



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2021 – 08:01 PM EDT

PDB ID : 4HHB
Title : THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT
1.74 ANGSTROMS RESOLUTION
Authors : Fermi, G.; Perutz, M.F.
Deposited on : 1984-03-07
Resolution : 1.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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) : 2.17.1

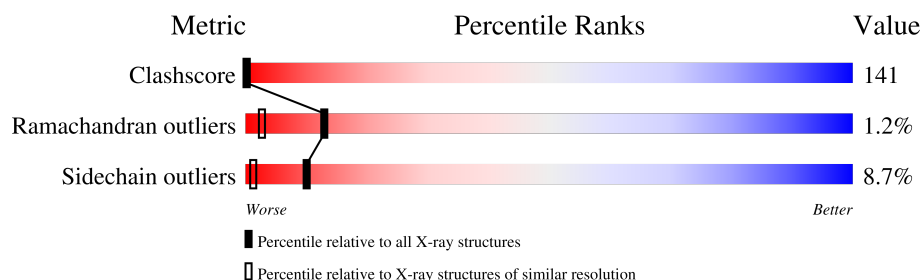
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 Å.





Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	
1	C	141	
2	B	146	
2	D	146	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4779 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemoglobin subunit alpha.

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

- Molecule 2 is a protein called Hemoglobin subunit beta.

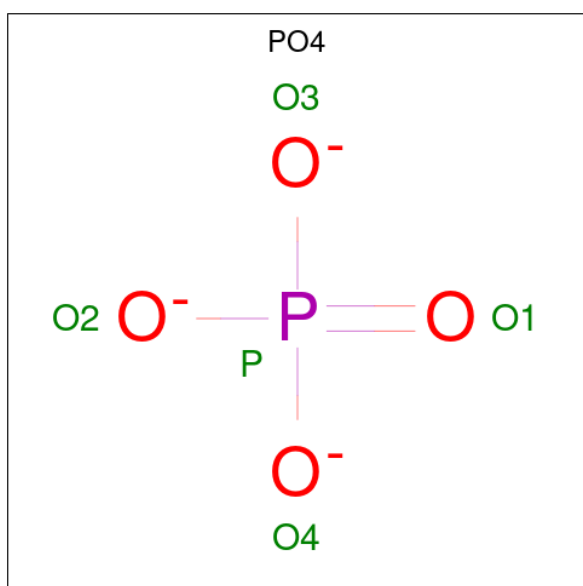
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (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	
			43	34	1	4	4	
3	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

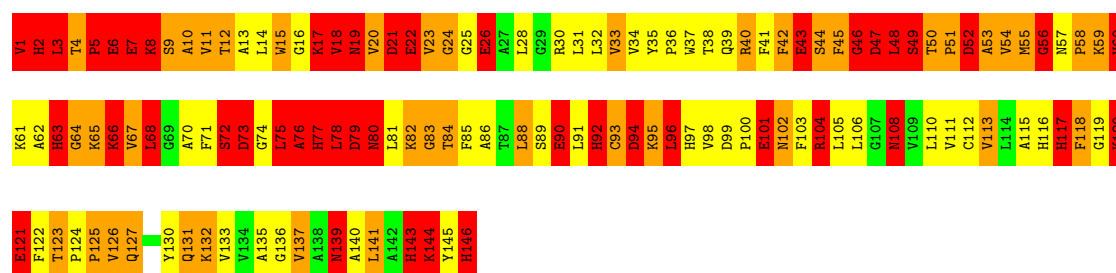


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	P		
			1	1	0	0
4	D	1	Total	P		
			1	1	0	0

- Molecule 5 is water.

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

Chain D: 8% 32% 28% 32%



4 Data and refinement statistics

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

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PO4

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	8.18	370/1097 (33.7%)	6.34	444/1491 (29.8%)
1	C	8.79	358/1097 (32.6%)	7.51	407/1491 (27.3%)
2	B	10.84	417/1153 (36.2%)	6.61	446/1566 (28.5%)
2	D	10.56	436/1153 (37.8%)	7.83	525/1566 (33.5%)
All	All	9.69	1581/4500 (35.1%)	7.11	1822/6114 (29.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	51
1	C	2	45
2	B	2	49
2	D	5	62
All	All	10	207

