:HG21	1.68	0.76
1:A:3:SER:O	1:A:4:ALA:HA	1.84	0.76
1:A:52:SER:C	1:A:54:GLN:N	2.39	0.76
1:C:134:THR:CG2	1:C:134:THR:CA	2.63	0.76
1:C:45:HIS:CE1	1:C:46:PHE:CE1	2.73	0.76
1:A:85:ASN:CA	1:A:85:ASN:CG	2.53	0.76
1:A:93:VAL:CA	1:A:93:VAL:CG1	2.64	0.76
1:A:12:ALA:O	1:A:13:ALA:N	2.19	0.75
1:A:39:THR:CG2	1:A:40:LYS:NZ	2.47	0.75
1:A:39:THR:CG2	1:A:40:LYS:HZ1	1.99	0.75
1:C:24:TYR:CG	1:C:24:TYR:CA	2.68	0.75
1:C:53:ALA:N	1:C:53:ALA:HA	1.95	0.75
2:D:100:GLN:HA	2:D:100:GLN:OE1	1.86	0.75
2:D:120:GLN:CA	2:D:120:GLN:CG	2.62	0.75
2:D:49:SER:O	2:D:53:VAL:HG12	1.85	0.75
2:D:76:HIS:CA	2:D:76:HIS:CG	2.69	0.75
1:A:50:HIS:ND1	1:A:50:HIS:CB	2.48	0.75
2:B:26:ALA:CA	2:B:27:LEU:N	2.46	0.75
2:B:5:GLU:CB	2:B:5:GLU:N	2.49	0.75
1:C:93:VAL:CG1	3:C:142:HEM:CAC	2.64	0.75
1:A:136:LEU:CD2	1:A:136:LEU:CD1	2.57	0.75
1:A:76:LEU:HB2	1:A:77:PRO:CD	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:VAL:CB	2:B:136:VAL:C	2.51	0.75
2:D:2:LEU:HD23	2:D:7:LYS:CD	2.16	0.75
2:D:43:HIS:CB	2:D:43:HIS:N	2.49	0.75
2:B:134:ALA:O	2:B:138:ASN:HB2	1.85	0.75
1:C:81:SER:N	1:C:81:SER:CB	2.46	0.75
2:D:103:ARG:NE	2:D:103:ARG:CG	2.48	0.75
2:D:59:VAL:HG13	2:D:59:VAL:HG21	1.68	0.75
2:D:95:LEU:HD12	2:D:97:VAL:HG21	1.67	0.75
1:A:81:SER:C	1:A:82:ASN:CA	2.49	0.75
2:B:103:ARG:HB3	2:B:103:ARG:HD2	1.69	0.75
2:B:81:LYS:NZ	2:B:142:HIS:CE1	2.55	0.75
2:B:77:LEU:C	2:B:77:LEU:HD13	2.07	0.75
1:C:88:ALA:HB1	1:C:139:LYS:CB	2.16	0.75
1:A:56:LYS:HE3	1:A:56:LYS:N	2.00	0.75
2:D:17:VAL:CB	2:D:17:VAL:C	2.55	0.75
1:A:29:LEU:HA	1:A:29:LEU:CB	2.12	0.75
1:C:138:SER:CB	1:C:138:SER:C	2.54	0.75
1:C:53:ALA:O	1:C:57:ALA:CB	2.35	0.75
2:D:81:LYS:NZ	2:D:81:LYS:CD	2.50	0.75
1:A:55:GLN:NE2	1:A:55:GLN:OE1	2.18	0.75
1:C:104:SER:N	1:C:104:SER:C	2.39	0.75
1:C:139:LYS:CD	1:C:139:LYS:CB	2.65	0.75
1:C:42:TYR:CD1	3:C:142:HEM:HBC1	2.22	0.75
2:D:101:ASN:C	3:D:146:HEM:HBB1	2.06	0.75
1:A:45:HIS:CG	1:A:45:HIS:CA	2.68	0.74
2:B:43:HIS:CE1	3:B:146:HEM:O2A	2.40	0.74
2:B:3:THR:O	2:B:4:ALA:CA	2.35	0.74
2:B:83:ALA:CB	2:B:83:ALA:N	2.50	0.74
1:C:3:SER:CB	1:C:4:ALA:N	2.50	0.74
2:D:55:ASN:O	2:D:60:LYS:CD	2.35	0.74
1:A:73:LEU:CD1	1:A:73:LEU:CD2	2.65	0.74
2:B:10:VAL:HG11	2:B:128:LEU:HD23	1.58	0.74
1:C:130:ALA:O	1:C:130:ALA:CA	2.35	0.74
1:C:17:VAL:HG13	1:C:24:TYR:CD2	2.22	0.74
2:D:93:ASN:CA	2:D:93:ASN:O	2.35	0.74
2:B:41:PHE:HB2	2:B:44:PHE:CD1	2.22	0.74
1:C:129:LEU:CB	1:C:129:LEU:HG	2.13	0.74
1:A:63:ALA:C	1:A:63:ALA:CB	2.53	0.74
1:A:88:ALA:N	1:A:88:ALA:C	2.41	0.74
2:B:37:THR:N	2:B:37:THR:CB	2.49	0.74
1:C:46:PHE:CD2	1:C:54:GLN:HB3	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MET:HG3	2:D:131:LYS:NZ	2.01	0.74
2:B:16:LYS:CE	2:B:16:LYS:CG	2.65	0.74
2:B:74:LEU:CD1	2:B:77:LEU:CG	2.65	0.74
2:B:80:LEU:HD22	2:B:82:GLY:CA	2.17	0.74
2:D:124:ASN:CA	2:D:124:ASN:CG	2.55	0.74
2:D:12:GLY:N	2:D:12:GLY:C	2.38	0.74
1:C:113:LEU:N	1:C:113:LEU:CD2	2.51	0.74
2:D:140:LEU:HD22	2:D:140:LEU:CD1	2.16	0.74
1:A:2:LEU:CG	1:A:2:LEU:CA	2.66	0.74
1:A:41:THR:HA	1:A:41:THR:CG2	2.16	0.74
2:B:140:LEU:O	2:B:141:ALA:CA	2.36	0.74
2:D:10:VAL:HG11	2:D:128:LEU:CD1	2.17	0.74
3:A:142:HEM:CHA	3:A:142:HEM:ND	2.50	0.74
1:A:3:SER:N	1:A:3:SER:CB	2.51	0.74
1:A:39:THR:HG23	1:A:40:LYS:HE2	1.69	0.74
1:A:46:PHE:HB2	1:A:48:LEU:CD2	2.18	0.74
2:B:123:PRO:HA	2:B:126:GLN:NE2	2.01	0.74
1:C:84:SER:C	1:C:84:SER:HB3	2.08	0.74
1:A:6:ASN:O	1:A:10:VAL:HG23	1.88	0.73
2:B:128:LEU:CG	2:B:128:LEU:CA	2.66	0.73
1:C:61:LYS:CD	1:C:61:LYS:HA	2.17	0.73
1:C:35:SER:HB3	2:D:127:ALA:HA	1.70	0.73
2:D:47:LEU:HB2	2:D:47:LEU:CA	2.09	0.73
1:A:73:LEU:CB	1:A:73:LEU:CD2	2.66	0.73
1:C:59:GLY:C	1:C:59:GLY:N	2.41	0.73
1:A:135:VAL:CA	1:A:136:LEU:N	2.49	0.73
2:B:41:PHE:CA	2:B:41:PHE:O	2.36	0.73
1:C:100:LEU:CB	1:C:100:LEU:CD2	2.65	0.73
1:C:67:THR:HA	1:C:67:THR:CG2	2.19	0.73
2:D:105:LEU:HD11	2:D:105:LEU:HD22	1.70	0.73
2:D:124:ASN:N	2:D:124:ASN:C	2.41	0.73
2:D:79:ASP:C	2:D:81:LYS:HD2	2.09	0.73
2:B:54:MET:N	2:B:54:MET:CB	2.51	0.73
1:C:137:THR:N	1:C:137:THR:C	2.42	0.73
1:C:89:HIS:CB	1:C:139:LYS:NZ	2.45	0.73
2:D:10:VAL:HG11	2:D:128:LEU:HD13	1.69	0.73
1:A:42:TYR:C	1:A:43:PHE:HA	2.08	0.73
2:B:2:LEU:CG	2:B:2:LEU:CA	2.67	0.73
2:B:41:PHE:HD2	2:B:44:PHE:HZ	1.30	0.73
1:C:45:HIS:CE1	3:C:142:HEM:CBD	2.64	0.73
2:D:124:ASN:CB	2:D:124:ASN:C	2.56	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:N	1:A:106:LEU:HB2	2.03	0.73
1:C:116:ASN:CA	1:C:117:PHE:N	2.45	0.73
2:B:103:ARG:HB3	2:B:103:ARG:CG	2.15	0.73
2:D:31:LEU:CB	2:D:31:LEU:HA	2.12	0.73
2:D:59:VAL:HG21	2:D:59:VAL:CG1	2.17	0.73
2:D:84:PHE:HB2	2:D:84:PHE:HD1	1.49	0.73
2:B:136:VAL:N	2:B:136:VAL:C	2.42	0.73
2:B:136:VAL:CA	2:B:136:VAL:O	2.37	0.73
2:B:53:VAL:O	2:B:59:VAL:CG2	2.37	0.73
2:D:19:VAL:O	2:D:21:VAL:N	2.22	0.73
1:A:52:SER:C	1:A:54:GLN:H	1.92	0.73
1:A:93:VAL:HA	1:A:93:VAL:CG1	2.18	0.73
2:B:102:PHE:CE2	2:B:141:ALA:HB2	2.24	0.73
1:A:31:ARG:HG2	2:B:126:GLN:NE2	2.02	0.73
2:B:62:HIS:HE1	3:B:146:HEM:CHA	2.02	0.73
1:C:103:HIS:CB	1:C:103:HIS:ND1	2.52	0.73
1:C:95:PRO:HG3	1:C:141:ARG:HH12	1.52	0.73
2:D:3:THR:N	2:D:3:THR:C	2.42	0.73
2:D:56:ASN:O	2:D:56:ASN:CA	2.36	0.73
2:B:98:ASN:CB	2:B:100:GLN:H	2.01	0.72
1:C:70:GLN:HB3	1:C:70:GLN:C	2.08	0.72
2:D:103:ARG:O	2:D:107:ASN:HB2	1.89	0.72
2:B:102:PHE:CD1	2:B:102:PHE:CB	2.54	0.72
1:C:80:LEU:HD23	1:C:135:VAL:HG22	1.70	0.72
2:D:76:HIS:CG	2:D:76:HIS:N	2.57	0.72
1:A:41:THR:OG1	1:A:41:THR:CG2	2.28	0.72
1:A:85:ASN:ND2	1:A:85:ASN:C	2.41	0.72
2:B:10:VAL:CG1	2:B:10:VAL:CA	2.67	0.72
2:B:22:VAL:CG2	2:B:22:VAL:CG1	2.67	0.72
2:B:22:VAL:N	2:B:23:GLY:N	2.37	0.72
2:B:47:LEU:HD12	2:B:53:VAL:HA	1.71	0.72
1:C:137:THR:O	1:C:138:SER:CA	2.37	0.72
2:D:103:ARG:HB3	2:D:103:ARG:O	1.89	0.72
2:B:103:ARG:HB2	2:B:103:ARG:CG	2.15	0.72
1:C:108:THR:HB	1:C:108:THR:HG22	1.68	0.72
2:D:126:GLN:NE2	2:D:126:GLN:OE1	2.22	0.72
2:D:6:GLU:CA	2:D:6:GLU:CG	2.64	0.72
1:A:89:HIS:CD2	1:A:139:LYS:HG2	2.25	0.72
2:B:39:ARG:CB	2:B:39:ARG:CD	2.67	0.72
1:C:131:ASN:N	1:C:131:ASN:CB	2.48	0.72
2:D:27:LEU:HD11	2:D:62:HIS:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:HD3	2:B:126:GLN:CG	2.18	0.72
2:B:106:GLY:HA2	2:B:133:VAL:CG2	2.18	0.72
2:B:140:LEU:O	2:B:141:ALA:HA	1.89	0.72
3:B:146:HEM:HHA	3:B:146:HEM:HAD2	1.71	0.72
2:D:144:TYR:OH	2:D:144:TYR:CE2	2.43	0.72
2:D:46:ASN:N	2:D:46:ASN:CB	2.52	0.72
2:B:62:HIS:N	2:B:62:HIS:C	2.43	0.72
2:D:25:GLN:NE2	2:D:115:ARG:HH22	1.88	0.72
2:D:34:TYR:HA	2:D:36:TRP:CZ3	2.25	0.72
1:A:126:ASN:N	1:A:127:LYS:N	2.38	0.72
2:B:55:ASN:CA	2:B:56:ASN:N	2.52	0.72
1:A:12:ALA:CA	1:A:13:ALA:N	2.52	0.72
1:A:32:MET:CB	1:A:32:MET:N	2.45	0.72
2:B:130:GLN:HE21	2:B:130:GLN:CG	1.89	0.72
1:C:32:MET:N	1:C:32:MET:CB	2.53	0.72
1:C:71:GLY:O	1:C:72:HIS:HB3	1.90	0.72
2:B:41:PHE:CB	2:B:44:PHE:CD1	2.73	0.71
2:B:80:LEU:HD13	2:B:80:LEU:CD2	2.20	0.71
2:B:81:LYS:NZ	2:B:142:HIS:CD2	2.58	0.71
1:C:14:TRP:CB	1:C:70:GLN:HE22	2.03	0.71
2:D:90:LEU:HD13	2:D:90:LEU:CB	2.20	0.71
1:A:35:SER:C	1:A:35:SER:CB	2.56	0.71
2:B:22:VAL:O	2:B:23:GLY:CA	2.38	0.71
2:B:76:HIS:C	2:B:78:ASP:HB3	2.10	0.71
1:C:56:LYS:HZ2	1:C:59:GLY:N	1.88	0.71
1:A:105:LEU:CB	1:A:105:LEU:N	2.52	0.71
2:B:75:LYS:HG2	2:B:76:HIS:ND1	2.05	0.71
2:B:8:ALA:CB	2:B:8:ALA:N	2.50	0.71
2:B:98:ASN:CB	2:B:101:ASN:H	2.03	0.71
1:C:17:VAL:CA	1:C:18:GLY:N	2.46	0.71
2:B:9:ALA:C	2:B:10:VAL:CA	2.57	0.71
1:C:108:THR:C	1:C:108:THR:HB	2.09	0.71
1:C:23:ALA:N	1:C:23:ALA:CB	2.53	0.71
2:D:84:PHE:CE1	2:D:136:VAL:HG13	2.26	0.71
1:A:127:LYS:HD2	1:A:127:LYS:HZ2	1.55	0.71
1:A:22:PRO:CG	1:A:22:PRO:CA	2.68	0.71
1:A:70:GLN:C	1:A:73:LEU:HD12	2.11	0.71
1:A:80:LEU:O	1:A:84:SER:N	2.23	0.71
2:D:145:HIS:CE1	2:D:145:HIS:CG	2.77	0.71
2:D:19:VAL:CG2	2:D:19:VAL:CG1	2.68	0.71
2:D:50:ALA:O	2:D:50:ALA:CA	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:C	1:A:85:ASN:HB3	2.11	0.71
1:A:94:ASN:O	1:A:95:PRO:N	2.18	0.71
1:C:21:ALA:C	1:C:22:PRO:CA	2.59	0.71
1:C:36:PHE:HA	1:C:37:PRO:CD	2.21	0.71
2:D:2:LEU:HD22	2:D:3:THR:C	2.11	0.71
2:D:6:GLU:HB2	2:D:128:LEU:CD2	2.12	0.71
2:D:90:LEU:CB	2:D:90:LEU:HD12	2.20	0.71
1:A:127:LYS:HA	1:A:127:LYS:O	1.91	0.71
1:A:11:LYS:CA	1:A:12:ALA:N	2.53	0.71
2:D:123:PRO:CA	2:D:124:ASN:N	2.53	0.71
2:D:67:LEU:O	2:D:71:THR:CB	2.38	0.71
2:D:77:LEU:CD1	2:D:77:LEU:CB	2.69	0.71
1:A:119:PRO:C	1:A:119:PRO:CB	2.57	0.71
2:B:101:ASN:CA	2:B:101:ASN:O	2.38	0.71
2:B:140:LEU:HB3	2:B:140:LEU:CD1	2.20	0.71
2:B:64:LYS:CB	2:B:64:LYS:NZ	2.49	0.71
2:D:87:LEU:HD12	2:D:90:LEU:HD12	1.71	0.71
1:A:109:LEU:HD12	1:A:117:PHE:CE1	2.24	0.71
2:B:103:ARG:NH2	2:B:103:ARG:NE	2.36	0.71
2:B:38:GLN:O	2:B:39:ARG:CA	2.39	0.71
2:B:2:LEU:HB2	2:B:6:GLU:CG	2.20	0.71
2:B:84:PHE:HD1	2:B:84:PHE:HB2	1.55	0.71
2:B:93:ASN:O	2:B:96:HIS:CE1	2.44	0.71
2:D:86:GLN:CG	2:D:86:GLN:CA	2.58	0.71
2:B:117:PHE:CD2	2:B:117:PHE:CD1	2.65	0.71
1:C:113:LEU:C	1:C:114:PRO:CA	2.59	0.71
1:A:87:HIS:CD2	1:A:87:HIS:CB	2.71	0.70
2:B:133:VAL:HA	2:B:133:VAL:O	1.91	0.70
2:B:144:TYR:HB3	2:B:144:TYR:CD2	2.26	0.70
1:A:118:THR:CG2	1:A:118:THR:OG1	2.39	0.70
1:A:29:LEU:HG	1:A:29:LEU:CB	2.17	0.70
1:A:40:LYS:CA	1:A:40:LYS:CG	2.65	0.70
1:A:57:ALA:HA	1:A:60:GLN:CG	2.21	0.70
1:C:80:LEU:O	1:C:81:SER:N	2.25	0.70
1:C:134:THR:C	1:C:134:THR:N	2.43	0.70
1:C:43:PHE:C	1:C:44:PRO:CA	2.58	0.70
2:D:70:PHE:HB3	2:D:71:THR:HB	1.73	0.70
2:B:10:VAL:CG1	2:B:128:LEU:HD22	1.98	0.70
1:C:86:LEU:CB	1:C:86:LEU:CD1	2.69	0.70
1:A:126:ASN:C	1:A:126:ASN:N	2.43	0.70
2:D:31:LEU:HA	2:D:31:LEU:CG	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HA	1:A:108:THR:CG2	2.18	0.70
1:A:76:LEU:O	1:A:77:PRO:O	2.10	0.70
2:B:6:GLU:CD	2:B:131:LYS:HZ1	1.95	0.70
2:B:94:LYS:N	2:B:95:LEU:H	1.89	0.70
1:C:56:LYS:NZ	1:C:59:GLY:N	2.39	0.70
2:D:25:GLN:HB3	2:D:112:VAL:CG2	2.21	0.70
2:D:48:SER:O	2:D:49:SER:HB3	1.91	0.70
1:A:13:ALA:CB	1:A:125:LEU:HD21	2.22	0.70
1:A:48:LEU:CA	1:A:48:LEU:HG	2.21	0.70
2:B:11:THR:CA	2:B:11:THR:OG1	2.40	0.70
2:B:11:THR:CB	2:B:11:THR:N	2.54	0.70
2:B:44:PHE:O	2:B:45:GLY:CA	2.38	0.70
2:B:76:HIS:CB	2:B:76:HIS:ND1	2.54	0.70
2:B:80:LEU:CB	2:B:82:GLY:HA3	2.22	0.70
2:B:94:LYS:N	2:B:95:LEU:N	2.40	0.70
1:C:98:PHE:CA	1:C:99:LYS:N	2.54	0.70
2:D:60:LYS:CD	2:D:60:LYS:NZ	2.55	0.70
2:D:70:PHE:CD2	2:D:136:VAL:HG11	2.27	0.70
2:B:121:PHE:CE2	2:B:126:GLN:HA	2.27	0.70
2:B:47:LEU:CD1	2:B:53:VAL:HG23	2.16	0.70
3:C:142:HEM:CAB	3:C:142:HEM:C4B	2.61	0.70
1:C:17:VAL:HG22	1:C:24:TYR:CE2	2.27	0.70
1:C:45:HIS:CB	1:C:45:HIS:C	2.51	0.70
1:C:9:ASN:HB3	1:C:124:ASN:HB2	1.74	0.70
2:D:109:LEU:CD1	2:D:109:LEU:CD2	2.69	0.70
2:D:2:LEU:CG	2:D:7:LYS:HD3	2.22	0.70
2:B:74:LEU:CD1	2:B:77:LEU:CB	2.57	0.70
1:C:45:HIS:NE2	1:C:46:PHE:HE1	1.89	0.70
2:D:93:ASN:CA	2:D:94:LYS:N	2.55	0.70
1:A:33:PHE:HB3	1:A:40:LYS:CG	2.22	0.69
1:A:14:TRP:HD1	1:A:70:GLN:HE21	1.39	0.69
1:A:86:LEU:C	1:A:87:HIS:CA	2.58	0.69
2:D:131:LYS:CB	2:D:131:LYS:N	2.54	0.69
2:D:99:PRO:O	2:D:102:PHE:HB2	1.90	0.69
2:B:25:GLN:OE1	2:B:112:VAL:HG11	1.90	0.69
2:D:78:ASP:CA	2:D:78:ASP:CG	2.52	0.69
2:B:95:LEU:HD11	3:B:146:HEM:CMA	2.22	0.69
2:B:3:THR:CB	2:B:6:GLU:HB2	2.22	0.69
1:C:44:PRO:N	1:C:44:PRO:CG	2.45	0.69
2:D:10:VAL:HG13	2:D:128:LEU:HD22	1.73	0.69
2:D:31:LEU:O	2:D:31:LEU:CA	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ASN:OD1	2:B:55:ASN:N	2.25	0.69
1:C:118:THR:CG2	1:C:118:THR:OG1	2.40	0.69
2:D:109:LEU:O	2:D:109:LEU:CA	2.37	0.69
2:D:2:LEU:HD13	2:D:3:THR:N	2.06	0.69
2:D:23:GLY:N	2:D:67:LEU:HD12	2.07	0.69
2:D:75:LYS:HG3	2:D:76:HIS:CD2	2.28	0.69
1:A:22:PRO:CD	1:A:22:PRO:CA	2.69	0.69
1:A:89:HIS:HD2	1:A:139:LYS:CD	2.04	0.69
2:B:2:LEU:CB	2:B:2:LEU:C	2.61	0.69
1:C:80:LEU:CD1	1:C:80:LEU:CD2	2.69	0.69
2:D:131:LYS:CA	2:D:131:LYS:HG3	2.22	0.69
2:B:22:VAL:HG12	2:B:67:LEU:CD2	2.20	0.69
1:C:104:SER:CA	1:C:105:LEU:N	2.56	0.69
1:C:14:TRP:CB	1:C:70:GLN:NE2	2.55	0.69
2:D:27:LEU:CD1	2:D:62:HIS:HB3	2.22	0.69
2:D:87:LEU:N	2:D:87:LEU:CB	2.48	0.69
1:A:132:ASP:OD1	1:A:136:LEU:HD11	1.93	0.69
1:A:57:ALA:O	1:A:60:GLN:CG	2.41	0.69
1:A:98:PHE:CE1	1:A:136:LEU:HD12	2.28	0.69
2:B:102:PHE:HE2	2:B:141:ALA:HB2	1.58	0.69
2:B:21:VAL:CG2	2:B:21:VAL:CA	2.70	0.69
2:B:27:LEU:CD2	2:B:66:VAL:HG11	2.23	0.69
1:C:89:HIS:O	1:C:90:LYS:CA	2.41	0.69
2:D:36:TRP:N	2:D:36:TRP:C	2.46	0.69
2:D:67:LEU:HA	2:D:67:LEU:CG	2.15	0.69
2:B:40:PHE:HB3	3:B:146:HEM:HMA2	1.74	0.69
2:B:20:ASP:CB	2:B:20:ASP:OD1	2.41	0.69
2:B:46:ASN:OD1	2:B:46:ASN:CB	2.40	0.69
1:C:36:PHE:HA	1:C:37:PRO:HD3	1.74	0.69
1:C:46:PHE:CB	1:C:46:PHE:CD1	2.74	0.69
2:D:59:VAL:CA	2:D:59:VAL:O	2.40	0.69
2:D:84:PHE:H	2:D:84:PHE:CB	2.06	0.69
1:A:106:LEU:CD2	1:A:106:LEU:CB	2.71	0.69
1:C:95:PRO:O	1:C:98:PHE:HB2	1.93	0.69
2:D:4:ALA:C	2:D:4:ALA:CB	2.61	0.69
1:A:124:ASN:CB	1:A:124:ASN:OD1	2.41	0.69
1:A:83:LEU:O	1:A:84:SER:CA	2.40	0.69
3:B:146:HEM:CMA	3:B:146:HEM:C4A	2.76	0.69
2:B:2:LEU:CB	2:B:3:THR:N	2.56	0.69
2:B:143:LYS:CD	2:B:143:LYS:NZ	2.56	0.68
2:B:86:GLN:CG	2:B:86:GLN:NE2	2.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:C	1:C:39:THR:CB	2.62	0.68
2:D:61:ALA:CB	2:D:62:HIS:N	2.55	0.68
2:D:79:ASP:CA	2:D:81:LYS:HD2	2.22	0.68
2:D:71:THR:C	2:D:71:THR:CG2	2.61	0.68
2:B:33:VAL:HG12	2:B:34:TYR:CZ	2.27	0.68
2:B:2:LEU:CB	2:B:6:GLU:OE2	2.42	0.68
2:D:95:LEU:HD11	3:D:146:HEM:CHB	2.24	0.68
2:D:61:ALA:N	2:D:61:ALA:CB	2.50	0.68
2:D:79:ASP:O	2:D:81:LYS:HD3	1.94	0.68
2:D:91:HIS:HA	2:D:95:LEU:HG	1.75	0.68
2:B:38:GLN:O	2:B:39:ARG:HA	1.91	0.68
1:C:136:LEU:HA	1:C:136:LEU:CB	2.14	0.68
2:D:100:GLN:C	2:D:101:ASN:CA	2.25	0.68
2:D:142:HIS:CG	2:D:142:HIS:HA	2.28	0.68
2:D:143:LYS:CB	2:D:143:LYS:N	2.56	0.68
2:B:43:HIS:HA	2:B:43:HIS:ND1	2.07	0.68
1:C:12:ALA:O	1:C:12:ALA:CA	2.42	0.68
1:C:131:ASN:CA	1:C:131:ASN:CG	2.62	0.68
1:C:84:SER:OG	1:C:136:LEU:CD2	2.42	0.68
1:C:72:HIS:CB	1:C:72:HIS:CD2	2.72	0.68
1:C:54:GLN:CA	1:C:54:GLN:O	2.42	0.68
1:C:87:HIS:HB3	1:C:93:VAL:CG2	2.23	0.68
2:D:104:LEU:CG	2:D:104:LEU:CA	2.71	0.68
2:D:79:ASP:OD1	2:D:79:ASP:O	2.11	0.68
1:A:127:LYS:HD3	1:A:127:LYS:NZ	2.03	0.68
1:A:43:PHE:HB3	1:A:43:PHE:CD2	2.27	0.68
2:B:75:LYS:C	2:B:76:HIS:CA	2.60	0.68
2:D:10:VAL:HG21	2:D:128:LEU:HB2	1.75	0.68
2:D:2:LEU:CG	2:D:7:LYS:CD	2.72	0.68
2:D:14:TRP:CE2	2:D:71:THR:HG23	2.28	0.68
2:D:14:TRP:CD1	2:D:74:LEU:HD23	2.29	0.68
1:A:16:LYS:CA	1:A:17:VAL:N	2.56	0.68
2:B:103:ARG:HE	2:B:103:ARG:CG	2.06	0.68
2:B:68:ASP:CA	2:B:68:ASP:CG	2.60	0.68
2:D:110:ALA:O	2:D:114:ALA:N	2.27	0.68
2:D:50:ALA:C	2:D:50:ALA:N	2.46	0.68
2:B:26:ALA:O	2:B:26:ALA:CA	2.40	0.68
2:B:6:GLU:C	2:B:6:GLU:N	2.45	0.68
2:B:75:LYS:O	2:B:76:HIS:O	2.11	0.68
1:C:84:SER:CA	1:C:84:SER:OG	2.42	0.68
2:D:102:PHE:N	2:D:102:PHE:CB	2.53	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HZ3	1:A:127:LYS:CD	2.00	0.68
3:A:142:HEM:HMD1	3:A:142:HEM:HHD	1.75	0.68
1:A:82:ASN:CB	1:A:82:ASN:N	2.54	0.68
2:B:46:ASN:C	2:B:47:LEU:HD13	2.14	0.68
2:B:57:PRO:CB	2:B:57:PRO:HD3	2.21	0.68
2:B:19:VAL:HG13	2:B:64:LYS:HE2	1.75	0.68
2:B:71:THR:H	2:B:71:THR:CA	1.33	0.68
1:C:68:LYS:CG	1:C:68:LYS:HA	2.22	0.68
2:D:103:ARG:NH2	2:D:130:GLN:O	2.24	0.68
2:D:79:ASP:CB	2:D:79:ASP:C	2.63	0.68
2:D:124:ASN:O	2:D:124:ASN:CA	2.43	0.67
2:B:41:PHE:HB2	2:B:44:PHE:CE1	2.30	0.67
2:B:54:MET:HA	2:B:54:MET:HG3	1.76	0.67
1:C:74:ASN:C	1:C:74:ASN:N	2.44	0.67
2:D:81:LYS:CB	2:D:81:LYS:CD	2.69	0.67
3:B:146:HEM:CMA	3:B:146:HEM:HHB	2.23	0.67
1:C:16:LYS:N	1:C:16:LYS:CB	2.56	0.67
2:D:28:GLY:CA	2:D:54:MET:CE	2.73	0.67
2:D:79:ASP:CG	2:D:81:LYS:HE2	2.14	0.67
2:D:86:GLN:HA	2:D:86:GLN:CB	2.15	0.67
2:D:92:CYS:CA	2:D:92:CYS:SG	2.81	0.67
2:D:94:LYS:HD2	2:D:95:LEU:CD2	2.24	0.67
1:A:126:ASN:C	1:A:126:ASN:HB3	2.14	0.67
1:A:72:HIS:O	1:A:72:HIS:ND1	2.25	0.67
1:A:86:LEU:CD2	1:A:86:LEU:CD1	2.70	0.67
2:B:34:TYR:CE2	2:B:34:TYR:OH	2.42	0.67
2:B:31:LEU:HB3	2:B:53:VAL:HG21	1.75	0.67
1:C:22:PRO:O	1:C:56:LYS:HE2	1.94	0.67
1:C:86:LEU:HD12	1:C:91:LEU:HD11	1.76	0.67
1:A:127:LYS:O	1:A:130:ALA:HB3	1.95	0.67
2:B:53:VAL:O	2:B:54:MET:CA	2.42	0.67
2:B:64:LYS:CE	2:B:64:LYS:CG	2.73	0.67
1:C:11:LYS:HG2	1:C:11:LYS:N	2.09	0.67
1:C:31:ARG:O	1:C:34:LEU:HB2	1.95	0.67
2:D:76:HIS:CB	2:D:76:HIS:CD2	2.78	0.67
2:B:131:LYS:O	2:B:134:ALA:HB3	1.95	0.67
2:B:138:ASN:ND2	2:B:138:ASN:CB	2.56	0.67
2:B:25:GLN:HA	2:B:25:GLN:N	1.99	0.67
2:B:33:VAL:C	2:B:35:PRO:CD	2.63	0.67
2:B:59:VAL:O	2:B:62:HIS:HB3	1.94	0.67
2:B:59:VAL:HG23	2:B:60:LYS:N	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:THR:HB	2:D:129:PHE:CZ	2.29	0.67
2:B:70:PHE:HD1	2:B:71:THR:HB	1.60	0.67
2:D:142:HIS:CG	2:D:142:HIS:CA	2.64	0.67
2:D:50:ALA:O	2:D:54:MET:HG2	1.94	0.67
2:D:75:LYS:HB3	2:D:76:HIS:CD2	2.29	0.67
1:A:100:LEU:CD2	1:A:100:LEU:HB3	2.23	0.67
1:A:76:LEU:CD2	1:A:76:LEU:H	2.06	0.67
2:B:33:VAL:C	2:B:35:PRO:HD2	2.14	0.67
2:D:128:LEU:CB	2:D:128:LEU:N	2.58	0.67
2:D:66:VAL:O	2:D:69:ALA:HB3	1.94	0.67
1:A:127:LYS:CB	1:A:127:LYS:CD	2.73	0.67
1:C:76:LEU:CD1	1:C:76:LEU:CB	2.73	0.67
1:A:105:LEU:CA	1:A:108:THR:HG22	2.21	0.67
1:A:114:PRO:HG2	2:B:115:ARG:HA	1.76	0.67
1:A:55:GLN:HB3	1:A:56:LYS:HZ3	1.59	0.67
1:A:87:HIS:CA	1:A:87:HIS:CG	2.77	0.67
1:A:89:HIS:HD2	1:A:139:LYS:CG	2.07	0.67
2:B:97:VAL:CA	2:B:97:VAL:CG1	2.70	0.67
1:C:86:LEU:HD11	3:C:142:HEM:CHA	2.25	0.67
1:A:110:ALA:O	1:A:114:PRO:CG	2.40	0.66
1:A:79:THR:CB	1:A:79:THR:C	2.62	0.66
2:B:49:SER:HB3	2:B:52:ALA:HB2	1.76	0.66
2:B:68:ASP:HA	2:B:71:THR:HG22	0.67	0.66
2:B:80:LEU:CD2	2:B:81:LYS:O	2.43	0.66
1:C:68:LYS:HG2	1:C:68:LYS:HA	1.77	0.66
2:D:39:ARG:HE	2:D:39:ARG:CG	2.06	0.66
2:D:49:SER:O	2:D:53:VAL:HG13	1.95	0.66
2:D:59:VAL:HA	2:D:59:VAL:HG23	1.73	0.66
2:B:140:LEU:CD2	2:B:140:LEU:CB	2.68	0.66
1:C:113:LEU:O	1:C:114:PRO:CA	2.43	0.66
2:D:130:GLN:CG	2:D:130:GLN:NE2	2.54	0.66
2:D:13:PHE:O	2:D:14:TRP:O	2.14	0.66
1:A:42:TYR:O	1:A:43:PHE:HA	1.95	0.66
2:D:88:SER:O	2:D:143:LYS:HE2	1.95	0.66
2:B:94:LYS:CD	2:B:94:LYS:HB3	2.23	0.66
2:D:95:LEU:CD2	2:D:95:LEU:N	2.58	0.66
1:A:43:PHE:HA	1:A:44:PRO:CD	2.25	0.66
2:B:105:LEU:N	2:B:105:LEU:C	2.48	0.66
2:B:34:TYR:N	2:B:35:PRO:HD2	2.10	0.66
1:C:101:LEU:CB	1:C:101:LEU:N	2.58	0.66
2:D:110:ALA:N	2:D:110:ALA:HA	2.02	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:LYS:C	2:D:131:LYS:CB	2.63	0.66
2:D:20:ASP:OD1	2:D:64:LYS:HB2	1.96	0.66
2:D:94:LYS:CD	2:D:95:LEU:HD23	2.25	0.66
1:A:136:LEU:H	1:A:136:LEU:CD2	1.94	0.66
1:A:9:ASN:OD1	1:A:9:ASN:CB	2.42	0.66
2:D:75:LYS:CB	2:D:76:HIS:N	2.59	0.66
1:A:42:TYR:O	1:A:44:PRO:HD2	1.96	0.66
2:B:125:VAL:CG1	2:B:125:VAL:CG2	2.72	0.66
1:C:132:ASP:O	1:C:136:LEU:HD23	1.95	0.66
2:D:145:HIS:CE1	2:D:145:HIS:CD2	2.84	0.66
2:D:27:LEU:CD1	2:D:27:LEU:CB	2.69	0.66
2:B:3:THR:CG2	2:B:5:GLU:CA	2.63	0.66
1:C:69:ALA:CA	1:C:70:GLN:N	2.54	0.66
1:C:83:LEU:CD2	1:C:83:LEU:CD1	2.70	0.66
2:D:14:TRP:CZ2	2:D:71:THR:HG23	2.31	0.66
2:D:19:VAL:HG12	2:D:64:LYS:HD2	1.78	0.66
2:B:63:GLY:HA2	2:B:66:VAL:CG1	2.21	0.66
1:C:64:ASN:N	1:C:64:ASN:CB	2.55	0.66
2:D:124:ASN:CB	2:D:124:ASN:OD1	2.44	0.66
1:A:44:PRO:N	1:A:45:HIS:CD2	2.63	0.66
2:B:13:PHE:HE1	2:B:120:GLN:HB2	1.61	0.66
3:B:146:HEM:CMA	3:B:146:HEM:CHB	2.74	0.66
1:C:61:LYS:HA	1:C:61:LYS:CG	2.18	0.66
2:D:101:ASN:O	2:D:104:LEU:HB2	1.96	0.66
2:D:124:ASN:HA	2:D:124:ASN:CG	2.14	0.66
2:D:95:LEU:CD2	2:D:95:LEU:CB	2.74	0.66
1:A:124:ASN:CA	1:A:124:ASN:CG	2.61	0.65
1:A:124:ASN:C	1:A:124:ASN:HB2	1.99	0.65
1:A:45:HIS:ND1	1:A:46:PHE:CD2	2.64	0.65
2:B:109:LEU:CD1	2:B:109:LEU:HB3	2.26	0.65
1:A:34:LEU:CD1	2:B:123:PRO:HB2	2.19	0.65
1:C:140:TYR:CA	1:C:140:TYR:CG	2.77	0.65
2:D:117:PHE:O	2:D:120:GLN:HB2	1.96	0.65
1:A:43:PHE:CZ	3:A:142:HEM:HMD1	2.31	0.65
2:B:2:LEU:CD2	2:B:2:LEU:CD1	2.72	0.65
2:D:32:VAL:HG11	2:D:50:ALA:HA	1.77	0.65
1:A:106:LEU:C	1:A:106:LEU:N	2.47	0.65
2:B:30:LEU:HD23	2:B:105:LEU:CA	2.18	0.65
1:C:26:ALA:HB2	1:C:56:LYS:HD2	1.76	0.65
1:C:66:LEU:CB	1:C:66:LEU:CD2	2.63	0.65
2:D:103:ARG:HB2	2:D:103:ARG:CD	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:CD2	3:A:142:HEM:C4D	2.66	0.65
1:C:118:THR:HG1	1:C:118:THR:CB	2.07	0.65
1:C:133:SER:O	1:C:133:SER:CA	2.41	0.65
1:C:3:SER:HB2	1:C:4:ALA:N	2.11	0.65
2:D:63:GLY:O	2:D:66:VAL:HB	1.95	0.65
1:A:80:LEU:CG	1:A:80:LEU:CA	2.74	0.65
1:A:31:ARG:HH21	2:B:126:GLN:HB2	1.60	0.65
2:B:57:PRO:HA	2:B:57:PRO:CD	2.20	0.65
2:B:78:ASP:HA	2:B:78:ASP:OD2	1.95	0.65
2:B:94:LYS:CA	2:B:95:LEU:N	2.59	0.65
2:D:34:TYR:HB3	2:D:36:TRP:CH2	2.31	0.65
2:D:68:ASP:HB3	2:D:68:ASP:C	2.16	0.65
2:D:70:PHE:O	2:D:73:GLY:HA3	1.96	0.65
1:A:20:ASN:OD1	1:A:20:ASN:CB	2.45	0.65
1:A:3:SER:HB3	1:A:6:ASN:ND2	2.11	0.65
2:B:75:LYS:N	2:B:75:LYS:O	2.29	0.65
1:C:43:PHE:HB3	1:C:46:PHE:CD1	2.28	0.65
2:D:105:LEU:HB2	3:D:146:HEM:HBB2	1.76	0.65
2:D:14:TRP:CB	2:D:14:TRP:C	2.63	0.65
2:B:1:MET:C	2:B:2:LEU:HD23	2.17	0.65