All (1581) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	GLU	CD-OE1	143.13	2.83	1.25
1	C	92	ARG	NE-CZ	126.10	2.96	1.33
2	D	6	GLU	CD-OE2	121.79	2.59	1.25
2	B	26	GLU	CD-OE2	106.90	2.43	1.25
1	C	23	GLU	CD-OE1	101.97	2.37	1.25
2	D	104	ARG	NE-CZ	96.15	2.58	1.33
1	A	92	ARG	NE-CZ	95.65	2.57	1.33
2	B	22	GLU	CD-OE2	78.69	2.12	1.25
2	B	104	ARG	NE-CZ	61.72	2.13	1.33
2	D	90	GLU	CG-CD	60.86	2.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	43	GLU	CG-CD	60.66	2.42	1.51
2	D	22	GLU	CG-CD	58.05	2.39	1.51
2	B	121	GLU	CD-OE1	56.01	1.87	1.25
2	D	52	ASP	CG-OD2	51.95	2.44	1.25
2	D	2	HIS	CG-ND1	49.81	2.48	1.38
2	B	104	ARG	CZ-NH2	49.80	1.97	1.33
2	D	26	GLU	CD-OE1	48.92	1.79	1.25
1	A	60	LYS	CE-NZ	47.93	2.68	1.49
1	A	90	LYS	CE-NZ	47.25	2.67	1.49
2	B	22	GLU	CD-OE1	46.75	1.77	1.25
1	C	1	VAL	CB-CG2	45.68	2.48	1.52
2	B	65	LYS	CE-NZ	44.03	2.59	1.49
2	D	73	ASP	CG-OD2	43.88	2.26	1.25
1	C	1	VAL	N-CA	43.63	2.33	1.46
1	C	116	GLU	CB-CG	42.97	2.33	1.52
1	C	23	GLU	CG-CD	42.51	2.15	1.51
1	A	23	GLU	CD-OE1	42.41	1.72	1.25
2	B	104	ARG	CZ-NH1	42.02	1.87	1.33
1	C	92	ARG	CZ-NH1	41.72	1.87	1.33
2	D	26	GLU	CD-OE2	41.28	1.71	1.25
1	C	30	GLU	CD-OE2	-41.18	0.80	1.25
2	B	2	HIS	CG-CD2	41.11	2.05	1.35
1	C	138	SER	CA-CB	40.95	2.14	1.52
2	D	22	GLU	CB-CG	-40.05	0.76	1.52
2	D	132	LYS	CE-NZ	39.97	2.48	1.49
1	A	75	ASP	CB-CG	-39.80	0.68	1.51
1	A	138	SER	CA-CB	39.62	2.12	1.52
2	D	43	GLU	CB-CG	-38.94	0.78	1.52
2	D	5	PRO	CA-CB	38.90	2.31	1.53
1	A	23	GLU	CG-CD	38.85	2.10	1.51
2	D	58	PRO	CG-CD	-38.65	0.23	1.50
2	B	117	HIS	CD2-NE2	37.97	2.21	1.42
1	A	78	ASN	CG-OD1	37.90	2.07	1.24
2	B	6	GLU	CD-OE1	37.86	1.67	1.25
2	B	6	GLU	CG-CD	36.95	2.07	1.51
2	B	121	GLU	CG-CD	36.90	2.07	1.51
2	B	2	HIS	CB-CG	-36.83	0.83	1.50
2	B	139	ASN	CB-CG	-36.83	0.66	1.51
2	B	43	GLU	CD-OE1	-36.77	0.85	1.25
2	B	90	GLU	CG-CD	36.68	2.06	1.51
2	D	101	GLU	CG-CD	36.62	2.06	1.51
1	A	92	ARG	CZ-NH2	-36.39	0.85	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	82	LYS	CD-CE	36.28	2.42	1.51
1	C	56	LYS	CD-CE	35.42	2.39	1.51
2	D	90	GLU	CD-OE1	35.18	1.64	1.25
2	B	65	LYS	CB-CG	-34.95	0.58	1.52
2	D	26	GLU	CB-CG	34.81	2.18	1.52
2	D	47	ASP	CA-C	34.66	2.43	1.52
1	C	23	GLU	CD-OE2	-34.47	0.87	1.25
2	B	82	LYS	CE-NZ	34.42	2.35	1.49
2	B	66	LYS	CD-CE	34.36	2.37	1.51
1	A	75	ASP	CG-OD2	34.26	2.04	1.25
2	B	59	LYS	CD-CE	34.19	2.36	1.51
2	B	101	GLU	CG-CD	33.84	2.02	1.51
2	B	65	LYS	CD-CE	33.62	2.35	1.51
2	B	2	HIS	ND1-CE1	33.32	2.18	1.34
1	C	1	VAL	CB-CG1	33.07	2.22	1.52
2	D	121	GLU	CG-CD	32.89	2.01	1.51
1	A	30	GLU	CG-CD	32.43	2.00	1.51
2	B	82	LYS	CD-CE	-32.40	0.70	1.51
2	D	120	LYS	CE-NZ	32.27	2.29	1.49
2	D	79	ASP	CG-OD1	32.20	1.99	1.25
2	B	2	HIS	CD2-NE2	32.02	2.09	1.42
2	D	79	ASP	CG-OD2	31.85	1.98	1.25
1	A	81	SER	CA-CB	31.84	2.00	1.52
2	D	43	GLU	CD-OE1	31.82	1.60	1.25
2	B	8	LYS	CE-NZ	31.50	2.27	1.49
2	D	47	ASP	N-CA	31.42	2.09	1.46
2	D	2	HIS	CA-CB	30.88	2.21	1.53
2	B	146	HIS	CB-CG	30.49	2.04	1.50
2	D	6	GLU	CB-CG	-30.44	0.94	1.52
2	D	66	LYS	CD-CE	30.42	2.27	1.51
2	D	6	GLU	CG-CD	30.34	1.97	1.51
2	D	43	GLU	CD-OE2	30.30	1.58	1.25
2	B	90	GLU	CD-OE1	-30.12	0.92	1.25
1	C	99	LYS	CD-CE	30.11	2.26	1.51
2	D	6	GLU	CA-C	30.01	2.31	1.52
1	A	127	LYS	CB-CG	-29.93	0.71	1.52
1	C	30	GLU	CG-CD	29.51	1.96	1.51
2	B	49	SER	C-O	29.47	1.79	1.23
1	A	92	ARG	CG-CD	29.45	2.25	1.51
2	D	2	HIS	CG-CD2	29.45	1.85	1.35
2	D	143	HIS	CG-CD2	29.09	1.85	1.35
1	C	99	LYS	CB-CG	-28.97	0.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	LYS	CD-CE	28.72	2.23	1.51
1	A	99	LYS	CE-NZ	28.60	2.20	1.49
2	B	65	LYS	CG-CD	28.60	2.49	1.52
2	B	12	THR	CB-CG2	-28.55	0.58	1.52
2	D	6	GLU	CD-OE1	-28.52	0.94	1.25
2	B	77	HIS	CG-CD2	28.39	1.84	1.35
2	D	3	LEU	C-O	28.24	1.77	1.23
2	D	65	LYS	CD-CE	27.80	2.20	1.51
1	A	61	LYS	CD-CE	-27.73	0.81	1.51
2	B	139	ASN	CG-ND2	27.55	2.01	1.32
2	B	6	GLU	CD-OE2	-27.46	0.95	1.25
1	A	15	GLY	C-O	27.29	1.67	1.23
2	D	144	LYS	CE-NZ	27.14	2.16	1.49
1	A	78	ASN	CB-CG	-27.09	0.88	1.51
2	D	146	HIS	ND1-CE1	-27.02	0.67	1.34
2	D	43	GLU	CG-CD	26.84	1.92	1.51
1	C	92	ARG	CZ-NH2	-26.47	0.98	1.33
2	D	20	VAL	CA-CB	26.29	2.10	1.54
1	C	40	LYS	CD-CE	-26.26	0.85	1.51
2	D	26	GLU	CG-CD	25.76	1.90	1.51
2	B	143	HIS	ND1-CE1	25.75	1.99	1.34
2	D	45	PHE	C-N	-25.51	0.87	1.33
2	B	117	HIS	CG-ND1	25.44	1.94	1.38
1	A	17	VAL	C-O	-25.43	0.75	1.23
2	D	2	HIS	CE1-NE2	25.33	1.91	1.32
2	B	6	GLU	CB-CG	-25.27	1.04	1.52
2	B	7	GLU	CA-CB	-25.13	0.98	1.53
2	B	1	VAL	C-O	24.89	1.70	1.23
2	D	2	HIS	CB-CG	-24.75	1.05	1.50
1	A	75	ASP	CG-OD1	24.71	1.82	1.25
1	A	49	SER	CB-OG	-24.50	1.10	1.42
2	B	5	PRO	N-CD	24.22	1.81	1.47
2	B	8	LYS	CB-CG	-24.20	0.87	1.52
1	C	49	SER	CB-OG	-24.15	1.10	1.42
2	D	121	GLU	CD-OE1	24.11	1.52	1.25
2	D	76	ALA	N-CA	24.06	1.94	1.46
1	A	96	VAL	CB-CG2	-24.05	1.02	1.52
2	B	1	VAL	CB-CG1	24.01	2.03	1.52
2	B	1	VAL	C-N	-23.87	0.79	1.34
2	B	43	GLU	CD-OE2	23.53	1.51	1.25
1	C	46	PHE	CD2-CE2	-23.52	0.92	1.39
2	B	47	ASP	CG-OD2	23.25	1.78	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	LYS	CE-NZ	23.11	2.06	1.49
2	B	121	GLU	CB-CG	-22.88	1.08	1.52
2	B	2	HIS	CG-ND1	22.82	1.89	1.38
2	D	121	GLU	CB-CG	-22.68	1.09	1.52
2	B	22	GLU	CG-CD	22.64	1.85	1.51
1	C	92	ARG	CD-NE	-22.63	1.07	1.46
2	D	77	HIS	ND1-CE1	22.61	1.91	1.34
2	B	45	PHE	CG-CD2	-22.55	1.04	1.38
2	D	2	HIS	ND1-CE1	22.27	1.90	1.34
2	D	50	THR	CA-CB	22.26	2.11	1.53
2	B	49	SER	CB-OG	22.20	1.71	1.42
2	D	104	ARG	CD-NE	22.18	1.84	1.46
2	D	77	HIS	CD2-NE2	22.18	1.88	1.42
1	C	56	LYS	CG-CD	21.99	2.27	1.52
2	D	65	LYS	CG-CD	21.96	2.27	1.52
2	B	58	PRO	N-CD	21.93	1.78	1.47
1	A	14	TRP	CG-CD1	21.88	1.67	1.36
1	A	50	HIS	CA-CB	21.85	2.02	1.53
2	D	5	PRO	N-CA	21.80	1.84	1.47
2	B	2	HIS	CA-CB	21.68	2.01	1.53
1	A	85	ASP	CG-OD1	-21.66	0.75	1.25
1	A	18	GLY	CA-C	21.65	1.86	1.51
1	A	21	ALA	CA-C	21.59	2.09	1.52
2	B	1	VAL	CA-C	21.57	2.09	1.52
2	D	21	ASP	CA-C	-21.48	0.97	1.52
1	C	15	GLY	C-O	21.34	1.57	1.23
2	D	146	HIS	CG-ND1	21.18	1.85	1.38
1	C	60	LYS	CE-NZ	21.16	2.02	1.49
1	A	72	HIS	CG-ND1	21.11	1.85	1.38
1	A	64	ASP	CB-CG	21.03	1.96	1.51
1	A	85	ASP	CG-OD2	20.96	1.73	1.25
2	D	8	LYS	CD-CE	20.93	2.03	1.51
2	B	49	SER	CA-CB	20.58	1.83	1.52
1	C	14	TRP	CZ3-CH2	20.53	1.72	1.40
1	A	50	HIS	C-N	-20.39	0.96	1.33
2	B	144	LYS	CE-NZ	20.24	1.99	1.49
2	B	42	PHE	CG-CD1	20.19	1.69	1.38
2	D	139	ASN	CG-OD1	20.14	1.68	1.24
2	D	42	PHE	CG-CD1	20.11	1.69	1.38
2	D	95	LYS	CE-NZ	20.00	1.99	1.49
2	B	144	LYS	CD-CE	19.96	2.01	1.51
1	A	75	ASP	CA-CB	19.91	1.97	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	146	HIS	ND1-CE1	19.85	1.84	1.34
2	D	17	LYS	CE-NZ	19.82	1.98	1.49
1	A	22	GLY	CA-C	-19.78	1.20	1.51
2	D	9	SER	CB-OG	-19.77	1.16	1.42
1	A	96	VAL	CB-CG1	-19.71	1.11	1.52
1	A	74	ASP	CG-OD1	-19.67	0.80	1.25
1	C	61	LYS	CE-NZ	19.65	1.98	1.49
2	D	13	ALA	CA-CB	-19.60	1.11	1.52
1	A	84	SER	CA-CB	19.59	1.82	1.52
1	C	22	GLY	CA-C	-19.50	1.20	1.51
2	D	4	THR	C-N	-19.46	0.97	1.34
1	A	24	TYR	CE1-CZ	-19.36	1.13	1.38
2	D	80	ASN	CG-OD1	19.27	1.66	1.24
2	D	7	GLU	CD-OE1	19.26	1.46	1.25
2	D	46	GLY	CA-C	19.23	1.82	1.51
1	C	114	PRO	CA-C	19.07	1.91	1.52
2	D	1	VAL	CA-C	19.05	2.02	1.52
2	D	95	LYS	CG-CD	18.98	2.17	1.52
2	D	7	GLU	CB-CG	18.89	1.88	1.52
2	B	45	PHE	CE1-CZ	-18.81	1.01	1.37
1	A	139	LYS	CE-NZ	18.78	1.96	1.49
1	C	72	HIS	CG-ND1	18.76	1.80	1.38
2	B	44	SER	CB-OG	-18.63	1.18	1.42
2	D	66	LYS	CE-NZ	18.57	1.95	1.49
2	D	47	ASP	CA-CB	18.49	1.94	1.53
1	A	14	TRP	CD2-CE2	18.40	1.63	1.41
2	B	79	ASP	CG-OD2	18.34	1.67	1.25
2	B	146	HIS	CG-ND1	-18.29	0.98	1.38
2	D	82	LYS	CE-NZ	18.27	1.94	1.49
1	C	84	SER	CB-OG	-18.21	1.18	1.42
1	A	15	GLY	C-N	-18.19	0.92	1.34
1	A	11	LYS	CD-CE	18.16	1.96	1.51
1	C	116	GLU	CD-OE2	18.14	1.45	1.25
1	C	112	HIS	CG-ND1	18.10	1.78	1.38
2	B	9	SER	N-CA	-18.09	1.10	1.46
2	D	8	LYS	CE-NZ	18.03	1.94	1.49
1	A	14	TRP	NE1-CE2	-18.00	1.14	1.37
2	D	101	GLU	CD-OE2	17.94	1.45	1.25
2	B	40	ARG	CZ-NH2	17.86	1.56	1.33
1	A	74	ASP	C-N	-17.86	0.93	1.34
2	B	117	HIS	CG-CD2	17.86	1.66	1.35
1	C	84	SER	CA-CB	17.82	1.79	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	20	VAL	CB-CG1	-17.81	1.15	1.52
1	C	139	LYS	CD-CE	17.80	1.95	1.51
2	D	53	ALA	C-O	-17.74	0.89	1.23
1	C	20	HIS	ND1-CE1	17.71	1.79	1.34
1	A	99	LYS	CD-CE	17.55	1.95	1.51
2	B	9	SER	CA-CB	17.51	1.79	1.52
2	D	76	ALA	CA-C	-17.40	1.07	1.52
2	B	59	LYS	CE-NZ	17.34	1.92	1.49
1	A	46	PHE	CG-CD2	-17.27	1.12	1.38
2	D	22	GLU	CD-OE1	17.19	1.44	1.25
2	D	78	LEU	CG-CD2	-17.10	0.88	1.51
1	C	11	LYS	CE-NZ	17.09	1.91	1.49
1	A	60	LYS	CD-CE	17.00	1.93	1.51
1	A	67	THR	CB-OG1	-16.96	1.09	1.43
1	A	37	PRO	N-CD	-16.94	1.24	1.47
1	C	74	ASP	C-O	-16.90	0.91	1.23
2	D	58	PRO	N-CD	16.84	1.71	1.47
2	D	1	VAL	CB-CG2	-16.76	1.17	1.52
2	B	76	ALA	C-O	-16.68	0.91	1.23
2	D	83	GLY	C-O	16.67	1.50	1.23
2	B	5	PRO	N-CA	-16.64	1.19	1.47
2	D	20	VAL	CB-CG2	-16.62	1.18	1.52
1	A	17	VAL	CA-C	16.61	1.96	1.52
1	A	116	GLU	CD-OE2	16.55	1.43	1.25
2	D	19	ASN	CG-OD1	16.47	1.60	1.24
1	A	16	LYS	CD-CE	16.40	1.92	1.51
2	D	2	HIS	C-O	16.37	1.54	1.23
1	C	105	LEU	CG-CD2	16.34	2.12	1.51
2	D	144	LYS	CD-CE	-16.26	1.10	1.51
2	B	117	HIS	ND1-CE1	16.21	1.75	1.34
2	D	117	HIS	CG-ND1	16.13	1.74	1.38
2	B	87	THR	CA-CB	16.13	1.95	1.53
2	B	79	ASP	CB-CG	-16.08	1.18	1.51
2	B	124	PRO	N-CD	16.08	1.70	1.47
2	D	59	LYS	CG-CD	-16.07	0.97	1.52
2	B	146	HIS	CG-CD2	16.06	1.63	1.35
2	D	43	GLU	CA-CB	-16.02	1.18	1.53
2	D	66	LYS	CG-CD	15.99	2.06	1.52
1	C	90	LYS	CD-CE	15.99	1.91	1.51
2	D	73	ASP	C-N	15.96	1.61	1.33
1	A	99	LYS	CB-CG	-15.95	1.09	1.52
2	B	74	GLY	C-N	15.91	1.70	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	145	TYR	C-N	-15.90	0.97	1.34
2	B	139	ASN	CG-OD1	15.86	1.58	1.24
2	D	43	GLU	CA-C	15.86	1.94	1.52
2	B	132	LYS	CE-NZ	15.84	1.88	1.49
1	A	56	LYS	CG-CD	15.83	2.06	1.52
1	C	72	HIS	CG-CD2	15.72	1.62	1.35
2	B	40	ARG	NE-CZ	15.64	1.53	1.33
1	C	72	HIS	CB-CG	-15.59	1.22	1.50
2	D	66	LYS	CB-CG	-15.54	1.10	1.52
1	A	131	SER	CB-OG	-15.53	1.22	1.42
1	A	137	THR	CB-CG2	-15.50	1.01	1.52
2	D	1	VAL	N-CA	15.50	1.77	1.46
2	D	19	ASN	CG-ND2	15.49	1.71	1.32
2	B	21	ASP	CB-CG	15.47	1.84	1.51
2	B	145	TYR	CD2-CE2	15.46	1.62	1.39
1	A	99	LYS	CG-CD	-15.38	1.00	1.52
2	D	12	THR	CA-CB	15.36	1.93	1.53
2	D	117	HIS	CE1-NE2	-15.32	0.97	1.32
1	C	16	LYS	CB-CG	15.31	1.93	1.52
2	D	130	TYR	CE1-CZ	15.31	1.58	1.38
1	C	82	ALA	C-N	15.31	1.69	1.34
2	D	52	ASP	N-CA	15.28	1.76	1.46
2	B	87	THR	CB-CG2	15.27	2.02	1.52
2	D	41	PHE	CE1-CZ	-15.25	1.08	1.37
1	A	84	SER	CB-OG	-15.24	1.22	1.42
2	B	59	LYS	CG-CD	-15.22	1.00	1.52
1	A	14	TRP	CB-CG	-15.21	1.22	1.50
1	C	70	VAL	C-N	-15.11	0.99	1.34
1	A	44	PRO	CA-C	15.08	1.83	1.52
2	B	1	VAL	CA-CB	15.08	1.86	1.54
1	A	50	HIS	CG-CD2	15.03	1.61	1.35
1	A	17	VAL	C-N	14.96	1.59	1.33
2	D	59	LYS	CD-CE	14.89	1.88	1.51
1	C	114	PRO	N-CA	14.86	1.72	1.47
1	A	3	SER	C-N	14.86	1.62	1.34
1	C	14	TRP	CG-CD1	14.86	1.57	1.36
1	A	23	GLU	CD-OE2	14.85	1.42	1.25
1	C	25	GLY	C-O	14.78	1.47	1.23
2	D	80	ASN	N-CA	14.77	1.75	1.46
1	A	1	VAL	N-CA	-14.73	1.16	1.46
2	D	73	ASP	CA-CB	14.72	1.86	1.53
1	C	78	ASN	CA-C	-14.71	1.14	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	HIS	CG-ND1	14.65	1.71	1.38
1	A	137	THR	CA-CB	14.64	1.91	1.53