1:C:36:PHE:HA	1:C:37:PRO:N	2.10	0.65
1:A:133:SER:O	1:A:137:THR:HB	1.97	0.65
1:A:39:THR:HG23	1:A:40:LYS:CE	2.26	0.65
2:B:68:ASP:CB	2:B:71:THR:CG2	2.36	0.65
1:C:66:LEU:CD2	1:C:66:LEU:HG	2.13	0.65
1:A:124:ASN:O	1:A:127:LYS:HB3	1.97	0.65
1:A:80:LEU:HG	1:A:80:LEU:CD2	2.16	0.65
2:B:113:VAL:HA	2:B:113:VAL:HG12	1.75	0.65
2:B:25:GLN:C	2:B:25:GLN:N	2.48	0.65
1:C:87:HIS:HA	1:C:91:LEU:CD1	2.11	0.65
2:D:14:TRP:HE3	2:D:14:TRP:HA	1.61	0.65
2:D:71:THR:C	2:D:71:THR:HG22	2.17	0.65
1:A:100:LEU:CB	1:A:100:LEU:HD13	2.22	0.65
1:A:88:ALA:O	1:A:92:ARG:CA	2.45	0.65
2:B:94:LYS:HD2	2:B:94:LYS:CB	2.25	0.65
1:C:32:MET:CG	1:C:39:THR:HG21	2.27	0.65
2:D:87:LEU:HD12	2:D:90:LEU:CD1	2.27	0.65
1:A:94:ASN:CA	1:A:94:ASN:CG	2.64	0.64
1:A:96:VAL:C	1:A:97:ASN:CA	2.62	0.64
1:A:31:ARG:CB	2:B:126:GLN:NE2	2.59	0.64
2:D:2:LEU:N	2:D:2:LEU:HB3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:THR:O	2:D:71:THR:HG22	1.97	0.64
1:A:89:HIS:C	1:A:89:HIS:ND1	2.51	0.64
1:A:35:SER:HB3	2:B:127:ALA:HA	1.78	0.64
2:B:144:TYR:O	2:B:145:HIS:O	2.14	0.64
1:C:79:THR:C	1:C:79:THR:CB	2.65	0.64
2:D:143:LYS:CB	2:D:143:LYS:C	2.60	0.64
2:D:19:VAL:HA	2:D:19:VAL:HG22	1.75	0.64
2:B:75:LYS:HE3	2:B:75:LYS:HG3	1.77	0.64
1:A:3:SER:O	1:A:4:ALA:C	2.35	0.64
1:A:58:HIS:CG	1:A:58:HIS:CA	2.74	0.64
1:C:109:LEU:O	1:C:113:LEU:HD22	1.97	0.64
1:A:100:LEU:CB	1:A:100:LEU:HD12	2.22	0.64
2:B:3:THR:HG23	2:B:5:GLU:HB3	0.65	0.64
2:B:5:GLU:N	2:B:6:GLU:N	2.45	0.64
2:B:79:ASP:HA	2:B:80:LEU:HG	1.78	0.64
2:B:81:LYS:HZ2	2:B:142:HIS:CD2	2.16	0.64
1:C:49:SER:HA	1:C:55:GLN:HE22	1.61	0.64
1:C:86:LEU:CD2	3:C:142:HEM:CBA	2.76	0.64
2:D:109:LEU:CD2	2:D:109:LEU:CB	2.74	0.64
1:A:118:THR:CG2	1:A:118:THR:HA	2.25	0.64
1:A:16:LYS:O	1:A:17:VAL:N	2.29	0.64
1:A:94:ASN:N	1:A:94:ASN:C	2.49	0.64
2:B:2:LEU:HG	2:B:6:GLU:HB3	1.78	0.64
1:C:32:MET:HG2	1:C:39:THR:HG21	1.80	0.64
2:D:16:LYS:HB2	2:D:16:LYS:CD	1.88	0.64
2:D:59:VAL:N	2:D:59:VAL:C	2.51	0.64
2:D:67:LEU:C	2:D:68:ASP:C	2.55	0.64
2:B:38:GLN:CA	2:B:38:GLN:O	2.44	0.64
1:C:105:LEU:CD1	1:C:105:LEU:HG	2.18	0.64
1:C:95:PRO:CG	1:C:141:ARG:HH12	2.09	0.64
2:D:28:GLY:CA	2:D:54:MET:HE1	2.27	0.64
2:B:24:ALA:CB	2:B:60:LYS:HA	2.27	0.64
2:B:77:LEU:N	2:B:78:ASP:HB3	2.13	0.64
1:C:94:ASN:ND2	1:C:94:ASN:N	2.46	0.64
2:D:115:ARG:CG	2:D:115:ARG:CA	2.75	0.64
2:B:124:ASN:O	2:B:125:VAL:HA	1.98	0.64
2:B:70:PHE:CD1	2:B:71:THR:HB	2.32	0.64
2:B:74:LEU:CD2	2:B:77:LEU:HG	2.28	0.64
1:C:93:VAL:CG1	1:C:93:VAL:CA	2.75	0.64
2:D:31:LEU:HA	2:D:37:THR:HG22	1.80	0.64
1:A:43:PHE:CE2	3:A:142:HEM:CMD	2.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:SER:HA	2:B:114:ALA:O	1.98	0.64
2:B:88:SER:HB2	2:B:143:LYS:HB3	1.79	0.64
2:B:97:VAL:C	2:B:97:VAL:CB	2.66	0.64
1:C:72:HIS:CB	1:C:74:ASN:ND2	2.54	0.64
2:D:32:VAL:HG13	2:D:53:VAL:HG21	1.80	0.64
1:A:127:LYS:C	1:A:128:PHE:C	2.56	0.63
1:A:37:PRO:HA	1:A:40:LYS:HD3	1.80	0.63
2:B:23:GLY:C	2:B:23:GLY:N	2.48	0.63
1:A:26:ALA:HB1	1:A:56:LYS:HE3	1.78	0.63
1:A:72:HIS:CE1	1:A:79:THR:HG21	2.33	0.63
1:C:119:PRO:HB2	1:C:119:PRO:C	2.16	0.63
1:C:137:THR:CB	1:C:137:THR:N	2.54	0.63
1:C:89:HIS:HB2	1:C:139:LYS:CD	2.28	0.63
2:D:74:LEU:CD1	2:D:132:VAL:HG21	2.27	0.63
1:A:31:ARG:NE	1:A:31:ARG:HG3	2.11	0.63
2:B:118:GLY:H	2:B:118:GLY:CA	1.29	0.63
2:B:80:LEU:HB3	2:B:82:GLY:CA	2.28	0.63
1:C:30:GLN:HB2	1:C:30:GLN:CD	2.17	0.63
2:D:38:GLN:CG	2:D:38:GLN:OE1	2.42	0.63
2:B:43:HIS:CD2	2:B:43:HIS:ND1	2.66	0.63
2:B:69:ALA:C	2:B:69:ALA:HB1	1.87	0.63
1:C:86:LEU:CD2	3:C:142:HEM:HBA2	2.28	0.63
2:D:19:VAL:CG2	2:D:19:VAL:N	2.62	0.63
2:D:64:LYS:NZ	2:D:68:ASP:OD1	2.28	0.63
2:D:94:LYS:CD	2:D:95:LEU:N	2.61	0.63
1:A:135:VAL:CB	1:A:135:VAL:C	2.64	0.63
2:B:128:LEU:C	2:B:128:LEU:N	2.45	0.63
2:B:21:VAL:HG12	2:B:25:GLN:NE2	2.14	0.63
2:B:41:PHE:CA	2:B:42:GLN:N	2.62	0.63
2:D:122:THR:H	2:D:125:VAL:HG12	1.63	0.63
2:D:28:GLY:HA3	2:D:54:MET:HE1	1.81	0.63
2:D:31:LEU:HD11	2:D:41:PHE:CD1	2.34	0.63
2:D:95:LEU:N	2:D:95:LEU:CG	2.62	0.63
1:A:105:LEU:HB2	1:A:105:LEU:N	2.12	0.63
1:A:57:ALA:O	1:A:60:GLN:CB	2.47	0.63
2:B:57:PRO:CA	2:B:57:PRO:HD3	2.17	0.63
2:B:60:LYS:HB2	2:B:60:LYS:HZ2	1.63	0.63
1:C:110:ALA:CB	1:C:110:ALA:C	2.66	0.63
1:A:47:ASP:C	1:A:49:SER:H	2.01	0.63
1:C:39:THR:O	1:C:42:TYR:HB2	1.98	0.63
1:C:76:LEU:HB3	1:C:80:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:LYS:CD	2:D:75:LYS:HG3	2.14	0.63
1:A:37:PRO:O	1:A:40:LYS:HD2	1.99	0.63
1:A:84:SER:O	1:A:88:ALA:HB2	1.99	0.63
2:B:24:ALA:C	2:B:25:GLN:CA	2.66	0.63
2:B:82:GLY:O	2:B:85:ALA:HB2	1.99	0.63
2:D:86:GLN:CA	2:D:87:LEU:N	2.58	0.63
1:A:79:THR:CA	1:A:79:THR:HG22	2.26	0.62
1:A:82:ASN:N	1:A:82:ASN:HB2	2.13	0.62
2:B:81:LYS:HZ3	2:B:142:HIS:CG	2.16	0.62
1:C:115:THR:OG1	1:C:115:THR:CG2	2.46	0.62
1:C:40:LYS:HD3	1:C:48:LEU:HD11	1.80	0.62
1:C:47:ASP:OD1	1:C:47:ASP:CB	2.47	0.62
2:D:22:VAL:HG13	2:D:109:LEU:HD21	1.81	0.62
2:D:56:ASN:O	2:D:57:PRO:C	2.38	0.62
2:D:74:LEU:O	2:D:75:LYS:O	2.17	0.62
2:D:84:PHE:HD2	2:D:87:LEU:HD23	1.63	0.62
2:B:81:LYS:HD2	2:B:142:HIS:HB3	1.81	0.62
2:B:91:HIS:O	2:B:96:HIS:HA	1.99	0.62
1:C:68:LYS:HD3	1:C:68:LYS:NZ	2.12	0.62
1:C:6:ASN:CA	1:C:7:LYS:N	2.54	0.62
2:D:2:LEU:HD13	2:D:2:LEU:C	2.18	0.62
2:D:96:HIS:CA	2:D:97:VAL:N	2.57	0.62
2:B:40:PHE:N	2:B:40:PHE:CD1	2.67	0.62
1:C:11:LYS:CB	1:C:11:LYS:N	2.60	0.62
2:D:75:LYS:O	2:D:77:LEU:HD11	1.99	0.62
1:A:76:LEU:O	1:A:77:PRO:CA	2.47	0.62
1:A:88:ALA:HB3	1:A:89:HIS:HB2	1.80	0.62
2:B:143:LYS:CG	2:B:143:LYS:HA	2.28	0.62
2:B:40:PHE:HB3	3:B:146:HEM:HMA3	1.81	0.62
2:B:5:GLU:N	2:B:5:GLU:C	2.51	0.62
1:C:103:HIS:CA	1:C:103:HIS:CG	2.82	0.62
1:C:42:TYR:CG	3:C:142:HEM:HBC1	2.34	0.62
2:D:26:ALA:C	2:D:26:ALA:N	2.51	0.62
1:C:89:HIS:CB	1:C:139:LYS:HG3	2.30	0.62
1:C:61:LYS:HD3	1:C:61:LYS:CG	2.16	0.62
2:D:61:ALA:HB3	2:D:62:HIS:H	1.65	0.62
2:D:6:GLU:O	2:D:6:GLU:HG3	1.99	0.62
2:D:84:PHE:H	2:D:84:PHE:HB2	1.63	0.62
1:A:27:GLN:O	1:A:30:GLN:HB3	2.00	0.62
2:B:98:ASN:HB3	2:B:101:ASN:N	2.15	0.62
2:B:125:VAL:HG12	2:B:125:VAL:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LEU:CD2	2:B:74:LEU:CD1	2.74	0.62
2:B:80:LEU:CB	2:B:81:LYS:O	2.43	0.62
1:C:115:THR:N	1:C:116:ASN:N	2.48	0.62
2:D:26:ALA:O	2:D:26:ALA:CA	2.45	0.62
2:D:78:ASP:N	2:D:79:ASP:N	2.47	0.62
1:A:27:GLN:OE1	1:A:112:HIS:HE1	1.83	0.62
1:A:42:TYR:O	1:A:43:PHE:N	2.28	0.62
2:B:1:MET:H1	2:B:77:LEU:HD11	1.64	0.62
2:D:27:LEU:HD12	2:D:63:GLY:N	2.15	0.62
2:B:70:PHE:HE2	2:B:133:VAL:HG23	1.65	0.62
1:A:116:ASN:N	1:A:116:ASN:C	2.53	0.62
1:A:31:ARG:CA	1:A:31:ARG:O	2.32	0.62
1:A:88:ALA:HB3	1:A:89:HIS:CB	2.30	0.62
2:D:7:LYS:N	2:D:10:VAL:HG22	2.15	0.62
2:D:83:ALA:C	2:D:83:ALA:N	2.51	0.62
2:B:103:ARG:NH2	2:B:103:ARG:NH1	2.44	0.62
2:B:144:TYR:CD1	2:B:144:TYR:CE2	2.87	0.62
1:C:116:ASN:CB	1:C:116:ASN:C	2.53	0.62
1:C:46:PHE:CE2	1:C:54:GLN:HG2	2.34	0.62
2:D:130:GLN:CA	2:D:130:GLN:HE21	2.13	0.62
1:A:43:PHE:CG	1:A:43:PHE:CA	2.76	0.61
1:A:46:PHE:HB3	1:A:48:LEU:HD23	1.82	0.61
2:B:40:PHE:C	2:B:40:PHE:N	2.53	0.61
2:D:19:VAL:CG1	2:D:64:LYS:HD2	2.29	0.61
1:A:2:LEU:CB	1:A:2:LEU:CD1	2.78	0.61
1:C:89:HIS:CD2	1:C:139:LYS:NZ	2.68	0.61
2:D:94:LYS:HD2	2:D:95:LEU:HD22	1.81	0.61
1:A:132:ASP:O	1:A:135:VAL:HG23	2.00	0.61
1:A:27:GLN:OE1	1:A:112:HIS:CE1	2.53	0.61
2:B:93:ASN:CG	2:B:93:ASN:HA	2.17	0.61
1:C:46:PHE:CD2	1:C:54:GLN:CB	2.83	0.61
2:D:36:TRP:CB	2:D:36:TRP:C	2.60	0.61
2:D:52:ALA:HA	2:D:55:ASN:H	1.63	0.61
2:B:17:VAL:CA	2:B:18:ASP:N	2.62	0.61
2:B:3:THR:C	2:B:5:GLU:H	2.01	0.61
2:D:130:GLN:CG	2:D:130:GLN:OE1	2.48	0.61
2:D:33:VAL:O	2:D:33:VAL:HG22	1.98	0.61
2:D:6:GLU:O	2:D:6:GLU:CG	2.48	0.61
1:A:104:SER:C	1:A:105:LEU:CA	2.66	0.61
1:C:84:SER:HA	1:C:136:LEU:HD13	1.83	0.61
1:C:95:PRO:HG3	1:C:141:ARG:NH2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:ARG:HG2	2:D:39:ARG:NE	2.09	0.61
1:A:105:LEU:HD11	1:A:105:LEU:CD2	2.25	0.61
1:A:43:PHE:N	1:A:43:PHE:CB	2.61	0.61
1:A:76:LEU:HD23	1:A:76:LEU:H	1.64	0.61
2:B:64:LYS:N	2:B:65:ARG:N	2.48	0.61
2:D:138:ASN:C	2:D:138:ASN:N	2.48	0.61
2:D:75:LYS:HG2	2:D:75:LYS:CD	2.14	0.61
2:B:43:HIS:CE1	3:B:146:HEM:CGA	2.83	0.61
2:B:97:VAL:HG12	2:B:101:ASN:HB2	1.83	0.61
1:C:90:LYS:N	1:C:90:LYS:CB	2.62	0.61
1:C:87:HIS:O	1:C:91:LEU:HB2	2.00	0.61
1:C:9:ASN:HB3	1:C:124:ASN:CB	2.31	0.61
3:D:146:HEM:C4C	3:D:146:HEM:CAC	2.74	0.61
2:D:88:SER:C	2:D:88:SER:CB	2.59	0.61
1:A:106:LEU:HD23	1:A:126:ASN:HD22	1.66	0.61
1:A:31:ARG:CD	2:B:126:GLN:HE21	2.14	0.61
1:A:52:SER:OG	1:A:52:SER:CA	2.48	0.61
2:B:39:ARG:CZ	2:B:40:PHE:CZ	2.82	0.61
2:B:43:HIS:CB	2:B:43:HIS:C	2.65	0.61
2:B:80:LEU:HB3	2:B:80:LEU:HD23	1.78	0.61
1:C:60:GLN:NE2	1:C:64:ASN:HD21	1.98	0.61
1:C:99:LYS:CB	1:C:99:LYS:CD	2.59	0.61
1:A:124:ASN:H	1:A:124:ASN:CB	2.06	0.61
1:A:43:PHE:HB2	1:A:48:LEU:HD22	1.83	0.61
1:A:86:LEU:O	1:A:91:LEU:HB2	2.00	0.61
2:B:126:GLN:CB	2:B:126:GLN:CD	2.69	0.61
2:B:140:LEU:CD2	2:B:140:LEU:CD1	2.79	0.61
1:C:44:PRO:O	1:C:45:HIS:C	2.40	0.61
2:D:79:ASP:OD1	2:D:81:LYS:CD	2.49	0.61
2:D:84:PHE:HB2	2:D:84:PHE:N	2.14	0.61
1:A:42:TYR:HB3	3:A:142:HEM:CMD	2.31	0.61
2:B:70:PHE:HD1	2:B:71:THR:CB	2.13	0.61
1:C:109:LEU:O	1:C:113:LEU:CD2	2.49	0.61
2:D:2:LEU:CG	2:D:7:LYS:CE	2.75	0.61
2:B:2:LEU:CB	2:B:131:LYS:HZ1	2.14	0.60
2:B:27:LEU:HD21	2:B:66:VAL:HG11	1.80	0.60
1:C:86:LEU:HD21	3:C:142:HEM:CBA	2.31	0.60
1:A:16:LYS:CG	1:A:16:LYS:CE	2.74	0.60
1:A:89:HIS:CD2	1:A:139:LYS:CD	2.77	0.60
2:B:121:PHE:CZ	2:B:126:GLN:HA	2.36	0.60
2:B:65:ARG:HH12	2:B:65:ARG:HH22	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:ALA:N	2:D:142:HIS:N	2.49	0.60
1:A:75:ASP:O	1:A:79:THR:N	2.35	0.60
1:A:14:TRP:O	1:A:17:VAL:HG23	2.01	0.60
1:A:50:HIS:CG	1:A:50:HIS:HA	2.35	0.60
1:C:113:LEU:N	1:C:113:LEU:HD23	2.10	0.60
1:C:114:PRO:CG	1:C:114:PRO:CA	2.78	0.60
1:C:129:LEU:O	1:C:130:ALA:CA	2.50	0.60
1:C:44:PRO:O	1:C:45:HIS:CA	2.49	0.60
2:D:72:GLN:HE22	2:D:73:GLY:HA2	1.61	0.60
2:B:104:LEU:O	2:B:107:ASN:HB2	2.01	0.60
2:B:55:ASN:HA	2:B:60:LYS:HZ1	1.66	0.60
1:C:61:LYS:HD2	1:C:61:LYS:CG	2.15	0.60
2:D:110:ALA:HB1	2:D:126:GLN:OE1	2.00	0.60
2:D:28:GLY:HA3	2:D:54:MET:CE	2.30	0.60
2:D:41:PHE:HB2	2:D:44:PHE:CE1	2.36	0.60
2:B:1:MET:HE3	2:B:78:ASP:OD2	2.00	0.60
2:D:79:ASP:OD1	2:D:81:LYS:HD3	2.02	0.60
2:D:5:GLU:CB	2:D:9:ALA:HB3	2.25	0.60
1:A:118:THR:CG2	1:A:118:THR:N	2.65	0.60
1:A:86:LEU:CA	1:A:87:HIS:N	2.62	0.60
2:B:80:LEU:CD1	2:B:80:LEU:HD21	2.32	0.60
2:B:82:GLY:O	2:B:85:ALA:CB	2.50	0.60
2:D:2:LEU:CD2	2:D:7:LYS:CD	2.78	0.60
1:A:36:PHE:CA	1:A:36:PHE:CG	2.81	0.60
1:A:76:LEU:HB2	1:A:77:PRO:HD3	1.82	0.60
1:A:94:ASN:OD1	1:A:96:VAL:CG2	2.49	0.60
1:C:89:HIS:CB	1:C:139:LYS:CG	2.80	0.60
2:D:137:ALA:CB	2:D:140:LEU:CD1	2.80	0.60
2:D:14:TRP:CE3	2:D:14:TRP:HA	2.34	0.60
2:D:84:PHE:C	2:D:84:PHE:CB	2.70	0.60
1:A:62:VAL:HG22	1:A:62:VAL:CG1	2.23	0.60
1:A:79:THR:HA	1:A:79:THR:CG2	2.24	0.60
2:B:123:PRO:CB	2:B:126:GLN:NE2	2.64	0.60
2:B:62:HIS:O	2:B:62:HIS:CD2	2.55	0.60
1:C:131:ASN:OD1	1:C:131:ASN:CB	2.49	0.60
2:D:116:ASN:CA	2:D:117:PHE:N	2.60	0.60
1:A:2:LEU:HB3	1:A:7:LYS:HD3	1.82	0.60
2:B:95:LEU:HD11	3:B:146:HEM:C2A	2.37	0.60
1:C:36:PHE:O	1:C:39:THR:HG22	2.01	0.60
1:C:26:ALA:CB	1:C:56:LYS:HD2	2.31	0.60
2:D:11:THR:CA	2:D:11:THR:HG1	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:PRO:HG3	2:D:123:PRO:CD	2.17	0.60
2:D:14:TRP:CB	2:D:15:GLY:N	2.65	0.60
1:A:106:LEU:HD11	1:A:106:LEU:CD2	2.32	0.59
1:A:31:ARG:HH21	2:B:126:GLN:HB3	1.66	0.59
2:B:137:ALA:CB	2:B:137:ALA:N	2.54	0.59
2:B:34:TYR:CE2	2:B:34:TYR:CD1	2.89	0.59
1:C:139:LYS:HD3	1:C:139:LYS:CB	2.31	0.59
2:D:142:HIS:CB	2:D:142:HIS:C	2.66	0.59
2:D:55:ASN:ND2	2:D:57:PRO:HD2	2.17	0.59
1:A:10:VAL:CA	1:A:11:LYS:N	2.54	0.59
2:B:105:LEU:CB	3:B:146:HEM:HBB2	2.32	0.59
3:B:146:HEM:CHB	3:B:146:HEM:HMA2	2.30	0.59
2:B:41:PHE:C	2:B:42:GLN:CA	2.68	0.59
2:B:43:HIS:O	2:B:43:HIS:CA	2.48	0.59
1:C:27:GLN:OE1	1:C:31:ARG:NH1	2.36	0.59
1:C:56:LYS:CE	1:C:59:GLY:HA3	2.32	0.59
2:D:10:VAL:CA	2:D:11:THR:N	2.64	0.59
2:D:87:LEU:CG	2:D:87:LEU:CA	2.71	0.59
2:B:22:VAL:O	2:B:23:GLY:HA2	2.03	0.59
2:B:5:GLU:C	2:B:8:ALA:HB3	2.22	0.59
2:B:3:THR:CG2	2:B:5:GLU:CD	2.70	0.59
2:D:94:LYS:HD3	2:D:94:LYS:C	2.22	0.59
1:A:29:LEU:HD23	1:A:29:LEU:O	2.02	0.59
2:B:26:ALA:N	2:B:26:ALA:C	2.55	0.59
1:C:70:GLN:O	1:C:73:LEU:HD11	2.02	0.59
2:D:129:PHE:N	2:D:129:PHE:CB	2.64	0.59
2:B:126:GLN:CA	2:B:127:ALA:N	2.60	0.59
2:B:16:LYS:HB3	2:B:16:LYS:N	2.18	0.59
2:B:2:LEU:HB2	2:B:6:GLU:HB2	1.83	0.59
2:B:19:VAL:CG2	2:B:68:ASP:OD2	2.46	0.59
2:B:7:LYS:HE3	2:B:74:LEU:HD11	1.84	0.59
2:D:59:VAL:HB	2:D:60:LYS:N	2.18	0.59
1:A:36:PHE:HB3	1:A:100:LEU:HD13	1.84	0.59
3:A:142:HEM:HMD1	3:A:142:HEM:CHD	2.32	0.59
1:A:26:ALA:CB	1:A:59:GLY:HA3	2.31	0.59
1:A:70:GLN:O	1:A:73:LEU:HD12	2.03	0.59
2:B:68:ASP:H	2:B:71:THR:HG21	1.61	0.59
2:B:78:ASP:OD2	2:B:79:ASP:HB2	2.02	0.59
1:C:87:HIS:O	1:C:93:VAL:HG23	2.01	0.59
2:D:103:ARG:NH2	2:D:130:GLN:NE2	2.50	0.59
2:B:58:LYS:CD	2:B:58:LYS:CB	2.77	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLY:CA	1:C:72:HIS:N	2.65	0.59
2:D:115:ARG:HH21	2:D:115:ARG:HG2	1.68	0.59
2:B:41:PHE:HB3	2:B:43:HIS:HB3	1.82	0.59
2:B:94:LYS:N	2:B:94:LYS:C	2.53	0.59
3:C:142:HEM:CAB	3:C:142:HEM:C2B	2.73	0.59
2:D:10:VAL:CG1	2:D:128:LEU:CD2	2.69	0.59
2:D:123:PRO:CD	2:D:123:PRO:HG2	2.17	0.59
2:D:126:GLN:NE2	2:D:130:GLN:CB	2.64	0.59
1:A:72:HIS:HB2	1:A:74:ASN:HD21	1.68	0.59
1:C:53:ALA:CB	1:C:53:ALA:C	2.71	0.59
1:A:116:ASN:N	1:A:116:ASN:CB	2.64	0.59
1:A:136:LEU:CA	1:A:137:THR:N	2.66	0.59
1:C:113:LEU:CD2	1:C:113:LEU:CD1	2.79	0.59
1:C:86:LEU:HD22	3:C:142:HEM:HBA2	1.84	0.59
2:D:30:LEU:CA	2:D:31:LEU:N	2.64	0.59
1:A:85:ASN:HA	1:A:139:LYS:HE3	1.85	0.58
1:C:89:HIS:HB2	1:C:139:LYS:HZ2	1.58	0.58
2:D:70:PHE:CA	2:D:71:THR:HB	2.32	0.58
2:D:86:GLN:HA	2:D:86:GLN:C	2.12	0.58
1:A:122:HIS:C	1:A:122:HIS:CB	2.66	0.58
1:A:91:LEU:HD23	3:A:142:HEM:C2D	2.37	0.58
2:B:42:GLN:O	2:B:43:HIS:N	2.35	0.58
2:B:22:VAL:CG1	2:B:67:LEU:HD21	2.30	0.58
1:C:43:PHE:CB	1:C:43:PHE:C	2.69	0.58
1:C:52:SER:C	1:C:53:ALA:HA	2.20	0.58
1:A:31:ARG:HE	1:A:31:ARG:HG3	1.66	0.58
2:B:109:LEU:O	2:B:110:ALA:CA	2.50	0.58
2:B:130:GLN:CB	2:B:130:GLN:N	2.65	0.58
1:A:36:PHE:CZ	2:B:130:GLN:HG3	2.37	0.58
2:B:55:ASN:HA	2:B:60:LYS:NZ	2.18	0.58
1:C:15:GLY:C	1:C:16:LYS:CA	2.69	0.58
1:C:46:PHE:CA	1:C:46:PHE:CG	2.86	0.58
1:C:76:LEU:CD2	1:C:76:LEU:CB	2.78	0.58
2:D:143:LYS:CE	2:D:143:LYS:CG	2.72	0.58
2:D:4:ALA:CA	2:D:5:GLU:CA	2.77	0.58
2:D:2:LEU:CD2	2:D:7:LYS:HB3	2.28	0.58
1:A:57:ALA:CA	1:A:60:GLN:NE2	2.61	0.58
2:B:75:LYS:CB	2:B:76:HIS:ND1	2.66	0.58
1:C:9:ASN:OD1	1:C:9:ASN:CB	2.50	0.58
1:A:52:SER:O	1:A:54:GLN:N	2.36	0.58
2:B:113:VAL:CG2	2:B:113:VAL:CG1	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:HIS:C	2:B:144:TYR:OH	2.42	0.58
1:C:32:MET:CA	1:C:32:MET:HB3	2.16	0.58
1:C:75:ASP:CB	1:C:75:ASP:C	2.72	0.58
1:A:79:THR:OG1	1:A:79:THR:CA	2.38	0.58
2:B:125:VAL:O	2:B:125:VAL:CG1	2.52	0.58
2:B:101:ASN:HB3	3:B:146:HEM:HAB	1.85	0.58
2:D:67:LEU:HA	2:D:67:LEU:HD23	1.84	0.58
2:D:79:ASP:OD1	2:D:81:LYS:HE2	2.02	0.58
2:B:18:ASP:O	2:B:20:ASP:OD2	2.22	0.58
2:B:39:ARG:HH12	2:B:40:PHE:HZ	0.62	0.58
2:B:97:VAL:CG1	3:B:146:HEM:HMB2	2.34	0.58
1:C:96:VAL:CG2	1:C:96:VAL:CG1	2.79	0.58
2:D:115:ARG:CA	2:D:115:ARG:HG3	2.32	0.58
2:D:87:LEU:CB	2:D:87:LEU:C	2.72	0.58
2:D:90:LEU:HD13	2:D:91:HIS:HD1	1.68	0.58
1:A:100:LEU:CG	1:A:100:LEU:HA	2.31	0.58
2:D:84:PHE:CG	2:D:84:PHE:CA	2.85	0.58
2:B:3:THR:N	2:B:6:GLU:CB	2.58	0.58
2:D:25:GLN:CD	2:D:25:GLN:CB	2.72	0.58
2:D:31:LEU:HG	2:D:31:LEU:HA	1.84	0.58
2:D:46:ASN:OD1	2:D:52:ALA:HB3	2.04	0.58
2:D:94:LYS:CD	2:D:94:LYS:C	2.72	0.58
1:A:10:VAL:HB	1:A:10:VAL:C	2.23	0.58
2:B:98:ASN:C	2:B:100:GLN:H	1.99	0.58
2:B:123:PRO:HB3	2:B:126:GLN:HE22	1.68	0.58
2:B:84:PHE:HE2	3:B:146:HEM:CBC	2.16	0.58
1:C:74:ASN:O	1:C:75:ASP:N	2.28	0.58
1:A:118:THR:O	1:A:122:HIS:N	2.28	0.57
1:A:109:LEU:CA	1:A:110:ALA:N	2.67	0.57
1:C:17:VAL:HG12	1:C:21:ALA:HB2	1.86	0.57
1:C:86:LEU:HD21	3:C:142:HEM:HBA1	1.85	0.57
2:D:30:LEU:HG	2:D:37:THR:HG21	1.84	0.57
2:B:105:LEU:HB3	3:B:146:HEM:HBB2	1.86	0.57
2:B:49:SER:HB3	2:B:52:ALA:HB3	1.86	0.57
2:B:7:LYS:HE3	2:B:74:LEU:CD1	2.34	0.57
1:C:20:ASN:O	1:C:21:ALA:N	2.30	0.57
1:A:127:LYS:HZ3	1:A:127:LYS:HD3	1.66	0.57
3:A:142:HEM:C1D	3:A:142:HEM:HMD1	2.36	0.57
1:A:79:THR:CA	1:A:79:THR:HG23	2.26	0.57
2:B:81:LYS:CE	2:B:142:HIS:ND1	2.67	0.57
2:B:20:ASP:O	2:B:21:VAL:HG22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LEU:O	1:C:130:ALA:C	2.43	0.57
1:A:112:HIS:HB2	1:A:112:HIS:ND1	2.16	0.57
1:A:136:LEU:HB2	1:A:136:LEU:C	2.25	0.57
1:A:80:LEU:CD1	1:A:80:LEU:CD2	2.79	0.57
2:B:13:PHE:CE1	2:B:120:GLN:HB2	2.40	0.57
1:C:9:ASN:CA	1:C:9:ASN:CG	2.70	0.57
1:A:100:LEU:CD1	1:A:100:LEU:HB2	2.27	0.57
1:A:32:MET:CA	1:A:33:PHE:N	2.65	0.57
1:A:53:ALA:CA	1:A:56:LYS:CG	2.82	0.57
2:B:4:ALA:C	2:B:8:ALA:HB2	2.24	0.57
2:B:55:ASN:C	2:B:55:ASN:HA	2.17	0.57
1:C:118:THR:OG1	1:C:121:VAL:HG23	2.05	0.57
2:D:95:LEU:CD1	3:D:146:HEM:CHB	2.82	0.57
2:D:67:LEU:O	2:D:71:THR:HB	2.04	0.57
2:D:79:ASP:OD1	2:D:81:LYS:CE	2.53	0.57
1:A:39:THR:C	1:A:40:LYS:HZ3	2.07	0.57
2:B:106:GLY:CA	2:B:133:VAL:HG21	2.35	0.57
2:B:20:ASP:HA	2:B:64:LYS:HG2	1.87	0.57
2:B:80:LEU:HB3	2:B:81:LYS:C	2.25	0.57
1:C:43:PHE:CE2	1:C:58:HIS:NE2	2.73	0.57
2:D:28:GLY:C	2:D:54:MET:CE	2.71	0.57
2:D:41:PHE:CB	2:D:44:PHE:CE1	2.88	0.57
1:A:33:PHE:HD1	1:A:40:LYS:CE	2.14	0.57
1:A:43:PHE:CD2	1:A:43:PHE:CD1	2.50	0.57
1:A:42:TYR:HB2	1:A:43:PHE:CE1	2.40	0.57
1:A:46:PHE:HB3	1:A:55:GLN:HE22	1.69	0.57
2:B:131:LYS:HD2	2:B:131:LYS:NZ	2.16	0.57
2:B:92:CYS:HB2	2:B:144:TYR:CZ	2.40	0.57
2:B:60:LYS:HB2	2:B:60:LYS:NZ	2.20	0.57
1:C:100:LEU:CB	1:C:100:LEU:CD1	2.80	0.57
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.87	0.57
2:B:1:MET:N	2:B:1:MET:C	2.58	0.57
2:B:6:GLU:OE1	2:B:131:LYS:CE	2.52	0.57
1:C:19:GLY:CA	1:C:20:ASN:N	2.56	0.57
2:D:50:ALA:C	2:D:53:VAL:HG13	2.24	0.57
2:B:16:LYS:O	2:B:117:PHE:HZ	1.86	0.57
1:C:70:GLN:HG2	1:C:128:PHE:CZ	2.39	0.57
1:C:117:PHE:HE2	2:D:111:LEU:HD11	1.69	0.57
1:A:105:LEU:C	1:A:106:LEU:CA	2.70	0.56
1:A:43:PHE:CD2	1:A:46:PHE:CE1	2.93	0.56
1:C:80:LEU:O	1:C:84:SER:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:TYR:HD1	2:D:145:HIS:N	1.86	0.56
1:A:73:LEU:HA	1:A:76:LEU:HD21	1.87	0.56
2:B:19:VAL:HG21	2:B:68:ASP:H	1.66	0.56
1:C:89:HIS:CD2	1:C:139:LYS:HZ3	2.22	0.56
1:C:54:GLN:O	1:C:57:ALA:HB3	2.05	0.56
1:A:29:LEU:N	1:A:29:LEU:CB	2.68	0.56
1:C:66:LEU:CD1	1:C:66:LEU:CD2	2.78	0.56
1:C:93:VAL:CG1	3:C:142:HEM:C3C	2.88	0.56
1:A:42:TYR:C	1:A:44:PRO:HD2	2.25	0.56
2:B:39:ARG:HD3	1:C:92:ARG:HB2	1.86	0.56
2:B:72:GLN:N	2:B:72:GLN:C	2.54	0.56
1:C:80:LEU:HD23	1:C:135:VAL:HG21	1.85	0.56
1:C:92:ARG:CD	1:C:92:ARG:HB2	2.35	0.56
2:D:1:MET:CG	2:D:131:LYS:NZ	2.67	0.56
2:D:54:MET:O	2:D:60:LYS:HD2	2.05	0.56
1:A:138:SER:CB	1:A:138:SER:HG	2.10	0.56
1:A:79:THR:HG1	1:A:79:THR:CA	2.19	0.56
2:B:94:LYS:H	2:B:95:LEU:HB2	1.70	0.56
1:C:141:ARG:CD	1:C:141:ARG:CB	2.81	0.56
1:C:17:VAL:HG22	1:C:24:TYR:HE2	1.67	0.56
2:D:25:GLN:NE2	2:D:115:ARG:NH2	2.53	0.56
2:D:65:ARG:HA	2:D:68:ASP:HB2	1.86	0.56
1:A:105:LEU:N	1:A:106:LEU:N	2.52	0.56
1:A:132:ASP:O	1:A:136:LEU:HG	2.05	0.56
1:A:31:ARG:NH2	2:B:126:GLN:HB2	2.21	0.56
1:A:14:TRP:CD1	1:A:67:THR:HG23	2.40	0.56
2:B:57:PRO:HB3	2:B:57:PRO:HD3	1.86	0.56
1:C:11:LYS:HD2	1:C:70:GLN:HE22	1.69	0.56
2:D:59:VAL:HB	2:D:59:VAL:C	2.23	0.56
2:D:56:ASN:O	2:D:59:VAL:N	2.39	0.56
2:B:14:TRP:O	2:B:17:VAL:HG23	2.05	0.56
2:B:24:ALA:O	2:B:28:GLY:HA3	2.05	0.56
1:C:93:VAL:O	1:C:140:TYR:OH	2.24	0.56
2:D:124:ASN:O	2:D:128:LEU:HD12	2.04	0.56
2:D:56:ASN:HD22	2:D:56:ASN:C	2.09	0.56
1:A:35:SER:CA	1:A:35:SER:OG	2.52	0.56
2:B:25:GLN:HG3	2:B:112:VAL:HG11	1.87	0.56
2:B:1:MET:H3	2:B:2:LEU:CD2	2.18	0.56
1:C:43:PHE:HE2	1:C:58:HIS:NE2	2.03	0.56
1:A:65:ALA:N	1:A:65:ALA:CB	2.59	0.56
1:A:9:ASN:N	1:A:9:ASN:C	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:VAL:CG1	2:B:21:VAL:CA	2.65	0.56
2:B:2:LEU:CB	2:B:131:LYS:NZ	2.62	0.56
2:B:134:ALA:O	2:B:138:ASN:ND2	2.37	0.56
2:B:97:VAL:HG11	3:B:146:HEM:CMB	2.36	0.56
2:B:1:MET:H3	2:B:2:LEU:HD23	1.68	0.56
2:B:70:PHE:HD1	2:B:71:THR:H	1.54	0.56
2:D:10:VAL:HG23	2:D:11:THR:HG22	1.87	0.56
2:D:61:ALA:CB	2:D:62:HIS:H	2.17	0.56
2:D:79:ASP:O	2:D:81:LYS:CD	2.54	0.56
1:A:26:ALA:CB	1:A:56:LYS:CE	2.72	0.56
1:A:63:ALA:HA	1:A:63:ALA:CB	2.16	0.56
2:B:53:VAL:C	2:B:54:MET:HA	2.17	0.56
2:B:87:LEU:CB	2:B:87:LEU:C	2.70	0.56
1:A:26:ALA:O	1:A:30:GLN:HB3	2.06	0.55
1:A:32:MET:HB3	1:A:32:MET:N	2.21	0.55
2:B:24:ALA:O	2:B:28:GLY:CA	2.53	0.55
2:B:46:ASN:C	2:B:46:ASN:CB	2.72	0.55
1:C:44:PRO:N	1:C:44:PRO:CB	2.59	0.55
1:C:88:ALA:HB3	1:C:139:LYS:HB2	1.87	0.55