2	D	21	ASP	CG-OD1	14.59	1.58	1.25
1	C	7	LYS	N-CA	14.55	1.75	1.46
2	B	108	ASN	CB-CG	14.55	1.84	1.51
2	D	117	HIS	CG-CD2	14.54	1.60	1.35
1	C	72	HIS	CA-CB	14.52	1.85	1.53
2	B	143	HIS	CG-ND1	14.50	1.70	1.38
1	C	68	ASN	CG-OD1	-14.47	0.92	1.24
2	D	21	ASP	C-O	14.42	1.50	1.23
2	D	8	LYS	CA-CB	14.40	1.85	1.53
2	D	73	ASP	CG-OD1	14.40	1.58	1.25
1	A	52	SER	N-CA	14.37	1.75	1.46
1	A	16	LYS	CG-CD	14.35	2.01	1.52
2	D	55	MET	CA-C	14.33	1.90	1.52
2	B	44	SER	C-O	14.33	1.50	1.23
1	A	14	TRP	CE2-CZ2	-14.28	1.15	1.39
2	B	145	TYR	CE1-CZ	14.27	1.57	1.38
1	A	1	VAL	CA-CB	14.26	1.84	1.54
1	C	118	THR	C-N	-14.24	1.07	1.34
2	B	125	PRO	N-CD	14.17	1.67	1.47
1	C	139	LYS	CE-NZ	14.16	1.84	1.49
2	D	15	TRP	CD2-CE2	14.15	1.58	1.41
1	C	37	PRO	N-CD	-14.10	1.28	1.47
1	A	74	ASP	CG-OD2	14.07	1.57	1.25
2	D	125	PRO	N-CD	14.06	1.67	1.47
2	B	90	GLU	CA-CB	14.03	1.84	1.53
2	D	108	ASN	CB-CG	14.03	1.83	1.51
2	D	117	HIS	CB-CG	-14.02	1.24	1.50
2	D	80	ASN	CA-CB	-13.95	1.16	1.53
2	B	81	LEU	C-N	13.94	1.66	1.34
1	C	1	VAL	CA-CB	-13.93	1.25	1.54
1	A	2	LEU	C-N	-13.92	1.02	1.34
2	D	40	ARG	CZ-NH1	-13.85	1.15	1.33
2	B	66	LYS	N-CA	-13.84	1.18	1.46
1	C	14	TRP	CD2-CE2	13.72	1.57	1.41
2	D	30	ARG	CD-NE	-13.72	1.23	1.46
2	B	102	ASN	CG-OD1	-13.68	0.93	1.24
2	D	76	ALA	C-O	13.68	1.49	1.23
2	D	79	ASP	CB-CG	-13.68	1.23	1.51
2	D	18	VAL	CA-CB	-13.62	1.26	1.54
2	B	130	TYR	CD2-CE2	13.59	1.59	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	ASP	CB-CG	13.56	1.80	1.51
2	B	143	HIS	CB-CG	13.55	1.74	1.50
1	A	1	VAL	CB-CG2	-13.50	1.24	1.52
2	B	1	VAL	CB-CG2	-13.43	1.24	1.52
1	C	131	SER	CA-CB	13.40	1.73	1.52
1	A	50	HIS	C-O	13.39	1.48	1.23
2	B	80	ASN	N-CA	13.38	1.73	1.46
1	A	127	LYS	CG-CD	13.37	1.97	1.52
1	A	56	LYS	CD-CE	13.35	1.84	1.51
2	B	7	GLU	CB-CG	13.35	1.77	1.52
1	A	90	LYS	CD-CE	13.26	1.84	1.51
1	A	14	TRP	CA-CB	13.22	1.83	1.53
1	A	92	ARG	CZ-NH1	13.20	1.50	1.33
2	B	9	SER	CA-C	13.17	1.87	1.52
2	D	95	LYS	C-N	13.07	1.64	1.34
1	C	7	LYS	CA-C	-13.07	1.19	1.52
2	B	76	ALA	C-N	13.06	1.64	1.34
2	B	40	ARG	CZ-NH1	-13.03	1.16	1.33
2	D	20	VAL	CA-C	-13.01	1.19	1.52
2	D	49	SER	CA-C	12.97	1.86	1.52
1	C	68	ASN	C-O	12.97	1.48	1.23
1	C	50	HIS	CG-ND1	12.96	1.67	1.38
1	A	26	ALA	N-CA	-12.93	1.20	1.46
2	D	48	LEU	N-CA	12.93	1.72	1.46
2	D	18	VAL	CB-CG2	12.93	1.79	1.52
1	C	14	TRP	CD2-CE3	-12.91	1.21	1.40
1	A	106	LEU	CB-CG	-12.90	1.15	1.52
2	B	5	PRO	CA-C	12.89	1.78	1.52
2	B	40	ARG	CD-NE	-12.88	1.24	1.46
2	B	46	GLY	C-O	12.86	1.44	1.23
1	A	20	HIS	CE1-NE2	-12.85	1.03	1.32
2	D	126	VAL	CA-CB	12.84	1.81	1.54
2	B	66	LYS	CE-NZ	12.82	1.81	1.49
1	A	33	PHE	CE2-CZ	-12.79	1.13	1.37
1	C	72	HIS	CA-C	-12.77	1.19	1.52
1	A	71	ALA	CA-C	-12.75	1.19	1.52
1	A	24	TYR	CE2-CZ	12.71	1.55	1.38
1	A	134	THR	CB-OG1	-12.71	1.17	1.43
1	C	140	TYR	CG-CD1	-12.71	1.22	1.39
2	B	89	SER	CB-OG	12.69	1.58	1.42
2	B	6	GLU	C-O	12.67	1.47	1.23
2	D	21	ASP	CB-CG	12.67	1.78	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ARG	CD-NE	12.67	1.68	1.46
2	D	44	SER	CB-OG	-12.66	1.25	1.42
2	B	71	PHE	C-N	-12.62	1.05	1.34
2	B	73	ASP	CA-C	-12.59	1.20	1.52
1	C	7	LYS	CG-CD	12.56	1.95	1.52
1	A	140	TYR	CE1-CZ	-12.50	1.22	1.38
2	B	2	HIS	CE1-NE2	12.49	1.61	1.32
1	A	56	LYS	C-N	12.49	1.55	1.33
2	D	50	THR	N-CA	12.46	1.71	1.46
2	D	139	ASN	CA-CB	-12.45	1.20	1.53
2	B	8	LYS	C-O	12.45	1.47	1.23
1	C	75	ASP	N-CA	12.44	1.71	1.46
1	A	19	ALA	C-O	12.42	1.47	1.23
2	B	43	GLU	CA-CB	-12.40	1.26	1.53
2	D	54	VAL	CB-CG2	-12.40	1.26	1.52
2	B	52	ASP	CB-CG	12.37	1.77	1.51
1	C	118	THR	CB-CG2	-12.37	1.11	1.52
2	D	40	ARG	C-O	12.33	1.46	1.23
2	B	80	ASN	CG-OD1	12.30	1.51	1.24
1	A	77	PRO	CA-C	-12.30	1.28	1.52
1	A	76	MET	CB-CG	-12.23	1.12	1.51
2	B	74	GLY	N-CA	-12.23	1.27	1.46
2	D	36	PRO	N-CD	-12.23	1.30	1.47
1	A	46	PHE	CB-CG	-12.22	1.30	1.51
1	C	73	VAL	CA-CB	12.21	1.80	1.54
2	D	77	HIS	CE1-NE2	-12.21	1.04	1.32
1	A	45	HIS	C-N	12.21	1.62	1.34
1	C	4	PRO	N-CA	-12.21	1.26	1.47
1	A	59	GLY	CA-C	-12.20	1.32	1.51
1	C	140	TYR	CE2-CZ	-12.17	1.22	1.38
2	D	73	ASP	CA-C	-12.16	1.21	1.52
2	B	2	HIS	CA-C	12.14	1.84	1.52
1	A	24	TYR	CB-CG	12.14	1.69	1.51
1	A	73	VAL	CA-C	-12.14	1.21	1.52
2	D	94	ASP	CG-OD2	12.11	1.53	1.25
2	D	44	SER	CA-CB	-12.10	1.34	1.52
2	D	117	HIS	ND1-CE1	12.09	1.65	1.34
2	B	74	GLY	CA-C	-12.06	1.32	1.51
2	D	63	HIS	CA-CB	-12.05	1.27	1.53
1	A	27	GLU	CG-CD	12.04	1.70	1.51
2	B	65	LYS	CA-CB	12.03	1.80	1.53
2	D	18	VAL	N-CA	12.03	1.70	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	LYS	CG-CD	12.01	1.93	1.52
1	A	52	SER	CA-C	-12.00	1.21	1.52
1	C	61	LYS	CD-CE	11.97	1.81	1.51
2	B	94	ASP	CG-OD2	-11.95	0.97	1.25
1	C	115	ALA	CA-C	-11.94	1.21	1.52
1	C	8	THR	CA-CB	11.94	1.84	1.53
2	D	146	HIS	CE1-NE2	11.93	1.60	1.32
2	D	104	ARG	CZ-NH1	11.92	1.48	1.33
2	B	63	HIS	CG-ND1	11.89	1.65	1.38
2	D	7	GLU	CD-OE2	11.86	1.38	1.25
1	C	7	LYS	CD-CE	-11.86	1.21	1.51
1	C	20	HIS	CG-ND1	11.84	1.64	1.38
1	A	12	ALA	C-O	11.82	1.45	1.23
2	D	145	TYR	CE2-CZ	-11.82	1.23	1.38
1	C	1	VAL	CA-C	11.80	1.83	1.52
2	D	79	ASP	CA-C	11.80	1.83	1.52
1	C	18	GLY	C-O	11.79	1.42	1.23
2	B	45	PHE	CD1-CE1	11.78	1.62	1.39
1	A	137	THR	CB-OG1	11.78	1.66	1.43
1	C	72	HIS	C-O	11.76	1.45	1.23
2	D	35	TYR	CG-CD2	-11.76	1.23	1.39
1	A	5	ALA	CA-CB	11.74	1.77	1.52
2	D	17	LYS	C-N	11.73	1.61	1.34
1	C	20	HIS	CB-CG	11.70	1.71	1.50
2	D	121	GLU	CA-CB	11.69	1.79	1.53
1	C	7	LYS	CE-NZ	-11.69	1.19	1.49
2	D	11	VAL	CB-CG1	-11.68	1.28	1.52
1	C	74	ASP	CG-OD1	11.64	1.52	1.25
2	D	22	GLU	CA-C	11.58	1.83	1.52
2	D	47	ASP	CB-CG	11.55	1.76	1.51
2	D	63	HIS	ND1-CE1	11.54	1.63	1.34
2	D	40	ARG	CB-CG	-11.50	1.21	1.52
2	D	82	LYS	C-N	11.45	1.53	1.33
1	A	14	TRP	CZ2-CH2	-11.43	1.15	1.37
1	C	133	SER	C-O	11.43	1.45	1.23
2	B	118	PHE	CD2-CE2	-11.43	1.16	1.39
2	B	104	ARG	CD-NE	11.41	1.65	1.46
2	D	131	GLN	CG-CD	11.41	1.77	1.51
2	D	52	ASP	CB-CG	11.40	1.75	1.51
2	B	142	ALA	CA-C	11.39	1.82	1.52
2	B	46	GLY	C-N	-11.37	1.07	1.34
2	B	90	GLU	CB-CG	-11.35	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	GLY	CA-C	11.35	1.70	1.51
1	A	64	ASP	CG-OD1	11.35	1.51	1.25
1	C	71	ALA	CA-CB	-11.34	1.28	1.52
1	C	116	GLU	CD-OE1	-11.32	1.13	1.25
2	B	1	VAL	N-CA	11.31	1.69	1.46
1	C	87	HIS	CA-C	11.31	1.82	1.52
1	C	119	PRO	N-CD	11.31	1.63	1.47
1	A	71	ALA	C-O	11.28	1.44	1.23
2	D	130	TYR	CD1-CE1	11.28	1.56	1.39
2	D	78	LEU	CA-CB	11.27	1.79	1.53
2	B	145	TYR	CA-CB	-11.27	1.29	1.53
2	D	78	LEU	C-O	-11.26	1.01	1.23
1	C	78	ASN	CB-CG	11.25	1.76	1.51
1	C	16	LYS	CA-C	11.23	1.82	1.52
1	A	7	LYS	C-N	11.23	1.59	1.34
2	B	69	GLY	N-CA	-11.22	1.29	1.46
2	D	12	THR	N-CA	11.22	1.68	1.46
1	C	72	HIS	ND1-CE1	-11.22	1.06	1.34
1	C	24	TYR	CD2-CE2	11.18	1.56	1.39
1	A	4	PRO	C-N	11.18	1.59	1.34
1	A	29	LEU	CA-CB	11.18	1.79	1.53
1	C	24	TYR	CG-CD1	11.17	1.53	1.39
2	D	19	ASN	C-O	11.15	1.44	1.23
2	B	81	LEU	N-CA	11.14	1.68	1.46
2	B	121	GLU	CD-OE2	-11.14	1.13	1.25
1	C	11	LYS	CA-C	-11.13	1.24	1.52
2	D	4	THR	CA-CB	11.10	1.82	1.53
2	B	79	ASP	C-O	-11.10	1.02	1.23
1	A	72	HIS	CA-CB	11.10	1.78	1.53
2	D	143	HIS	ND1-CE1	11.08	1.62	1.34
1	C	90	LYS	CG-CD	11.07	1.90	1.52
2	D	6	GLU	C-O	-11.07	1.02	1.23
2	D	7	GLU	CG-CD	-11.07	1.35	1.51
1	C	10	VAL	CA-C	11.05	1.81	1.52
2	D	102	ASN	C-O	11.03	1.44	1.23
2	D	8	LYS	N-CA	11.02	1.68	1.46
1	A	128	PHE	CG-CD2	-11.01	1.22	1.38
2	D	73	ASP	CB-CG	-10.99	1.28	1.51
2	B	118	PHE	CG-CD2	10.98	1.55	1.38
1	C	128	PHE	CG-CD2	-10.98	1.22	1.38
1	C	75	ASP	C-N	10.96	1.59	1.34
1	C	19	ALA	C-O	10.96	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	GLU	CB-CG	10.96	1.73	1.52
2	D	18	VAL	CB-CG1	-10.95	1.29	1.52
1	A	33	PHE	CG-CD2	10.92	1.55	1.38
1	C	70	VAL	N-CA	10.89	1.68	1.46
2	D	94	ASP	N-CA	10.89	1.68	1.46
2	D	82	LYS	CG-CD	10.85	1.89	1.52
2	D	45	PHE	CD1-CE1	10.83	1.60	1.39
2	D	4	THR	N-CA	-10.82	1.24	1.46
2	D	53	ALA	CA-CB	-10.82	1.29	1.52
2	B	49	SER	N-CA	10.79	1.68	1.46
1	A	141	ARG	NE-CZ	10.78	1.47	1.33
1	A	112	HIS	ND1-CE1	10.77	1.61	1.34
2	D	40	ARG	NE-CZ	10.77	1.47	1.33
1	C	20	HIS	CE1-NE2	10.73	1.57	1.32
1	C	49	SER	C-N	10.72	1.58	1.34
2	B	2	HIS	C-O	10.71	1.43	1.23
1	A	58	HIS	CB-CG	10.69	1.69	1.50
2	D	144	LYS	CA-CB	-10.69	1.30	1.53
2	B	7	GLU	CD-OE2	10.68	1.37	1.25
1	C	15	GLY	C-N	-10.68	1.09	1.34
1	A	49	SER	C-N	10.66	1.58	1.34
1	C	38	THR	CA-CB	10.65	1.81	1.53
2	B	80	ASN	CB-CG	10.65	1.75	1.51
2	B	22	GLU	CB-CG	-10.61	1.31	1.52
2	D	101	GLU	CB-CG	10.61	1.72	1.52
2	D	93	CYS	CB-SG	10.60	2.00	1.82
1	C	24	TYR	CE1-CZ	-10.59	1.24	1.38
1	C	114	PRO	CA-CB	-10.58	1.32	1.53
2	B	47	ASP	N-CA	10.56	1.67	1.46
2	D	46	GLY	C-O	10.56	1.40	1.23
2	D	80	ASN	CB-CG	-10.55	1.26	1.51
1	C	117	PHE	CD1-CE1	10.54	1.60	1.39
2	D	40	ARG	CZ-NH2	10.54	1.46	1.33
2	B	143	HIS	CG-CD2	-10.53	1.17	1.35
2	D	40	ARG	CD-NE	-10.53	1.28	1.46
1	A	89	HIS	CG-CD2	10.52	1.53	1.35
2	D	45	PHE	CG-CD2	-10.49	1.23	1.38
1	A	49	SER	CA-CB	-10.49	1.37	1.52
2	B	61	LYS	CB-CG	-10.49	1.24	1.52
1	C	137	THR	CB-OG1	-10.47	1.22	1.43
2	B	73	ASP	CG-OD2	-10.47	1.01	1.25
1	C	46	PHE	CE2-CZ	10.46	1.57	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	80	ASN	CA-C	10.46	1.80	1.52
2	D	63	HIS	CB-CG	10.45	1.68	1.50
2	B	61	LYS	CE-NZ	10.41	1.75	1.49
2	B	143	HIS	CE1-NE2	10.41	1.56	1.32
1	C	71	ALA	N-CA	10.41	1.67	1.46
2	D	113	VAL	CB-CG2	10.38	1.74	1.52
1	A	20	HIS	CG-CD2	10.36	1.53	1.35
1	C	50	HIS	CB-CG	-10.33	1.31	1.50
2	D	60	VAL	N-CA	10.32	1.67	1.46
2	D	136	GLY	N-CA	-10.31	1.30	1.46
2	D	67	VAL	CA-CB	10.31	1.76	1.54
1	C	112	HIS	CB-CG	-10.31	1.31	1.50
2	B	3	LEU	CA-CB	10.30	1.77	1.53
1	A	83	LEU	CB-CG	-10.30	1.22	1.52
2	D	78	LEU	N-CA	-10.26	1.25	1.46
1	A	36	PHE	CG-CD2	10.25	1.54	1.38
2	B	12	THR	CB-OG1	-10.25	1.22	1.43
2	D	19	ASN	CA-C	-10.25	1.26	1.52
1	A	61	LYS	CE-NZ	10.23	1.74	1.49
1	C	2	LEU	CA-C	10.23	1.79	1.52
1	A	77	PRO	C-O	10.21	1.43	1.23
1	C	24	TYR	CZ-OH	10.20	1.55	1.37
2	D	58	PRO	C-O	10.19	1.43	1.23
2	B	46	GLY	CA-C	10.19	1.68	1.51
2	B	41	PHE	CG-CD2	10.18	1.54	1.38
1	A	3	SER	CB-OG	-10.17	1.29	1.42
1	C	92	ARG	C-O	-10.15	1.04	1.23
2	B	51	PRO	N-CD	10.15	1.62	1.47
2	D	84	THR	CB-OG1	-10.14	1.23	1.43
1	A	4	PRO	CA-CB	10.11	1.73	1.53
1	C	127	LYS	C-O	10.11	1.42	1.23
2	D	61	LYS	CE-NZ	-10.09	1.23	1.49
2	D	58	PRO	CB-CG	10.08	2.00	1.50
1	A	72	HIS	CD2-NE2	10.06	1.63	1.42
1	C	41	THR	C-O	10.04	1.42	1.23
1	C	14	TRP	NE1-CE2	-10.03	1.24	1.37
1	A	141	ARG	CB-CG	10.02	1.79	1.52
2	B	4	THR	CA-C	-9.97	1.27	1.52
2	D	42	PHE	CE2-CZ	9.96	1.56	1.37
1	C	128	PHE	CB-CG	9.95	1.68	1.51
1	C	17	VAL	CB-CG1	-9.94	1.31	1.52
2	B	113	VAL	C-O	9.94	1.42	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	VAL	C-N	9.94	1.50	1.33
2	D	8	LYS	CB-CG	9.94	1.79	1.52
1	A	122	HIS	N-CA	9.93	1.66	1.46
2	D	77	HIS	CA-CB	9.92	1.75	1.53
2	D	37	TRP	CE2-CZ2	9.92	1.56	1.39
1	A	33	PHE	CG-CD1	-9.90	1.24	1.38
1	C	47	ASP	CB-CG	9.88	1.72	1.51
1	C	50	HIS	CE1-NE2	9.87	1.55	1.32
1	A	140	TYR	CG-CD1	9.86	1.51	1.39
1	A	40	LYS	CA-CB	9.86	1.75	1.53
1	C	44	PRO	C-N	-9.85	1.11	1.34
2	B	103	PHE	CE1-CZ	-9.84	1.18	1.37
1	A	140	TYR	CZ-OH	-9.84	1.21	1.37
1	C	51	GLY	N-CA	-9.84	1.31	1.46
1	A	1	VAL	CB-CG1	-9.83	1.32	1.52
2	B	17	LYS	C-O	9.83	1.42	1.23
2	B	132	LYS	CA-CB	-9.82	1.32	1.53
1	C	36	PHE	CG-CD2	9.81	1.53	1.38
2	B	10	ALA	CA-C	9.79	1.78	1.52
1	C	46	PHE	CE1-CZ	-9.78	1.18	1.37