3:A:142:HEM:HHB	3:A:142:HEM:HMA2	1.87	0.55
1:A:2:LEU:CD1	1:A:2:LEU:HD22	2.32	0.55
1:A:34:LEU:C	1:A:34:LEU:CB	2.70	0.55
2:B:21:VAL:HB	2:B:22:VAL:N	2.20	0.55
2:B:65:ARG:HD3	3:B:146:HEM: CBD	2.35	0.55
2:B:6:GLU:O	2:B:9:ALA:HB3	2.05	0.55
1:C:101:LEU:HD12	3:C:142:HEM:HHC	1.88	0.55
1:C:32:MET:CE	1:C:101:LEU:HG	2.36	0.55
1:C:88:ALA:HB2	1:C:136:LEU:O	2.07	0.55
2:D:67:LEU:CD2	2:D:67:LEU:HA	2.36	0.55
2:D:88:SER:N	2:D:88:SER:CB	2.65	0.55
2:B:102:PHE:CD1	2:B:140:LEU:HD12	2.42	0.55
2:B:24:ALA:HB2	2:B:60:LYS:HA	1.89	0.55
2:B:80:LEU:CB	2:B:82:GLY:CA	2.84	0.55
2:D:138:ASN:N	2:D:138:ASN:CB	2.64	0.55
3:D:146:HEM:CAA	3:D:146:HEM:CHA	2.83	0.55
1:A:32:MET:SD	1:A:101:LEU:HB2	2.46	0.55
1:A:85:ASN:C	1:A:85:ASN:CG	2.65	0.55
1:A:31:ARG:NH2	2:B:126:GLN:CB	2.65	0.55
2:B:92:CYS:HB2	2:B:144:TYR:CE2	2.41	0.55
1:C:93:VAL:CG1	3:C:142:HEM:HAC	2.30	0.55
2:D:25:GLN:CD	2:D:115:ARG:NH2	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:GLY:O	2:D:54:MET:HB2	2.06	0.55
1:A:74:ASN:N	1:A:74:ASN:HD22	2.04	0.55
2:B:97:VAL:HG21	3:B:146:HEM:C1B	2.41	0.55
1:A:139:LYS:CD	1:A:139:LYS:NZ	2.70	0.55
2:B:4:ALA:O	2:B:8:ALA:HB2	2.06	0.55
1:C:47:ASP:CB	1:C:47:ASP:OD2	2.48	0.55
1:A:140:TYR:HB2	1:A:140:TYR:CD1	2.40	0.55
1:A:72:HIS:HE1	1:A:79:THR:OG1	1.89	0.55
2:B:106:GLY:CA	2:B:107:ASN:N	2.63	0.55
2:B:97:VAL:CG1	3:B:146:HEM:CMB	2.85	0.55
1:C:117:PHE:O	1:C:117:PHE:CD2	2.59	0.55
2:D:47:LEU:HD12	2:D:53:VAL:HA	1.87	0.55
2:B:101:ASN:CA	2:B:102:PHE:N	2.59	0.55
2:B:113:VAL:HG12	2:B:117:PHE:CE2	2.42	0.55
2:B:70:PHE:HA	2:B:84:PHE:HZ	1.72	0.55
1:C:60:GLN:CA	1:C:60:GLN:HG2	2.35	0.55
1:A:1:VAL:C	1:A:1:VAL:CB	2.70	0.55
2:B:3:THR:CG2	2:B:5:GLU:CG	2.78	0.55
1:C:7:LYS:O	1:C:11:LYS:HB2	2.06	0.55
1:C:15:GLY:N	1:C:16:LYS:N	2.53	0.55
1:C:23:ALA:HA	1:C:56:LYS:HD3	1.89	0.55
1:C:48:LEU:HA	1:C:55:GLN:CD	2.27	0.55
2:B:13:PHE:HE1	2:B:120:GLN:CB	2.20	0.55
2:B:125:VAL:CG1	2:B:125:VAL:CA	2.81	0.55
2:B:18:ASP:CG	2:B:18:ASP:CA	2.71	0.55
2:B:47:LEU:CD1	2:B:53:VAL:HA	2.37	0.55
1:C:32:MET:CA	1:C:32:MET:HB2	2.16	0.55
1:A:43:PHE:HA	1:A:44:PRO:HD2	1.89	0.54
1:A:55:GLN:HB3	1:A:56:LYS:NZ	2.21	0.54
2:B:109:LEU:CA	2:B:109:LEU:CD2	2.80	0.54
2:B:54:MET:O	2:B:59:VAL:CG2	2.56	0.54
2:B:24:ALA:HB1	2:B:60:LYS:HA	1.89	0.54
2:B:85:ALA:O	2:B:88:SER:HB2	2.06	0.54
1:C:17:VAL:O	1:C:18:GLY:CA	2.54	0.54
1:C:84:SER:HA	1:C:87:HIS:HD1	1.72	0.54
1:C:83:LEU:HB3	1:C:84:SER:OG	2.07	0.54
2:D:65:ARG:N	2:D:66:VAL:N	2.55	0.54
2:D:83:ALA:C	2:D:83:ALA:CB	2.76	0.54
2:D:90:LEU:HD12	2:D:90:LEU:HB3	1.85	0.54
1:A:17:VAL:CG2	1:A:17:VAL:CA	2.78	0.54
1:A:43:PHE:HA	1:A:45:HIS:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:CD2	1:A:48:LEU:HG	2.22	0.54
1:C:83:LEU:CD1	3:C:142:HEM:HMA1	2.35	0.54
2:D:10:VAL:HG23	2:D:11:THR:CG2	2.35	0.54
2:D:112:VAL:CG1	2:D:112:VAL:HA	2.37	0.54
2:D:128:LEU:N	2:D:128:LEU:C	2.58	0.54
1:A:119:PRO:HD3	2:B:29:ARG:NH1	2.23	0.54
1:A:26:ALA:O	1:A:30:GLN:CB	2.55	0.54
1:A:41:THR:HG23	1:A:41:THR:CA	2.35	0.54
1:A:7:LYS:N	1:A:7:LYS:C	2.60	0.54
1:A:93:VAL:HG21	3:A:142:HEM:C3C	2.42	0.54
2:B:63:GLY:CA	2:B:66:VAL:HG13	2.24	0.54
1:C:85:ASN:OD1	1:C:89:HIS:HB3	2.08	0.54
2:D:104:LEU:CD1	2:D:104:LEU:CB	2.85	0.54
2:D:70:PHE:CE2	2:D:136:VAL:HG11	2.42	0.54
1:A:26:ALA:CA	1:A:29:LEU:HD22	2.21	0.54
1:C:49:SER:HG	1:C:49:SER:CB	2.09	0.54
3:D:146:HEM:CAA	3:D:146:HEM:CGA	2.85	0.54
2:D:70:PHE:CD1	2:D:71:THR:OG1	2.13	0.54
2:B:128:LEU:HA	2:B:128:LEU:CB	2.21	0.54
2:B:143:LYS:CA	2:B:143:LYS:CG	2.83	0.54
1:C:39:THR:N	1:C:39:THR:HB	2.17	0.54
2:D:95:LEU:HD11	3:D:146:HEM:C4A	2.43	0.54
2:D:52:ALA:CB	2:D:52:ALA:C	2.70	0.54
1:A:19:GLY:O	1:A:22:PRO:HG2	2.08	0.54
1:A:1:VAL:CG1	1:A:1:VAL:HG22	2.35	0.54
1:A:42:TYR:O	1:A:43:PHE:CA	2.55	0.54
1:A:26:ALA:CB	1:A:56:LYS:HE3	2.37	0.54
1:A:62:VAL:HG23	3:A:142:HEM:C1B	2.42	0.54
2:B:27:LEU:HD23	2:B:66:VAL:CG1	2.38	0.54
1:C:86:LEU:O	1:C:91:LEU:N	2.26	0.54
2:D:14:TRP:HB3	2:D:15:GLY:N	2.22	0.54
2:B:30:LEU:CD2	2:B:105:LEU:HB2	2.37	0.54
2:B:36:TRP:C	2:B:37:THR:CA	2.75	0.54
1:C:99:LYS:HB3	1:C:99:LYS:CD	2.37	0.54
2:D:16:LYS:CB	2:D:16:LYS:O	2.55	0.54
2:B:38:GLN:N	2:B:38:GLN:C	2.59	0.54
2:B:19:VAL:HA	2:B:67:LEU:HD23	1.90	0.54
2:B:75:LYS:CD	2:B:75:LYS:CB	2.83	0.54
1:C:42:TYR:CG	3:C:142:HEM:CBC	2.90	0.54
1:C:86:LEU:CD2	3:C:142:HEM:HBA1	2.37	0.54
2:D:14:TRP:O	2:D:17:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:VAL:CG1	2:D:53:VAL:HG21	2.38	0.54
1:A:96:VAL:HG11	2:D:100:GLN:CG	2.36	0.54
2:D:115:ARG:NH2	2:D:115:ARG:HG2	2.16	0.54
2:D:129:PHE:CG	2:D:129:PHE:N	2.75	0.54
1:A:72:HIS:CE1	1:A:79:THR:OG1	2.61	0.53
2:B:114:ALA:O	2:B:118:GLY:HA2	2.07	0.53
2:B:39:ARG:CG	2:B:39:ARG:CA	2.82	0.53
2:B:49:SER:O	2:B:49:SER:CA	2.57	0.53
1:C:128:PHE:O	1:C:131:ASN:HB2	2.09	0.53
1:C:91:LEU:CD2	1:C:91:LEU:CD1	2.76	0.53
2:D:101:ASN:HB2	3:D:146:HEM:HAB	1.90	0.53
2:D:79:ASP:C	2:D:81:LYS:CD	2.76	0.53
1:A:115:THR:CB	1:A:115:THR:HG1	2.10	0.53
1:A:132:ASP:HB2	1:A:132:ASP:OD2	2.07	0.53
2:B:94:LYS:HD2	2:B:94:LYS:HB3	1.85	0.53
1:C:99:LYS:CG	1:C:99:LYS:HE3	2.37	0.53
2:D:17:VAL:CG2	2:D:17:VAL:C	2.76	0.53
1:A:110:ALA:HB2	1:A:117:PHE:CE2	2.44	0.53
1:A:40:LYS:CE	1:A:40:LYS:N	2.71	0.53
1:A:44:PRO:CA	1:A:45:HIS:HD2	2.21	0.53
2:B:70:PHE:CE2	2:B:133:VAL:HG23	2.44	0.53
2:D:34:TYR:N	2:D:34:TYR:CG	2.77	0.53
2:D:67:LEU:CD2	2:D:67:LEU:CA	2.87	0.53
1:A:37:PRO:HA	1:A:40:LYS:CD	2.38	0.53
2:B:125:VAL:O	2:B:125:VAL:CA	2.46	0.53
2:B:34:TYR:HB3	2:B:36:TRP:CZ2	2.44	0.53
1:C:83:LEU:HD11	3:C:142:HEM:CMA	2.36	0.53
1:A:127:LYS:CB	1:A:128:PHE:N	2.71	0.53
2:B:10:VAL:HG12	2:B:129:PHE:CE2	2.43	0.53
1:C:108:THR:O	1:C:108:THR:CA	2.54	0.53
1:A:10:VAL:N	1:A:10:VAL:C	2.59	0.53
1:A:72:HIS:C	1:A:72:HIS:HD1	2.12	0.53
2:B:133:VAL:CG2	2:B:133:VAL:HG11	2.36	0.53
2:B:80:LEU:HD22	2:B:80:LEU:HB3	1.82	0.53
1:A:100:LEU:HA	1:A:100:LEU:CD2	2.38	0.53
1:A:113:LEU:O	1:A:117:PHE:HB2	2.08	0.53
1:A:21:ALA:HB3	1:A:22:PRO:CD	2.38	0.53
2:B:128:LEU:H	2:B:128:LEU:CB	2.16	0.53
2:B:43:HIS:HD1	2:B:43:HIS:HA	1.72	0.53
2:B:86:GLN:HA	2:B:86:GLN:CG	2.38	0.53
1:C:60:GLN:NE2	1:C:64:ASN:ND2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:GLN:HB2	1:C:70:GLN:N	2.19	0.53
1:C:76:LEU:O	1:C:80:LEU:N	2.34	0.53
2:D:76:HIS:ND1	2:D:76:HIS:O	2.41	0.53
2:D:77:LEU:N	2:D:77:LEU:HD12	2.24	0.53
2:D:7:LYS:O	2:D:7:LYS:CB	2.56	0.53
2:D:85:ALA:N	2:D:85:ALA:CB	2.72	0.53
2:B:134:ALA:C	2:B:138:ASN:HD22	2.09	0.53
2:B:30:LEU:HG	2:B:105:LEU:HD23	1.90	0.53
2:B:2:LEU:HB2	2:B:6:GLU:CD	2.28	0.53
2:B:70:PHE:CD1	2:B:71:THR:N	2.77	0.53
2:D:12:GLY:O	2:D:13:PHE:C	2.47	0.53
1:A:73:LEU:HD21	1:A:128:PHE:HD2	1.73	0.53
2:B:55:ASN:CA	2:B:60:LYS:HZ1	2.21	0.53
1:C:107:VAL:HG23	2:D:114:ALA:HB3	1.91	0.53
1:C:43:PHE:HE2	1:C:58:HIS:CE1	2.27	0.53
2:D:90:LEU:HD13	2:D:90:LEU:HB3	1.86	0.53
1:A:140:TYR:CA	1:A:140:TYR:CG	2.79	0.53
1:A:63:ALA:HA	1:A:66:LEU:HB2	1.89	0.53
1:A:74:ASN:CB	1:A:74:ASN:ND2	2.72	0.53
3:B:146:HEM:CMB	3:B:146:HEM:C3B	2.61	0.53
2:B:41:PHE:HB3	2:B:44:PHE:CD1	2.41	0.53
2:B:52:ALA:C	2:B:52:ALA:N	2.60	0.53
2:B:97:VAL:HG11	3:B:146:HEM:C2B	2.44	0.53
1:C:29:LEU:CB	1:C:29:LEU:CD2	2.79	0.53
2:D:20:ASP:CG	2:D:64:LYS:HB2	2.29	0.53
1:A:61:LYS:CB	1:A:61:LYS:C	2.74	0.52
2:B:95:LEU:HD11	3:B:146:HEM:HMA1	1.91	0.52
2:B:34:TYR:CB	2:B:34:TYR:N	2.64	0.52
2:D:92:CYS:CA	2:D:92:CYS:O	2.42	0.52
1:C:91:LEU:C	1:C:91:LEU:N	2.57	0.52
1:A:127:LYS:CG	1:A:127:LYS:CE	2.84	0.52
1:A:41:THR:C	1:A:41:THR:HB	2.27	0.52
2:B:140:LEU:HB2	2:B:140:LEU:CD1	2.37	0.52
2:B:41:PHE:CD2	2:B:44:PHE:HZ	2.05	0.52
2:B:53:VAL:O	2:B:54:MET:HA	2.09	0.52
2:B:80:LEU:O	2:B:81:LYS:N	2.41	0.52
2:D:81:LYS:HD3	2:D:82:GLY:H	1.75	0.52
1:A:34:LEU:CB	1:A:34:LEU:HA	2.24	0.52
2:B:74:LEU:CD1	2:B:77:LEU:HG	2.38	0.52
1:C:65:ALA:O	1:C:68:LYS:HB2	2.10	0.52
2:D:77:LEU:CA	2:D:77:LEU:CG	2.79	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:LYS:CG	2:D:95:LEU:N	2.69	0.52
2:B:124:ASN:O	2:B:125:VAL:CA	2.56	0.52
2:B:64:LYS:HB3	2:B:64:LYS:HZ3	1.64	0.52
2:B:70:PHE:HD1	2:B:71:THR:N	2.07	0.52
1:C:43:PHE:CB	1:C:43:PHE:CD1	2.85	0.52
1:C:45:HIS:CG	1:C:45:HIS:N	2.77	0.52
2:D:140:LEU:HD13	2:D:140:LEU:HB2	1.88	0.52
2:D:37:THR:O	2:D:40:PHE:HD1	1.93	0.52
1:A:14:TRP:HD1	1:A:70:GLN:NE2	2.08	0.52
1:C:3:SER:HB2	1:C:5:ALA:H	1.73	0.52
1:C:89:HIS:ND1	1:C:89:HIS:O	2.42	0.52
2:D:79:ASP:CB	2:D:79:ASP:O	2.58	0.52
1:A:116:ASN:H	1:A:116:ASN:CA	2.05	0.52
1:A:137:THR:HG1	1:A:137:THR:CG2	2.15	0.52
1:A:33:PHE:HB3	1:A:40:LYS:HE3	1.90	0.52
2:B:59:VAL:CG2	2:B:60:LYS:N	2.72	0.52
1:C:111:SER:O	1:C:114:PRO:CG	2.57	0.52
1:A:53:ALA:CA	1:A:53:ALA:O	2.54	0.52
1:A:2:LEU:O	1:A:7:LYS:HE2	2.09	0.52
1:A:80:LEU:CG	1:A:80:LEU:N	2.72	0.52
2:B:31:LEU:CD1	2:B:31:LEU:HD21	2.39	0.52
2:B:62:HIS:HE1	3:B:146:HEM:C1A	2.27	0.52
1:C:137:THR:O	1:C:139:LYS:N	2.42	0.52
1:C:57:ALA:O	1:C:60:GLN:CB	2.58	0.52
1:C:86:LEU:HA	1:C:90:LYS:HB2	1.91	0.52
1:C:110:ALA:HB1	2:D:115:ARG:HB2	1.92	0.52
2:D:59:VAL:HB	2:D:60:LYS:H	1.75	0.52
2:D:67:LEU:CA	2:D:67:LEU:HD23	2.39	0.52
2:D:79:ASP:CB	2:D:79:ASP:N	2.61	0.52
3:A:142:HEM:CMD	3:A:142:HEM:CHD	2.87	0.52
1:A:42:TYR:O	1:A:45:HIS:NE2	2.42	0.52
1:C:129:LEU:C	1:C:130:ALA:CA	2.67	0.52
2:D:11:THR:CA	2:D:14:TRP:H	2.17	0.52
2:D:1:MET:C	2:D:1:MET:H3	2.10	0.52
2:D:6:GLU:CA	2:D:6:GLU:O	2.57	0.52
2:D:99:PRO:O	2:D:102:PHE:N	2.38	0.52
1:A:100:LEU:CB	1:A:100:LEU:HD23	2.36	0.52
1:A:83:LEU:O	1:A:84:SER:HA	2.10	0.52
2:B:122:THR:HG1	2:B:125:VAL:H	1.55	0.52
1:C:28:ALA:N	1:C:29:LEU:N	2.58	0.52
2:D:37:THR:O	2:D:41:PHE:CE1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HB2	1:A:136:LEU:CD1	2.36	0.51
2:B:59:VAL:CG1	2:B:59:VAL:HA	2.39	0.51
1:C:83:LEU:C	1:C:83:LEU:CB	2.70	0.51
2:D:103:ARG:HD3	2:D:103:ARG:HB2	1.92	0.51
1:A:32:MET:N	1:A:33:PHE:N	2.58	0.51
2:B:6:GLU:OE1	2:B:131:LYS:NZ	2.43	0.51
2:B:33:VAL:C	2:B:35:PRO:HD3	2.30	0.51
2:B:56:ASN:O	2:B:58:LYS:N	2.44	0.51
1:C:29:LEU:HB2	1:C:29:LEU:CD2	2.41	0.51
1:C:95:PRO:HA	1:C:98:PHE:HD2	1.74	0.51
1:C:96:VAL:CA	1:C:96:VAL:CG2	2.87	0.51
2:D:44:PHE:C	2:D:44:PHE:CB	2.79	0.51
3:B:146:HEM:CHA	3:B:146:HEM:HAD2	2.37	0.51
2:B:6:GLU:OE1	2:B:131:LYS:HE2	2.10	0.51
1:C:55:GLN:O	1:C:56:LYS:O	2.28	0.51
2:D:101:ASN:N	2:D:102:PHE:H	2.05	0.51
2:D:141:ALA:CA	2:D:142:HIS:N	2.74	0.51
2:B:62:HIS:CB	2:B:62:HIS:N	2.64	0.51
2:D:91:HIS:HD2	2:D:102:PHE:CE1	2.28	0.51
2:D:3:THR:O	2:D:5:GLU:HA	2.10	0.51
2:D:86:GLN:N	2:D:86:GLN:CB	2.67	0.51
1:A:32:MET:CE	1:A:32:MET:CG	2.87	0.51
1:A:72:HIS:HE1	1:A:79:THR:CB	2.23	0.51
1:A:87:HIS:HE1	3:A:142:HEM:C4A	2.27	0.51
2:B:2:LEU:HD13	2:B:131:LYS:NZ	2.25	0.51
2:B:55:ASN:O	2:B:57:PRO:N	2.43	0.51
1:C:57:ALA:O	1:C:60:GLN:HB3	2.10	0.51
2:D:56:ASN:C	2:D:57:PRO:HG2	2.25	0.51
2:B:136:VAL:CG1	2:B:136:VAL:C	2.79	0.51
1:C:138:SER:CA	1:C:138:SER:OG	2.59	0.51
3:C:142:HEM:CAC	3:C:142:HEM:HHD	2.40	0.51
1:C:72:HIS:HE1	1:C:79:THR:OG1	1.92	0.51
1:A:33:PHE:HB3	1:A:40:LYS:CD	2.41	0.51
1:A:97:ASN:HD22	1:A:100:LEU:HD11	1.76	0.51
2:B:123:PRO:CB	2:B:126:GLN:HE22	2.22	0.51
2:B:7:LYS:HD2	2:B:77:LEU:HD12	1.91	0.51
1:C:111:SER:CA	1:C:112:HIS:N	2.74	0.51
1:A:131:ASN:HB2	1:A:131:ASN:N	2.26	0.51
1:A:43:PHE:C	1:A:43:PHE:CB	2.74	0.51
2:B:117:PHE:O	2:B:118:GLY:CA	2.46	0.51
2:B:97:VAL:HG11	3:B:146:HEM:HMB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:LEU:HA	2:B:108:VAL:HG21	1.93	0.51
1:C:84:SER:OG	1:C:136:LEU:CD1	2.58	0.51
2:D:75:LYS:C	2:D:75:LYS:HB3	2.21	0.51
2:D:76:HIS:CD2	2:D:76:HIS:H	2.28	0.51
2:D:7:LYS:O	2:D:8:ALA:C	2.40	0.51
2:D:91:HIS:O	2:D:95:LEU:HG	2.10	0.51
3:A:142:HEM:CMA	3:A:142:HEM:HHB	2.41	0.51
1:A:14:TRP:HB3	1:A:70:GLN:NE2	2.26	0.51
2:B:14:TRP:HZ2	2:B:67:LEU:HG	1.76	0.51
2:B:84:PHE:CE2	3:B:146:HEM:CBC	2.94	0.51
1:C:55:GLN:O	1:C:56:LYS:NZ	2.44	0.51
2:D:145:HIS:O	2:D:145:HIS:OXT	2.28	0.51
2:D:93:ASN:HB3	2:D:93:ASN:O	2.09	0.51
1:A:100:LEU:HD12	1:A:100:LEU:HB2	1.88	0.51
1:C:10:VAL:HG11	1:C:10:VAL:CG2	2.36	0.51
1:C:121:VAL:C	1:C:122:HIS:C	2.68	0.51
1:C:89:HIS:HB2	1:C:139:LYS:CG	2.41	0.51
1:A:89:HIS:ND1	1:A:90:LYS:N	2.58	0.50
1:A:93:VAL:C	1:A:94:ASN:CA	2.66	0.50
2:B:11:THR:CB	2:B:11:THR:HG1	2.12	0.50
1:C:45:HIS:CG	1:C:46:PHE:CE1	2.99	0.50
1:C:90:LYS:C	1:C:90:LYS:N	2.58	0.50
2:D:44:PHE:H	2:D:44:PHE:CB	2.24	0.50
1:A:131:ASN:N	1:A:131:ASN:C	2.63	0.50
1:A:1:VAL:HG22	1:A:1:VAL:HG13	1.90	0.50
1:A:4:ALA:O	1:A:8:SER:HB2	2.10	0.50
2:B:36:TRP:CG	1:C:94:ASN:HA	2.46	0.50
2:B:41:PHE:HA	2:B:42:GLN:N	2.26	0.50
2:B:6:GLU:CG	2:B:6:GLU:CA	2.72	0.50
2:D:120:GLN:HA	2:D:120:GLN:CG	2.40	0.50
2:B:98:ASN:OD1	2:B:98:ASN:HB2	2.09	0.50
3:C:142:HEM:CAC	3:C:142:HEM:CHD	2.89	0.50
1:C:68:LYS:HD3	1:C:79:THR:CG2	2.38	0.50
1:A:44:PRO:N	1:A:45:HIS:HD2	2.08	0.50
1:A:72:HIS:CE1	1:A:79:THR:CB	2.94	0.50
2:B:80:LEU:C	2:B:81:LYS:C	2.69	0.50
1:C:140:TYR:C	1:C:141:ARG:HD3	2.31	0.50
2:B:36:TRP:HA	1:C:92:ARG:HB3	1.92	0.50
2:D:130:GLN:CA	2:D:130:GLN:NE2	2.75	0.50
1:A:105:LEU:C	1:A:105:LEU:N	2.51	0.50
1:A:56:LYS:CD	1:A:56:LYS:NZ	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:CB	1:A:85:ASN:ND2	2.74	0.50
1:C:114:PRO:CD	1:C:114:PRO:CA	2.87	0.50
1:C:56:LYS:HA	1:C:56:LYS:CD	2.41	0.50
1:C:61:LYS:HD2	1:C:61:LYS:HA	1.90	0.50
2:D:110:ALA:N	2:D:110:ALA:C	2.65	0.50
2:D:145:HIS:C	2:D:145:HIS:HB2	2.30	0.50
1:A:53:ALA:N	1:A:56:LYS:HG2	2.26	0.50
1:A:99:LYS:CD	1:A:99:LYS:CB	2.90	0.50
2:B:101:ASN:C	3:B:146:HEM:CBB	2.79	0.50
1:C:99:LYS:C	1:C:100:LEU:CA	2.71	0.50
1:C:110:ALA:O	1:C:110:ALA:CA	2.58	0.50
1:C:14:TRP:CG	1:C:70:GLN:NE2	2.79	0.50
1:C:74:ASN:H	1:C:75:ASP:N	2.10	0.50
1:C:89:HIS:CA	1:C:139:LYS:HG3	2.42	0.50
2:D:141:ALA:O	2:D:143:LYS:CA	2.60	0.50
1:A:41:THR:CA	1:A:41:THR:HG22	2.35	0.50
2:B:80:LEU:CA	2:B:81:LYS:O	2.59	0.50
1:A:67:THR:HG22	1:A:70:GLN:NE2	2.27	0.50
1:C:39:THR:H	1:C:39:THR:CB	2.22	0.50
1:C:94:ASN:ND2	1:C:97:ASN:OD1	2.45	0.50
2:D:81:LYS:CE	2:D:81:LYS:CG	2.90	0.50
1:A:121:VAL:HG23	1:A:121:VAL:O	2.12	0.50
1:A:42:TYR:CA	1:A:43:PHE:N	2.65	0.50
1:A:49:SER:HB3	1:A:52:SER:HB3	1.83	0.50
2:B:1:MET:O	2:B:2:LEU:CD2	2.58	0.50
2:B:31:LEU:O	2:B:32:VAL:CA	2.59	0.50
1:C:107:VAL:HG23	2:D:114:ALA:CB	2.42	0.50
2:D:106:GLY:HA3	2:D:133:VAL:CG1	2.42	0.50
2:D:56:ASN:ND2	2:D:56:ASN:C	2.64	0.50
1:A:4:ALA:CB	1:A:4:ALA:N	2.71	0.49
3:B:146:HEM:CAD	3:B:146:HEM:CHA	2.90	0.49
2:B:3:THR:HB	2:B:6:GLU:CB	2.39	0.49
2:B:46:ASN:O	2:B:46:ASN:CB	2.60	0.49
1:C:32:MET:CB	1:C:32:MET:C	2.77	0.49
1:C:60:GLN:O	1:C:64:ASN:N	2.45	0.49
2:D:75:LYS:HG2	2:D:75:LYS:HB2	1.32	0.49
2:D:95:LEU:CD1	2:D:97:VAL:CG2	2.87	0.49
1:A:126:ASN:HB3	1:A:127:LYS:N	2.26	0.49
1:A:88:ALA:CB	1:A:89:HIS:HB2	2.42	0.49
1:C:18:GLY:N	1:C:18:GLY:C	2.57	0.49
1:A:100:LEU:HD22	1:A:100:LEU:HB3	1.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:HG23	2:B:111:LEU:HD22	1.93	0.49
2:B:55:ASN:O	2:B:57:PRO:CD	2.61	0.49
2:B:94:LYS:HG3	2:B:94:LYS:CE	2.39	0.49
1:C:123:ALA:HB3	1:C:124:ASN:HD22	1.77	0.49
2:D:42:GLN:HG2	2:D:42:GLN:CA	2.01	0.49
2:D:70:PHE:HB3	2:D:71:THR:CB	2.40	0.49
1:A:57:ALA:CA	1:A:60:GLN:CG	2.90	0.49
2:B:23:GLY:N	2:B:24:ALA:N	2.60	0.49
2:B:65:ARG:O	2:B:67:LEU:N	2.44	0.49
2:B:66:VAL:CA	2:B:66:VAL:CG1	2.76	0.49
2:D:25:GLN:HE22	2:D:115:ARG:NH2	2.00	0.49
2:D:54:MET:CE	2:D:54:MET:CG	2.90	0.49
2:D:70:PHE:CB	2:D:71:THR:HB	2.42	0.49
2:D:83:ALA:CA	2:D:84:PHE:N	2.70	0.49
1:A:44:PRO:CD	1:A:45:HIS:CD2	2.96	0.49
1:A:67:THR:C	1:A:67:THR:CB	2.76	0.49
1:C:104:SER:O	1:C:107:VAL:HG13	2.13	0.49
1:C:126:ASN:CB	1:C:126:ASN:C	2.73	0.49
2:D:71:THR:CG2	2:D:71:THR:OG1	2.61	0.49
1:A:27:GLN:HE22	1:A:31:ARG:HH11	1.60	0.49
2:B:81:LYS:CD	2:B:142:HIS:HB3	2.42	0.49
1:C:30:GLN:HB2	1:C:30:GLN:NE2	2.27	0.49
2:D:139:ALA:O	2:D:142:HIS:N	2.45	0.49
2:D:50:ALA:O	2:D:53:VAL:CG1	2.59	0.49
1:A:2:LEU:CG	1:A:2:LEU:HA	2.43	0.49
1:A:53:ALA:O	1:A:53:ALA:HA	2.12	0.49
1:A:56:LYS:CE	1:A:56:LYS:N	2.72	0.49
1:C:21:ALA:O	1:C:22:PRO:HA	2.09	0.49
1:C:29:LEU:CD1	1:C:59:GLY:HA2	2.42	0.49
1:C:85:ASN:HA	1:C:88:ALA:HB3	1.95	0.49
2:D:29:ARG:HG3	2:D:112:VAL:HG11	1.94	0.49
2:D:69:ALA:CB	2:D:70:PHE:N	2.70	0.49
1:A:103:HIS:ND1	1:A:103:HIS:CB	2.59	0.49
1:A:43:PHE:HB3	1:A:46:PHE:CD1	2.47	0.49
1:A:43:PHE:HD2	1:A:46:PHE:CE1	2.30	0.49
2:B:62:HIS:O	2:B:66:VAL:HG12	2.13	0.49
1:C:89:HIS:C	1:C:90:LYS:CA	2.78	0.49
2:D:58:LYS:O	2:D:61:ALA:HB3	2.12	0.49
1:A:85:ASN:CG	1:A:90:LYS:HE3	2.32	0.49
1:A:94:ASN:N	1:A:94:ASN:O	2.45	0.49
2:B:124:ASN:O	2:B:127:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:MET:C	2:B:55:ASN:OD1	2.51	0.49
1:C:113:LEU:O	1:C:117:PHE:N	2.46	0.49
1:C:45:HIS:ND1	3:C:142:HEM:CGD	2.75	0.49
1:C:16:LYS:CD	1:C:16:LYS:CB	2.89	0.49
1:C:64:ASN:CA	1:C:64:ASN:CG	2.70	0.49
2:D:130:GLN:HA	2:D:130:GLN:CD	2.31	0.49
2:D:130:GLN:NE2	2:D:130:GLN:HA	2.28	0.49
2:D:78:ASP:OD2	2:D:78:ASP:CB	2.54	0.49
2:B:115:ARG:CA	2:B:115:ARG:CG	2.90	0.49
2:B:74:LEU:O	2:B:75:LYS:HG2	2.13	0.49
1:C:45:HIS:CE1	1:C:46:PHE:CZ	3.00	0.49
1:C:65:ALA:HB1	1:C:83:LEU:CD2	2.43	0.49
2:D:10:VAL:HG11	2:D:128:LEU:HD11	1.95	0.49
2:D:14:TRP:CZ2	2:D:71:THR:CG2	2.96	0.49
1:A:16:LYS:HB2	1:A:113:LEU:HD21	1.95	0.48
1:A:47:ASP:C	1:A:49:SER:N	2.56	0.48
1:A:70:GLN:OE1	1:A:70:GLN:NE2	2.46	0.48
2:B:144:TYR:HB3	2:B:145:HIS:NE2	2.23	0.48
2:B:23:GLY:O	2:B:24:ALA:CA	2.58	0.48
2:B:44:PHE:HD2	2:B:58:LYS:HG2	1.77	0.48
1:C:140:TYR:CE1	1:C:141:ARG:NH2	2.81	0.48
1:A:32:MET:N	1:A:33:PHE:H	2.10	0.48
2:B:19:VAL:CG1	2:B:20:ASP:N	2.75	0.48
2:B:66:VAL:HG11	2:B:66:VAL:CG2	2.39	0.48
1:C:76:LEU:HB3	1:C:80:LEU:CD2	2.43	0.48
2:D:95:LEU:HD13	3:D:146:HEM:HMA2	1.94	0.48
1:A:17:VAL:HG11	1:A:17:VAL:CG2	2.40	0.48
2:B:77:LEU:C	2:B:77:LEU:CD1	2.78	0.48
2:B:95:LEU:C	2:B:95:LEU:CB	2.75	0.48
1:C:17:VAL:CG1	1:C:24:TYR:CD2	2.95	0.48
2:D:121:PHE:O	2:D:122:THR:O	2.32	0.48
2:D:43:HIS:CE1	3:D:146:HEM:CGA	2.96	0.48
1:A:37:PRO:C	1:A:40:LYS:HD2	2.34	0.48
2:B:27:LEU:CD2	2:B:66:VAL:CG1	2.92	0.48
2:B:43:HIS:N	2:B:44:PHE:N	2.61	0.48
2:B:44:PHE:CD2	2:B:58:LYS:HG2	2.49	0.48
1:C:17:VAL:HG13	1:C:24:TYR:CE2	2.48	0.48
1:A:106:LEU:HB3	2:B:111:LEU:HD11	1.94	0.48
1:A:91:LEU:CD2	3:A:142:HEM:C2D	2.95	0.48
1:A:16:LYS:N	1:A:17:VAL:N	2.53	0.48
2:B:26:ALA:HB2	2:B:112:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:GLN:CB	2:B:130:GLN:CD	2.79	0.48
2:B:97:VAL:HG11	3:B:146:HEM:HAB	1.95	0.48
1:C:109:LEU:O	1:C:112:HIS:N	2.44	0.48
2:D:59:VAL:CA	2:D:59:VAL:HG23	2.29	0.48
1:A:84:SER:OG	1:A:136:LEU:HA	2.13	0.48
2:B:92:CYS:CB	2:B:144:TYR:CZ	2.96	0.48
2:B:92:CYS:N	2:B:144:TYR:OH	2.45	0.48
1:C:12:ALA:O	1:C:16:LYS:HB2	2.14	0.48
1:C:11:LYS:HD3	1:C:70:GLN:OE1	2.14	0.48
1:C:7:LYS:HE2	1:C:7:LYS:HB2	1.95	0.48
1:C:99:LYS:HG2	1:C:99:LYS:HE3	1.95	0.48
2:D:104:LEU:CG	2:D:104:LEU:HA	2.43	0.48
2:D:62:HIS:ND1	2:D:62:HIS:CB	2.67	0.48
2:D:75:LYS:O	2:D:77:LEU:CD1	2.60	0.48
2:D:95:LEU:CD1	2:D:95:LEU:CB	2.91	0.48
2:B:107:ASN:ND2	2:B:107:ASN:HB2	2.23	0.48
2:B:86:GLN:CB	2:B:86:GLN:CD	2.75	0.48
1:C:130:ALA:O	1:C:131:ASN:N	2.36	0.48
1:C:22:PRO:O	1:C:56:LYS:HE3	2.11	0.48
2:D:11:THR:CG2	2:D:11:THR:OG1	2.56	0.48
2:D:119:GLY:N	2:D:120:GLN:N	2.62	0.48
2:D:94:LYS:CD	2:D:95:LEU:CD2	2.87	0.48
1:A:114:PRO:HB3	2:B:115:ARG:HG2	1.96	0.48
1:A:43:PHE:O	1:A:48:LEU:HD21	2.14	0.48
1:A:72:HIS:CE1	1:A:79:THR:CG2	2.96	0.48
1:A:97:ASN:C	1:A:97:ASN:N	2.61	0.48
2:B:74:LEU:HD12	2:B:75:LYS:O	2.14	0.48
2:B:92:CYS:O	2:B:96:HIS:ND1	2.33	0.48
1:C:45:HIS:CD2	1:C:45:HIS:N	2.82	0.48
1:C:46:PHE:CE2	1:C:54:GLN:HB3	2.49	0.48
1:C:58:HIS:C	1:C:59:GLY:C	2.72	0.48
2:D:14:TRP:CE3	2:D:14:TRP:CA	2.93	0.48
2:D:55:ASN:O	2:D:55:ASN:ND2	2.45	0.48
1:A:57:ALA:H	1:A:57:ALA:HB3	1.74	0.48
1:A:84:SER:HA	1:A:84:SER:N	2.12	0.48
1:C:117:PHE:N	1:C:117:PHE:C	2.62	0.48
1:C:36:PHE:N	1:C:36:PHE:CB	2.69	0.48
2:D:74:LEU:HD12	2:D:132:VAL:HG21	1.95	0.48
1:A:19:GLY:CA	1:A:20:ASN:N	2.68	0.48
2:D:102:PHE:N	2:D:103:ARG:N	2.61	0.48
2:D:43:HIS:CA	2:D:43:HIS:HB2	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:GLU:CD	2:D:5:GLU:CB	2.75	0.48
2:D:99:PRO:O	2:D:100:GLN:C	2.52	0.48
1:A:40:LYS:CB	1:A:40:LYS:CD	2.88	0.47
1:C:45:HIS:CE1	3:C:142:HEM:O2D	2.67	0.47
1:C:47:ASP:O	1:C:52:SER:OG	2.31	0.47
2:D:101:ASN:N	2:D:102:PHE:N	2.62	0.47
2:D:104:LEU:CD2	2:D:104:LEU:HA	2.43	0.47
2:D:106:GLY:HA3	2:D:133:VAL:HG12	1.96	0.47
2:D:36:TRP:N	2:D:37:THR:N	2.62	0.47
2:D:72:GLN:C	2:D:72:GLN:HE21	2.11	0.47
2:D:81:LYS:HZ2	2:D:81:LYS:CD	2.27	0.47
1:A:43:PHE:CE2	3:A:142:HEM:HMD1	2.48	0.47
1:A:69:ALA:N	1:A:70:GLN:N	2.62	0.47
2:B:66:VAL:HG21	2:B:66:VAL:CG1	2.39	0.47
1:C:104:SER:C	1:C:104:SER:HB3	2.34	0.47
1:C:135:VAL:O	1:C:136:LEU:N	2.44	0.47
2:D:84:PHE:O	2:D:88:SER:N	2.44	0.47
1:A:21:ALA:HB1	1:A:63:ALA:HB1	1.95	0.47
1:A:70:GLN:C	1:A:73:LEU:CD1	2.81	0.47
2:B:1:MET:N	2:B:2:LEU:HD21	2.23	0.47
2:B:33:VAL:H	2:B:35:PRO:HD3	1.79	0.47
1:C:23:ALA:HB1	1:C:23:ALA:C	2.29	0.47
1:C:85:ASN:OD1	1:C:89:HIS:CB	2.62	0.47
1:A:79:THR:HA	1:A:79:THR:HG23	1.93	0.47
2:B:130:GLN:HG2	2:B:130:GLN:HE21	1.75	0.47
2:B:93:ASN:O	2:B:96:HIS:HE1	1.93	0.47
1:C:137:THR:O	1:C:137:THR:CA	2.59	0.47
2:D:27:LEU:HD12	2:D:63:GLY:CA	2.45	0.47
2:D:61:ALA:O	2:D:64:LYS:HB3	2.14	0.47
2:B:91:HIS:HA	2:B:95:LEU:CD2	2.41	0.47
1:C:25:GLY:N	1:C:25:GLY:C	2.53	0.47
2:D:31:LEU:N	2:D:31:LEU:CB	2.66	0.47
2:B:118:GLY:H	2:B:118:GLY:HA2	1.26	0.47
2:B:46:ASN:ND2	2:B:46:ASN:HA	2.30	0.47
2:B:54:MET:O	2:B:59:VAL:HG23	2.15	0.47
1:C:113:LEU:O	1:C:116:ASN:HB3	2.15	0.47
2:D:6:GLU:N	2:D:6:GLU:CB	2.66	0.47
2:B:31:LEU:HB3	2:B:53:VAL:CG2	2.44	0.47
2:B:49:SER:C	2:B:49:SER:N	2.58	0.47
1:C:110:ALA:O	1:C:114:PRO:CB	2.59	0.47
1:C:141:ARG:N	1:C:141:ARG:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LEU:O	1:C:81:SER:CA	2.62	0.47
2:D:30:LEU:CG	2:D:37:THR:HG21	2.44	0.47
2:D:70:PHE:N	2:D:71:THR:HB	2.28	0.47
2:D:84:PHE:C	2:D:85:ALA:CA	2.81	0.47
1:A:32:MET:CE	1:A:32:MET:HG2	2.44	0.47
1:A:46:PHE:HA	1:A:54:GLN:OE1	2.14	0.47
2:B:52:ALA:C	2:B:54:MET:N	2.61	0.47
2:B:87:LEU:O	2:B:88:SER:C	2.53	0.47
2:B:95:LEU:CG	2:B:95:LEU:HA	2.24	0.47
1:C:32:MET:HE2	1:C:101:LEU:HG	1.96	0.47
1:A:141:ARG:OXT	1:C:1:VAL:O	2.32	0.47
1:C:46:PHE:CE2	1:C:54:GLN:CG	2.98	0.47
2:D:105:LEU:HD11	2:D:105:LEU:CD2	2.29	0.47
2:D:47:LEU:N	2:D:47:LEU:CB	2.68	0.47
2:D:7:LYS:NZ	2:D:78:ASP:OD2	2.44	0.47
1:A:42:TYR:HB2	1:A:43:PHE:CD1	2.50	0.47
2:B:77:LEU:N	2:B:78:ASP:CB	2.78	0.47
2:B:7:LYS:CB	2:B:7:LYS:C	2.81	0.47
2:D:19:VAL:CG2	2:D:19:VAL:HG13	2.44	0.47
1:A:60:GLN:N	1:A:61:LYS:N	2.62	0.47
2:B:32:VAL:HG11	2:B:50:ALA:CB	2.45	0.47
2:B:59:VAL:O	2:B:62:HIS:CB	2.60	0.47
2:B:7:LYS:NZ	2:B:7:LYS:CD	2.78	0.47
2:B:87:LEU:O	2:B:89:GLY:N	2.48	0.47
1:C:86:LEU:HD22	1:C:86:LEU:CD1	2.39	0.47
2:D:84:PHE:HD2	2:D:87:LEU:CD2	2.28	0.47
1:A:86:LEU:CD1	1:A:91:LEU:HD22	2.45	0.47
2:B:106:GLY:HA3	2:B:133:VAL:CG2	2.28	0.47
2:B:133:VAL:O	2:B:134:ALA:CA	2.60	0.47
2:B:14:TRP:CZ2	2:B:67:LEU:HG	2.49	0.47
2:B:77:LEU:C	2:B:77:LEU:HB3	2.27	0.47
1:C:11:LYS:HD2	1:C:70:GLN:NE2	2.30	0.47
1:C:1:VAL:C	1:C:1:VAL:N	2.68	0.47
1:C:29:LEU:HD13	1:C:29:LEU:HD22	1.91	0.47
2:D:101:ASN:O	2:D:104:LEU:CB	2.63	0.47
2:D:90:LEU:HD13	2:D:91:HIS:ND1	2.30	0.47
1:A:26:ALA:CB	1:A:56:LYS:NZ	2.66	0.46
2:B:123:PRO:HA	2:B:126:GLN:CD	2.35	0.46
2:B:92:CYS:N	2:B:144:TYR:CZ	2.83	0.46
2:B:21:VAL:HG12	2:B:25:GLN:HE21	1.79	0.46
2:B:78:ASP:O	2:B:80:LEU:O	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:GLN:C	2:B:86:GLN:CG	2.83	0.46
1:C:26:ALA:N	1:C:56:LYS:CE	2.67	0.46
1:A:85:ASN:O	1:A:87:HIS:N	2.48	0.46
2:B:16:LYS:CD	2:B:117:PHE:CE1	2.85	0.46
2:B:70:PHE:CZ	2:B:109:LEU:HD11	2.49	0.46
1:C:10:VAL:HG11	1:C:128:PHE:CG	2.50	0.46
2:D:105:LEU:HB3	2:D:105:LEU:CD1	2.25	0.46
2:D:81:LYS:O	2:D:85:ALA:HB2	2.15	0.46
1:A:64:ASN:CB	1:A:64:ASN:C	2.77	0.46
1:A:114:PRO:CG	2:B:115:ARG:HG3	2.46	0.46
2:D:55:ASN:CG	2:D:55:ASN:CA	2.77	0.46
2:D:69:ALA:O	2:D:69:ALA:CA	2.49	0.46
2:D:94:LYS:CG	2:D:95:LEU:CD2	2.82	0.46
1:A:31:ARG:CA	1:A:32:MET:N	2.54	0.46
1:A:41:THR:H	1:A:41:THR:CB	2.23	0.46
2:B:125:VAL:C	2:B:126:GLN:C	2.74	0.46
2:B:13:PHE:N	2:B:13:PHE:C	2.65	0.46
2:B:94:LYS:H	2:B:95:LEU:H	1.59	0.46
1:C:75:ASP:CA	1:C:76:LEU:N	2.74	0.46
1:A:1:VAL:C	1:A:1:VAL:N	2.63	0.46
1:A:25:GLY:C	1:A:29:LEU:HD22	2.36	0.46
1:A:33:PHE:CB	1:A:40:LYS:HE3	2.45	0.46
3:B:146:HEM:C3D	3:B:146:HEM:HBD2	2.48	0.46
2:B:16:LYS:O	2:B:117:PHE:CZ	2.68	0.46
2:D:55:ASN:CB	2:D:55:ASN:C	2.81	0.46
1:A:126:ASN:CB	1:A:127:LYS:N	2.66	0.46
1:A:77:PRO:CA	1:A:77:PRO:O	2.60	0.46
1:A:94:ASN:HD21	1:A:96:VAL:HG22	1.81	0.46
2:B:74:LEU:HD22	2:B:77:LEU:HG	1.94	0.46
1:C:83:LEU:N	1:C:83:LEU:CB	2.67	0.46
2:D:28:GLY:O	2:D:54:MET:CE	2.60	0.46
1:A:135:VAL:HB	1:A:135:VAL:C	2.35	0.46
2:B:102:PHE:CD1	2:B:140:LEU:CD1	2.99	0.46
2:B:141:ALA:O	2:B:144:TYR:HB2	2.16	0.46
2:B:19:VAL:CG1	2:B:19:VAL:CA	2.84	0.46
2:B:98:ASN:HA	2:B:99:PRO:HD2	1.44	0.46
1:C:10:VAL:HG11	1:C:128:PHE:CD1	2.50	0.46
2:D:110:ALA:HB3	2:D:110:ALA:C	2.34	0.46
1:A:14:TRP:CE3	1:A:14:TRP:HA	2.51	0.46
1:A:27:GLN:O	1:A:31:ARG:HB2	2.16	0.46
2:B:136:VAL:HG12	2:B:136:VAL:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:SER:C	2:B:49:SER:CB	2.78	0.46
2:B:67:LEU:O	2:B:69:ALA:HB3	2.14	0.46
2:B:3:THR:CA	2:B:6:GLU:HB2	2.45	0.46
1:C:130:ALA:O	1:C:130:ALA:HA	2.14	0.46
2:D:25:GLN:HE22	2:D:116:ASN:CG	2.18	0.46
2:D:69:ALA:HB1	2:D:69:ALA:C	2.34	0.46
1:A:104:SER:CB	1:A:104:SER:HA	2.21	0.46
1:A:3:SER:HB2	1:A:6:ASN:HD22	1.75	0.46
1:C:15:GLY:N	1:C:15:GLY:C	2.58	0.46
1:C:54:GLN:CA	1:C:54:GLN:HG3	2.43	0.46
1:C:73:LEU:C	1:C:74:ASN:CA	2.71	0.46
2:B:39:ARG:NE	1:C:92:ARG:O	2.49	0.46
2:D:138:ASN:O	2:D:139:ALA:C	2.54	0.46
2:D:19:VAL:HG12	2:D:64:LYS:HA	1.97	0.46
1:A:11:LYS:O	1:A:12:ALA:CA	2.63	0.45
1:A:26:ALA:HB1	1:A:56:LYS:HZ2	1.76	0.45
2:B:19:VAL:C	2:B:19:VAL:CG1	2.83	0.45
2:B:27:LEU:HD23	2:B:66:VAL:HG11	1.94	0.45
2:B:46:ASN:CG	2:B:46:ASN:HA	2.32	0.45
1:C:106:LEU:HD23	2:D:111:LEU:HD21	1.97	0.45
1:A:36:PHE:CZ	2:B:130:GLN:CG	2.99	0.45
2:B:66:VAL:O	2:B:66:VAL:CG2	2.64	0.45
2:B:74:LEU:C	2:B:75:LYS:C	2.68	0.45
1:C:85:ASN:OD1	1:C:85:ASN:O	2.34	0.45
2:D:126:GLN:O	2:D:127:ALA:O	2.34	0.45
2:D:132:VAL:N	2:D:133:VAL:N	2.64	0.45
3:D:146:HEM:HHB	3:D:146:HEM:HMA2	1.79	0.45
2:D:94:LYS:HD3	2:D:95:LEU:N	2.26	0.45
1:A:12:ALA:CB	1:A:12:ALA:C	2.84	0.45
1:A:5:ALA:O	1:A:8:SER:C	2.54	0.45
1:C:58:HIS:O	1:C:59:GLY:C	2.55	0.45
1:C:93:VAL:HG11	3:C:142:HEM:C2C	2.51	0.45
2:D:17:VAL:HG23	2:D:17:VAL:C	2.35	0.45
1:A:3:SER:O	1:A:4:ALA:N	2.38	0.45
1:A:49:SER:CB	1:A:52:SER:CB	2.61	0.45
1:A:79:THR:CB	1:A:80:LEU:CD2	2.63	0.45
2:B:24:ALA:N	2:B:25:GLN:N	2.64	0.45
1:C:84:SER:CA	1:C:136:LEU:HD13	2.46	0.45
1:A:98:PHE:CZ	1:A:136:LEU:HB2	2.52	0.45
2:B:46:ASN:ND2	2:B:46:ASN:CA	2.77	0.45
2:B:61:ALA:C	2:B:62:HIS:CA	2.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LYS:O	1:C:56:LYS:NZ	2.48	0.45
2:D:56:ASN:C	2:D:57:PRO:CD	2.74	0.45
2:D:75:LYS:HG3	2:D:75:LYS:HB3	1.34	0.45
1:A:127:LYS:HB3	1:A:128:PHE:N	2.32	0.45
2:B:16:LYS:CE	2:B:16:LYS:HG3	2.47	0.45
1:C:26:ALA:HA	1:C:56:LYS:NZ	2.31	0.45
2:D:112:VAL:CG1	2:D:112:VAL:CG2	2.75	0.45
2:D:22:VAL:CG1	2:D:22:VAL:CA	2.71	0.45
1:A:95:PRO:HB3	1:A:137:THR:CG2	2.46	0.45
2:B:106:GLY:C	2:B:133:VAL:HG21	2.36	0.45
2:B:29:ARG:HB3	2:B:108:VAL:CG1	2.46	0.45
2:B:115:ARG:C	2:B:115:ARG:CB	2.81	0.45
2:B:3:THR:C	2:B:5:GLU:N	2.65	0.45
1:C:17:VAL:CG1	1:C:24:TYR:HD2	2.30	0.45
2:D:14:TRP:O	2:D:14:TRP:N	2.43	0.45
2:D:2:LEU:CD2	2:D:4:ALA:CA	2.78	0.45
1:A:106:LEU:CD2	1:A:126:ASN:HD22	2.30	0.45
2:B:104:LEU:O	2:B:108:VAL:N	2.50	0.45
2:B:62:HIS:CG	2:B:62:HIS:C	2.90	0.45
2:B:74:LEU:O	2:B:76:HIS:HB2	2.17	0.45
2:D:122:THR:N	2:D:125:VAL:HG12	2.29	0.45
2:D:122:THR:OG1	2:D:125:VAL:N	2.47	0.45
1:A:109:LEU:C	1:A:109:LEU:HB3	2.37	0.45
1:A:16:LYS:HD2	1:A:116:ASN:HB3	1.99	0.45
2:B:11:THR:O	2:B:12:GLY:CA	2.64	0.45
2:B:47:LEU:HB3	2:B:53:VAL:HG23	1.99	0.45
1:C:74:ASN:N	1:C:75:ASP:N	2.65	0.45
1:C:83:LEU:C	1:C:83:LEU:HG	2.37	0.45
2:D:94:LYS:HD3	2:D:95:LEU:CA	2.47	0.45
1:A:116:ASN:N	1:A:117:PHE:N	2.64	0.45
1:A:33:PHE:CG	1:A:48:LEU:HD13	2.52	0.45
2:B:109:LEU:HD22	2:B:109:LEU:CA	2.46	0.45
2:B:94:LYS:NZ	2:B:94:LYS:HE2	2.14	0.45
2:D:110:ALA:CB	2:D:126:GLN:OE1	2.65	0.45
2:D:140:LEU:HD11	2:D:140:LEU:CD2	2.38	0.45
2:D:4:ALA:CA	2:D:5:GLU:HA	2.45	0.45
2:D:74:LEU:HD13	2:D:132:VAL:HG21	1.97	0.45
1:C:38:THR:OG1	1:C:38:THR:CG2	2.63	0.44
1:C:61:LYS:CA	1:C:61:LYS:CD	2.92	0.44
2:D:6:GLU:HA	2:D:6:GLU:CB	2.22	0.44
2:D:94:LYS:HD3	2:D:95:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:THR:O	2:B:126:GLN:HB3	2.18	0.44
2:B:43:HIS:ND1	2:B:43:HIS:CA	2.76	0.44
2:B:84:PHE:CD2	2:B:84:PHE:CA	3.00	0.44
1:C:27:GLN:OE1	1:C:112:HIS:HE1	2.00	0.44
2:D:131:LYS:HG3	2:D:131:LYS:HA	1.96	0.44
2:D:14:TRP:CD1	2:D:74:LEU:CD2	2.98	0.44
1:A:85:ASN:CA	1:A:139:LYS:HE3	2.47	0.44
2:B:104:LEU:N	2:B:104:LEU:CB	2.76	0.44
1:C:20:ASN:O	1:C:22:PRO:N	2.51	0.44
2:D:33:VAL:CG2	2:D:33:VAL:O	2.62	0.44
2:B:33:VAL:HG12	2:B:34:TYR:CD1	2.51	0.44
2:B:54:MET:HB3	2:B:55:ASN:CG	2.35	0.44
1:C:52:SER:CB	1:C:55:GLN:NE2	2.61	0.44
1:A:132:ASP:O	1:A:136:LEU:CD2	2.65	0.44
2:B:50:ALA:O	2:B:51:GLY:C	2.56	0.44
1:C:39:THR:H	1:C:39:THR:HB	1.80	0.44
1:C:45:HIS:CG	1:C:45:HIS:CA	2.83	0.44
1:C:73:LEU:O	1:C:74:ASN:CA	2.65	0.44
1:C:87:HIS:HB2	1:C:87:HIS:ND1	2.27	0.44
1:C:89:HIS:ND1	1:C:90:LYS:HG2	2.27	0.44
3:D:146:HEM:HAA2	3:D:146:HEM:CHA	2.46	0.44
1:A:128:PHE:O	1:A:131:ASN:N	2.50	0.44
3:A:142:HEM:HHD	3:A:142:HEM:CMD	2.43	0.44
1:A:122:HIS:NE2	2:B:29:ARG:HG2	2.33	0.44
2:B:71:THR:HG23	2:B:71:THR:O	2.17	0.44
1:C:31:ARG:CA	1:C:31:ARG:O	2.55	0.44
1:C:32:MET:HG3	1:C:39:THR:HG21	1.98	0.44
1:C:46:PHE:HB3	1:C:47:ASP:O	2.18	0.44
2:D:137:ALA:HA	2:D:140:LEU:HD12	1.99	0.44
1:A:26:ALA:HB1	1:A:56:LYS:HZ1	1.74	0.44
1:A:32:MET:C	1:A:32:MET:N	2.64	0.44
1:A:79:THR:CG2	1:A:80:LEU:HD23	2.39	0.44
2:D:137:ALA:CB	2:D:140:LEU:HD12	2.48	0.44
2:B:62:HIS:CE1	3:B:146:HEM:C1A	3.06	0.44
2:B:97:VAL:CG2	2:B:97:VAL:CG1	2.90	0.44
1:C:102:SER:O	1:C:103:HIS:CA	2.65	0.44
1:C:15:GLY:N	1:C:16:LYS:H	2.16	0.44
1:C:84:SER:N	1:C:84:SER:C	2.66	0.44
2:D:141:ALA:O	2:D:143:LYS:C	2.56	0.44
2:D:32:VAL:CG1	2:D:50:ALA:HA	2.44	0.44
2:B:11:THR:CG2	2:B:11:THR:OG1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ASP:HB3	2:B:64:LYS:HE2	1.94	0.44
2:B:70:PHE:HA	2:B:84:PHE:CZ	2.52	0.44
2:B:98:ASN:C	2:B:100:GLN:N	2.63	0.44
1:C:130:ALA:N	1:C:130:ALA:C	2.59	0.44
1:C:36:PHE:C	1:C:37:PRO:CD	2.76	0.44
1:C:69:ALA:N	1:C:70:GLN:N	2.64	0.44
1:C:6:ASN:C	1:C:7:LYS:CA	2.82	0.44
2:D:10:VAL:CG2	2:D:11:THR:HG22	2.48	0.44
2:D:31:LEU:CD1	2:D:41:PHE:CE1	2.96	0.44
2:D:56:ASN:HD22	2:D:57:PRO:HG2	1.83	0.44
1:A:35:SER:HB3	2:B:126:GLN:OE1	2.17	0.43
1:A:45:HIS:O	1:A:45:HIS:CB	2.66	0.43
1:A:72:HIS:C	1:A:72:HIS:ND1	2.65	0.43
2:B:145:HIS:C	2:B:145:HIS:CB	2.72	0.43
2:B:62:HIS:C	2:B:62:HIS:CD2	2.92	0.43
2:B:64:LYS:CE	2:B:64:LYS:HA	2.49	0.43
2:B:84:PHE:O	2:B:85:ALA:C	2.57	0.43
1:C:42:TYR:HB3	1:C:43:PHE:CD1	2.53	0.43
2:D:14:TRP:HZ2	2:D:71:THR:CG2	2.30	0.43
2:D:79:ASP:HA	2:D:81:LYS:HD2	1.99	0.43
1:A:87:HIS:CD2	3:A:142:HEM:NC	2.86	0.43
2:B:26:ALA:HB2	2:B:112:VAL:HG21	2.01	0.43
2:B:2:LEU:CB	2:B:6:GLU:CD	2.86	0.43
1:C:11:LYS:O	1:C:12:ALA:C	2.55	0.43
1:C:45:HIS:ND1	3:C:142:HEM:O2D	2.51	0.43
1:C:80:LEU:HB2	1:C:80:LEU:CD1	2.46	0.43
2:D:55:ASN:O	2:D:60:LYS:HD2	2.15	0.43
1:A:45:HIS:ND1	1:A:46:PHE:CE2	2.81	0.43
2:B:39:ARG:HD3	1:C:92:ARG:O	2.18	0.43
2:B:81:LYS:NZ	2:B:142:HIS:NE2	2.65	0.43
1:C:105:LEU:CD1	1:C:105:LEU:CD2	2.90	0.43
1:C:44:PRO:HD3	1:C:44:PRO:CB	2.40	0.43
1:C:60:GLN:CG	1:C:60:GLN:HA	2.43	0.43
2:D:122:THR:HA	2:D:123:PRO:CD	2.47	0.43
1:A:1:VAL:CG2	1:A:1:VAL:HG13	2.36	0.43
1:A:52:SER:CA	1:A:52:SER:HG	2.30	0.43
1:A:73:LEU:HD21	1:A:128:PHE:CD2	2.52	0.43
2:B:110:ALA:C	2:B:111:LEU:CA	2.74	0.43
1:C:133:SER:C	1:C:134:THR:C	2.72	0.43
3:C:142:HEM:CMB	3:C:142:HEM:HBB2	2.48	0.43
2:D:55:ASN:ND2	2:D:57:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:PRO:O	2:D:58:LYS:C	2.54	0.43
2:D:75:LYS:CD	2:D:75:LYS:NZ	2.81	0.43
2:B:109:LEU:CB	2:B:109:LEU:HD13	2.40	0.43
2:B:32:VAL:O	2:B:32:VAL:CG1	2.64	0.43
2:B:66:VAL:HG21	2:B:66:VAL:HG11	1.99	0.43
1:C:17:VAL:CG2	1:C:17:VAL:HA	2.44	0.43
1:C:36:PHE:CZ	2:D:130:GLN:OE1	2.72	0.43
2:D:18:ASP:O	2:D:19:VAL:O	2.31	0.43
2:D:19:VAL:O	2:D:20:ASP:C	2.54	0.43
1:A:21:ALA:O	1:A:22:PRO:C	2.50	0.43
2:B:53:VAL:CG1	2:B:54:MET:N	2.82	0.43
1:C:49:SER:CA	1:C:55:GLN:HE22	2.29	0.43
1:C:122:HIS:HD2	2:D:29:ARG:HD3	1.83	0.43
2:D:30:LEU:HB3	2:D:30:LEU:C	2.35	0.43
2:D:30:LEU:O	2:D:37:THR:CG2	2.66	0.43
1:A:105:LEU:O	1:A:108:THR:HG22	2.19	0.43
2:B:1:MET:CB	2:B:1:MET:SD	3.01	0.43
2:B:21:VAL:CG1	2:B:21:VAL:C	2.70	0.43
2:B:2:LEU:CD1	2:B:6:GLU:CG	2.90	0.43
2:B:84:PHE:CZ	3:B:146:HEM:HBC1	2.54	0.43
2:B:92:CYS:CA	2:B:144:TYR:CZ	3.02	0.43
1:C:140:TYR:CG	1:C:140:TYR:N	2.85	0.43
1:C:94:ASN:HD22	1:C:94:ASN:N	2.16	0.43
1:C:94:ASN:ND2	1:C:94:ASN:O	2.40	0.43
2:D:141:ALA:N	2:D:141:ALA:C	2.66	0.43
1:A:135:VAL:CG2	1:A:135:VAL:HG13	2.45	0.43
2:B:21:VAL:CB	2:B:21:VAL:O	2.59	0.43
2:B:28:GLY:O	2:B:31:LEU:HB2	2.18	0.43
1:C:10:VAL:CG1	1:C:128:PHE:CD1	3.02	0.43
1:C:39:THR:CA	1:C:39:THR:OG1	2.54	0.43
1:C:46:PHE:HA	1:C:54:GLN:OE1	2.19	0.43
1:C:70:GLN:CA	1:C:72:HIS:H	2.31	0.43
2:D:124:ASN:HA	2:D:124:ASN:ND2	2.34	0.43
2:D:95:LEU:CD1	3:D:146:HEM:C4A	3.02	0.43
2:D:96:HIS:N	2:D:96:HIS:C	2.72	0.43
1:A:10:VAL:C	1:A:10:VAL:CG1	2.84	0.43
1:A:14:TRP:CD1	1:A:70:GLN:NE2	2.86	0.43
2:D:25:GLN:NE2	2:D:116:ASN:OD1	2.52	0.43
1:A:70:GLN:HA	1:A:73:LEU:HD11	2.01	0.43
2:B:101:ASN:HA	2:B:101:ASN:HD22	1.67	0.43
2:B:106:GLY:HA2	2:B:133:VAL:HG21	1.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:THR:O	2:B:4:ALA:HA	2.17	0.43
2:B:49:SER:O	2:B:49:SER:N	2.52	0.43
1:C:89:HIS:CG	1:C:139:LYS:HZ3	2.33	0.43
3:D:146:HEM:NA	3:D:146:HEM:CHA	2.70	0.43
1:A:98:PHE:HE2	1:A:137:THR:HG1	1.63	0.42
1:A:2:LEU:CG	1:A:73:LEU:HD23	2.32	0.42
2:B:5:GLU:CB	2:B:5:GLU:H	2.28	0.42
2:B:84:PHE:HA	2:B:84:PHE:CD2	2.54	0.42
2:D:109:LEU:HD13	2:D:113:VAL:CG2	2.49	0.42
2:D:77:LEU:N	2:D:77:LEU:CG	2.81	0.42
1:A:2:LEU:HD11	1:A:2:LEU:CD2	2.44	0.42
1:A:70:GLN:HG2	1:A:70:GLN:CD	2.19	0.42
1:A:7:LYS:O	1:A:7:LYS:CA	2.45	0.42
2:B:97:VAL:HG13	3:B:146:HEM:CMB	2.49	0.42
1:C:46:PHE:HD2	1:C:54:GLN:CG	2.32	0.42
1:C:83:LEU:HG	1:C:83:LEU:CA	2.47	0.42
2:D:141:ALA:C	2:D:142:HIS:HA	2.34	0.42
1:A:26:ALA:O	1:A:30:GLN:HB2	2.20	0.42
2:B:34:TYR:N	2:B:35:PRO:HD3	2.29	0.42
2:B:43:HIS:CD2	2:B:43:HIS:CE1	3.04	0.42
1:C:60:GLN:HA	1:C:60:GLN:HG2	2.00	0.42
2:D:19:VAL:N	2:D:19:VAL:HG23	2.33	0.42
1:A:6:ASN:HD21	1:A:127:LYS:NZ	2.17	0.42
2:B:26:ALA:N	2:B:27:LEU:N	2.67	0.42
2:B:2:LEU:HB3	2:B:131:LYS:HZ3	1.75	0.42
2:B:62:HIS:CE1	3:B:146:HEM:C4D	3.08	0.42
1:C:117:PHE:O	1:C:117:PHE:HD2	2.00	0.42
2:D:67:LEU:O	2:D:68:ASP:C	2.57	0.42
1:A:53:ALA:HA	1:A:56:LYS:CG	2.49	0.42
1:A:86:LEU:HD21	3:A:142:HEM:HBA2	2.01	0.42
2:B:30:LEU:HD21	2:B:105:LEU:HB2	2.00	0.42
2:B:109:LEU:HD23	2:B:109:LEU:HA	2.01	0.42
2:B:73:GLY:C	2:B:74:LEU:O	2.58	0.42
1:C:131:ASN:H	1:C:131:ASN:CB	2.28	0.42
1:C:68:LYS:CB	1:C:68:LYS:HD3	2.49	0.42
1:C:70:GLN:CB	1:C:71:GLY:N	2.78	0.42
1:C:86:LEU:CD2	1:C:86:LEU:HD11	2.40	0.42
2:D:65:ARG:NH2	2:D:65:ARG:NH1	2.57	0.42
2:D:70:PHE:O	2:D:84:PHE:CZ	2.72	0.42
1:A:100:LEU:CB	1:A:100:LEU:HD22	2.36	0.42
2:B:105:LEU:HB2	3:B:146:HEM:HBB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:TYR:CB	1:C:140:TYR:CD1	2.63	0.42
1:C:32:MET:HG2	1:C:39:THR:CG2	2.49	0.42
3:D:146:HEM:CGD	3:D:146:HEM:CAD	2.90	0.42
2:D:81:LYS:HD3	2:D:82:GLY:N	2.34	0.42
2:B:22:VAL:CG2	2:B:113:VAL:HG13	2.50	0.42
2:B:64:LYS:CB	2:B:64:LYS:CE	2.97	0.42
2:B:1:MET:CB	2:B:77:LEU:HD11	2.45	0.42
2:B:74:LEU:HD21	2:B:77:LEU:HG	2.02	0.42
2:B:91:HIS:HE1	3:B:146:HEM:ND	2.18	0.42
1:C:33:PHE:O	1:C:37:PRO:HG3	2.19	0.42
1:C:85:ASN:OD1	1:C:85:ASN:CB	2.67	0.42
2:D:95:LEU:HD13	3:D:146:HEM:CMA	2.50	0.42
1:A:139:LYS:O	1:A:140:TYR:C	2.58	0.42
1:A:31:ARG:HH21	2:B:126:GLN:CG	2.33	0.42
1:A:95:PRO:HB3	1:A:137:THR:HG23	2.01	0.42
2:B:106:GLY:O	2:B:133:VAL:HG21	2.20	0.42
2:B:1:MET:CA	2:B:2:LEU:HD23	2.50	0.42
2:B:62:HIS:HE1	3:B:146:HEM:C4D	2.38	0.42
1:C:49:SER:HA	1:C:55:GLN:NE2	2.31	0.42
1:C:56:LYS:CB	1:C:56:LYS:CD	2.98	0.42
1:A:141:ARG:C	1:A:141:ARG:HA	2.22	0.42
2:B:98:ASN:HB2	2:B:101:ASN:H	1.81	0.42
1:C:10:VAL:CG1	1:C:10:VAL:HG22	2.40	0.42
1:C:17:VAL:HG13	1:C:24:TYR:HD2	1.77	0.42
2:D:100:GLN:N	2:D:100:GLN:CB	2.73	0.42
2:D:90:LEU:HD22	2:D:90:LEU:O	2.19	0.42
2:B:78:ASP:OD2	2:B:78:ASP:CB	2.47	0.42
1:C:130:ALA:CA	1:C:133:SER:HB2	2.50	0.42
1:C:43:PHE:CB	1:C:43:PHE:O	2.67	0.42
1:C:61:LYS:HD3	1:C:61:LYS:HA	2.00	0.42
1:C:68:LYS:HZ2	1:C:68:LYS:CD	2.30	0.42
2:D:141:ALA:O	2:D:144:TYR:HB2	2.20	0.42
2:D:33:VAL:C	2:D:34:TYR:CA	2.76	0.42
1:A:43:PHE:HB2	1:A:48:LEU:CD2	2.50	0.41
1:A:93:VAL:HB	1:A:93:VAL:HG23	1.90	0.41
2:B:109:LEU:C	2:B:110:ALA:HA	2.33	0.41
2:B:109:LEU:O	2:B:110:ALA:HA	2.19	0.41
2:B:70:PHE:O	2:B:73:GLY:N	2.52	0.41
3:A:142:HEM:CMA	3:A:142:HEM:CHB	2.98	0.41
1:A:42:TYR:C	1:A:44:PRO:CD	2.88	0.41
2:B:133:VAL:HG21	2:B:133:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ALA:C	2:B:142:HIS:C	2.78	0.41
2:B:53:VAL:HG13	2:B:54:MET:N	2.35	0.41
1:C:29:LEU:CD1	1:C:59:GLY:CA	2.98	0.41
2:D:43:HIS:CE1	3:D:146:HEM:CBA	3.03	0.41
2:D:27:LEU:HD12	2:D:62:HIS:C	2.40	0.41
2:D:2:LEU:CB	2:D:7:LYS:HD3	2.50	0.41
2:D:98:ASN:O	2:D:100:GLN:N	2.52	0.41
1:A:135:VAL:CG2	1:A:135:VAL:CA	2.90	0.41
1:A:14:TRP:C	1:A:17:VAL:HG23	2.40	0.41
2:B:109:LEU:HD23	2:B:109:LEU:CA	2.48	0.41
1:A:31:ARG:HG2	2:B:123:PRO:HB3	2.01	0.41
2:D:37:THR:O	2:D:40:PHE:CD1	2.73	0.41
2:D:59:VAL:CB	2:D:60:LYS:N	2.76	0.41
2:D:75:LYS:NZ	2:D:76:HIS:HD2	2.18	0.41
1:A:119:PRO:HG3	2:B:54:MET:SD	2.61	0.41
1:A:74:ASN:CA	1:A:74:ASN:O	2.57	0.41
2:B:115:ARG:HD2	2:B:115:ARG:HH21	1.36	0.41
2:B:80:LEU:HB3	2:B:82:GLY:N	2.34	0.41
1:C:102:SER:C	1:C:103:HIS:C	2.79	0.41
1:C:36:PHE:CE1	2:D:103:ARG:NH1	2.89	0.41
1:C:44:PRO:O	1:C:46:PHE:N	2.54	0.41
1:C:95:PRO:HD3	1:C:141:ARG:HH22	1.85	0.41
2:D:105:LEU:HD13	2:D:105:LEU:HB3	1.97	0.41
2:D:43:HIS:HB2	2:D:43:HIS:N	2.31	0.41
1:A:132:ASP:O	1:A:136:LEU:HD21	2.21	0.41
2:B:126:GLN:N	2:B:127:ALA:N	2.65	0.41
2:B:6:GLU:HA	2:B:6:GLU:CB	2.23	0.41
2:D:109:LEU:CA	2:D:110:ALA:N	2.66	0.41
2:D:102:PHE:HB3	2:D:137:ALA:CB	2.51	0.41
1:A:46:PHE:HD1	1:A:55:GLN:OE1	2.04	0.41
1:A:48:LEU:HG	1:A:48:LEU:N	2.35	0.41
2:B:10:VAL:CG2	2:B:10:VAL:CG1	2.88	0.41
1:C:97:ASN:N	1:C:98:PHE:N	2.67	0.41
2:D:131:LYS:O	2:D:132:VAL:CA	2.63	0.41
2:D:41:PHE:HB3	2:D:44:PHE:CE1	2.56	0.41
1:A:32:MET:HG2	1:A:32:MET:HE2	2.03	0.41
1:A:60:GLN:HE21	1:A:61:LYS:CD	2.33	0.41
1:A:62:VAL:CG2	3:A:142:HEM:C1B	3.03	0.41
1:A:14:TRP:HD1	1:A:67:THR:HG23	1.84	0.41
2:D:127:ALA:HB3	2:D:127:ALA:C	2.34	0.41
1:A:43:PHE:CE2	3:A:142:HEM:C2D	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:TYR:N	1:A:43:PHE:N	2.69	0.41
1:A:50:HIS:CD2	1:A:50:HIS:HA	2.56	0.41
1:A:91:LEU:C	1:A:91:LEU:N	2.66	0.41
2:B:74:LEU:O	2:B:75:LYS:CA	2.69	0.41
2:B:84:PHE:HA	2:B:84:PHE:CG	2.52	0.41
1:C:42:TYR:CB	1:C:43:PHE:CD1	3.03	0.41
1:C:54:GLN:CG	1:C:54:GLN:HA	2.43	0.41
1:C:89:HIS:CE1	1:C:90:LYS:CG	2.94	0.41
2:D:131:LYS:C	2:D:132:VAL:HA	2.33	0.41
1:A:64:ASN:N	1:A:64:ASN:C	2.66	0.41
2:B:113:VAL:CG2	2:B:113:VAL:HB	2.30	0.41
2:B:128:LEU:CD1	2:B:128:LEU:HB3	2.46	0.41
2:B:40:PHE:HE2	2:B:95:LEU:O	2.03	0.41
2:B:41:PHE:CB	2:B:41:PHE:C	2.85	0.41
2:B:62:HIS:C	2:B:66:VAL:HG12	2.41	0.41
1:C:18:GLY:N	1:C:18:GLY:O	2.54	0.41
1:A:124:ASN:CA	1:A:124:ASN:O	2.62	0.41
1:A:45:HIS:CE1	1:A:46:PHE:CE2	3.09	0.41
1:A:73:LEU:C	1:A:74:ASN:HD22	2.24	0.41
2:B:70:PHE:CD1	2:B:71:THR:CB	2.94	0.41
1:C:129:LEU:CD2	1:C:129:LEU:HB3	2.49	0.41
1:C:134:THR:CB	1:C:134:THR:N	2.81	0.41
1:C:95:PRO:CG	1:C:141:ARG:NH1	2.68	0.41
3:C:142:HEM:HBB2	3:C:142:HEM:HMB1	2.03	0.41
1:C:7:LYS:CB	1:C:7:LYS:HG2	2.21	0.41
1:A:48:LEU:O	1:A:50:HIS:N	2.53	0.41
2:B:19:VAL:HG13	2:B:20:ASP:N	2.36	0.41
2:B:34:TYR:HB3	2:B:36:TRP:CH2	2.56	0.41
2:B:57:PRO:HD3	2:B:57:PRO:HA	1.96	0.41
1:C:130:ALA:C	1:C:133:SER:HB2	2.42	0.41
2:D:11:THR:HG22	2:D:11:THR:N	2.30	0.41
2:D:41:PHE:O	2:D:42:GLN:HA	2.21	0.41
2:D:53:VAL:CG2	2:D:54:MET:HE1	2.45	0.41
1:A:31:ARG:NH2	2:B:126:GLN:HB3	2.34	0.40
2:B:141:ALA:HA	2:B:144:TYR:CD1	2.56	0.40
2:B:25:GLN:O	2:B:29:ARG:N	2.54	0.40
1:C:116:ASN:HA	1:C:116:ASN:O	2.17	0.40
1:C:13:ALA:HB2	1:C:121:VAL:HG11	2.02	0.40
2:D:43:HIS:CA	2:D:43:HIS:HB3	2.23	0.40
2:B:126:GLN:CD	2:B:126:GLN:HB3	2.42	0.40
2:B:105:LEU:HB2	3:B:146:HEM:CBB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:LEU:HD23	2:B:105:LEU:CB	2.50	0.40
1:C:17:VAL:O	1:C:18:GLY:HA3	2.20	0.40
1:C:32:MET:N	1:C:32:MET:HB3	2.30	0.40
1:C:46:PHE:CD2	1:C:54:GLN:CG	3.04	0.40
1:A:39:THR:CA	1:A:40:LYS:NZ	2.73	0.40
2:B:36:TRP:HE1	2:B:101:ASN:HD21	1.69	0.40
1:C:84:SER:HB3	1:C:136:LEU:HA	2.02	0.40
1:C:48:LEU:HA	1:C:55:GLN:NE2	2.36	0.40
1:C:22:PRO:C	1:C:56:LYS:HD3	2.42	0.40
2:D:64:LYS:CE	2:D:64:LYS:CG	2.83	0.40
2:B:44:PHE:HD2	2:B:58:LYS:CG	2.34	0.40
2:B:76:HIS:HB2	2:B:76:HIS:N	2.27	0.40
1:C:48:LEU:HD13	1:C:49:SER:HB2	1.96	0.40
2:B:138:ASN:HB2	2:B:138:ASN:ND2	2.33	0.40
2:B:34:TYR:HB3	2:B:36:TRP:CE2	2.56	0.40
1:C:131:ASN:ND2	1:C:131:ASN:CA	2.84	0.40
1:C:16:LYS:C	1:C:17:VAL:C	2.80	0.40
1:C:2:LEU:HD12	1:C:7:LYS:HG3	2.02	0.40
2:D:91:HIS:HD2	2:D:102:PHE:HE1	1.68	0.40
1:C:35:SER:CB	2:D:127:ALA:HA	2.47	0.40
2:D:95:LEU:CD1	2:D:97:VAL:HG21	2.43	0.40