2	D	1	VAL	CB-CG1	9.76	1.73	1.52
1	A	90	LYS	CG-CD	-9.75	1.19	1.52
2	B	126	VAL	C-O	9.74	1.41	1.23
2	D	139	ASN	CG-ND2	9.72	1.57	1.32
1	A	44	PRO	N-CD	-9.71	1.34	1.47
2	B	104	ARG	CG-CD	9.70	1.76	1.51
1	C	138	SER	CB-OG	-9.69	1.29	1.42
2	B	50	THR	CA-CB	-9.68	1.28	1.53
1	A	72	HIS	CB-CG	-9.67	1.32	1.50
1	A	33	PHE	CD2-CE2	9.64	1.58	1.39
2	B	73	ASP	CB-CG	9.64	1.72	1.51
2	D	4	THR	C-O	9.60	1.41	1.23
2	B	118	PHE	CB-CG	-9.59	1.35	1.51
1	C	44	PRO	CA-CB	9.59	1.72	1.53
2	D	53	ALA	C-N	9.59	1.56	1.34
1	C	18	GLY	CA-C	-9.59	1.36	1.51
1	A	2	LEU	CA-C	9.58	1.77	1.52
2	B	41	PHE	CA-C	9.57	1.77	1.52
1	A	17	VAL	N-CA	-9.56	1.27	1.46
2	B	42	PHE	CE1-CZ	-9.56	1.19	1.37
2	B	82	LYS	CA-C	-9.55	1.28	1.52
1	C	56	LYS	CE-NZ	9.53	1.72	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	LYS	CA-CB	9.51	1.74	1.53
1	C	46	PHE	CB-CG	-9.50	1.35	1.51
2	B	73	ASP	CG-OD1	9.48	1.47	1.25
2	D	46	GLY	N-CA	-9.48	1.31	1.46
1	C	20	HIS	CD2-NE2	-9.48	1.17	1.38
2	B	2	HIS	C-N	-9.47	1.12	1.34
2	B	6	GLU	CA-C	9.46	1.77	1.52
2	D	72	SER	CA-CB	9.45	1.67	1.52
1	A	77	PRO	CA-CB	9.43	1.72	1.53
1	C	76	MET	CG-SD	9.40	2.05	1.81
2	B	44	SER	C-N	9.38	1.55	1.34
1	C	128	PHE	CD2-CE2	9.38	1.58	1.39
1	C	52	SER	CA-C	-9.38	1.28	1.52
1	A	137	THR	N-CA	9.38	1.65	1.46
2	D	83	GLY	C-N	9.37	1.55	1.34
1	C	132	VAL	CB-CG2	9.35	1.72	1.52
2	D	15	TRP	CZ3-CH2	9.33	1.54	1.40
2	D	36	PRO	N-CA	9.32	1.63	1.47
1	A	14	TRP	CD1-NE1	9.30	1.53	1.38
1	C	71	ALA	CA-C	-9.28	1.28	1.52
1	A	46	PHE	CE1-CZ	9.26	1.54	1.37
1	C	81	SER	CB-OG	9.26	1.54	1.42
2	B	83	GLY	N-CA	9.25	1.59	1.46
2	D	77	HIS	C-N	9.24	1.55	1.34
1	C	47	ASP	CG-OD1	-9.23	1.04	1.25
1	A	90	LYS	N-CA	-9.23	1.27	1.46
2	D	19	ASN	CB-CG	9.23	1.72	1.51
2	B	146	HIS	N-CA	9.22	1.64	1.46
1	C	61	LYS	CA-C	9.22	1.76	1.52
2	B	143	HIS	CA-C	9.21	1.76	1.52
1	A	50	HIS	CB-CG	-9.21	1.33	1.50
2	D	93	CYS	C-O	-9.19	1.05	1.23
1	C	22	GLY	C-O	9.19	1.38	1.23
2	B	51	PRO	C-O	9.18	1.41	1.23
1	A	104	CYS	N-CA	9.17	1.64	1.46
2	B	63	HIS	ND1-CE1	9.16	1.57	1.34
1	C	12	ALA	C-N	9.16	1.55	1.34
1	C	43	PHE	CG-CD2	9.16	1.52	1.38
1	C	38	THR	CB-OG1	9.16	1.61	1.43
1	C	103	HIS	CG-ND1	9.14	1.58	1.38
2	B	21	ASP	CG-OD2	9.12	1.46	1.25
2	D	42	PHE	CE1-CZ	-9.12	1.20	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	81	SER	CA-CB	9.12	1.66	1.52
1	A	58	HIS	CA-C	9.11	1.76	1.52
1	C	69	ALA	N-CA	9.11	1.64	1.46
2	D	53	ALA	CA-C	9.11	1.76	1.52
2	D	15	TRP	NE1-CE2	9.10	1.49	1.37
1	C	42	TYR	CG-CD1	9.09	1.50	1.39
1	A	86	LEU	CB-CG	-9.07	1.26	1.52
2	B	37	TRP	NE1-CE2	-9.05	1.25	1.37
2	D	137	VAL	CA-CB	9.04	1.73	1.54
1	C	95	PRO	CA-C	-9.04	1.34	1.52
1	A	67	THR	C-O	9.02	1.40	1.23
2	B	40	ARG	C-N	-9.02	1.13	1.34
2	D	49	SER	C-O	9.02	1.40	1.23
1	A	88	ALA	C-O	-9.01	1.06	1.23
2	B	117	HIS	CE1-NE2	9.01	1.53	1.32
2	B	7	GLU	CG-CD	-8.99	1.38	1.51
1	C	72	HIS	N-CA	-8.98	1.28	1.46
2	B	18	VAL	CB-CG2	8.98	1.71	1.52
1	C	14	TRP	CZ2-CH2	-8.98	1.20	1.37
2	D	59	LYS	CA-C	8.97	1.76	1.52
2	B	77	HIS	CB-CG	8.97	1.66	1.50
2	D	79	ASP	CA-CB	8.96	1.73	1.53
1	C	48	LEU	C-O	8.93	1.40	1.23
1	C	16	LYS	CE-NZ	8.92	1.71	1.49
2	D	92	HIS	CA-C	8.91	1.76	1.52
2	B	26	GLU	CG-CD	-8.90	1.38	1.51
1	C	131	SER	CA-C	8.90	1.76	1.52
1	C	56	LYS	CA-C	-8.89	1.29	1.52
2	D	146	HIS	C-OXT	8.88	1.40	1.23
1	C	99	LYS	CG-CD	8.87	1.82	1.52
1	C	141	ARG	CZ-NH2	8.86	1.44	1.33
2	D	5	PRO	CB-CG	-8.86	1.05	1.50
1	C	21	ALA	C-N	-8.85	1.17	1.33
2	D	97	HIS	CB-CG	8.85	1.66	1.50
1	C	77	PRO	CA-C	-8.84	1.35	1.52
1	C	126	ASP	CB-CG	8.84	1.70	1.51
1	C	42	TYR	CE2-CZ	8.82	1.50	1.38
1	C	57	GLY	C-O	8.82	1.37	1.23
2	B	94	ASP	CB-CG	8.82	1.70	1.51
2	D	10	ALA	CA-C	8.82	1.75	1.52
1	C	113	LEU	CA-CB	-8.82	1.33	1.53
1	C	115	ALA	CA-CB	8.81	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	HIS	CA-C	8.80	1.75	1.52
1	A	4	PRO	N-CA	-8.79	1.32	1.47
1	A	85	ASP	N-CA	8.79	1.64	1.46
1	A	47	ASP	C-N	-8.78	1.13	1.34
1	A	73	VAL	CA-CB	-8.78	1.36	1.54
1	A	138	SER	CB-OG	-8.74	1.30	1.42
1	A	33	PHE	CA-C	-8.74	1.30	1.52
2	D	143	HIS	CB-CG	-8.73	1.34	1.50
1	A	57	GLY	CA-C	8.73	1.65	1.51
1	C	68	ASN	CG-ND2	8.73	1.54	1.32
2	D	71	PHE	N-CA	8.72	1.63	1.46
2	D	12	THR	C-O	8.71	1.40	1.23
1	A	78	ASN	C-O	8.71	1.39	1.23
2	D	61	LYS	CD-CE	8.71	1.73	1.51
1	A	68	ASN	C-O	8.70	1.39	1.23
2	B	50	THR	N-CA	-8.69	1.28	1.46
2	D	4	THR	CB-CG2	-8.69	1.23	1.52
1	A	45	HIS	CE1-NE2	8.69	1.52	1.32
1	C	46	PHE	C-N	8.68	1.54	1.34
2	B	73	ASP	C-O	8.68	1.39	1.23
2	D	20	VAL	N-CA	8.67	1.63	1.46
1	C	85	ASP	CG-OD1	-8.67	1.05	1.25
1	C	115	ALA	N-CA	-8.67	1.29	1.46
2	D	8	LYS	CG-CD	-8.66	1.23	1.52
2	D	82	LYS	CB-CG	-8.66	1.29	1.52
1	A	27	GLU	CD-OE1	-8.66	1.16	1.25
1	A	105	LEU	CG-CD2	-8.65	1.19	1.51
2	D	121	GLU	N-CA	-8.65	1.29	1.46
1	A	29	LEU	N-CA	8.64	1.63	1.46
1	A	8	THR	CB-OG1	-8.64	1.25	1.43
2	B	145	TYR	CA-C	8.61	1.75	1.52
2	B	44	SER	CA-CB	-8.61	1.40	1.52
2	D	146	HIS	CA-CB	8.60	1.72	1.53
2	D	6	GLU	CA-CB	8.59	1.72	1.53
1	A	37	PRO	N-CA	8.58	1.61	1.47
2	D	80	ASN	C-O	-8.58	1.07	1.23
2	D	85	PHE	N-CA	8.57	1.63	1.46
1	C	16	LYS	CG-CD	8.57	1.81	1.52
1	C	118	THR	CA-CB	8.57	1.75	1.53
2	B	69	GLY	C-N	8.56	1.53	1.34
2	D	23	VAL	CB-CG1	-8.55	1.34	1.52
1	A	42	TYR	CE1-CZ	-8.53	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	20	VAL	CA-C	-8.53	1.30	1.52
2	B	47	ASP	CA-C	8.52	1.75	1.52
1	C	54	GLN	CA-C	8.51	1.75	1.52
2	D	43	GLU	C-O	-8.51	1.07	1.23
1	A	10	VAL	CB-CG2	-8.50	1.34	1.52
1	C	95	PRO	N-CA	8.50	1.61	1.47
2	B	10	ALA	N-CA	-8.49	1.29	1.46
2	D	7	GLU	CA-C	8.49	1.75	1.52
1	A	62	VAL	CA-C	8.48	1.75	1.52
2	D	145	TYR	CD2-CE2	8.47	1.52	1.39
1	A	46	PHE	CD2-CE2	8.47	1.56	1.39
1	A	30	GLU	CB-CG	-8.46	1.36	1.52
1	C	26	ALA	C-N	8.45	1.53	1.34
2	B	42	PHE	CB-CG	-8.45	1.36	1.51
1	C	47	ASP	CA-CB	8.44	1.72	1.53
2	B	75	LEU	CB-CG	-8.43	1.28	1.52
2	D	125	PRO	N-CA	-8.43	1.32	1.47
2	B	95	LYS	CA-CB	8.41	1.72	1.53
2	D	123	THR	CB-CG2	8.39	1.80	1.52
2	B	134	VAL	N-CA	-8.38	1.29	1.46
1	C	137	THR	CA-C	8.38	1.74	1.52
1	C	59	GLY	N-CA	-8.38	1.33	1.46
1	C	131	SER	N-CA	8.38	1.63	1.46
1	A	3	SER	N-CA	8.36	1.63	1.46
2	D	146	HIS	N-CA	8.36	1.63	1.46
1	C	70	VAL	CA-C	8.34	1.74	1.52
2	B	54	VAL	CA-C	-8.33	1.31	1.52
1	A	141	ARG	CA-CB	-8.32	1.35	1.53
1	C	140	TYR	CG-CD2	8.30	1.50	1.39
2	D	70	ALA	C-O	8.30	1.39	1.23
2	D	30	ARG	CZ-NH2	8.29	1.43	1.33
1	A	21	ALA	C-O	-8.28	1.07	1.23
2	B	41	PHE	C-O	-8.28	1.07	1.23
2	B	69	GLY	CA-C	8.27	1.65	1.51
1	C	114	PRO	N-CD	8.27	1.59	1.47
2	D	41	PHE	CG-CD2	-8.25	1.26	1.38
1	C	50	HIS	CA-CB	8.25	1.72	1.53
2	B	52	ASP	CG-OD1	-8.24	1.06	1.25
2	B	37	TRP	CG-CD1	8.24	1.48	1.36
2	B	49	SER	CA-C	-8.24	1.31	1.52
2	B	95	LYS	CA-C	-8.24	1.31	1.52
1	A	47	ASP	CA-C	8.23	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	110	LEU	C-N	8.23	1.52	1.34
1	A	70	VAL	CA-CB	-8.22	1.37	1.54
2	D	48	LEU	CA-CB	-8.22	1.34	1.53
1	C	40	LYS	CE-NZ	8.22	1.69	1.49
2	B	94	ASP	C-O	8.21	1.39	1.23
1	A	134	THR	CA-C	-8.20	1.31	1.52
2	B	93	CYS	CB-SG	8.20	1.96	1.82
2	B	20	VAL	C-O	8.20	1.39	1.23
2	D	14	LEU	CA-CB	8.19	1.72	1.53
2	D	94	ASP	CG-OD1	-8.18	1.06	1.25
2	B	84	THR	CB-OG1	8.17	1.59	1.43
1	C	96	VAL	CB-CG2	-8.17	1.35	1.52
1	C	14	TRP	C-O	8.16	1.38	1.23
2	B	84	THR	CB-CG2	-8.15	1.25	1.52
2	B	77	HIS	ND1-CE1	-8.15	1.14	1.34
2	D	11	VAL	CB-CG2	8.15	1.70	1.52
2	D	13	ALA	C-N	8.15	1.52	1.34
2	B	142	ALA	C-N	-8.13	1.15	1.34
2	B	69	GLY	C-O	-8.12	1.10	1.23
2	D	55	MET	CB-CG	-8.10	1.25	1.51
1	A	78	ASN	CG-ND2	-8.10	1.12	1.32
2	D	51	PRO	N-CD	8.09	1.59	1.47
1	A	76	MET	CG-SD	8.09	2.02	1.81
2	D	19	ASN	C-N	-8.08	1.15	1.34
2	D	58	PRO	CA-C	8.08	1.69	1.52
1	C	25	GLY	N-CA	-8.07	1.33	1.46
1	C	113	LEU	CG-CD2	-8.07	1.22	1.51
2	B	59	LYS	CA-CB	-8.06	1.36	1.53
2	D	80	ASN	CA-C	8.05	1.73	1.52
2	B	16	GLY	N-CA	8.04	1.58	1.46
2	B	7	GLU	N-CA	8.04	1.62	1.46
1	A	105	LEU	CB-CG	-8.03	1.29	1.52
2	B	118	PHE	CE1-CZ	8.03	1.52	1.37
1	C	3	SER	CA-CB	-8.03	1.41	1.52
2	D	104	ARG	CZ-NH2	-8.02	1.22	1.33
2	D	54	VAL	C-O	8.02	1.38	1.23
1	A	17	VAL	CA-CB	-8.01	1.38	1.54
2	D	76	ALA	CA-CB	-8.00	1.35	1.52
1	C	58	HIS	CG-CD2	-8.00	1.22	1.35
2	D	3	LEU	C-N	8.00	1.52	1.34
2	D	130	TYR	CE2-CZ	-7.99	1.28	1.38
1	A	88	ALA	CA-C	7.99	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	GLU	C-N	7.98	1.52	1.34
1	C	17	VAL	C-O	7.98	1.38	1.23
1	C	45	HIS	ND1-CE1	-7.98	1.14	1.34
2	D	41	PHE	CA-C	7.97	1.73	1.52
1	A	114	PRO	N-CA	7.97	1.60	1.47
2	D	132	LYS	CD-CE	7.95	1.71	1.51
2	D	41	PHE	CB-CG	7.95	1.64	1.51
2	B	45	PHE	CB-CG	7.94	1.64	1.51
2	D	122	PHE	CG-CD1	-7.93	1.26	1.38
2	D	122	PHE	CG-CD2	7.93	1.50	1.38
2	B	80	ASN	C-O	-7.92	1.08	1.23
1	A	132	VAL	C-O	7.90	1.38	1.23
2	B	81	LEU	CA-C	-7.90	1.32	1.52
1	A	141	ARG	N-CA	7.89	1.62	1.46
2	D	39	GLN	CD-OE1	7.88	1.41	1.24
2	B	121	GLU	N-CA	-7.86	1.30	1.46
2	B	143	HIS	CA-CB	-7.86	1.36	1.53
1	C	48	LEU	CA-C	-7.85	1.32	1.52
2	D	116	HIS	CE1-NE2	7.85	1.50	1.32
1	A	7	LYS	N-CA	7.84	1.62	1.46
1	A	16	LYS	C-O	-7.84	1.08	1.23
1	C	11	LYS	CD-CE	-7.84	1.31	1.51
1	A	44	PRO	CA-CB	-7.84	1.37	1.53
2	B	117	HIS	CB-CG	-7.83	1.35	1.50
2	D	54	VAL	N-CA	7.82	1.61	1.46
2	D	135	ALA	CA-C	7.82	1.73	1.52
2	B	15	TRP	CG-CD1	-7.82	1.25	1.36
2	D	18	VAL	CA-C	7.82	1.73	1.52
1	C	74	ASP	CB-CG	-7.81	1.35	1.51
1	A	16	LYS	C-N	7.81	1.52	1.34
1	A	8	THR	C-N	7.80	1.51	1.34
2	B	22	GLU	N-CA	7.79	1.61	1.46
2	D	146	HIS	CD2-NE2	7.79	1.58	1.42
1	C	64	ASP	CG-OD2	-7.79	1.07	1.25
2	D	16	GLY	CA-C	-7.76	1.39	1.51
2	B	19	ASN	CG-OD1	-7.76	1.06	1.24
1	C	128	PHE	CA-C	7.75	1.73	1.52
2	B	8	LYS	CG-CD	7.75	1.78	1.52
2	D	16	GLY	C-O	7.74	1.36	1.23
1	A	13	ALA	CA-C	7.74	1.73	1.52
2	D	8	LYS	CA-C	-7.73	1.32	1.52
1	A	49	SER	N-CA	7.72	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	123	THR	C-N	-7.72	1.19	1.34
2	B	95	LYS	C-N	7.71	1.51	1.34
2	B	35	TYR	CE2-CZ	-7.70	1.28	1.38
1	C	31	ARG	CD-NE	7.69	1.59	1.46
1	A	43	PHE	CG-CD2	-7.69	1.27	1.38
2	B	42	PHE	CE2-CZ	7.69	1.51	1.37
1	A	132	VAL	CA-CB	-7.68	1.38	1.54
2	B	64	GLY	C-O	-7.67	1.11	1.23
1	C	23	GLU	N-CA	-7.67	1.31	1.46
2	D	97	HIS	ND1-CE1	7.67	1.53	1.34
1	C	8	THR	CA-C	-7.67	1.33	1.52
1	C	49	SER	CA-C	-7.67	1.33	1.52
1	A	53	ALA	CA-CB	7.66	1.68	1.52
1	A	20	HIS	CA-CB	-7.65	1.37	1.53
1	C	52	SER	N-CA	7.65	1.61	1.46
2	D	45	PHE	CA-C	7.65	1.72	1.52
2	D	118	PHE	CD2-CE2	7.65	1.54	1.39
1	C	114	PRO	C-O	7.64	1.38	1.23
2	D	92	HIS	CG-ND1	7.63	1.55	1.38
2	B	15	TRP	NE1-CE2	7.62	1.47	1.37
2	B	101	GLU	CD-OE1	-7.61	1.17	1.25
2	D	48	LEU	C-N	7.61	1.51	1.34
2	D	2	HIS	CD2-NE2	7.61	1.57	1.42
1	A	99	LYS	CA-C	-7.60	1.33	1.52
1	A	60	LYS	C-N	7.60	1.51	1.34
2	B	112	CYS	CA-CB	-7.60	1.37	1.53
2	D	25	GLY	CA-C	-7.59	1.39	1.51
2	B	66	LYS	CA-C	7.58	1.72	1.52
1	C	55	VAL	N-CA	7.58	1.61	1.46
2	D	58	PRO	C-N	-7.58	1.16	1.34
1	C	18	GLY	N-CA	7.56	1.57	1.46
2	D	17	LYS	CB-CG	-7.56	1.32	1.52
1	A	42	TYR	CA-C	7.55	1.72	1.52
2	B	97	HIS	CB-CG	7.55	1.63	1.50
2	B	61	LYS	CD-CE	7.54	1.70	1.51
1	C	76	MET	CA-C	-7.53	1.33	1.52
1	A	127	LYS	C-N	-7.53	1.16	1.34
2	D	60	VAL	CA-C	-7.52	1.33	1.52
2	B	134	VAL	C-O	7.52	1.37	1.23
2	B	71	PHE	CG-CD2	7.51	1.50	1.38
1	C	24	TYR	CD1-CE1	7.51	1.50	1.39
1	A	122	HIS	ND1-CE1	7.50	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	15	TRP	CZ2-CH2	-7.50	1.23	1.37
1	C	90	LYS	N-CA	-7.49	1.31	1.46
2	B	120	LYS	CB-CG	-7.49	1.32	1.52
1	C	94	ASP	CG-OD1	-7.48	1.08	1.25