All (80) 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:A:2:LEU:O	2:D:49:SER:CB[4_555]	0.51	1.69
1:A:75:ASP:C	2:D:55:ASN:CG[4_555]	0.81	1.39
1:A:74:ASN:CG	2:D:54:MET:CA[4_555]	0.92	1.28
1:A:2:LEU:O	2:D:49:SER:CA[4_555]	1.05	1.15
1:A:7:LYS:NZ	2:D:51:GLY:N[4_555]	1.06	1.14
1:A:1:VAL:N	2:D:48:SER:O[4_555]	1.09	1.11
1:A:74:ASN:CG	2:D:54:MET:C[4_555]	1.10	1.10
1:A:75:ASP:N	2:D:55:ASN:CB[4_555]	1.13	1.07
1:A:2:LEU:C	2:D:49:SER:CB[4_555]	1.13	1.07
1:A:75:ASP:CG	2:D:55:ASN:O[4_555]	1.14	1.06
1:A:75:ASP:CA	2:D:55:ASN:CB[4_555]	1.19	1.01
1:A:75:ASP:C	2:D:55:ASN:OD1[4_555]	1.22	0.98
1:A:75:ASP:CB	2:D:55:ASN:O[4_555]	1.27	0.93
1:A:74:ASN:OD1	2:D:54:MET:CA[4_555]	1.28	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:N	2:D:55:ASN:CA[4_555]	1.29	0.91
1:A:75:ASP:O	2:D:55:ASN:OD1[4_555]	1.31	0.89
1:A:75:ASP:CB	2:D:55:ASN:C[4_555]	1.36	0.84
1:A:7:LYS:NZ	2:D:51:GLY:CA[4_555]	1.38	0.82
1:A:75:ASP:CA	2:D:55:ASN:CG[4_555]	1.42	0.78
1:A:73:LEU:O	2:D:51:GLY:O[4_555]	1.44	0.76
1:A:74:ASN:C	2:D:55:ASN:N[4_555]	1.45	0.75
1:A:74:ASN:C	2:D:55:ASN:CA[4_555]	1.49	0.71
1:A:75:ASP:OD1	2:D:60:LYS:CD[4_555]	1.50	0.70
1:A:75:ASP:CB	2:D:55:ASN:ND2[4_555]	1.50	0.70
1:A:75:ASP:C	2:D:55:ASN:CB[4_555]	1.52	0.68
1:A:75:ASP:OD2	2:D:57:PRO:CA[4_555]	1.56	0.64
1:A:90:LYS:NZ	1:C:82:ASN:ND2[4_545]	1.57	0.63
1:A:74:ASN:CA	2:D:52:ALA:CA[4_555]	1.59	0.61
1:A:74:ASN:CG	2:D:54:MET:CB[4_555]	1.59	0.61
1:A:75:ASP:OD2	2:D:57:PRO:N[4_555]	1.63	0.57
1:A:74:ASN:OD1	2:D:54:MET:CB[4_555]	1.64	0.56
1:A:74:ASN:CB	2:D:54:MET:N[4_555]	1.65	0.55
1:A:74:ASN:CA	2:D:55:ASN:N[4_555]	1.66	0.54
1:A:74:ASN:N	2:D:51:GLY:O[4_555]	1.67	0.53
1:A:75:ASP:OD1	2:D:55:ASN:O[4_555]	1.69	0.51
1:A:7:LYS:NZ	2:D:50:ALA:C[4_555]	1.70	0.50
1:A:90:LYS:CD	1:C:82:ASN:ND2[4_545]	1.71	0.49
1:A:76:LEU:N	2:D:55:ASN:OD1[4_555]	1.73	0.47
1:A:76:LEU:N	2:D:55:ASN:CB[4_555]	1.74	0.46
1:A:74:ASN:CB	2:D:51:GLY:O[4_555]	1.74	0.46
1:A:74:ASN:CB	2:D:55:ASN:N[4_555]	1.74	0.46
1:A:74:ASN:CB	2:D:54:MET:C[4_555]	1.76	0.44
1:A:76:LEU:N	2:D:55:ASN:CG[4_555]	1.78	0.42
1:A:74:ASN:O	2:D:56:ASN:N[4_555]	1.80	0.40
1:A:73:LEU:C	2:D:51:GLY:O[4_555]	1.80	0.40
1:A:7:LYS:NZ	2:D:51:GLY:C[4_555]	1.81	0.39
1:A:75:ASP:N	2:D:55:ASN:N[4_555]	1.82	0.38
1:A:73:LEU:O	2:D:51:GLY:C[4_555]	1.84	0.36
1:A:2:LEU:O	2:D:49:SER:OG[4_555]	1.84	0.36
1:A:75:ASP:OD2	2:D:57:PRO:CD[4_555]	1.85	0.35
1:A:74:ASN:O	2:D:52:ALA:O[4_555]	1.87	0.33
1:A:75:ASP:CA	2:D:55:ASN:C[4_555]	1.88	0.32
1:A:90:LYS:CE	1:C:82:ASN:ND2[4_545]	1.89	0.31
1:A:74:ASN:CA	2:D:51:GLY:O[4_555]	1.89	0.31
1:A:74:ASN:OD1	2:D:54:MET:C[4_555]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:CB	2:D:55:ASN:CA[4_555]	1.90	0.30
1:A:7:LYS:CE	2:D:51:GLY:CA[4_555]	1.91	0.29
1:A:76:LEU:CA	2:D:55:ASN:OD1[4_555]	1.91	0.29
1:A:2:LEU:CA	2:D:49:SER:OG[4_555]	1.92	0.28
1:A:75:ASP:CA	2:D:55:ASN:CA[4_555]	1.92	0.28
1:A:75:ASP:O	2:D:55:ASN:CG[4_555]	1.94	0.26
1:A:75:ASP:O	2:D:55:ASN:ND2[4_555]	1.95	0.25
1:A:7:LYS:CE	2:D:51:GLY:N[4_555]	1.95	0.25
1:A:74:ASN:CB	2:D:54:MET:CA[4_555]	1.98	0.22
1:A:75:ASP:OD1	2:D:60:LYS:CG[4_555]	2.00	0.20
1:A:74:ASN:C	2:D:55:ASN:CB[4_555]	2.01	0.19
1:A:75:ASP:CA	2:D:55:ASN:ND2[4_555]	2.01	0.19
1:A:75:ASP:C	2:D:55:ASN:ND2[4_555]	2.02	0.18
1:A:1:VAL:CA	2:D:48:SER:O[4_555]	2.04	0.16
1:A:76:LEU:C	2:D:55:ASN:OD1[4_555]	2.04	0.16
1:A:74:ASN:CA	2:D:52:ALA:C[4_555]	2.06	0.14
1:A:2:LEU:C	2:D:49:SER:OG[4_555]	2.06	0.14
1:A:75:ASP:N	2:D:55:ASN:CG[4_555]	2.07	0.13
1:A:75:ASP:CB	2:D:56:ASN:N[4_555]	2.07	0.13
1:A:74:ASN:CG	2:D:54:MET:N[4_555]	2.09	0.11
1:A:75:ASP:CG	2:D:57:PRO:CD[4_555]	2.09	0.11
1:A:2:LEU:CB	2:D:49:SER:OG[4_555]	2.11	0.09
1:A:74:ASN:O	2:D:55:ASN:C[4_555]	2.13	0.07
1:A:75:ASP:CB	2:D:55:ASN:CG[4_555]	2.17	0.03
1:A:1:VAL:N	2:D:48:SER:C[4_555]	2.17	0.03