1	C	83	LEU	C-O	7.48	1.37	1.23
2	D	45	PHE	C-O	7.47	1.37	1.23
1	C	7	LYS	C-N	7.47	1.51	1.34
2	D	104	ARG	CG-CD	7.46	1.70	1.51
2	D	75	LEU	CG-CD2	-7.45	1.24	1.51
2	D	68	LEU	CG-CD1	-7.45	1.24	1.51
1	C	105	LEU	CG-CD1	7.44	1.79	1.51
1	A	106	LEU	C-O	7.43	1.37	1.23
1	A	8	THR	CB-CG2	-7.43	1.27	1.52
2	B	53	ALA	CA-CB	-7.43	1.36	1.52
1	A	90	LYS	CB-CG	7.42	1.72	1.52
2	B	16	GLY	CA-C	-7.41	1.40	1.51
1	C	106	LEU	CA-C	-7.41	1.33	1.52
2	D	86	ALA	CA-CB	7.41	1.68	1.52
2	B	136	GLY	N-CA	7.40	1.57	1.46
2	D	5	PRO	N-CD	7.39	1.58	1.47
2	D	43	GLU	N-CA	7.39	1.61	1.46
1	C	12	ALA	C-O	7.38	1.37	1.23
1	C	2	LEU	CG-CD2	-7.37	1.24	1.51
2	D	130	TYR	CD2-CE2	7.37	1.50	1.39
1	C	12	ALA	N-CA	-7.37	1.31	1.46
1	A	72	HIS	CG-CD2	7.35	1.48	1.35
2	B	13	ALA	CA-CB	7.35	1.67	1.52
1	A	76	MET	N-CA	7.34	1.61	1.46
2	B	17	LYS	CD-CE	7.34	1.69	1.51
1	A	131	SER	CA-CB	7.33	1.64	1.52
2	B	72	SER	N-CA	7.32	1.60	1.46
2	B	28	LEU	CB-CG	7.32	1.73	1.52
2	D	10	ALA	N-CA	7.32	1.60	1.46
2	B	124	PRO	C-N	-7.32	1.20	1.34
1	A	106	LEU	CA-C	-7.31	1.33	1.52
2	B	112	CYS	CB-SG	7.31	1.94	1.82
2	B	145	TYR	CB-CG	7.31	1.62	1.51
1	C	112	HIS	C-N	-7.30	1.17	1.34
2	B	57	ASN	CG-OD1	-7.29	1.07	1.24
2	D	6	GLU	N-CA	-7.29	1.31	1.46
2	B	144	LYS	C-O	7.29	1.37	1.23
2	D	61	LYS	CG-CD	-7.29	1.27	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	ALA	C-N	-7.28	1.17	1.34
1	A	24	TYR	CG-CD1	-7.28	1.29	1.39
2	D	1	VAL	CA-CB	7.27	1.70	1.54
2	D	119	GLY	CA-C	7.27	1.63	1.51
1	A	74	ASP	N-CA	7.26	1.60	1.46
1	A	11	LYS	CB-CG	-7.25	1.32	1.52
1	A	48	LEU	CA-CB	7.25	1.70	1.53
2	D	50	THR	CA-C	7.24	1.71	1.52
1	C	59	GLY	C-O	7.24	1.35	1.23
2	D	81	LEU	CG-CD1	-7.24	1.25	1.51
2	B	72	SER	CB-OG	-7.23	1.32	1.42
1	C	2	LEU	CG-CD1	-7.23	1.25	1.51
2	D	44	SER	CA-C	-7.21	1.34	1.52
1	C	2	LEU	CA-CB	-7.20	1.37	1.53
1	A	69	ALA	C-O	-7.18	1.09	1.23
1	A	20	HIS	CB-CG	-7.17	1.37	1.50
1	C	29	LEU	CA-C	-7.17	1.34	1.52
2	D	67	VAL	CA-C	-7.17	1.34	1.52
2	B	46	GLY	N-CA	-7.16	1.35	1.46
1	A	43	PHE	CG-CD1	7.16	1.49	1.38
1	A	64	ASP	C-N	7.16	1.50	1.34
2	B	73	ASP	CA-CB	7.14	1.69	1.53
1	C	78	ASN	C-N	7.14	1.50	1.34
2	B	85	PHE	CB-CG	-7.13	1.39	1.51
1	C	122	HIS	CG-CD2	7.13	1.47	1.35
1	A	109	LEU	CG-CD2	-7.13	1.25	1.51
2	D	51	PRO	C-O	7.13	1.37	1.23
2	D	126	VAL	C-N	7.12	1.50	1.34
2	D	145	TYR	CE1-CZ	7.11	1.47	1.38
1	C	50	HIS	CA-C	7.10	1.71	1.52
2	B	54	VAL	CA-CB	7.10	1.69	1.54
2	B	11	VAL	CA-CB	-7.09	1.39	1.54
2	D	141	LEU	CG-CD2	7.09	1.78	1.51
1	A	90	LYS	CA-CB	7.08	1.69	1.53
1	A	79	ALA	CA-CB	-7.08	1.37	1.52
2	B	15	TRP	CD2-CE2	7.08	1.49	1.41
1	C	117	PHE	CG-CD1	7.08	1.49	1.38
1	C	20	HIS	CA-CB	-7.06	1.38	1.53
2	D	99	ASP	CB-CG	7.06	1.66	1.51
2	D	72	SER	CB-OG	-7.06	1.33	1.42
2	D	64	GLY	C-N	7.05	1.50	1.34
1	A	59	GLY	N-CA	7.05	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	TRP	CZ3-CH2	-7.04	1.28	1.40
2	D	26	GLU	CA-C	7.03	1.71	1.52
2	D	103	PHE	CG-CD1	7.03	1.49	1.38
1	A	48	LEU	CG-CD2	-7.02	1.25	1.51
2	B	95	LYS	C-O	-7.01	1.10	1.23
1	C	61	LYS	CB-CG	-7.01	1.33	1.52
2	D	126	VAL	C-O	-7.00	1.10	1.23
1	A	62	VAL	N-CA	7.00	1.60	1.46
1	A	71	ALA	CA-CB	-7.00	1.37	1.52
1	A	96	VAL	CA-CB	7.00	1.69	1.54
2	D	146	HIS	CG-CD2	-7.00	1.23	1.35
1	C	64	ASP	CB-CG	7.00	1.66	1.51
1	A	98	PHE	CD1-CE1	-6.99	1.25	1.39
1	C	23	GLU	CA-C	6.98	1.71	1.52
2	D	98	VAL	CB-CG2	6.98	1.67	1.52
2	D	78	LEU	C-N	6.97	1.50	1.34
1	A	77	PRO	N-CA	-6.96	1.35	1.47
1	A	114	PRO	CA-C	6.96	1.66	1.52
2	B	50	THR	CB-CG2	6.96	1.75	1.52
1	C	52	SER	C-O	6.96	1.36	1.23
1	C	74	ASP	N-CA	6.95	1.60	1.46
2	D	143	HIS	CG-ND1	-6.93	1.23	1.38
1	A	56	LYS	CA-C	-6.93	1.34	1.52
1	A	92	ARG	CD-NE	-6.92	1.34	1.46
2	D	10	ALA	CA-CB	-6.92	1.38	1.52
1	A	60	LYS	C-O	-6.92	1.10	1.23
2	B	145	TYR	CD1-CE1	-6.92	1.28	1.39
1	C	133	SER	C-N	-6.91	1.18	1.34
2	D	105	LEU	CA-CB	-6.89	1.37	1.53
2	D	122	PHE	CD1-CE1	6.89	1.53	1.39
2	B	41	PHE	CE1-CZ	-6.89	1.24	1.37
2	B	142	ALA	C-O	6.89	1.36	1.23
1	C	130	ALA	C-O	6.89	1.36	1.23
1	A	76	MET	C-N	-6.87	1.21	1.34
1	A	26	ALA	C-N	6.86	1.49	1.34
1	C	65	ALA	C-N	6.86	1.49	1.34
1	A	8	THR	CA-CB	6.86	1.71	1.53
1	A	98	PHE	CE2-CZ	-6.86	1.24	1.37
1	A	119	PRO	CA-C	-6.86	1.39	1.52
1	C	110	ALA	C-O	6.86	1.36	1.23
1	C	87	HIS	CE1-NE2	-6.85	1.17	1.32
1	C	40	LYS	N-CA	6.84	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	75	LEU	CA-CB	6.84	1.69	1.53
1	C	131	SER	CB-OG	6.83	1.51	1.42
2	D	28	LEU	C-N	6.82	1.45	1.33
2	D	131	GLN	C-O	-6.82	1.10	1.23
2	B	32	LEU	CG-CD1	-6.81	1.26	1.51
2	B	79	ASP	N-CA	6.81	1.59	1.46
2	D	7	GLU	C-N	-6.81	1.18	1.34
2	D	77	HIS	N-CA	-6.81	1.32	1.46
2	D	86	ALA	N-CA	6.81	1.59	1.46
2	B	34	VAL	N-CA	6.80	1.59	1.46
2	D	51	PRO	CA-C	-6.80	1.39	1.52
1	C	132	VAL	CA-CB	-6.79	1.40	1.54
2	B	54	VAL	C-O	6.79	1.36	1.23
1	A	41	THR	CA-C	-6.78	1.35	1.52
1	A	80	LEU	N-CA	6.78	1.59	1.46
2	B	121	GLU	CA-CB	6.78	1.68	1.53
2	B	120	LYS	CE-NZ	-6.77	1.32	1.49
2	B	123	THR	CB-OG1	-6.77	1.29	1.43
2	D	13	ALA	C-O	-6.77	1.10	1.23
1	A	79	ALA	CA-C	6.77	1.70	1.52
2	B	67	VAL	N-CA	6.75	1.59	1.46
1	C	14	TRP	C-N	-6.75	1.20	1.33
1	C	48	LEU	N-CA	6.75	1.59	1.46
2	B	13	ALA	N-CA	-6.74	1.32	1.46
2	D	95	LYS	N-CA	6.74	1.59	1.46
1	C	98	PHE	CG-CD2	-6.73	1.28	1.38
2	D	18	VAL	C-N	-6.73	1.18	1.34
1	C	124	SER	CA-CB	6.72	1.63	1.52
2	D	91	LEU	C-N	6.72	1.49	1.34
2	D	32	LEU	C-O	6.72	1.36	1.23
2	B	39	GLN	N-CA	6.72	1.59	1.46
2	B	12	THR	CA-CB	6.71	1.70	1.53
1	C	38	THR	CA-C	-6.71	1.35	1.52
1	A	8	THR	CA-C	-6.70	1.35	1.52
2	B	13	ALA	C-N	6.70	1.49	1.34
1	C	139	LYS	CG-CD	-6.70	1.29	1.52
2	D	15	TRP	CG-CD2	6.70	1.55	1.43
2	B	37	TRP	CD2-CE2	6.69	1.49	1.41
1	A	117	PHE	CD2-CE2	6.69	1.52	1.39
2	B	35	TYR	CD2-CE2	-6.69	1.29	1.39
2	B	73	ASP	N-CA	6.69	1.59	1.46
2	D	1	VAL	C-N	-6.68	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	94	ASP	CB-CG	6.68	1.65	1.51
1	A	139	LYS	N-CA	6.67	1.59	1.46
2	D	110	LEU	CA-CB	-6.67	1.38	1.53
1	A	12	ALA	N-CA	-6.67	1.33	1.46
1	A	73	VAL	CB-CG2	-6.66	1.38	1.52
2	B	19	ASN	CG-ND2	6.66	1.49	1.32
1	A	81	SER	C-O	6.66	1.35	1.23
2	D	84	THR	N-CA	-6.66	1.33	1.46
1	C	60	LYS	CD-CE	-6.65	1.34	1.51
2	B	119	GLY	C-O	6.64	1.34	1.23
2	B	124	PRO	C-O	6.63	1.36	1.23
2	B	83	GLY	CA-C	-6.63	1.41	1.51
1	A	120	ALA	N-CA	-6.62	1.33	1.46
1	A	33	PHE	C-N	6.62	1.49	1.34
2	D	68	LEU	CB-CG	-6.62	1.33	1.52
1	A	22	GLY	C-N	6.62	1.49	1.34
2	D	44	SER	C-N	6.61	1.49	1.34
2	B	144	LYS	CA-C	-6.61	1.35	1.52
1	C	109	LEU	C-N	6.60	1.49	1.34
2	D	93	CYS	N-CA	6.60	1.59	1.46
2	B	63	HIS	C-N	-6.59	1.21	1.33
2	D	54	VAL	CB-CG1	6.59	1.66	1.52
1	C	43	PHE	N-CA	6.59	1.59	1.46
1	A	41	THR	C-O	6.58	1.35	1.23
2	B	63	HIS	CA-CB	-6.58	1.39	1.53
1	C	87	HIS	CG-CD2	6.58	1.47	1.35
2	B	8	LYS	N-CA	-6.58	1.33	1.46
1	C	52	SER	CA-CB	-6.57	1.43	1.52
2	B	120	LYS	CA-CB	6.56	1.68	1.53
1	A	42	TYR	CG-CD2	6.56	1.47	1.39
2	B	3	LEU	N-CA	6.56	1.59	1.46
1	A	11	LYS	N-CA	6.55	1.59	1.46
2	B	76	ALA	N-CA	-6.55	1.33	1.46
1	C	78	ASN	CA-CB	6.55	1.70	1.53
1	C	68	ASN	N-CA	-6.55	1.33	1.46
2	B	123	THR	CA-C	6.55	1.70	1.52
1	A	20	HIS	CD2-NE2	6.55	1.55	1.42
1	A	113	LEU	CB-CG	6.54	1.71	1.52
2	B	58	PRO	CB-CG	-6.54	1.17	1.50
1	A	18	GLY	C-O	6.54	1.34	1.23
2	D	117	HIS	CD2-NE2	-6.53	1.23	1.38
1	A	5	ALA	N-CA	-6.52	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	68	LEU	CG-CD2	-6.52	1.27	1.51
1	A	40	LYS	C-O	-6.51	1.10	1.23
2	B	47	ASP	C-N	6.51	1.49	1.34
2	B	77	HIS	CA-CB	-6.51	1.39	1.53
2	D	14	LEU	N-CA	-6.51	1.33	1.46
2	D	32	LEU	CG-CD2	-6.51	1.27	1.51
2	B	102	ASN	CG-ND2	6.51	1.49	1.32
2	B	93	CYS	C-O	-6.50	1.11	1.23
2	B	123	THR	C-O	-6.50	1.11	1.23
1	C	27	GLU	CD-OE2	6.50	1.32	1.25
2	D	47	ASP	C-N	-6.49	1.19	1.34
1	A	92	ARG	CB-CG	-6.49	1.35	1.52
2	D	126	VAL	CB-CG1	-6.49	1.39	1.52
1	C	36	PHE	CD2-CE2	-6.49	1.26	1.39
1	C	46	PHE	CA-CB	6.46	1.68	1.53
1	A	113	LEU	CA-CB	-6.46	1.39	1.53
1	C	95	PRO	C-O	6.44	1.36	1.23
2	B	35	TYR	CG-CD1	6.43	1.47	1.39
1	C	58	HIS	CA-C	6.43	1.69	1.52
2	D	48	LEU	CG-CD1	6.42	1.75	1.51
2	B	48	LEU	N-CA	6.42	1.59	1.46
1	A	60	LYS	CA-CB	6.42	1.68	1.53
2	B	53	ALA	C-N	6.42	1.48	1.34
2	D	83	GLY	CA-C	-6.42	1.41	1.51
2	B	8	LYS	CD-CE	-6.41	1.35	1.51
2	B	90	GLU	C-N	6.41	1.48	1.34
1	A	68	ASN	C-N	6.40	1.48	1.34
1	C	113	LEU	CG-CD1	6.39	1.75	1.51
1	A	74	ASP	C-O	6.39	1.35	1.23
1	A	35	SER	N-CA	-6.39	1.33	1.46
2	D	66	LYS	C-N	6.38	1.48	1.34
1	A	72	HIS	CA-C	-6.38	1.36	1.52
1	A	45	HIS	CA-CB	-6.38	1.40	1.53
2	D	71	PHE	CE1-CZ	-6.38	1.25	1.37
1	C	120	ALA	C-O	6.37	1.35	1.23
1	A	63	ALA	CA-C	-6.37	1.36	1.52
2	B	104	ARG	CA-CB	6.36	1.68	1.53
1	A	95	PRO	C-O	6.35	1.35	1.23
1	C	45	HIS	CB-CG	6.34	1.61	1.50
2	D	55	MET	CA-CB	6.34	1.67	1.53
2	B	133	VAL	CB-CG1	-6.34	1.39	1.52
1	A	44	PRO	C-N	-6.33	1.19	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	VAL	N-CA	6.33	1.59	1.46
1	A	94	ASP	CA-C	6.33	1.69	1.52
1	C	63	ALA	CA-C	-6.33	1.36	1.52
2	B	145	TYR	C-O	6.33	1.35	1.23
2	B	140	ALA	CA-CB	6.32	1.65	1.52
1	A	61	LYS	CA-C	6.32	1.69	1.52
1	C	50	HIS	CG-CD2	-6.31	1.25	1.35
2	B	98	VAL	CA-C	6.31	1.69	1.52
2	B	120	LYS	CD-CE	6.31	1.67	1.51
1	C	130	ALA	CA-CB	-6.31	1.39	1.52
1	C	128	PHE	CE2-CZ	-6.31	1.25	1.37
1	C	122	HIS	CA-CB	-6.30	1.40	1.53
2	B	109	VAL	CB-CG2	6.29	1.66	1.52
2	B	15	TRP	CB-CG	6.29	1.61	1.50
1	A	60	LYS	CA-C	-6.28	1.36	1.52
2	B	80	ASN	CA-CB	-6.27	1.36	1.53
2	B	98	VAL	CB-CG2	6.26	1.66	1.52
1	C	17	VAL	CB-CG2	6.25	1.66	1.52
1	C	73	VAL	CA-C	6.25	1.69	1.52
1	A	108	THR	CA-CB	6.25	1.69	1.53
1	A	11	LYS	CA-CB	-6.25	1.40	1.53
2	B	92	HIS	CD2-NE2	-6.24	1.24	1.38
2	D	30	ARG	C-N	-6.24	1.19	1.34
1	A	128	PHE	CD2-CE2	6.22	1.51	1.39
1	C	73	VAL	N-CA	-6.22	1.33	1.46
2	B	106	LEU	CG-CD2	-6.21	1.28	1.51
1	A	60	LYS	CB-CG	-6.21	1.35	1.52
1	A	25	GLY	CA-C	-6.21	1.42	1.51
2	D	85	PHE	CE1-CZ	6.21	1.49	1.37
2	D	112	CYS	C-O	-6.21	1.11	1.23
2	D	120	LYS	CB-CG	-6.21	1.35	1.52
2	B	48	LEU	CA-CB	-6.20	1.39	1.53
2	B	118	PHE	CD1-CE1	6.20	1.51	1.39
1	C	99	LYS	C-O	-6.20	1.11	1.23
1	C	10	VAL	CB-CG1	6.20	1.65	1.52
1	A	128	PHE	CG-CD1	6.17	1.48	1.38
2	D	118	PHE	CG-CD2	6.17	1.48	1.38
1	C	128	PHE	CE1-CZ	-6.17	1.25	1.37
2	B	103	PHE	CG-CD2	-6.17	1.29	1.38
2	D	48	LEU	CA-C	6.17	1.69	1.52
1	C	41	THR	N-CA	6.16	1.58	1.46
2	D	47	ASP	C-O	6.16	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	48	LEU	CG-CD2	6.16	1.74	1.51
1	C	106	LEU	N-CA	6.16	1.58	1.46
2	B	130	TYR	CE1-CZ	-6.15	1.30	1.38
1	A	97	ASN	CG-ND2	6.15	1.48	1.32
1	A	10	VAL	CA-C	6.15	1.69	1.52
2	D	37	TRP	CD2-CE2	-6.15	1.33	1.41
2	D	116	HIS	CG-ND1	-6.14	1.25	1.38
2	B	91	LEU	CG-CD2	-6.13	1.29	1.51
1	A	30	GLU	CD-OE2	6.13	1.32	1.25
1	A	52	SER	CB-OG	-6.13	1.34	1.42
2	B	35	TYR	C-N	-6.13	1.22	1.34
2	D	95	LYS	CA-C	-6.12	1.37	1.52
2	D	59	LYS	N-CA	-6.12	1.34	1.46
2	D	118	PHE	CE1-CZ	6.12	1.49	1.37
2	B	90	GLU	N-CA	-6.12	1.34	1.46
2	B	6	GLU	C-N	-6.11	1.20	1.34
1	C	19	ALA	N-CA	-6.11	1.34	1.46
2	B	44	SER	N-CA	6.11	1.58	1.46
2	B	132	LYS	CD-CE	6.11	1.66	1.51
2	D	140	ALA	C-N	-6.10	1.20	1.34
1	A	16	LYS	CB-CG	6.09	1.69	1.52
1	C	4	PRO	CA-C	6.09	1.65	1.52
2	D	60	VAL	C-N	6.08	1.48	1.34
1	C	73	VAL	CB-CG1	-6.08	1.40	1.52
2	D	144	LYS	CB-CG	6.08	1.69	1.52
1	C	2	LEU	C-N	-6.08	1.20	1.34
2	D	84	THR	CA-C	6.07	1.68	1.52
1	A	11	LYS	CG-CD	-6.06	1.31	1.52
2	D	74	GLY	N-CA	-6.06	1.36	1.46
1	C	50	HIS	C-N	-6.05	1.22	1.33
2	D	23	VAL	C-N	-6.05	1.22	1.33
1	A	87	HIS	CB-CG	6.04	1.60	1.50