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%)	74 (53%)	34 (24%)	31 (22%)	0 0
1	C	139/141 (99%)	78 (56%)	28 (20%)	33 (24%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	143/145 (99%)	75 (52%)	28 (20%)	40 (28%)	0	0
2	D	143/145 (99%)	78 (54%)	26 (18%)	39 (27%)	0	0
All	All	564/572 (99%)	305 (54%)	116 (21%)	143 (25%)	0	0

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	6	ASN
1	A	13	ALA
1	A	15	GLY
1	A	17	VAL
1	A	30	GLN
1	A	31	ARG
1	A	40	LYS
1	A	47	ASP
1	A	53	ALA
1	A	72	HIS
1	A	74	ASN
1	A	89	HIS
1	A	109	LEU
1	A	110	ALA
2	B	7	LYS
2	B	19	VAL
2	B	20	ASP
2	B	21	VAL
2	B	33	VAL
2	B	46	ASN
2	B	56	ASN
2	B	57	PRO
2	B	66	VAL
2	B	68	ASP
2	B	72	GLN
2	B	74	LEU
2	B	76	HIS
2	B	85	ALA
2	B	86	GLN
2	B	93	ASN
2	B	96	HIS
2	B	122	THR
2	B	137	ALA

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Mol	Chain	Res	Type
1	C	3	SER
1	C	21	ALA
1	C	45	HIS
1	C	48	LEU
1	C	63	ALA
1	C	64	ASN
1	C	75	ASP
1	C	83	LEU
1	C	84	SER
1	C	86	LEU
1	C	102	SER
1	C	110	ALA
1	C	138	SER
2	D	2	LEU
2	D	6	GLU
2	D	7	LYS
2	D	14	TRP
2	D	20	ASP
2	D	43	HIS
2	D	46	ASN
2	D	49	SER
2	D	59	VAL
2	D	72	GLN
2	D	73	GLY
2	D	75	LYS
2	D	78	ASP
2	D	124	ASN
2	D	144	TYR
1	A	14	TRP
1	A	25	GLY
1	A	29	LEU
1	A	49	SER
1	A	86	LEU
1	A	88	ALA
1	A	99	LYS
1	A	132	ASP
1	A	140	TYR
2	B	15	GLY
2	B	28	GLY
2	B	43	HIS
2	B	52	ALA
2	B	69	ALA

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Mol	Chain	Res	Type
2	B	81	LYS
2	B	89	GLY
2	B	95	LEU
2	B	118	GLY
1	C	7	LYS
1	C	10	VAL
1	C	44	PRO
1	C	61	LYS
1	C	130	ALA
2	D	8	ALA
2	D	9	ALA
2	D	12	GLY
2	D	16	LYS
2	D	44	PHE
2	D	58	LYS
2	D	60	LYS
2	D	61	ALA
2	D	64	LYS
2	D	71	THR
2	D	82	GLY
2	D	110	ALA
2	D	116	ASN
2	D	134	ALA
2	D	143	LYS
1	A	66	LEU
1	A	82	ASN
1	A	136	LEU
1	A	139	LYS
2	B	60	LYS
2	B	67	LEU
2	B	75	LYS
2	B	112	VAL
2	B	143	LYS
1	C	24	TYR
1	C	31	ARG
1	C	68	LYS
1	C	124	ASN
1	C	139	LYS
2	D	92	CYS
2	D	128	LEU
2	D	139	ALA
1	A	37	PRO

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Mol	Chain	Res	Type
2	B	2	LEU
2	B	31	LEU
2	B	83	ALA
2	B	127	ALA
1	C	57	ALA
1	C	109	LEU
2	D	3	THR
2	D	99	PRO
2	D	122	THR
1	A	50	HIS
1	A	128	PHE
1	C	9	ASN
1	C	17	VAL
1	C	37	PRO
1	C	74	ASN
1	C	118	THR
1	C	133	SER
2	D	62	HIS
1	C	56	LYS
2	D	86	GLN
2	D	19	VAL
1	C	96	VAL
2	B	17	VAL
2	B	82	GLY
2	B	132	VAL

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	115/115 (100%)	57 (50%)	58 (50%)	0	0
1	C	115/115 (100%)	64 (56%)	51 (44%)	0	0
2	B	113/113 (100%)	50 (44%)	63 (56%)	0	0
2	D	113/113 (100%)	53 (47%)	60 (53%)	0	0
All	All	456/456 (100%)	224 (49%)	232 (51%)	0	0

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	14	TRP
1	A	16	LYS
1	A	17	VAL
1	A	22	PRO
1	A	24	TYR
1	A	27	GLN
1	A	29	LEU
1	A	30	GLN
1	A	32	MET
1	A	33	PHE
1	A	34	LEU
1	A	37	PRO
1	A	38	THR
1	A	39	THR
1	A	40	LYS
1	A	41	THR
1	A	43	PHE
1	A	45	HIS
1	A	50	HIS
1	A	52	SER
1	A	55	GLN
1	A	56	LYS
1	A	60	GLN
1	A	61	LYS
1	A	62	VAL
1	A	68	LYS
1	A	70	GLN
1	A	73	LEU
1	A	74	ASN
1	A	76	LEU
1	A	79	THR
1	A	80	LEU
1	A	82	ASN
1	A	84	SER
1	A	85	ASN
1	A	90	LYS
1	A	93	VAL
1	A	99	LYS
1	A	100	LEU
1	A	104	SER
1	A	105	LEU

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Mol	Chain	Res	Type
1	A	106	LEU
1	A	108	THR
1	A	109	LEU
1	A	111	SER
1	A	113	LEU
1	A	114	PRO
1	A	118	THR
1	A	121	VAL
1	A	122	HIS
1	A	124	ASN
1	A	133	SER
1	A	135	VAL
1	A	136	LEU
1	A	137	THR
1	A	138	SER
1	A	139	LYS
2	B	2	LEU
2	B	3	THR
2	B	5	GLU
2	B	7	LYS
2	B	13	PHE
2	B	16	LYS
2	B	19	VAL
2	B	22	VAL
2	B	25	GLN
2	B	27	LEU
2	B	30	LEU
2	B	31	LEU
2	B	34	TYR
2	B	37	THR
2	B	38	GLN
2	B	39	ARG
2	B	41	PHE
2	B	42	GLN
2	B	47	LEU
2	B	54	MET
2	B	55	ASN
2	B	56	ASN
2	B	58	LYS
2	B	59	VAL
2	B	60	LYS
2	B	64	LYS

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Mol	Chain	Res	Type
2	B	65	ARG
2	B	66	VAL
2	B	68	ASP
2	B	70	PHE
2	B	71	THR
2	B	72	GLN
2	B	74	LEU
2	B	75	LYS
2	B	77	LEU
2	B	80	LEU
2	B	81	LYS
2	B	84	PHE
2	B	87	LEU
2	B	88	SER
2	B	92	CYS
2	B	94	LYS
2	B	95	LEU
2	B	97	VAL
2	B	98	ASN
2	B	99	PRO
2	B	104	LEU
2	B	105	LEU
2	B	109	LEU
2	B	111	LEU
2	B	112	VAL
2	B	113	VAL
2	B	116	ASN
2	B	120	GLN
2	B	121	PHE
2	B	122	THR
2	B	124	ASN
2	B	126	GLN
2	B	128	LEU
2	B	129	PHE
2	B	130	GLN
2	B	132	VAL
2	B	138	ASN
1	C	1	VAL
1	C	2	LEU
1	C	3	SER
1	C	6	ASN
1	C	7	LYS

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Mol	Chain	Res	Type
1	C	11	LYS
1	C	14	TRP
1	C	16	LYS
1	C	20	ASN
1	C	22	PRO
1	C	35	SER
1	C	36	PHE
1	C	39	THR
1	C	45	HIS
1	C	47	ASP
1	C	48	LEU
1	C	52	SER
1	C	55	GLN
1	C	56	LYS
1	C	60	GLN
1	C	61	LYS
1	C	66	LEU
1	C	68	LYS
1	C	72	HIS
1	C	73	LEU
1	C	74	ASN
1	C	76	LEU
1	C	79	THR
1	C	81	SER
1	C	82	ASN
1	C	86	LEU
1	C	89	HIS
1	C	90	LYS
1	C	92	ARG
1	C	94	ASN
1	C	99	LYS
1	C	100	LEU
1	C	101	LEU
1	C	104	SER
1	C	106	LEU
1	C	107	VAL
1	C	113	LEU
1	C	115	THR
1	C	117	PHE
1	C	124	ASN
1	C	127	LYS
1	C	129	LEU

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Mol	Chain	Res	Type
1	C	131	ASN
1	C	132	ASP
1	C	139	LYS
1	C	140	TYR
2	D	1	MET
2	D	2	LEU
2	D	3	THR
2	D	7	LYS
2	D	10	VAL
2	D	11	THR
2	D	14	TRP
2	D	20	ASP
2	D	21	VAL
2	D	25	GLN
2	D	27	LEU
2	D	31	LEU
2	D	33	VAL
2	D	37	THR
2	D	40	PHE
2	D	41	PHE
2	D	43	HIS
2	D	47	LEU
2	D	48	SER
2	D	53	VAL
2	D	55	ASN
2	D	56	ASN
2	D	58	LYS
2	D	64	LYS
2	D	65	ARG
2	D	68	ASP
2	D	72	GLN
2	D	75	LYS
2	D	78	ASP
2	D	80	LEU
2	D	81	LYS
2	D	84	PHE
2	D	87	LEU
2	D	90	LEU
2	D	94	LYS
2	D	95	LEU
2	D	96	HIS
2	D	100	GLN

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Mol	Chain	Res	Type
2	D	101	ASN
2	D	103	ARG
2	D	104	LEU
2	D	107	ASN
2	D	109	LEU
2	D	111	LEU
2	D	113	VAL
2	D	115	ARG
2	D	116	ASN
2	D	121	PHE
2	D	124	ASN
2	D	125	VAL
2	D	126	GLN
2	D	128	LEU
2	D	130	GLN
2	D	131	LYS
2	D	133	VAL
2	D	138	ASN
2	D	140	LEU
2	D	142	HIS
2	D	143	LYS
2	D	145	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	60	GLN
1	A	70	GLN
1	A	74	ASN
1	A	85	ASN
1	A	97	ASN
1	A	112	HIS
1	A	126	ASN
2	B	62	HIS
2	B	101	ASN
2	B	116	ASN
2	B	120	GLN
2	B	126	GLN
2	B	138	ASN
2	B	145	HIS
1	C	45	HIS

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Mol	Chain	Res	Type
1	C	55	GLN
1	C	60	GLN
1	C	70	GLN
1	C	72	HIS
1	C	74	ASN
1	C	89	HIS
2	D	25	GLN
2	D	43	HIS
2	D	55	ASN
2	D	56	ASN
2	D	62	HIS
2	D	72	GLN
2	D	76	HIS
2	D	126	GLN
2	D	130	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	B	146	2	27,50,50	10.55	22 (81%)	17,82,82	8.98	10 (58%)
3	HEM	D	146	-	27,50,50	10.88	23 (85%)	17,82,82	9.27	15 (88%)
3	HEM	A	142	1	27,50,50	9.67	21 (77%)	17,82,82	11.88	15 (88%)
3	HEM	C	142	1	27,50,50	8.96	20 (74%)	17,82,82	6.87	11 (64%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	146	2	-	2/6/54/54	-
3	HEM	D	146	-	-	3/6/54/54	-
3	HEM	A	142	1	-	2/6/54/54	-
3	HEM	C	142	1	-	1/6/54/54	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	146	HEM	CAD-C3D	-27.74	1.03	1.52
3	B	146	HEM	C4D-C3D	23.91	1.96	1.42
3	B	146	HEM	C3B-C2B	-23.74	1.07	1.40
3	D	146	HEM	CMD-C2D	-23.16	1.03	1.51
3	B	146	HEM	CMA-C3A	20.85	1.95	1.51
3	C	142	HEM	CMA-C3A	-20.46	1.09	1.51
3	D	146	HEM	C1A-CHA	19.36	1.94	1.41
3	A	142	HEM	C4A-NA	-18.72	0.97	1.36
3	A	142	HEM	C1B-C2B	-18.47	1.00	1.42
3	D	146	HEM	C4A-NA	18.02	1.73	1.36
3	A	142	HEM	C3B-C2B	16.25	1.62	1.40
3	C	142	HEM	C3B-CAB	15.76	1.80	1.47
3	B	146	HEM	C4A-NA	15.50	1.68	1.36
3	A	142	HEM	C4B-CHC	-15.31	0.98	1.41
3	A	142	HEM	CAD-C3D	-15.24	1.25	1.52
3	A	142	HEM	C4B-NB	15.21	1.67	1.36
3	D	146	HEM	CMC-C2C	-14.92	1.16	1.51
3	A	142	HEM	C3D-C2D	-14.92	0.93	1.37
3	B	146	HEM	CAD-C3D	14.47	1.77	1.52
3	C	142	HEM	CMD-C2D	-13.94	1.22	1.51
3	B	146	HEM	CMB-C2B	13.71	1.84	1.51
3	B	146	HEM	C3C-C2C	-13.60	1.21	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	C4D-C3D	-13.07	1.13	1.42
3	B	146	HEM	C1C-C2C	12.89	1.71	1.42
3	C	142	HEM	C1C-C2C	12.67	1.71	1.42
3	C	142	HEM	CAA-C2A	12.32	1.70	1.52
3	C	142	HEM	C3C-C2C	12.11	1.57	1.40
3	D	146	HEM	CMB-C2B	12.10	1.80	1.51
3	A	142	HEM	CMA-C3A	11.67	1.75	1.51
3	D	146	HEM	C1D-ND	11.63	1.60	1.36
3	D	146	HEM	C4D-C3D	11.06	1.67	1.42
3	D	146	HEM	CAA-C2A	-10.52	1.36	1.52
3	B	146	HEM	C1B-C2B	9.98	1.65	1.42
3	C	142	HEM	C4B-NB	9.77	1.56	1.36
3	A	142	HEM	C3C-C2C	9.51	1.53	1.40
3	C	142	HEM	C4A-CHB	9.46	1.67	1.41
3	C	142	HEM	C1A-NA	9.21	1.55	1.36
3	D	146	HEM	CMA-C3A	-8.72	1.33	1.51
3	D	146	HEM	C4B-NB	8.63	1.53	1.36
3	A	142	HEM	C4A-CHB	8.62	1.64	1.41
3	C	142	HEM	C1A-CHA	8.45	1.64	1.41
3	C	142	HEM	CAD-C3D	7.78	1.65	1.52
3	C	142	HEM	CMC-C2C	7.71	1.69	1.51
3	D	146	HEM	C3C-C2C	7.61	1.50	1.40
3	A	142	HEM	CAA-C2A	7.37	1.62	1.52
3	A	142	HEM	C2A-C3A	7.33	1.59	1.37
3	C	142	HEM	C3D-C2D	7.33	1.59	1.37
3	B	146	HEM	C3D-C2D	7.32	1.59	1.37
3	B	146	HEM	C4A-CHB	-7.20	1.21	1.41
3	C	142	HEM	C2A-C3A	7.08	1.58	1.37
3	A	142	HEM	C4D-C3D	7.02	1.58	1.42
3	B	146	HEM	C4B-CHC	6.53	1.59	1.41
3	B	146	HEM	C1A-CHA	-6.43	1.23	1.41
3	D	146	HEM	C3D-C2D	6.21	1.56	1.37
3	A	142	HEM	C3C-CAC	-6.03	1.35	1.47
3	D	146	HEM	C3B-CAB	-5.98	1.35	1.47
3	A	142	HEM	CMC-C2C	5.72	1.65	1.51
3	A	142	HEM	CMB-C2B	5.70	1.65	1.51
3	D	146	HEM	C1B-C2B	-5.50	1.30	1.42
3	C	142	HEM	C4B-CHC	-5.49	1.25	1.41
3	B	146	HEM	CAA-C2A	5.47	1.60	1.52
3	D	146	HEM	C1D-CHD	-5.33	1.26	1.41
3	A	142	HEM	CBC-CAC	-5.17	0.94	1.29
3	B	146	HEM	C4B-NB	-5.12	1.25	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	146	HEM	C3B-C2B	4.85	1.47	1.40
3	B	146	HEM	C1D-ND	4.79	1.46	1.36
3	C	142	HEM	C4A-NA	4.78	1.46	1.36
3	D	146	HEM	CBC-CAC	-4.66	0.98	1.29
3	C	142	HEM	C3C-CAC	4.55	1.57	1.47
3	D	146	HEM	C4A-CHB	4.33	1.53	1.41
3	C	142	HEM	CBB-CAB	-4.20	1.01	1.29
3	A	142	HEM	C3B-CAB	-4.18	1.39	1.47
3	D	146	HEM	C1C-C2C	4.05	1.51	1.42
3	B	146	HEM	C2A-C3A	-3.98	1.25	1.37
3	B	146	HEM	CBB-CAB	3.97	1.55	1.29
3	A	142	HEM	CMD-C2D	-3.95	1.43	1.51
3	B	146	HEM	CMD-C2D	3.88	1.59	1.51
3	B	146	HEM	C3C-CAC	-3.65	1.40	1.47
3	C	142	HEM	C1D-CHD	3.43	1.50	1.41
3	D	146	HEM	CBA-CAA	3.34	1.77	1.53
3	A	142	HEM	CBA-CAA	3.09	1.75	1.53
3	A	142	HEM	CBD-CAD	3.01	1.74	1.53
3	B	146	HEM	C3B-CAB	2.97	1.54	1.47
3	B	146	HEM	CBD-CAD	-2.72	1.34	1.53
3	D	146	HEM	C4B-CHC	-2.68	1.33	1.41
3	D	146	HEM	C3C-CAC	-2.06	1.43	1.47

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	CBD-CAD-C3D	27.20	162.59	112.48
3	D	146	HEM	C4A-C3A-C2A	25.96	125.06	107.00
3	A	142	HEM	C4C-C3C-C2C	-24.18	90.01	106.90
3	B	146	HEM	CMA-C3A-C4A	-20.36	97.18	128.46
3	B	146	HEM	CMC-C2C-C3C	17.94	158.24	124.68
3	B	146	HEM	C4A-C3A-C2A	17.94	119.47	107.00
3	A	142	HEM	CMD-C2D-C1D	-17.37	101.77	128.46
3	A	142	HEM	CMD-C2D-C3D	15.12	153.45	124.94
3	C	142	HEM	CAD-CBD-CGD	15.03	137.88	112.67
3	C	142	HEM	C4C-C3C-C2C	14.27	116.86	106.90
3	D	146	HEM	CMA-C3A-C4A	-13.30	108.03	128.46
3	C	142	HEM	CBD-CAD-C3D	12.52	135.55	112.48
3	A	142	HEM	C4A-C3A-C2A	-11.87	98.73	107.00
3	D	146	HEM	C4C-C3C-C2C	-11.78	98.67	106.90
3	A	142	HEM	C3C-C4C-NC	9.79	129.42	110.94
3	B	146	HEM	C1D-C2D-C3D	-9.64	100.29	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	146	HEM	CMA-C3A-C2A	9.56	142.96	124.94
3	D	146	HEM	CAA-C2A-C3A	9.46	154.43	127.25
3	D	146	HEM	CMD-C2D-C1D	-8.69	115.10	128.46
3	D	146	HEM	CAA-CBA-CGA	-8.18	98.95	112.67
3	A	142	HEM	CBA-CAA-C2A	-8.13	97.49	112.49
3	C	142	HEM	CAA-CBA-CGA	-8.12	99.04	112.67
3	A	142	HEM	CMB-C2B-C3B	-8.12	109.48	124.68
3	D	146	HEM	CBA-CAA-C2A	-7.49	98.67	112.49
3	A	142	HEM	CAA-C2A-C3A	7.49	148.76	127.25
3	D	146	HEM	C3B-C4B-NB	7.15	118.46	109.21
3	A	142	HEM	CAA-CBA-CGA	-7.09	100.77	112.67
3	C	142	HEM	CMD-C2D-C1D	-6.67	118.22	128.46
3	D	146	HEM	CBD-CAD-C3D	6.65	124.73	112.48
3	B	146	HEM	C3B-C4B-NB	6.24	117.27	109.21
3	B	146	HEM	C4C-C3C-C2C	5.88	111.01	106.90
3	B	146	HEM	CAD-C3D-C2D	5.32	142.54	127.25
3	C	142	HEM	C3C-C4C-NC	-5.04	101.44	110.94
3	A	142	HEM	C1D-C2D-C3D	-5.02	103.50	107.00
3	D	146	HEM	C1D-C2D-C3D	4.80	110.34	107.00
3	C	142	HEM	CAD-C3D-C2D	-4.80	113.45	127.25
3	D	146	HEM	CMD-C2D-C3D	4.45	133.33	124.94
3	C	142	HEM	CAA-C2A-C3A	-4.24	115.05	127.25
3	D	146	HEM	CAD-CBD-CGD	-3.91	106.12	112.67
3	A	142	HEM	C3B-C4B-NB	-3.77	104.33	109.21
3	C	142	HEM	C3B-C4B-NB	-3.63	104.51	109.21
3	D	146	HEM	CMC-C2C-C3C	3.53	131.27	124.68
3	A	142	HEM	CMA-C3A-C2A	3.45	131.44	124.94
3	C	142	HEM	CBA-CAA-C2A	-3.20	106.59	112.49
3	D	146	HEM	CAD-C3D-C2D	3.06	136.04	127.25
3	A	142	HEM	CAD-C3D-C2D	2.82	135.35	127.25
3	B	146	HEM	CAD-CBD-CGD	-2.76	108.04	112.67
3	C	142	HEM	CMC-C2C-C3C	2.67	129.68	124.68
3	A	142	HEM	CMC-C2C-C3C	-2.67	119.69	124.68
3	D	146	HEM	CMB-C2B-C3B	2.52	129.39	124.68
3	B	146	HEM	CMD-C2D-C1D	2.43	132.20	128.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	146	HEM	C2D-C3D-CAD-CBD
3	B	146	HEM	C4D-C3D-CAD-CBD