1	A	92	ARG	CA-C	-6.04	1.37	1.52
1	A	40	LYS	CD-CE	-6.04	1.36	1.51
1	C	128	PHE	C-O	6.04	1.34	1.23
2	D	145	TYR	N-CA	-6.03	1.34	1.46
1	A	46	PHE	CG-CD1	6.03	1.47	1.38
2	B	145	TYR	CE2-CZ	6.02	1.46	1.38
2	B	82	LYS	CG-CD	6.02	1.73	1.52
2	D	12	THR	CA-C	-6.01	1.37	1.52
1	C	88	ALA	CA-C	6.00	1.68	1.52
2	D	51	PRO	C-N	5.99	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ASP	C-O	-5.99	1.11	1.23
1	A	76	MET	SD-CE	-5.99	1.44	1.77
2	B	118	PHE	CA-CB	-5.98	1.40	1.53
2	B	23	VAL	C-O	5.97	1.34	1.23
2	B	40	ARG	CG-CD	5.96	1.66	1.51
2	D	78	LEU	CA-C	-5.96	1.37	1.52
1	A	86	LEU	C-N	5.96	1.47	1.34
1	C	17	VAL	CA-CB	5.96	1.67	1.54
2	B	52	ASP	CG-OD2	5.96	1.39	1.25
1	C	3	SER	C-N	5.95	1.45	1.34
2	B	129	ALA	C-O	5.95	1.34	1.23
1	A	12	ALA	CA-CB	5.95	1.65	1.52
1	A	34	LEU	CB-CG	-5.94	1.35	1.52
2	B	117	HIS	CA-CB	5.93	1.67	1.53
2	D	125	PRO	CG-CD	-5.93	1.31	1.50
2	B	94	ASP	CG-OD1	-5.93	1.11	1.25
1	C	2	LEU	C-O	5.92	1.34	1.23
1	A	26	ALA	CA-C	5.92	1.68	1.52
1	A	58	HIS	CE1-NE2	-5.92	1.19	1.32
1	C	25	GLY	CA-C	-5.91	1.42	1.51
2	B	34	VAL	CB-CG2	-5.91	1.40	1.52
2	B	7	GLU	CD-OE1	5.91	1.32	1.25
2	B	146	HIS	CA-C	-5.91	1.37	1.52
1	C	6	ASP	CG-OD1	5.90	1.39	1.25
1	A	140	TYR	N-CA	-5.90	1.34	1.46
2	D	121	GLU	CA-C	5.90	1.68	1.52
2	D	68	LEU	C-N	5.90	1.43	1.33
2	B	58	PRO	CA-CB	5.89	1.65	1.53
2	D	11	VAL	N-CA	5.89	1.58	1.46
1	A	114	PRO	N-CD	-5.89	1.39	1.47
2	D	58	PRO	CA-CB	5.88	1.65	1.53
1	C	24	TYR	C-O	-5.88	1.12	1.23
2	D	85	PHE	CD2-CE2	5.87	1.50	1.39
1	C	14	TRP	CD1-NE1	5.87	1.48	1.38
2	D	72	SER	C-O	5.87	1.34	1.23
1	C	51	GLY	CA-C	-5.86	1.42	1.51
2	D	71	PHE	CD2-CE2	5.86	1.50	1.39
1	A	71	ALA	N-CA	5.86	1.58	1.46
2	B	116	HIS	CG-ND1	5.85	1.51	1.38
2	B	92	HIS	CA-C	5.85	1.68	1.52
2	D	126	VAL	CA-C	5.85	1.68	1.52
1	A	64	ASP	N-CA	-5.84	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	66	LYS	CA-CB	5.84	1.66	1.53
1	C	26	ALA	C-O	-5.84	1.12	1.23
2	B	29	GLY	N-CA	-5.82	1.37	1.46
1	C	57	GLY	N-CA	-5.82	1.37	1.46
1	C	89	HIS	CE1-NE2	-5.81	1.19	1.32
2	B	84	THR	C-N	5.81	1.47	1.34
2	D	37	TRP	N-CA	-5.81	1.34	1.46
2	B	63	HIS	CG-CD2	5.81	1.45	1.35
2	D	63	HIS	CE1-NE2	-5.81	1.19	1.32
1	C	105	LEU	N-CA	-5.81	1.34	1.46
1	A	43	PHE	CE1-CZ	-5.80	1.26	1.37
2	D	92	HIS	CB-CG	5.80	1.60	1.50
2	B	84	THR	C-O	-5.80	1.12	1.23
1	A	20	HIS	C-N	-5.79	1.20	1.34
1	A	51	GLY	C-O	-5.79	1.14	1.23
2	B	35	TYR	CZ-OH	5.79	1.47	1.37
2	B	14	LEU	CG-CD1	-5.79	1.30	1.51
2	B	26	GLU	CA-CB	-5.79	1.41	1.53
2	B	92	HIS	CG-ND1	5.79	1.51	1.38
2	D	118	PHE	C-O	5.78	1.34	1.23
1	C	33	PHE	CA-C	-5.78	1.38	1.52
1	A	6	ASP	CA-CB	-5.78	1.41	1.53
2	D	139	ASN	CB-CG	-5.78	1.37	1.51
1	A	24	TYR	CD1-CE1	5.77	1.48	1.39
1	C	47	ASP	CA-C	5.77	1.68	1.52
1	C	29	LEU	CA-CB	5.76	1.67	1.53
1	C	61	LYS	C-N	5.76	1.47	1.34
2	D	60	VAL	CB-CG1	5.76	1.65	1.52
1	C	121	VAL	CA-CB	-5.75	1.42	1.54
1	A	28	ALA	C-O	-5.75	1.12	1.23
2	D	103	PHE	CB-CG	5.75	1.61	1.51
1	A	47	ASP	CA-CB	5.74	1.66	1.53
2	B	72	SER	C-O	5.74	1.34	1.23
2	D	97	HIS	C-N	5.74	1.47	1.34
2	D	115	ALA	C-O	-5.74	1.12	1.23
2	D	51	PRO	CG-CD	5.74	1.69	1.50
2	D	21	ASP	N-CA	5.73	1.57	1.46
2	B	33	VAL	CB-CG2	-5.72	1.40	1.52
1	A	112	HIS	CA-CB	5.72	1.66	1.53
1	A	33	PHE	CD1-CE1	5.72	1.50	1.39
2	B	71	PHE	CE1-CZ	-5.71	1.26	1.37
1	C	124	SER	CB-OG	5.71	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	9	ASN	CG-ND2	-5.70	1.18	1.32
1	A	92	ARG	N-CA	5.70	1.57	1.46
2	B	87	THR	CB-OG1	-5.70	1.31	1.43
1	A	21	ALA	CA-CB	-5.70	1.40	1.52
1	A	37	PRO	CA-C	-5.69	1.41	1.52
2	D	90	GLU	C-O	-5.69	1.12	1.23
2	D	145	TYR	CG-CD2	5.69	1.46	1.39
1	A	36	PHE	C-O	5.69	1.34	1.23
1	A	59	GLY	C-O	5.69	1.32	1.23
1	A	5	ALA	CA-C	5.68	1.67	1.52
1	A	34	LEU	CA-CB	-5.68	1.40	1.53
1	C	141	ARG	CA-C	5.68	1.67	1.52
1	C	141	ARG	CZ-NH1	-5.67	1.25	1.33
1	C	136	LEU	C-O	5.67	1.34	1.23
2	B	126	VAL	C-N	-5.66	1.21	1.34
1	C	31	ARG	CZ-NH2	-5.66	1.25	1.33
1	C	33	PHE	CE1-CZ	-5.66	1.26	1.37
1	A	78	ASN	N-CA	-5.66	1.35	1.46
2	B	140	ALA	C-O	5.66	1.34	1.23
1	C	134	THR	CB-OG1	-5.65	1.31	1.43
2	D	85	PHE	CG-CD1	5.65	1.47	1.38
1	C	46	PHE	CA-C	-5.65	1.38	1.52
1	C	84	SER	C-N	5.65	1.47	1.34
1	C	54	GLN	CA-CB	-5.64	1.41	1.53
2	B	62	ALA	C-O	-5.64	1.12	1.23
1	A	109	LEU	CG-CD1	-5.64	1.30	1.51
1	A	75	ASP	N-CA	5.63	1.57	1.46
1	C	141	ARG	CG-CD	5.63	1.66	1.51
1	A	46	PHE	N-CA	-5.62	1.35	1.46
2	D	30	ARG	CG-CD	-5.62	1.38	1.51
1	C	129	LEU	CA-CB	-5.62	1.40	1.53
1	C	28	ALA	N-CA	5.61	1.57	1.46
1	C	113	LEU	C-N	-5.61	1.23	1.34
2	D	14	LEU	CG-CD2	-5.61	1.31	1.51
2	B	17	LYS	CB-CG	5.59	1.67	1.52
1	C	8	THR	CB-CG2	-5.59	1.33	1.52
1	C	134	THR	C-O	5.59	1.33	1.23
2	B	9	SER	CB-OG	5.58	1.49	1.42
2	D	49	SER	CA-CB	5.58	1.61	1.52
1	A	63	ALA	CA-CB	5.57	1.64	1.52
1	A	2	LEU	N-CA	5.57	1.57	1.46
1	A	115	ALA	C-O	-5.57	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	71	PHE	CD1-CE1	5.57	1.50	1.39
1	C	92	ARG	C-N	5.57	1.46	1.34
2	B	37	TRP	CB-CG	-5.56	1.40	1.50
2	B	114	LEU	CA-CB	-5.56	1.41	1.53
2	D	102	ASN	CG-OD1	-5.55	1.11	1.24
2	B	47	ASP	CB-CG	-5.55	1.40	1.51
1	C	53	ALA	CA-CB	-5.55	1.40	1.52
2	D	51	PRO	N-CA	-5.54	1.37	1.47
2	B	92	HIS	ND1-CE1	5.54	1.48	1.34
1	C	19	ALA	CA-CB	-5.54	1.40	1.52
1	C	14	TRP	CE3-CZ3	5.54	1.47	1.38
1	A	105	LEU	CA-CB	5.54	1.66	1.53
1	A	54	GLN	CA-C	5.54	1.67	1.52
1	C	13	ALA	C-O	5.54	1.33	1.23
1	C	30	GLU	N-CA	-5.53	1.35	1.46
1	C	140	TYR	C-O	5.53	1.33	1.23
1	A	93	VAL	CA-C	-5.53	1.38	1.52
2	B	43	GLU	C-N	5.53	1.46	1.34
2	B	120	LYS	C-N	-5.53	1.21	1.34
1	A	9	ASN	C-O	-5.52	1.12	1.23
1	A	48	LEU	CG-CD1	5.52	1.72	1.51
2	D	99	ASP	C-N	-5.51	1.23	1.34
2	B	119	GLY	CA-C	-5.51	1.43	1.51
1	C	141	ARG	NE-CZ	5.50	1.40	1.33
2	B	28	LEU	C-N	5.50	1.43	1.33
2	B	116	HIS	ND1-CE1	5.49	1.48	1.34
2	B	57	ASN	N-CA	-5.49	1.35	1.46
1	A	123	ALA	C-O	5.49	1.33	1.23
1	C	97	ASN	CA-CB	-5.49	1.38	1.53
2	D	71	PHE	CG-CD2	5.48	1.47	1.38
2	B	30	ARG	NE-CZ	-5.48	1.25	1.33
2	D	31	LEU	C-N	5.48	1.46	1.34
1	A	112	HIS	C-O	5.47	1.33	1.23
2	D	50	THR	CB-OG1	5.47	1.54	1.43
1	A	72	HIS	N-CA	-5.47	1.35	1.46
2	B	23	VAL	C-N	-5.46	1.23	1.33
1	A	3	SER	CA-C	-5.46	1.38	1.52
1	C	12	ALA	CA-C	-5.46	1.38	1.52
1	C	135	VAL	C-N	5.46	1.46	1.34
1	A	43	PHE	CB-CG	5.46	1.60	1.51
2	D	59	LYS	CE-NZ	5.45	1.62	1.49
2	B	70	ALA	N-CA	-5.45	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	74	GLY	C-N	5.45	1.46	1.34
2	D	17	LYS	N-CA	-5.43	1.35	1.46
1	A	139	LYS	CD-CE	-5.43	1.37	1.51
2	B	17	LYS	CG-CD	-5.43	1.34	1.52
2	B	41	PHE	C-N	-5.42	1.21	1.34
1	A	140	TYR	C-N	-5.42	1.21	1.34
1	A	87	HIS	CG-ND1	5.42	1.50	1.38
2	B	68	LEU	C-O	5.42	1.33	1.23
1	C	46	PHE	C-O	5.42	1.33	1.23
1	A	129	LEU	CA-C	-5.41	1.38	1.52
2	D	92	HIS	N-CA	5.41	1.57	1.46
2	D	60	VAL	CB-CG2	-5.41	1.41	1.52
2	B	109	VAL	C-O	5.39	1.33	1.23
2	B	23	VAL	CA-C	5.39	1.67	1.52
2	B	144	LYS	CB-CG	5.39	1.67	1.52
1	A	61	LYS	CB-CG	5.39	1.67	1.52
1	A	141	ARG	CZ-NH2	5.38	1.40	1.33
1	C	37	PRO	CA-C	5.38	1.63	1.52
2	D	42	PHE	CD1-CE1	5.38	1.50	1.39
1	A	39	THR	C-N	-5.38	1.21	1.34
2	B	100	PRO	C-O	5.38	1.34	1.23
1	C	139	LYS	CB-CG	5.38	1.67	1.52
2	D	104	ARG	CB-CG	-5.38	1.38	1.52
1	C	109	LEU	CG-CD2	-5.38	1.31	1.51
2	B	6	GLU	CA-CB	5.37	1.65	1.53
2	B	33	VAL	CA-C	5.37	1.66	1.52
1	C	38	THR	N-CA	5.37	1.57	1.46
1	A	91	LEU	CG-CD1	-5.36	1.32	1.51
1	C	89	HIS	C-N	-5.36	1.21	1.34
1	A	85	ASP	C-O	-5.36	1.13	1.23
1	C	4	PRO	CA-CB	5.36	1.64	1.53
1	A	91	LEU	CA-CB	5.36	1.66	1.53
1	C	46	PHE	N-CA	-5.36	1.35	1.46
1	C	35	SER	C-N	5.35	1.46	1.34
2	B	17	LYS	CA-C	-5.35	1.39	1.52
2	D	49	SER	N-CA	5.34	1.57	1.46
2	B	48	LEU	CG-CD2	-5.34	1.32	1.51
2	B	15	TRP	CA-CB	-5.34	1.42	1.53
2	B	57	ASN	C-O	5.34	1.33	1.23
2	B	112	CYS	C-N	-5.33	1.21	1.34
2	D	35	TYR	CD1-CE1	5.33	1.47	1.39
2	D	102	ASN	CG-ND2	5.32	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	SER	C-N	5.32	1.46	1.34
2	B	13	ALA	CA-C	-5.32	1.39	1.52
1	C	85	ASP	CG-OD2	5.32	1.37	1.25
2	B	43	GLU	N-CA	5.31	1.56	1.46
1	C	115	ALA	C-O	5.31	1.33	1.23
1	C	12	ALA	CA-CB	-5.31	1.41	1.52
1	A	21	ALA	N-CA	5.30	1.56	1.46
2	B	86	ALA	CA-C	-5.29	1.39	1.52
1	C	54	GLN	N-CA	5.29	1.56	1.46
1	A	107	VAL	CB-CG2	5.29	1.64	1.52
2	B	108	ASN	CG-OD1	5.28	1.35	1.24
2	D	12	THR	CB-OG1	5.28	1.53	1.43
1	A	84	SER	C-O	-5.28	1.13	1.23
1	C	94	ASP	N-CA	-5.27	1.35	1.46
2	B	101	GLU	CA-CB	-5.27	1.42	1.53
1	C	5	ALA	CA-C	5.26	1.66	1.52
1	A	27	GLU	CD-OE2	-5.26	1.19	1.25
2	B	28	LEU	CA-C	-5.26	1.39	1.52
2	B	63	HIS	CE1-NE2	-5.26	1.20	1.32
2	D	102	ASN	N-CA	5.26	1.56	1.46
1	A	14	TRP	CA-C	5.25	1.66	1.52
2	B	3	LEU	CG-CD1	-5.25	1.32	1.51
2	B	79	ASP	C-N	5.25	1.46	1.34
1	A	114	PRO	C-O	-5.25	1.12	1.23
1	C	54	GLN	CB-CG	-5.25	1.38	1.52
1	C	56	LYS	C-N	5.24	1.42	1.33
2	D	68	LEU	CG-CD2	-5.24	1.32	1.51
1	C	27	GLU	C-N	5.23	1.46	1.34
1	C	45	HIS	CG-ND1	5.23	1.50	1.38
2	B	85	PHE	CD2-CE2	5.22	1.49	1.39
1	C	29	LEU	N-CA	5.22	1.56	1.46
2	B	42	PHE	C-N	-5.22	1.22	1.34
2	B	119	GLY	C-N	-5.22	1.22	1.34
2	B	24	GLY	N-CA	-5.22	1.38	1.46
1	C	82	ALA	CA-C	-5.22	1.39	1.52
2	B	71	PHE	CG-CD1	-5.22	1.30	1.38
2	B	78	LEU	CB-CG	5.21	1.67	1.52
1	C	116	GLU	C-N	-5.21	1.22	1.34
2	D	42	PHE	CB-CG	5.21	1.60	1.51
2	D	131	GLN	CB-CG	-5.21	1.38	1.52
1	A	46	PHE	C-N	5.20	1.46	1.34
2	D	145	TYR	CD1-CE1	-5.19	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	116	HIS	CB-CG	-5.19	1.40	1.50
2	D	91	LEU	CG-CD1	5.19	1.71	1.51
2	B	122	PHE	CE2-CZ	5.18	1.47	1.37
1	A	107	VAL	CB-CG1	-5.18	1.42	1.52
2	D	112	CYS	CA-C	5.18	1.66	1.52
2	D	119	GLY	C-N	5.18	1.46	1.34
1	C	86	LEU	N-CA	-5.17	1.36	1.46
1	A	88	ALA	N-CA	5.16	1.56	1.46
1	C	124	SER	C-N	-5.16	1.22	1.34
2	D	31	LEU	C-O	-5.16	1.13	1.23
2	D	102	ASN	CA-CB	-5.16	1.39	1.53
1	C	114	PRO	CG-CD	5.15	1.67	1.50
1	A	79	ALA	C-N	-5.14	1.22	1.34
2	D	77	HIS	CA-C	5.14	1.66	1.52
1	A	35	SER	CA-CB	5.14	1.60	1.52
1	C	55	VAL	CB-CG2	-5.14	1.42	1.52
2	D	16	GLY	N-CA	5.14	1.53	1.46
2	D	118	PHE	CB-CG	5.14	1.60	1.51
1	A	93	VAL	C-O	5.12	1.33	1.23
1	A	117	PHE	CB-CG	5.12	1.60	1.51
1	A	9	ASN	CA-C	5.12	1.66	1.52
1	A	135	VAL	C-O	5.12	1.33	1.23
2	B	67	VAL	C-O	5.12	1.33	1.23
1	A	75	ASP	C-O	5.11	1.33	1.23
2	B	30	ARG	CZ-NH1	5.11	1.39	1.33
1	A	115	ALA	N-CA	5.11	1.56	1.46
2	D	144	LYS	CA-C	-5.11	1.39	1.52
2	B	68	LEU	CA-CB	-5.10	1.42	1.53
2	D	111	VAL	C-N	5.10	1.45	1.34
2	B	105	LEU	CA-CB	-5.10	1.42	1.53
2	D	125	PRO	C-N	5.10	1.45	1.34
1	C	43	PHE	CE1-CZ	5.09	1.47	1.37
1	C	4	PRO	C-N	-5.09	1.22	1.34
1	A	19	ALA	CA-C	5.09	1.66	1.52
1	C	73	VAL	CB-CG2	-5.09	1.42	1.52
1	A	121	VAL	CB-CG1	5.09	1.63	1.52
1	C	58	HIS	CA-CB	-5.09	1.42	1.53
1	C	85	ASP	C-N	5.08	1.45	1.34
1	A	63	ALA	C-O	5.08	1.33	1.23
1	C	66	LEU	CG-CD1	-5.07	1.33	1.51
2	B	64	GLY	CA-C	-5.07	1.43	1.51
2	D	63	HIS	CG-CD2	5.06	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	52	ASP	CG-OD1	-5.06	1.13	1.25
2	B	85	PHE	N-CA	5.05	1.56	1.46
2	D	57	ASN	CG-ND2	-5.05	1.20	1.32
1	C	86	LEU	C-O	-5.05	1.13	1.23
1	A	69	ALA	C-N	5.04	1.45	1.34
1	A	112	HIS	C-N	-5.04	1.22	1.34
1	A	137	THR	C-N	-5.03	1.22	1.34
2	B	107	GLY	C-O	5.03	1.31	1.23
2	B	132	LYS	C-N	5.03	1.45	1.34
1	A	129	LEU	CG-CD2	5.02	1.70	1.51
1	A	85	ASP	C-N	5.02	1.45	1.34
1	A	68	ASN	CG-OD1	-5.02	1.12	1.24
1	C	113	LEU	CA-C	5.02	1.66	1.52
1	C	43	PHE	CG-CD1	5.01	1.46	1.38
1	A	54	GLN	CD-NE2	5.01	1.45	1.32
2	B	103	PHE	CD2-CE2	5.00	1.49	1.39
2	D	116	HIS	C-O	5.00	1.32	1.23

All (1822) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ARG	NE-CZ-NH2	-165.65	37.48	120.30
2	D	104	ARG	NE-CZ-NH2	-86.93	76.83	120.30
2	D	6	GLU	OE1-CD-OE2	-66.27	43.78	123.30
2	D	104	ARG	NE-CZ-NH1	-58.44	91.08	120.30
1	A	92	ARG	NE-CZ-NH2	-57.11	91.75	120.30
1	C	92	ARG	NE-CZ-NH1	-56.22	92.19	120.30
1	A	92	ARG	CD-NE-CZ	-51.91	50.92	123.60
2	B	26	GLU	OE1-CD-OE2	-50.93	62.19	123.30
2	B	101	GLU	OE1-CD-OE2	46.02	178.53	123.30
1	A	75	ASP	CB-CG-OD2	-43.83	78.85	118.30
2	B	22	GLU	OE1-CD-OE2	-43.42	71.19	123.30
2	D	73	ASP	CB-CG-OD1	43.24	157.21	118.30
1	A	92	ARG	NE-CZ-NH1	-40.84	99.88	120.30
2	D	40	ARG	NE-CZ-NH2	-38.42	101.09	120.30
1	A	75	ASP	CB-CG-OD1	38.31	152.78	118.30
2	B	104	ARG	CD-NE-CZ	-37.22	71.50	123.60
1	C	1	VAL	CG1-CB-CG2	-35.84	53.56	110.90
2	B	40	ARG	NE-CZ-NH2	-35.62	102.49	120.30
2	B	104	ARG	NE-CZ-NH2	-34.69	102.95	120.30
2	B	143	HIS	CG-ND1-CE1	-34.66	59.68	108.20
1	C	141	ARG	NE-CZ-NH2	-34.61	103.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ARG	CD-NE-CZ	-34.45	75.38	123.60
2	D	26	GLU	OE1-CD-OE2	-34.40	82.02	123.30
2	B	143	HIS	ND1-CG-CD2	32.83	154.76	108.80
2	B	26	GLU	CG-CD-OE2	-32.52	53.26	118.30
2	D	20	VAL	CG1-CB-CG2	32.43	162.78	110.90
1	C	75	ASP	CB-CG-OD2	-32.33	89.20	118.30
1	C	30	GLU	OE1-CD-OE2	32.31	162.07	123.30
2	D	73	ASP	CB-CG-OD2	-31.97	89.53	118.30
2	B	30	ARG	NE-CZ-NH2	31.85	136.23	120.30
2	D	52	ASP	CB-CG-OD2	-31.76	89.72	118.30
2	B	43	GLU	OE1-CD-OE2	31.63	161.26	123.30
1	A	92	ARG	CG-CD-NE	-31.16	46.35	111.80
2	D	58	PRO	N-CD-CG	-30.97	56.75	103.20
2	D	30	ARG	NE-CZ-NH1	29.94	135.27	120.30
2	B	5	PRO	N-CA-CB	29.91	139.19	103.30
1	A	92	ARG	NH1-CZ-NH2	29.46	151.81	119.40
2	D	43	GLU	OE1-CD-OE2	-29.30	88.14	123.30
2	D	3	LEU	O-C-N	-29.20	75.98	122.70
2	D	79	ASP	CB-CG-OD2	-29.16	92.06	118.30
1	C	23	GLU	OE1-CD-OE2	-28.52	89.08	123.30
2	D	80	ASN	CA-CB-CG	28.39	175.86	113.40
2	D	101	GLU	OE1-CD-OE2	28.06	156.98	123.30
2	B	42	PHE	CB-CG-CD2	27.91	140.34	120.80
2	D	73	ASP	OD1-CG-OD2	-27.45	71.14	123.30
2	B	45	PHE	CG-CD2-CE2	27.02	150.52	120.80
2	D	104	ARG	CD-NE-CZ	-26.61	86.35	123.60
2	D	20	VAL	CA-CB-CG2	-26.26	71.51	110.90
1	C	74	ASP	CB-CG-OD2	25.98	141.69	118.30
1	A	75	ASP	OD1-CG-OD2	-25.96	73.98	123.30
1	C	1	VAL	CA-CB-CG1	-25.93	72.00	110.90
2	B	44	SER	O-C-N	-25.83	81.38	122.70
2	D	52	ASP	CB-CG-OD1	-25.80	95.08	118.30
2	D	47	ASP	O-C-N	25.76	163.91	122.70
2	B	139	ASN	OD1-CG-ND2	-25.63	62.94	121.90
2	D	26	GLU	CG-CD-OE1	-25.55	67.20	118.30
1	A	31	ARG	NE-CZ-NH2	-25.32	107.64	120.30
2	D	26	GLU	CB-CG-CD	-25.23	46.06	114.20
1	A	141	ARG	NE-CZ-NH1	25.18	132.89	120.30
1	C	46	PHE	CB-CG-CD2	25.10	138.37	120.80
2	B	43	GLU	CG-CD-OE2	-24.55	69.20	118.30
1	A	47	ASP	CB-CG-OD2	-24.55	96.21	118.30
2	D	94	ASP	CB-CG-OD1	-24.43	96.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	HIS	ND1-CG-CD2	-24.25	72.06	106.00
2	D	43	GLU	CA-CB-CG	23.84	165.85	113.40
2	D	82	LYS	CD-CE-NZ	-23.77	57.02	111.70
2	D	47	ASP	N-CA-CB	-23.76	67.83	110.60
2	B	45	PHE	CZ-CE2-CD2	-23.48	91.93	120.10
1	A	141	ARG	NE-CZ-NH2	-23.44	108.58	120.30
1	C	38	THR	OG1-CB-CG2	-23.39	56.20	110.00
2	B	12	THR	OG1-CB-CG2	23.36	163.74	110.00
2	B	94	ASP	CB-CG-OD1	-23.18	97.44	118.30
1	A	64	ASP	CB-CG-OD1	-23.16	97.46	118.30
2	D	146	HIS	ND1-CG-CD2	-23.13	73.62	106.00
2	D	145	TYR	CB-CG-CD1	23.04	134.83	121.00
2	D	47	ASP	CB-CG-OD1	-22.89	97.70	118.30
1	C	46	PHE	CZ-CE2-CD2	22.88	147.55	120.10
1	C	1	VAL	CA-CB-CG2	-22.79	76.72	110.90
2	B	145	TYR	CB-CG-CD2	-22.52	107.48	121.00
2	D	6	GLU	O-C-N	22.45	158.63	122.70
1	A	46	PHE	CB-CG-CD2	22.39	136.47	120.80
2	D	5	PRO	N-CA-CB	-22.35	76.48	103.30
1	C	24	TYR	CG-CD1-CE1	-22.27	103.48	121.30
2	B	40	ARG	NH1-CZ-NH2	22.23	143.86	119.40
2	D	90	GLU	CG-CD-OE1	-22.02	74.26	118.30
2	D	71	PHE	CG-CD2-CE2	-22.01	96.59	120.80
1	A	14	TRP	CD1-NE1-CE2	21.98	128.78	109.00
2	D	42	PHE	CB-CG-CD1	-21.92	105.46	120.80
2	B	40	ARG	NE-CZ-NH1	-21.87	109.36	120.30
2	D	55	MET	O-C-N	21.86	160.37	123.20
2	D	26	GLU	CG-CD-OE2	-21.76	74.78	118.30
2	B	52	ASP	CB-CG-OD2	-21.74	98.73	118.30
2	D	17	LYS	O-C-N	-21.70	87.99	122.70
1	A	138	SER	CA-CB-OG	-21.69	52.63	111.20
2	D	79	ASP	OD1-CG-OD2	-21.68	82.10	123.30
1	C	73	VAL	CG1-CB-CG2	21.66	145.56	110.90
2	B	1	VAL	CG1-CB-CG2	21.62	145.49	110.90
2	B	49	SER	O-C-N	-21.42	88.43	122.70
2	D	76	ALA	N-CA-CB	-21.36	80.19	110.10
1	C	138	SER	CA-CB-OG	-21.29	53.73	111.20
2	B	101	GLU	CG-CD-OE2	-21.23	75.83	118.30
1	C	14	TRP	CD1-NE1-CE2	21.02	127.91	109.00
2	D	45	PHE	CB-CG-CD2	20.98	135.49	120.80
2	D	55	MET	C-N-CA	-20.95	78.31	122.30
1	A	64	ASP	CB-CG-OD2	-20.92	99.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	GLU	CB-CG-CD	20.80	170.36	114.20
2	B	42	PHE	CD1-CE1-CZ	20.70	144.95	120.10
2	D	41	PHE	CG-CD1-CE1	-20.56	98.18	120.80
2	D	118	PHE	CB-CG-CD1	20.55	135.19	120.80
1	C	128	PHE	CB-CG-CD2	-20.23	106.64	120.80
1	C	14	TRP	CG-CD1-NE1	-20.13	89.97	110.10
1	C	23	GLU	CG-CD-OE1	-20.04	78.22	118.30
2	D	72	SER	N-CA-CB	19.95	140.43	110.50
1	A	12	ALA	CB-CA-C	-19.65	80.62	110.10
1	C	47	ASP	CB-CG-OD2	-19.45	100.79	118.30
1	C	1	VAL	N-CA-CB	-19.31	69.02	111.50
1	C	24	TYR	CZ-CE2-CD2	-19.11	102.60	119.80
2	B	21	ASP	CB-CG-OD2	-18.95	101.24	118.30
1	A	90	LYS	CD-CE-NZ	-18.86	68.32	111.70
1	A	2	LEU	O-C-N	18.85	152.86	122.70
2	D	118	PHE	CG-CD1-CE1	18.84	141.52	120.80
1	C	128	PHE	CD1-CG-CD2	18.79	142.72	118.30
2	D	19	ASN	OD1-CG-ND2	-18.78	78.71	121.90
2	D	101	GLU	CG-CD-OE2	-18.71	80.88	118.30
2	D	94	ASP	CB-CG-OD2	-18.70	101.47	118.30
1	A	75	ASP	CA-CB-CG	-18.58	72.52	113.40
2	D	78	LEU	CB-CG-CD2	18.57	142.56	111.00
2	D	42	PHE	CG-CD1-CE1	-18.55	100.40	120.80
2	D	41	PHE	CD1-CE1-CZ	18.47	142.26	120.10
2	D	145	TYR	CB-CG-CD2	-18.45	109.93	121.00
2	B	108	ASN	OD1-CG-ND2	18.43	164.28	121.90
2	D	56	GLY	O-C-N	-18.39	93.28	122.70
1	C	128	PHE	CG-CD1-CE1	-18.19	100.80	120.80
2	B	22	GLU	CG-CD-OE2	-18.14	82.02	118.30
1	C	47	ASP	CB-CG-OD1	-18.10	102.01	118.30
2	D	46	GLY	C-N-CA	-18.04	76.60	121.70
1	A	85	ASP	CB-CG-OD1	17.99	134.49	118.30
1	A	17	VAL	O-C-N	17.92	153.67	123.20
2	B	144	LYS	CG-CD-CE	17.88	165.54	111.90
2	B	45	PHE	CB-CG-CD2	17.87	133.31	120.80
1	A	49	SER	CB-CA-C	17.80	143.92	110.10
1	C	74	ASP	OD1-CG-OD2	-17.77	89.54	123.30
1	C	116	GLU	CG-CD-OE2	-17.75	82.79	118.30
1	C	16	LYS	N-CA-CB	17.66	142.39	110.60
2	B	65	LYS	CD-CE-NZ	-17.59	71.24	111.70
2	B	50	THR	CA-CB-CG2	17.58	137.02	112.40
2	B	6	GLU	OE1-CD-OE2	-17.57	102.21	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	GLY	O-C-N	-17.57	94.58	122.70
2	D	44	SER	O-C-N	-17.49	94.72	122.70
1	A	30	GLU	OE1-CD-OE2	17.45	144.24	123.30
2	B	59	LYS	CD-CE-NZ	-17.45	71.57	111.70
2	D	132	LYS	CD-CE-NZ	-17.44	71.58	111.70
1	A	128	PHE	CZ-CE2-CD2	-17.39	99.23	120.10
1	A	31	ARG	NE-CZ-NH1	17.39	129.00	120.30
2	D	17	LYS	CA-C-O	17.32	156.46	120.10
1	A	1	VAL	CA-CB-CG2	-17.30	84.96	110.90
2	B	21	ASP	CB-CG-OD1	-17.20	102.82	118.30
1	A	1	VAL	CG1-CB-CG2	17.16	138.36	110.90
2	D	130	TYR	CG-CD1-CE1	17.12	135.00	121.30
1	A	33	PHE	CB-CG-CD1	17.08	132.76	120.80
1	A	23	GLU	CG-CD-OE1	-17.05	84.20	118.30
2	D	58	PRO	CA-CB-CG	-16.98	71.73	104.00
2	B	139	ASN	CB-CG-OD1	16.96	155.53	121.60
2	B	2	HIS	CB-CA-C	-16.86	76.68	110.40
1	A	72	HIS	CA-CB-CG	-16.82	85.01	113.60
2	D	18	VAL	O-C-N	16.82	149.60	122.70
2	B	4	THR	CA-CB-CG2	16.73	135.82	112.40
1	C	22	GLY	O-C-N	-16.72	95.94	122.70
2	D	130	TYR	CD1-CE1-CZ	-16.62	104.84	119.80
2	B	74	GLY	CA-C-O	16.59	150.46	120.60
1	C	14	TRP	CE3-CZ3-CH2	-16.59	102.95	121.20
2	B	94	ASP	OD1-CG-OD2	16.57	154.79	123.30
1	C	139	LYS	CD-CE-NZ	-16.57	73.59	111.70
2	B	121	GLU	CG-CD-OE2	-16.55	85.20	118.30
1	A	60	LYS	CD-CE-NZ	-16.50	73.75	111.70
1	C	64	ASP	CB-CG-OD2	-16.48	103.47	118.30
2	B	20	VAL	O-C-N	-16.43	96.41	122.70
1	C	14	TRP	C-N-CA	16.34	156.60	122.30
1	C	61	LYS	CD-CE-NZ	-16.32	74.17	111.70
1	C	46	PHE	CE1-CZ-CE2	-16.29	90.68	120.00
1	A	17	VAL	CA-C-N	-16.28	83.64	116.20
1	A	16	LYS	CG-CD-CE	-16.18	63.34	111.90
1	A	12	ALA	O-C-N	-16.17	96.83	122.70
2	B	118	PHE	CB-CG-CD2	16.17	132.12	120.80
2	D	8	LYS	CA-CB-CG	-16.15	77.88	113.40
1	C	128	PHE	CG-CD2-CE2	-16.07	103.12	120.80
1	C	14	TRP	O-C-N	-16.05	95.92	123.20
1	A	78	ASN	OD1-CG-ND2	-16.05	84.99	121.90
1	C	56	LYS	CD-CE-NZ	-16.03	74.83	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	VAL	C-N-CA	-16.02	81.66	121.70
2	D	78	LEU	CA-C-O	16.02	153.73	120.10
2	B	85	PHE	CZ-CE2-CD2	16.01	139.31	120.10
2	D	47	ASP	CA-C-N	-16.00	82.00	117.20
2	D	46	GLY	CA-C-O	-15.99	91.81	120.60
2	D	13	ALA	N-CA-CB	15.97	132.46	110.10
2	D	94	ASP	OD1-CG-OD2	15.88	153.46	123.30
2	B	65	LYS	CG-CD-CE	-15.84	64.38	111.90
2	D	12	THR	CA-CB-CG2	-15.73	90.38	112.40
1	C	24	TYR	CE1-CZ-CE2	15.68	144.88	119.80
1	A	18	GLY	O-C-N	15.67	147.77	122.70
1	A	43	PHE	CB-CG-CD2	15.66	131.76	120.80
2	B	32	LEU	CB-CG-CD1	15.64	137.60	111.00
2	D	76	ALA	CA-C-N	15.57	151.46	117.20
2	D	76	ALA	O-C-N	-15.56	97.80	122.70
1	C	23	GLU	CG-CD-OE2	-15.53	87.24	118.30
2	B	73	ASP	O-C-N	-15.52	96.82	123.20
1	C	71	ALA	CB-CA-C	15.47	133.31	110.10
2	D	71	PHE	CD1-CG-CD2	15.47	138.41	118.30
2	B	117	HIS	CG-CD2-NE2	-15.46	79.82	109.20
2	D	71	PHE	CB-CG-CD2	-15.45	109.98	120.80
2	D	2	HIS	CE1-NE2-CD2	15.45	145.22	106.60
2	D	77	HIS	CG-CD2-NE2	-15.44	79.87	109.20
2	B	74	GLY	O-C-N	-15.42	98.03	122.70
1	C	7	LYS	CD-CE-NZ	15.42	147.16	111.70
1	C	75	ASP	OD1-CG-OD2	15.41	152.58	123.30
2	D	43	GLU	O-C-N	15.41	147.35	122.70
2	D	6	GLU	CG-CD-OE2	-15.40	87.49	118.30
1	C	85	ASP	CB-CG-OD1	15.40	132.16	118.30
1	A	98	PHE	CB-CG-CD1	-15.40	110.02	120.80
1	A	33	PHE	CB-CG-CD2	-15.32	110.08	120.80
2	D	146	HIS	CG-CD2-NE2	15.29	138.24	109.20
2	D	47	ASP	N-CA-C	-15.28	69.75	111.00
2	B	2	HIS	CG-ND1-CE1	-15.25	85.88	105.70
2	D	139	ASN	CB-CG-OD1	-15.19	91.22	121.60
1	C	56	LYS	CG-CD-CE	-15.18	66.36	111.90
1	A	81	SER	N-CA-CB	-15.14	87.78	110.50
1	C	45	HIS	CG-ND1-CE1	-15.08	86.09	105.70
2	D	47	ASP	CB-CA-C	-15.08	80.24	110.40
2	D	1	VAL	CA-C-N	-15.07	84.04	117.20
2	B	37	TRP	CD1-NE1-CE2	15.07	122.56	109.00
2	D	1	VAL	O-C-N	14.88	146.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	121	GLU	OE1-CD-OE2	-14.85	105.48	123.30
2	D	41	PHE	O-C-N	14.82	146.41	122.70
1	A	137	THR	CA-CB-OG1	-14.81	77.90	109.00
2	D	79	ASP	CB-CA-C	-14.74	80.92	110.40
2	B	56	GLY	O-C-N	-14.70	99.19	122.70
2	D	90	GLU	OE1-CD-OE2	-14.68	105.68	123.30
2	D	50	THR	N-CA-CB	-14.67	82.42	110.30
1	C	73	VAL	CA-CB-CG1	-14.66	88.90	110.90
2	B	58	PRO	N-CD-CG	-14.64	81.24	103.20
1	C	128	PHE	CB-CG-CD1	-14.64	110.55	120.80
1	C	98	PHE	CZ-CE2-CD2	14.63	137.65	120.10
1	C	72	HIS	ND1-CG-CD2	-14.60	85.56	106.00
2	D	59	LYS	O-C-N	14.53	145.94	122.70
1	C	12	ALA	CA-C-O	14.50	150.54	120.10
2	B	145	TYR	CG-CD2-CE2	-14.45	109.74	121.30
2	D	30	ARG	NH1-CZ-NH2	-14.43	103.53	119.40
1	A	46	PHE	CG-CD2-CE2	14.40	136.64	120.80
2	D	101	GLU	CG-CD-OE1	-14.37	89.56	118.30
2	D	71	PHE	CB-CG-CD1	-14.35	110.75	120.80
1	A	116	GLU	OE1-CD-OE2	-14.33	106.10	123.30
1	C	71	ALA	O-C-N	-14.28	99.85	122.70
1	A	85	ASP	CB-CG-OD2	-14.27	105.46	118.30
2	B	132	LYS	CD-CE-NZ	-14.19	79.06	111.70
2	B	49	SER	C-N-CA	14.17	157.13	121.70
2	D	77	HIS	ND1-CG-CD2	14.17	128.64	108.80
2	D	80	ASN	OD1-CG-ND2	14.13	154.40	121.90
2	B	87	THR	OG1-CB-CG2	-14.12	77.53	110.00
1	A	47	ASP	CB-CG-OD1	14.09	130.98	118.30
2	B	26	GLU	CG-CD-OE1	-14.09	90.13	118.30
1	A	50	HIS	N-CA-CB	-14.07	85.28	110.60
1	C	43	PHE	CG-CD2-CE2	-14.04	105.36	120.80
2	B	146	HIS	CG-CD2-NE2	-14.03	82.54	109.20
1	A	62	VAL	O-C-N	14.02	145.12	122.70
2	B	146	HIS	ND1-CE1-NE2	-14.00	79.09	109.90
2	D	73	ASP	O-C-N	-13.94	99.50	123.20
2	B	94	ASP	CB-CG-OD2	-13.93	105.76	118.30
1	A	21	ALA	CA-C-N	-13.89	88.42	116.20
1	C	43	PHE	CZ-CE2-CD2	13.85	136.72	120.10
2	B	77	HIS	CG-CD2-NE2	-13.84	82.91	109.20
2	D	20	VAL	CA-C-O	13.76	148.99	120.10
2	B	145	TYR	CD1-CG-CD2	13.75	133.03	117.90
2	D	43	GLU	CG-CD-OE2	13.75	145.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	TRP	NE1-CE2-CZ2	13.74	145.51	130.40
1	C	78	ASN	CA-C-O	13.74	148.95	120.10
1	A	21	ALA	C-N-CA	-13.72	93.49	122.30
2	D	66	LYS	CA-CB-CG	13.70	143.54	113.40
1	C	25	GLY	O-C-N	-13.69	100.80	122.70
2	B	28	LEU	CB-CG-CD2	-13.69	87.73	111.00
1	A	33	PHE	CG-CD2-CE2	-13.68	105.75	120.80
2	B	121	GLU	CG-CD-OE1	-13.68	90.95	118.30
1	A	58	HIS	O-C-N	13.68	146.45	123.20
2	D	73	ASP	CA-CB-CG	-13.58	83.52	113.40
1	C	48	LEU	O-C-N	-13.57	100.99	122.70
1	A	14	TRP	CG-CD1-NE1	-13.54	96.56	110.10
2	B	22	GLU	CG-CD-OE1	-13.54	91.22	118.30
1	C	33	PHE	CB-CG-CD1	-13.54	111.32	120.80
2	B	41	PHE	O-C-N	13.51	144.31	122.70
1	A	50	HIS	C-N-CA	13.46	150.57	122.30
2	B	44	SER	CA-CB-OG	13.45	147.52	111.20
2	B	45	PHE	CB-CG-CD1	-13.44	111.39	120.80
2	D	32	LEU	CB-CG-CD2	13.44	133.84	111.00
2	B	108	ASN	CB-CG-ND2	-13.42	84.50	116.70
2	D	146	HIS	CE1-NE2-CD2	-13.41	73.07	106.60
2	D	46	GLY	O-C-N	13.41	144.15	122.70
2	B	143	HIS	CB-CG-ND1	-13.41	89.68	123.20
2	D	118	PHE	CD1-CE1-CZ	-13.40	104.02	120.10
2	D	2	HIS	O-C-N	13.40	144.13	122.70
2	D	8	LYS	O-C-N	-13.39	101.28	122.70
1	C	16	LYS	CB-CG-CD	-13.38	76.81	111.60
2	B	49	SER	CA-C-O	-13.37	92.03	120.10
1	A	21	ALA	CB-CA-C	13.36	130.14	110.10
1	C	46	PHE	CD1-CG-CD2	-13.35	100.94	118.30
1	C	24	TYR	CD1-CG-CD2	13.34	132.57	117.90
2	D	67	VAL	CG1-CB-CG2	13.34	132.24	110.90
2	B	49	SER	CB-CA-C	-13.33	84.78	110.10
2	D	10	ALA	CB-CA-C	-13.31	90.14	110.10
2	D	22	GLU	CG-CD-OE2	-13.28	91.74	118.30
2	B	117	HIS	CB-CG-ND1	-13.23	90.12	123.20
1	A	140	TYR	CB-CG-CD2	13.23	128.94	121.00
1	A	14	TRP	CH2-CZ2-CE2	13.21	130.61	117.40
1	A	110	ALA	O-C-N	-13.19	101.60	122.70
2	D	37	TRP	CZ3-CH2-CZ2	13.11	137.34	121.60
2	B	5	PRO	CA-N-CD	-13.09	93.17	111.50
2	B	125	PRO	N-CA-CB	13.08	119.00	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	121	GLU	CG-CD-OE2	-13.07	92.16	118.30
2	D	76	ALA	CB-CA-C	13.05	129.67	110.10
2	D	77	HIS	CB-CA-C	-13.01	84.38	110.40
2	D	73	ASP	CA-C-O	12.96	147.31	120.10
1	C	140	TYR	CB-CG-CD1	12.93	128.76	121.00
2	B	146	HIS	ND1-CG-CD2	-12.92	87.91	106.00
2	D	45	PHE	CG-CD2-CE2	12.91	135.00	120.80
2	B	8	LYS	O-C-N	-12.88	102.09	122.70
2	D	79	ASP	N-CA-CB	-12.88	87.41	110.60
1	C	46	PHE	O-C-N	-12.88	102.10	122.70
1	C	85	ASP	CB-CG-OD2	-12.87	106.71	118.30
1	C	19	ALA	O-C-N	-12.85	102.14	122.70
2	D	99	ASP	CB-CG-OD1	-12.84	106.74	118.30
1	C	15	GLY	C-N-CA	12.82	153.75	121.70
2	B	37	TRP	CH2-CZ2-CE2	-12.79	104.61	117.40
1	C	31	ARG	NE-CZ-NH2	-12.79	113.90	120.30
1	A	61	LYS	O-C-N	12.79	143.17	122.70
2	B	76	ALA	CB-CA-C	-12.78	90.93	110.10
1	A	48	LEU	CB-CG-CD2	12.72	132.62	111.00