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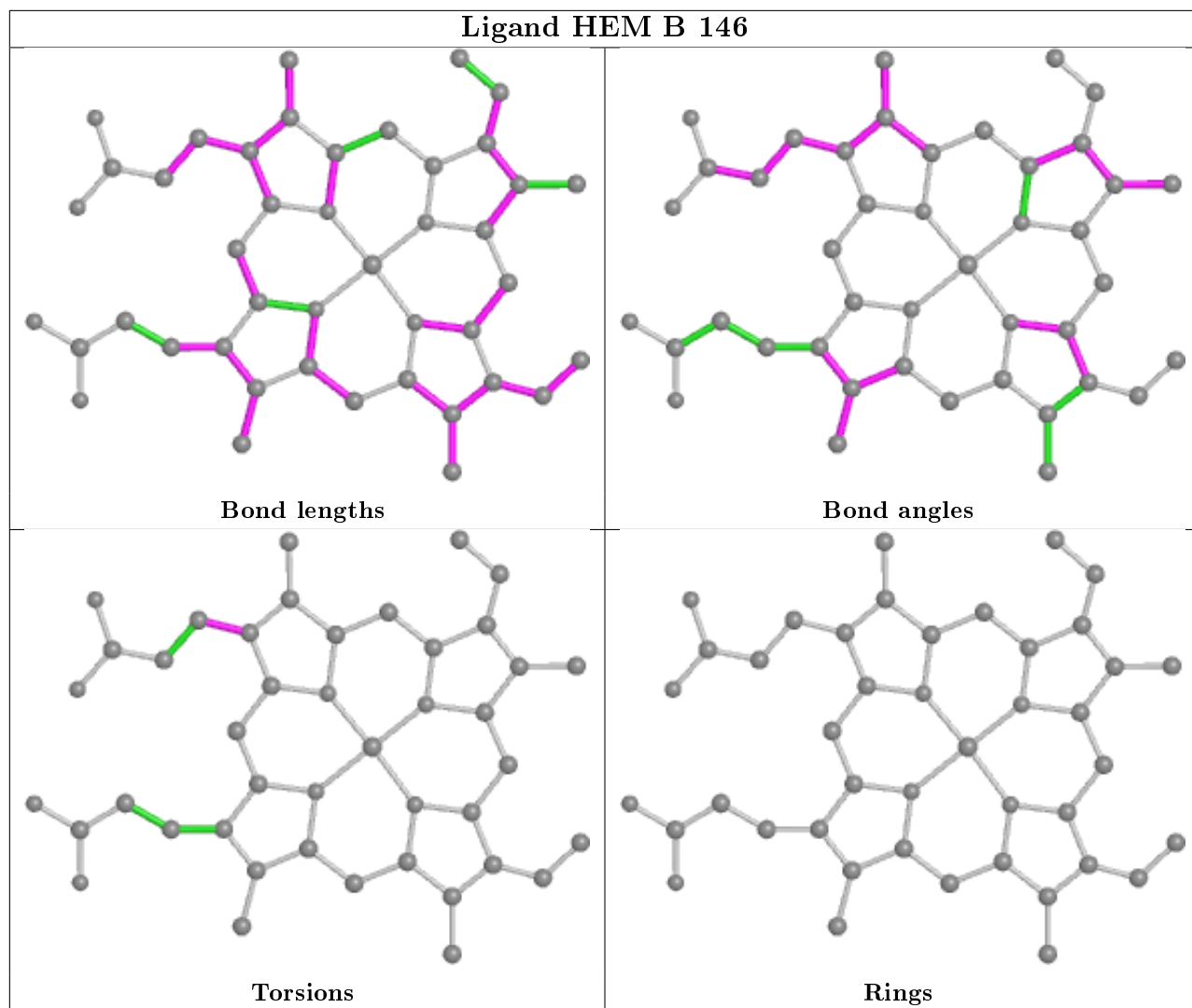
Mol	Chain	Res	Type	Atoms
3	D	146	HEM	C1A-C2A-CAA-CBA
3	D	146	HEM	C3A-C2A-CAA-CBA
3	D	146	HEM	C3D-CAD-CBD-CGD
3	A	142	HEM	C1A-C2A-CAA-CBA
3	A	142	HEM	C3A-C2A-CAA-CBA
3	C	142	HEM	C4D-C3D-CAD-CBD

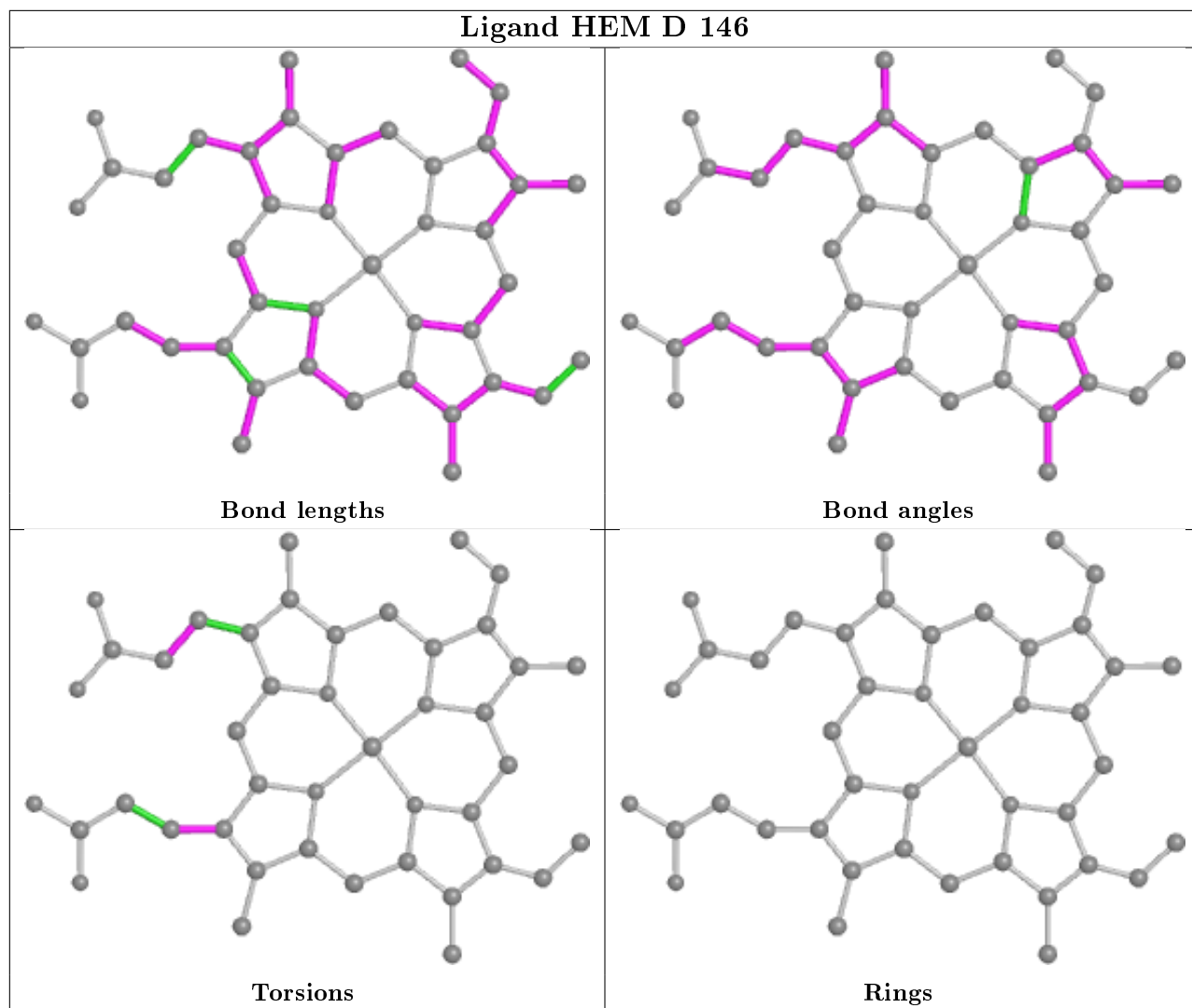
There are no ring outliers.

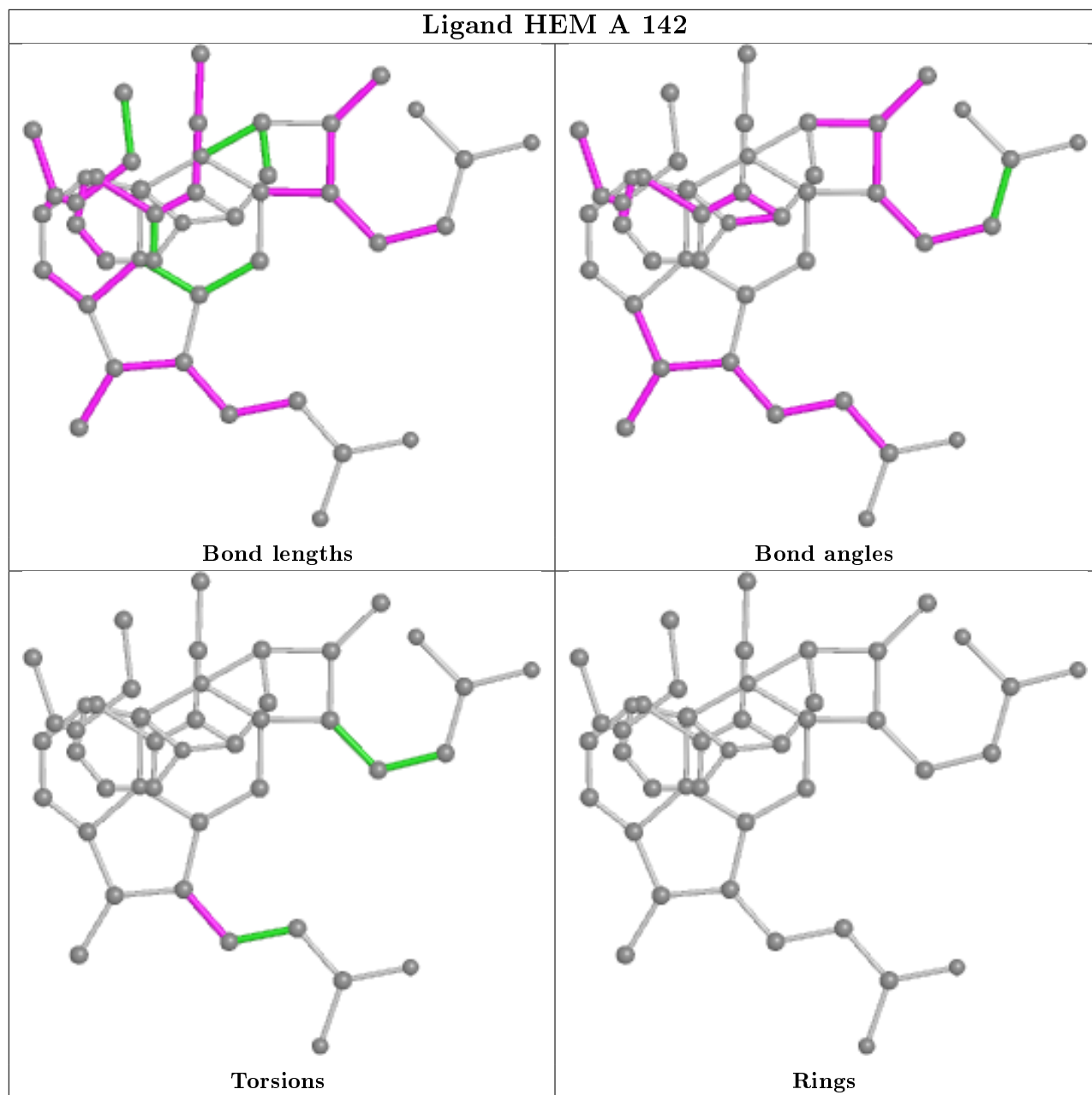
4 monomers are involved in 176 short contacts:

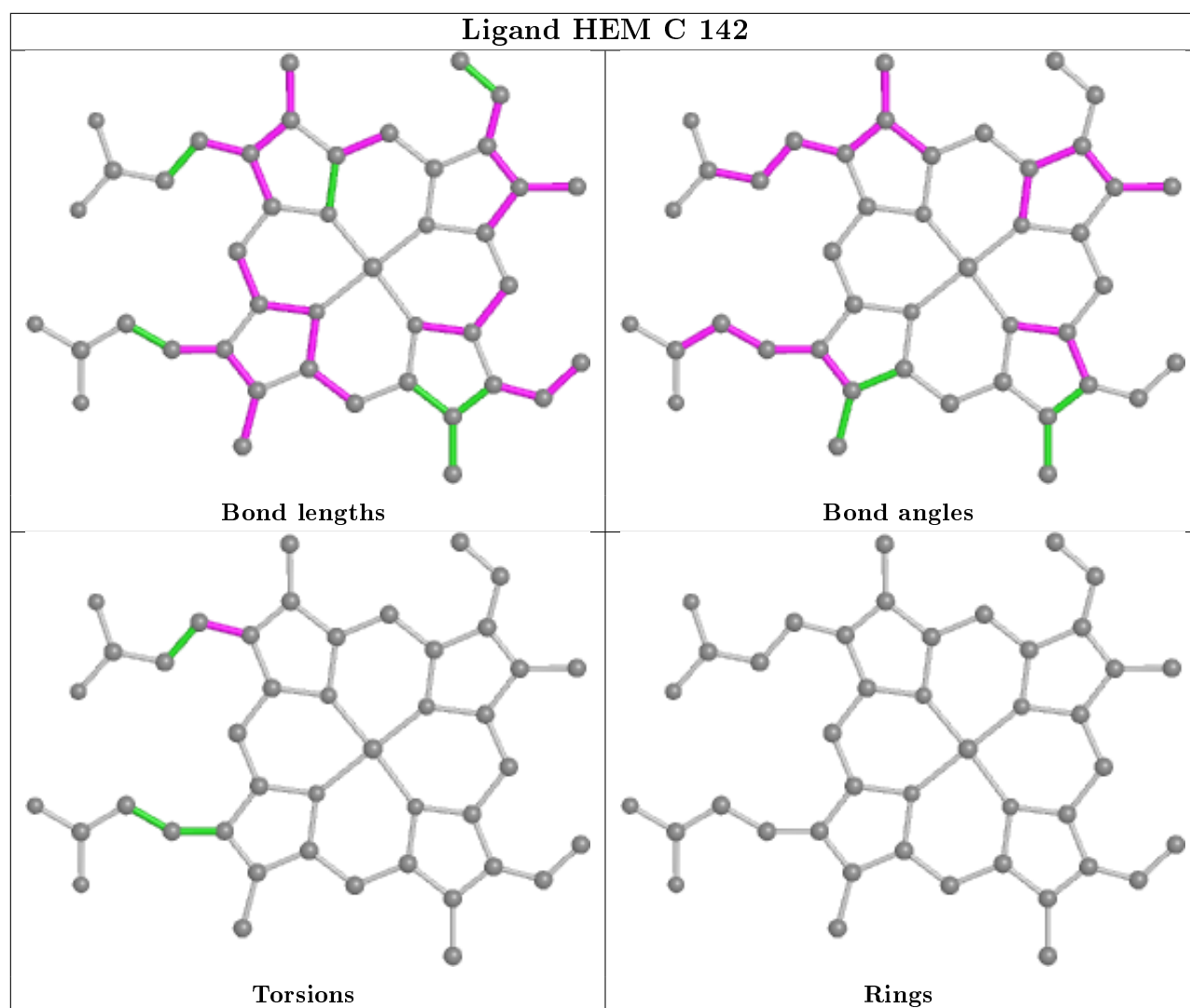
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	146	HEM	56	0
3	D	146	HEM	29	0
3	A	142	HEM	49	0
3	C	142	HEM	42	0

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









5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	53
1	A	51
2	B	47
1	C	47

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	98:PHE	C	99:LYS	N	1.99
1	B	42:GLN	C	43:HIS	N	1.93
1	D	51:GLY	C	52:ALA	N	1.87
1	B	41:PHE	C	42:GLN	N	1.85
1	C	74:ASN	C	75:ASP	N	1.84
1	D	41:PHE	C	42:GLN	N	1.83
1	A	31:ARG	C	32:MET	N	1.81
1	A	43:PHE	C	44:PRO	N	1.78
1	B	55:ASN	C	56:ASN	N	1.78
1	C	102:SER	C	103:HIS	N	1.78
1	A	16:LYS	C	17:VAL	N	1.76
1	C	36:PHE	C	37:PRO	N	1.76
1	C	6:ASN	C	7:LYS	N	1.75
1	B	110:ALA	C	111:LEU	N	1.74
1	C	121:VAL	C	122:HIS	N	1.74
1	A	42:TYR	C	43:PHE	N	1.73
1	A	58:HIS	C	59:GLY	N	1.71
1	B	58:LYS	C	59:VAL	N	1.71
1	B	80:LEU	C	81:LYS	N	1.71
1	C	20:ASN	C	21:ALA	N	1.71
1	D	116:ASN	C	117:PHE	N	1.71
1	D	141:ALA	C	142:HIS	N	1.71
1	D	20:ASP	C	21:VAL	N	1.70
1	A	11:LYS	C	12:ALA	N	1.69
1	A	32:MET	C	33:PHE	N	1.69
1	A	119:PRO	C	120:ALA	N	1.69
1	A	77:PRO	C	78:GLY	N	1.68
1	A	86:LEU	C	87:HIS	N	1.68
1	B	124:ASN	C	125:VAL	N	1.68
1	B	141:ALA	C	142:HIS	N	1.68
1	C	33:PHE	C	34:LEU	N	1.67
1	B	102:PHE	C	103:ARG	N	1.66
1	B	139:ALA	C	140:LEU	N	1.66
1	C	28:ALA	C	29:LEU	N	1.66
1	D	13:PHE	C	14:TRP	N	1.66
1	A	2:LEU	C	3:SER	N	1.65
1	C	113:LEU	C	114:PRO	N	1.65
1	D	73:GLY	C	74:LEU	N	1.65
1	A	12:ALA	C	13:ALA	N	1.64
1	B	92:CYS	C	93:ASN	N	1.64
1	C	10:VAL	C	11:LYS	N	1.64
1	C	81:SER	C	82:ASN	N	1.64
1	C	111:SER	C	112:HIS	N	1.64

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	51:GLY	C	52:ALA	N	1.63
1	B	56:ASN	C	57:PRO	N	1.63
1	A	40:LYS	C	41:THR	N	1.62
1	B	99:PRO	C	100:GLN	N	1.62
1	D	10:VAL	C	11:THR	N	1.62
1	D	131:LYS	C	132:VAL	N	1.62
1	A	87:HIS	C	88:ALA	N	1.61
1	A	112:HIS	C	113:LEU	N	1.61
1	A	121:VAL	C	122:HIS	N	1.61
1	D	54:MET	C	55:ASN	N	1.61
1	D	115:ARG	C	116:ASN	N	1.61
1	A	70:GLN	C	71:GLY	N	1.60
1	A	3:SER	C	4:ALA	N	1.20
1	A	91:LEU	C	92:ARG	N	1.20
1	A	106:LEU	C	107:VAL	N	1.20
1	A	139:LYS	C	140:TYR	N	1.20
1	B	7:LYS	C	8:ALA	N	1.20
1	C	3:SER	C	4:ALA	N	1.20
1	A	28:ALA	C	29:LEU	N	1.19
1	A	109:LEU	C	110:ALA	N	1.19
1	A	131:ASN	C	132:ASP	N	1.19
1	B	67:LEU	C	68:ASP	N	1.19
1	C	62:VAL	C	63:ALA	N	1.19
1	C	133:SER	C	134:THR	N	1.19
1	D	34:TYR	C	35:PRO	N	1.19
1	D	35:PRO	C	36:TRP	N	1.19
1	D	85:ALA	C	86:GLN	N	1.19
1	C	78:GLY	C	79:THR	N	1.18
1	C	131:ASN	C	132:ASP	N	1.18
1	D	56:ASN	C	57:PRO	N	1.18
1	D	71:THR	C	72:GLN	N	1.18
1	D	110:ALA	C	111:LEU	N	1.18
1	D	127:ALA	C	128:LEU	N	1.18
1	A	39:THR	C	40:LYS	N	1.17
1	A	74:ASN	C	75:ASP	N	1.17
1	A	132:ASP	C	133:SER	N	1.17
1	B	77:LEU	C	78:ASP	N	1.17
1	D	57:PRO	C	58:LYS	N	1.17
1	A	45:HIS	C	46:PHE	N	1.16
1	A	107:VAL	C	108:THR	N	1.16
1	B	125:VAL	C	126:GLN	N	1.16
1	B	143:LYS	C	144:TYR	N	1.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	13:ALA	C	14:TRP	N	1.16
1	C	19:GLY	C	20:ASN	N	1.16
1	D	109:LEU	C	110:ALA	N	1.16
1	A	59:GLY	C	60:GLN	N	1.15
1	B	27:LEU	C	28:GLY	N	1.15
1	C	35:SER	C	36:PHE	N	1.15
1	C	129:LEU	C	130:ALA	N	1.15
1	A	37:PRO	C	38:THR	N	1.14
1	B	93:ASN	C	94:LYS	N	1.14
1	B	101:ASN	C	102:PHE	N	1.14
1	B	104:LEU	C	105:LEU	N	1.14
1	C	107:VAL	C	108:THR	N	1.14
1	C	134:THR	C	135:VAL	N	1.14
1	C	137:THR	C	138:SER	N	1.14
1	D	19:VAL	C	20:ASP	N	1.14
1	D	44:PHE	C	45:GLY	N	1.14
1	D	132:VAL	C	133:VAL	N	1.14
1	A	103:HIS	C	104:SER	N	1.13
1	A	122:HIS	C	123:ALA	N	1.13
1	B	71:THR	C	72:GLN	N	1.13
1	B	116:ASN	C	117:PHE	N	1.13
1	B	130:GLN	C	131:LYS	N	1.13
1	C	47:ASP	C	48:LEU	N	1.13
1	C	60:GLN	C	61:LYS	N	1.13
1	D	2:LEU	C	3:THR	N	1.13
1	D	31:LEU	C	32:VAL	N	1.13
1	A	44:PRO	C	45:HIS	N	1.12
1	A	83:LEU	C	84:SER	N	1.12
1	A	134:THR	C	135:VAL	N	1.12
1	B	34:TYR	C	35:PRO	N	1.12
1	C	69:ALA	C	70:GLN	N	1.12
1	C	101:LEU	C	102:SER	N	1.12
1	C	126:ASN	C	127:LYS	N	1.12
1	C	136:LEU	C	137:THR	N	1.12
1	D	32:VAL	C	33:VAL	N	1.12
1	A	10:VAL	C	11:LYS	N	1.11
1	A	14:TRP	C	15:GLY	N	1.11
1	A	99:LYS	C	100:LEU	N	1.11
1	B	23:GLY	C	24:ALA	N	1.11
1	B	38:GLN	C	39:ARG	N	1.11
1	D	100:GLN	C	101:ASN	N	1.11
1	A	73:LEU	C	74:ASN	N	1.10

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	5:GLU	C	6:GLU	N	1.10
1	C	61:LYS	C	62:VAL	N	1.10
1	C	88:ALA	C	89:HIS	N	1.10
1	C	132:ASP	C	133:SER	N	1.10
1	D	95:LEU	C	96:HIS	N	1.10
1	D	97:VAL	C	98:ASN	N	1.10
1	B	136:VAL	C	137:ALA	N	1.09
1	C	42:TYR	C	43:PHE	N	1.09
1	C	58:HIS	C	59:GLY	N	1.09
1	D	102:PHE	C	103:ARG	N	1.09
1	B	118:GLY	C	119:GLY	N	1.08
1	C	115:THR	C	116:ASN	N	1.08
1	D	50:ALA	C	51:GLY	N	1.08
1	A	55:GLN	C	56:LYS	N	1.07
1	A	60:GLN	C	61:LYS	N	1.07
1	A	116:ASN	C	117:PHE	N	1.07
1	C	128:PHE	C	129:LEU	N	1.07
1	D	15:GLY	C	16:LYS	N	1.07
1	B	53:VAL	C	54:MET	N	1.06
1	C	108:THR	C	109:LEU	N	1.06
1	D	88:SER	C	89:GLY	N	1.05
1	D	104:LEU	C	105:LEU	N	1.05
1	A	68:LYS	C	69:ALA	N	1.04
1	B	33:VAL	C	34:TYR	N	1.04
1	B	115:ARG	C	116:ASN	N	1.04
1	C	93:VAL	C	94:ASN	N	1.04
1	A	21:ALA	C	22:PRO	N	1.03
1	B	66:VAL	C	67:LEU	N	1.03
1	B	133:VAL	C	134:ALA	N	1.03
1	D	67:LEU	C	68:ASP	N	1.03
1	D	114:ALA	C	115:ARG	N	1.03
1	D	7:LYS	C	8:ALA	N	1.02
1	D	68:ASP	C	69:ALA	N	1.02
1	C	17:VAL	C	18:GLY	N	1.01
1	D	4:ALA	C	5:GLU	N	1.01
1	A	126:ASN	C	127:LYS	N	1.00
1	B	72:GLN	C	73:GLY	N	1.00
1	D	46:ASN	C	47:LEU	N	1.00
1	D	70:PHE	C	71:THR	N	1.00
1	A	78:GLY	C	79:THR	N	0.99
1	B	25:GLN	C	26:ALA	N	0.99
1	B	142:HIS	C	143:LYS	N	0.99

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	40:LYS	C	41:THR	N	0.99
1	C	116:ASN	C	117:PHE	N	0.99
1	D	14:TRP	C	15:GLY	N	0.99
1	D	137:ALA	C	138:ASN	N	0.99
1	A	7:LYS	C	8:SER	N	0.98
1	A	81:SER	C	82:ASN	N	0.98
1	B	1:MET	C	2:LEU	N	0.98
1	C	59:GLY	C	60:GLN	N	0.98
1	D	6:GLU	C	7:LYS	N	0.98
1	D	39:ARG	C	40:PHE	N	0.98
1	C	110:ALA	C	111:SER	N	0.97
1	D	63:GLY	C	64:LYS	N	0.97
1	D	55:ASN	C	56:ASN	N	0.96
1	D	89:GLY	C	90:LEU	N	0.96
1	A	67:THR	C	68:LYS	N	0.95
1	B	109:LEU	C	110:ALA	N	0.95
1	D	28:GLY	C	29:ARG	N	0.95
1	B	82:GLY	C	83:ALA	N	0.94
1	B	128:LEU	C	129:PHE	N	0.94
1	C	83:LEU	C	84:SER	N	0.94
1	D	42:GLN	C	43:HIS	N	0.94
1	D	65:ARG	C	66:VAL	N	0.93
1	B	19:VAL	C	20:ASP	N	0.92
1	B	45:GLY	C	46:ASN	N	0.92
1	D	94:LYS	C	95:LEU	N	0.92
1	B	74:LEU	C	75:LYS	N	0.91
1	C	117:PHE	C	118:THR	N	0.90
1	D	111:LEU	C	112:VAL	N	0.84
1	A	127:LYS	C	128:PHE	N	0.82

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.