1	A	74	ASP	CA-C-N	12.70	145.14	117.20
2	B	87	THR	CA-CB-CG2	-12.70	94.63	112.40
1	C	30	GLU	CG-CD-OE1	-12.70	92.91	118.30
1	C	113	LEU	CB-CG-CD1	-12.69	89.42	111.00
2	D	7	GLU	CG-CD-OE1	-12.69	92.93	118.30
1	C	70	VAL	O-C-N	12.67	142.98	122.70
1	C	64	ASP	CB-CG-OD1	-12.67	106.89	118.30
2	D	20	VAL	O-C-N	-12.63	102.50	122.70
2	D	118	PHE	CB-CG-CD2	-12.62	111.97	120.80
1	A	46	PHE	CD1-CG-CD2	-12.60	101.92	118.30
1	C	50	HIS	CG-CD2-NE2	12.60	133.14	109.20
2	D	49	SER	C-N-CA	-12.58	90.26	121.70
2	D	71	PHE	CG-CD1-CE1	-12.54	107.00	120.80
2	D	37	TRP	CH2-CZ2-CE2	-12.54	104.86	117.40
2	D	145	TYR	CG-CD1-CE1	12.54	131.33	121.30
1	A	24	TYR	CZ-CE2-CD2	-12.53	108.52	119.80
2	D	7	GLU	CG-CD-OE2	12.52	143.34	118.30
1	C	14	TRP	CB-CG-CD1	-12.52	110.73	127.00
1	C	84	SER	N-CA-CB	12.51	129.27	110.50
2	B	1	VAL	CA-C-N	-12.51	89.69	117.20
2	D	63	HIS	CG-CD2-NE2	-12.49	85.46	109.20
2	B	146	HIS	CB-CG-CD2	-12.49	92.09	130.80
1	C	33	PHE	CG-CD2-CE2	-12.49	107.06	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	TRP	CD1-CG-CD2	12.46	116.27	106.30
2	D	97	HIS	CG-CD2-NE2	-12.46	85.54	109.20
2	B	68	LEU	CB-CG-CD1	-12.42	89.88	111.00
1	A	4	PRO	CB-CA-C	-12.41	80.97	112.00
1	C	126	ASP	CB-CG-OD1	-12.41	107.13	118.30
1	A	36	PHE	CB-CG-CD2	-12.41	112.11	120.80
2	D	65	LYS	CB-CG-CD	-12.41	79.34	111.60
2	D	45	PHE	O-C-N	12.40	144.28	123.20
1	A	111	ALA	N-CA-CB	12.39	127.45	110.10
1	C	20	HIS	CG-ND1-CE1	-12.36	89.63	105.70
1	A	65	ALA	O-C-N	12.34	142.45	122.70
1	C	24	TYR	CB-CG-CD1	-12.32	113.61	121.00
1	C	24	TYR	CB-CG-CD2	-12.32	113.61	121.00
2	B	64	GLY	CA-C-O	12.32	142.77	120.60
2	D	24	GLY	O-C-N	-12.30	102.29	123.20
2	D	75	LEU	CB-CG-CD2	12.30	131.91	111.00
1	A	89	HIS	CE1-NE2-CD2	12.29	137.32	106.60
2	D	53	ALA	N-CA-CB	12.29	127.30	110.10
1	A	89	HIS	ND1-CE1-NE2	-12.28	82.88	109.90
1	C	105	LEU	CB-CG-CD2	-12.28	90.12	111.00
1	A	75	ASP	CB-CA-C	-12.25	85.89	110.40
1	A	34	LEU	CB-CG-CD1	12.25	131.82	111.00
1	C	52	SER	O-C-N	-12.24	103.12	122.70
2	D	77	HIS	CA-C-O	12.23	145.78	120.10
2	D	42	PHE	CB-CG-CD2	12.22	129.35	120.80
2	D	130	TYR	CB-CG-CD2	12.19	128.31	121.00
1	C	113	LEU	CB-CG-CD2	12.17	131.68	111.00
2	B	53	ALA	CA-C-O	12.15	145.62	120.10
2	D	93	CYS	O-C-N	12.15	142.14	122.70
2	B	4	THR	N-CA-CB	-12.15	87.22	110.30
2	B	22	GLU	CB-CG-CD	12.14	146.99	114.20
1	A	141	ARG	CD-NE-CZ	-12.09	106.67	123.60
2	D	65	LYS	CD-CE-NZ	-12.07	83.95	111.70
2	D	121	GLU	CG-CD-OE1	-12.07	94.17	118.30
2	B	85	PHE	CG-CD2-CE2	-12.06	107.53	120.80
1	C	14	TRP	CH2-CZ2-CE2	12.06	129.46	117.40
2	D	79	ASP	CA-C-N	-12.05	90.69	117.20
2	D	52	ASP	OD1-CG-OD2	-12.05	100.41	123.30
1	A	42	TYR	CD1-CE1-CZ	12.01	130.60	119.80
2	D	78	LEU	N-CA-C	11.99	143.39	111.00
1	C	116	GLU	CB-CG-CD	-11.99	81.84	114.20
2	B	43	GLU	O-C-N	-11.98	103.53	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	GLY	CA-C-O	-11.98	99.04	120.60
2	D	2	HIS	CB-CG-CD2	11.98	167.93	130.80
1	A	20	HIS	CG-ND1-CE1	-11.97	90.13	105.70
2	B	18	VAL	CA-CB-CG2	-11.97	92.95	110.90
1	C	48	LEU	CB-CG-CD1	11.96	131.34	111.00
1	C	53	ALA	CB-CA-C	11.96	128.03	110.10
2	D	80	ASN	CA-C-N	-11.96	90.90	117.20
1	A	7	LYS	CD-CE-NZ	-11.93	84.27	111.70
1	A	24	TYR	CD1-CE1-CZ	11.93	130.53	119.80
2	D	83	GLY	O-C-N	-11.91	103.64	122.70
2	B	82	LYS	N-CA-CB	-11.89	89.19	110.60
1	C	116	GLU	CG-CD-OE1	11.89	142.09	118.30
2	D	52	ASP	N-CA-CB	-11.88	89.21	110.60
2	B	44	SER	CB-CA-C	11.86	132.63	110.10
1	A	26	ALA	N-CA-CB	11.84	126.68	110.10
1	C	114	PRO	O-C-N	-11.83	103.78	122.70
2	D	42	PHE	CD1-CE1-CZ	11.82	134.28	120.10
2	D	65	LYS	CG-CD-CE	-11.82	76.44	111.90
2	B	1	VAL	CA-C-O	-11.81	95.30	120.10
2	D	20	VAL	CA-CB-CG1	-11.81	93.19	110.90
2	D	21	ASP	N-CA-C	11.79	142.84	111.00
2	D	120	LYS	O-C-N	-11.78	103.85	122.70
1	A	14	TRP	CA-CB-CG	-11.77	91.34	113.70
2	D	58	PRO	CB-CG-CD	11.77	152.38	106.50
2	D	41	PHE	CZ-CE2-CD2	-11.76	105.99	120.10
1	A	47	ASP	O-C-N	11.75	141.50	122.70
1	C	41	THR	O-C-N	-11.75	103.90	122.70
2	D	2	HIS	CA-C-O	-11.74	95.44	120.10
2	B	79	ASP	O-C-N	-11.74	103.92	122.70
1	C	12	ALA	O-C-N	-11.74	103.92	122.70
2	D	4	THR	CA-C-O	-11.74	95.44	120.10
1	A	21	ALA	CA-C-O	-11.72	95.49	120.10
1	C	112	HIS	ND1-CG-CD2	-11.71	89.61	106.00
2	D	63	HIS	CA-CB-CG	11.69	133.48	113.60
1	A	19	ALA	N-CA-CB	11.69	126.46	110.10
2	D	21	ASP	CB-CG-OD2	-11.69	107.78	118.30
2	D	78	LEU	CA-C-N	-11.68	91.50	117.20
1	A	141	ARG	CG-CD-NE	-11.68	87.28	111.80
1	C	98	PHE	CG-CD2-CE2	-11.68	107.95	120.80
1	A	112	HIS	CG-ND1-CE1	-11.67	90.52	105.70
2	B	42	PHE	CG-CD2-CE2	11.67	133.63	120.80
1	C	89	HIS	CG-ND1-CE1	-11.65	90.55	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	GLY	CA-C-N	11.64	142.80	117.20
1	C	16	LYS	CD-CE-NZ	-11.64	84.94	111.70
2	B	2	HIS	CA-CB-CG	11.63	133.37	113.60
2	D	47	ASP	OD1-CG-OD2	11.62	145.39	123.30
1	A	73	VAL	O-C-N	-11.62	104.11	122.70
1	A	89	HIS	CG-ND1-CE1	11.57	124.40	108.20
2	B	78	LEU	CB-CG-CD2	11.55	130.64	111.00
2	D	6	GLU	CB-CA-C	-11.55	87.31	110.40
1	A	140	TYR	CD1-CE1-CZ	11.54	130.18	119.80
2	D	2	HIS	CB-CG-ND1	-11.53	94.37	123.20
1	C	53	ALA	O-C-N	11.52	141.14	122.70
2	D	45	PHE	CA-C-O	-11.46	96.03	120.10
2	B	43	GLU	N-CA-CB	-11.43	90.02	110.60
1	A	64	ASP	OD1-CG-OD2	11.43	145.01	123.30
2	B	42	PHE	CG-CD1-CE1	-11.41	108.25	120.80
2	D	40	ARG	NE-CZ-NH1	-11.41	114.59	120.30
1	C	114	PRO	CB-CA-C	11.39	140.48	112.00
2	B	145	TYR	N-CA-CB	11.38	131.08	110.60
2	D	82	LYS	CG-CD-CE	-11.37	77.78	111.90
2	B	73	ASP	CB-CG-OD2	-11.37	108.07	118.30
1	C	72	HIS	ND1-CE1-NE2	11.35	134.88	109.90
2	B	9	SER	CA-CB-OG	-11.35	80.55	111.20
2	D	58	PRO	CA-N-CD	-11.34	95.62	111.50
2	D	2	HIS	ND1-CE1-NE2	-11.30	85.04	109.90
2	D	43	GLU	CB-CA-C	-11.30	87.80	110.40
2	B	96	LEU	CB-CG-CD2	-11.28	91.83	111.00
2	B	117	HIS	ND1-CG-CD2	11.27	124.57	108.80
2	D	50	THR	CB-CA-C	-11.26	81.21	111.60
1	C	45	HIS	ND1-CE1-NE2	11.23	134.61	109.90
2	D	97	HIS	CE1-NE2-CD2	11.23	134.69	106.60
1	A	74	ASP	CA-C-O	-11.23	96.52	120.10
1	C	118	THR	CA-CB-CG2	11.22	128.10	112.40
2	D	57	ASN	CA-C-O	11.18	143.58	120.10
1	C	49	SER	CB-CA-C	11.16	131.31	110.10
1	A	25	GLY	O-C-N	-11.16	104.84	122.70
1	C	90	LYS	CD-CE-NZ	-11.15	86.05	111.70
2	D	63	HIS	CG-ND1-CE1	-11.15	91.20	105.70
1	A	57	GLY	O-C-N	11.13	140.51	122.70
2	B	43	GLU	CA-CB-CG	11.13	137.88	113.40
1	C	81	SER	N-CA-CB	-11.13	93.80	110.50
2	B	17	LYS	CD-CE-NZ	-11.12	86.12	111.70
1	A	120	ALA	N-CA-CB	11.11	125.66	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	LEU	CA-C-O	-11.11	96.76	120.10
1	A	73	VAL	CA-C-O	11.10	143.41	120.10
2	D	49	SER	CB-CA-C	-11.08	89.04	110.10
1	C	20	HIS	CB-CG-ND1	-11.08	95.50	123.20
2	B	144	LYS	O-C-N	-11.07	104.99	122.70
2	D	117	HIS	ND1-CG-CD2	-11.07	90.50	106.00
2	D	122	PHE	CZ-CE2-CD2	-11.06	106.83	120.10
2	D	105	LEU	CB-CG-CD1	11.04	129.78	111.00
1	A	71	ALA	CA-C-N	11.04	141.49	117.20
1	A	46	PHE	CE1-CZ-CE2	-11.04	100.14	120.00
2	B	5	PRO	CA-CB-CG	-11.02	83.06	104.00
2	D	18	VAL	CA-CB-CG1	11.02	127.43	110.90
2	B	17	LYS	O-C-N	-11.01	105.09	122.70
2	D	55	MET	CA-C-N	-11.01	94.19	116.20
2	D	85	PHE	CB-CG-CD1	-11.00	113.10	120.80
1	C	41	THR	CA-C-N	10.98	141.37	117.20
2	B	85	PHE	CB-CG-CD2	-10.98	113.11	120.80
1	A	128	PHE	CG-CD2-CE2	10.98	132.88	120.80
2	D	21	ASP	OD1-CG-OD2	-10.96	102.47	123.30
1	C	29	LEU	O-C-N	-10.96	105.17	122.70
2	D	12	THR	O-C-N	-10.96	105.17	122.70
1	A	45	HIS	CA-CB-CG	10.95	132.22	113.60
2	B	104	ARG	NH1-CZ-NH2	10.95	131.45	119.40
2	B	6	GLU	CA-CB-CG	10.94	137.46	113.40
1	C	89	HIS	ND1-CE1-NE2	10.93	133.94	109.90
2	D	126	VAL	CA-CB-CG2	-10.92	94.52	110.90
2	D	45	PHE	CB-CG-CD1	-10.89	113.17	120.80
1	A	26	ALA	CB-CA-C	-10.89	93.77	110.10
2	B	80	ASN	CB-CG-OD1	-10.88	99.84	121.60
1	C	115	ALA	O-C-N	-10.88	105.29	122.70
2	B	60	VAL	O-C-N	-10.84	105.35	122.70
2	B	49	SER	N-CA-CB	-10.84	94.24	110.50
2	D	67	VAL	CA-CB-CG1	-10.84	94.64	110.90
2	B	23	VAL	CA-CB-CG2	-10.83	94.66	110.90
1	C	45	HIS	CA-CB-CG	10.80	131.96	113.60
2	B	43	GLU	CG-CD-OE1	-10.79	96.71	118.30
1	C	30	GLU	CG-CD-OE2	-10.79	96.71	118.30
1	A	122	HIS	CB-CA-C	10.77	131.94	110.40
1	C	14	TRP	CA-C-N	10.77	137.74	116.20
2	D	90	GLU	CG-CD-OE2	-10.77	96.76	118.30
1	C	44	PRO	N-CA-CB	-10.77	90.38	103.30
1	A	49	SER	C-N-CA	-10.76	94.79	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	134	VAL	N-CA-CB	10.76	135.18	111.50
1	C	63	ALA	O-C-N	-10.74	105.52	122.70
1	C	10	VAL	O-C-N	10.73	139.87	122.70
1	C	78	ASN	O-C-N	-10.73	105.52	122.70
1	A	42	TYR	CB-CG-CD1	10.72	127.43	121.00
1	A	116	GLU	CG-CD-OE1	10.71	139.71	118.30
2	D	104	ARG	CG-CD-NE	-10.71	89.32	111.80
2	B	48	LEU	CB-CG-CD2	10.68	129.16	111.00
2	D	9	SER	O-C-N	10.67	139.78	122.70
2	D	79	ASP	C-N-CA	-10.66	95.05	121.70
2	B	3	LEU	C-N-CA	-10.63	95.12	121.70
2	B	45	PHE	CG-CD1-CE1	-10.63	109.11	120.80
2	B	45	PHE	CA-C-N	10.62	137.45	116.20
2	D	7	GLU	O-C-N	10.62	139.70	122.70
2	B	78	LEU	CB-CA-C	-10.61	90.04	110.20
2	B	81	LEU	CB-CA-C	10.60	130.35	110.20
1	C	72	HIS	N-CA-C	10.56	139.53	111.00
1	C	73	VAL	O-C-N	10.56	139.60	122.70
1	C	17	VAL	CG1-CB-CG2	10.55	127.79	110.90
1	A	20	HIS	ND1-CE1-NE2	10.53	133.06	109.90
2	D	77	HIS	CE1-NE2-CD2	10.52	132.91	106.60
2	D	80	ASN	CB-CG-ND2	-10.51	91.49	116.70
2	D	3	LEU	CA-C-O	-10.50	98.04	120.10
1	A	41	THR	O-C-N	-10.50	105.90	122.70
1	C	113	LEU	CA-C-O	-10.50	98.06	120.10
2	D	3	LEU	N-CA-C	-10.47	82.74	111.00
2	D	54	VAL	CA-CB-CG1	-10.46	95.21	110.90
2	B	72	SER	CB-CA-C	10.46	129.97	110.10
1	C	116	GLU	CB-CA-C	-10.43	89.54	110.40
2	D	72	SER	CA-C-O	10.43	142.00	120.10
2	D	12	THR	CA-CB-OG1	-10.42	87.12	109.00
1	A	22	GLY	CA-C-O	10.42	139.35	120.60
1	A	131	SER	O-C-N	10.42	139.37	122.70
2	D	3	LEU	N-CA-CB	10.40	131.20	110.40
2	B	85	PHE	CD1-CE1-CZ	10.40	132.58	120.10
1	A	43	PHE	CG-CD2-CE2	10.40	132.24	120.80
2	D	63	HIS	ND1-CG-CD2	10.40	123.36	108.80
1	C	22	GLY	CA-C-N	10.38	140.04	117.20
1	A	2	LEU	CA-C-O	-10.37	98.33	120.10
2	D	21	ASP	CB-CG-OD1	10.35	127.62	118.30
1	A	12	ALA	N-CA-CB	-10.35	95.61	110.10
1	C	56	LYS	O-C-N	-10.34	105.62	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ALA	CA-C-O	10.34	141.81	120.10
1	A	72	HIS	CG-CD2-NE2	10.34	128.84	109.20
2	B	1	VAL	CA-CB-CG1	-10.31	95.43	110.90
2	B	35	TYR	CB-CG-CD2	10.31	127.19	121.00
1	A	43	PHE	CZ-CE2-CD2	-10.31	107.73	120.10
1	A	81	SER	CA-CB-OG	-10.29	83.41	111.20
1	A	141	ARG	CB-CA-C	10.29	130.97	110.40
2	D	60	VAL	CG1-CB-CG2	10.25	127.30	110.90
2	B	2	HIS	ND1-CE1-NE2	10.25	132.44	109.90
1	C	7	LYS	CA-C-O	10.23	141.58	120.10
2	B	85	PHE	CE1-CZ-CE2	-10.23	101.59	120.00
2	B	90	GLU	N-CA-C	10.20	138.54	111.00
2	D	35	TYR	CD1-CE1-CZ	-10.19	110.63	119.80
1	C	84	SER	CA-CB-OG	-10.19	83.70	111.20
2	D	73	ASP	N-CA-C	10.17	138.46	111.00
1	A	106	LEU	CA-CB-CG	10.15	138.65	115.30
1	A	14	TRP	NE1-CE2-CZ2	10.15	141.56	130.40
1	A	8	THR	CA-C-O	10.14	141.41	120.10
2	B	47	ASP	OD1-CG-OD2	-10.14	104.03	123.30
2	D	19	ASN	CA-C-N	10.14	139.51	117.20
2	B	68	LEU	CD1-CG-CD2	10.12	140.87	110.50
2	D	3	LEU	CA-CB-CG	-10.11	92.04	115.30
1	C	2	LEU	O-C-N	10.10	138.86	122.70
1	A	74	ASP	CB-CG-OD1	10.10	127.39	118.30
2	D	8	LYS	N-CA-CB	-10.09	92.43	110.60
2	D	5	PRO	CB-CA-C	-10.08	86.80	112.00
2	D	146	HIS	ND1-CE1-NE2	10.07	132.06	109.90
2	D	117	HIS	CG-ND1-CE1	-10.07	92.61	105.70
1	A	87	HIS	O-C-N	10.05	138.79	122.70
2	B	42	PHE	CD1-CG-CD2	-10.05	105.23	118.30
2	D	84	THR	CA-CB-CG2	10.05	126.47	112.40
1	C	131	SER	O-C-N	10.03	138.74	122.70
2	B	30	ARG	NH1-CZ-NH2	-10.02	108.38	119.40
2	B	30	ARG	NE-CZ-NH1	-10.01	115.29	120.30
2	D	82	LYS	O-C-N	-10.01	106.18	123.20
2	D	14	LEU	CB-CG-CD1	-10.01	93.98	111.00
1	A	53	ALA	CB-CA-C	-10.00	95.10	110.10
2	B	94	ASP	O-C-N	-9.99	106.72	122.70
1	C	43	PHE	CB-CG-CD2	-9.98	113.81	120.80
1	A	126	ASP	O-C-N	-9.95	106.78	122.70
2	B	58	PRO	CB-CG-CD	9.94	145.28	106.50
2	D	133	VAL	CG1-CB-CG2	9.92	126.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	GLU	CA-C-O	-9.91	99.29	120.10
2	B	142	ALA	O-C-N	9.91	138.55	122.70
2	D	11	VAL	O-C-N	9.90	138.55	122.70
1	C	79	ALA	CB-CA-C	-9.90	95.25	110.10
1	A	76	MET	CG-SD-CE	9.89	116.03	100.20
1	A	50	HIS	CB-CA-C	-9.87	90.66	110.40
1	A	105	LEU	CB-CG-CD2	9.87	127.78	111.00
2	B	81	LEU	N-CA-CB	-9.85	90.70	110.40
2	D	60	VAL	CB-CA-C	9.84	130.10	111.40
2	D	95	LYS	O-C-N	-9.84	106.95	122.70
2	B	90	GLU	CG-CD-OE1	-9.82	98.66	118.30
1	A	88	ALA	O-C-N	9.82	138.41	122.70
2	B	42	PHE	CB-CG-CD1	-9.82	113.93	120.80
2	B	125	PRO	CA-N-CD	-9.81	97.76	111.50
1	C	4	PRO	O-C-N	9.81	138.40	122.70
2	B	61	LYS	CD-CE-NZ	-9.80	89.16	111.70
1	A	43	PHE	CB-CG-CD1	-9.79	113.95	120.80
2	B	87	THR	CA-CB-OG1	-9.78	88.45	109.00
1	A	82	ALA	N-CA-CB	9.78	123.79	110.10
2	D	97	HIS	ND1-CE1-NE2	-9.78	88.39	109.90
1	A	6	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	C	71	ALA	C-N-CA	9.76	146.09	121.70
2	B	8	LYS	CB-CG-CD	9.74	136.94	111.60
2	B	45	PHE	CE1-CZ-CE2	9.74	137.54	120.00
2	D	30	ARG	CD-NE-CZ	9.73	137.23	123.60
1	A	15	GLY	N-CA-C	-9.72	88.80	113.10
1	C	90	LYS	N-CA-CB	9.69	128.04	110.60
2	B	145	TYR	CA-C-O	-9.69	99.76	120.10
1	C	90	LYS	CB-CG-CD	-9.68	86.44	111.60
1	C	58	HIS	CG-ND1-CE1	-9.67	93.12	105.70
2	B	60	VAL	CA-C-O	9.67	140.40	120.10
2	D	78	LEU	CB-CG-CD1	-9.66	94.58	111.00
1	A	33	PHE	CZ-CE2-CD2	9.65	131.68	120.10
1	C	60	LYS	CD-CE-NZ	-9.65	89.51	111.70
1	A	78	ASN	N-CA-CB	9.64	127.95	110.60
1	C	49	SER	CA-C-O	9.64	140.34	120.10
1	C	82	ALA	O-C-N	-9.63	107.29	122.70
2	D	137	VAL	O-C-N	-9.63	107.30	122.70
2	D	144	LYS	CD-CE-NZ	9.62	133.84	111.70
1	C	14	TRP	CD2-CE2-CZ2	-9.62	110.76	122.30
1	C	56	LYS	CB-CG-CD	-9.61	86.61	111.60
2	B	47	ASP	CA-C-N	-9.60	96.08	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	ASP	OD1-CG-OD2	9.60	141.54	123.30
2	D	54	VAL	O-C-N	-9.60	107.35	122.70
1	C	70	VAL	CA-C-O	-9.58	99.97	120.10
2	D	65	LYS	CA-CB-CG	-9.58	92.33	113.40
2	B	53	ALA	O-C-N	-9.57	107.39	122.70
1	A	76	MET	CA-CB-CG	-9.55	97.06	113.30
1	A	89	HIS	O-C-N	-9.55	107.42	122.70
2	B	122	PHE	CB-CG-CD2	-9.54	114.12	120.80
1	C	138	SER	N-CA-CB	-9.52	96.22	110.50
2	D	18	VAL	CA-C-O	-9.52	100.11	120.10
2	D	85	PHE	CZ-CE2-CD2	9.52	131.52	120.10
2	D	143	HIS	CG-ND1-CE1	-9.52	93.33	105.70
2	B	139	ASN	CB-CA-C	-9.52	91.37	110.40
1	C	38	THR	CA-CB-CG2	-9.50	99.09	112.40
1	C	109	LEU	CB-CA-C	9.50	128.25	110.20
1	A	42	TYR	CG-CD1-CE1	-9.48	113.71	121.30
1	C	138	SER	O-C-N	9.48	137.87	122.70
2	D	19	ASN	CB-CG-OD1	-9.47	102.66	121.60
1	A	96	VAL	CA-CB-CG2	-9.45	96.72	110.90
2	B	126	VAL	CG1-CB-CG2	-9.45	95.78	110.90
2	B	73	ASP	CB-CG-OD1	9.45	126.80	118.30
2	B	134	VAL	CA-CB-CG1	-9.45	96.72	110.90
2	D	79	ASP	CB-CG-OD1	-9.45	109.80	118.30
2	B	130	TYR	CB-CG-CD1	9.43	126.66	121.00
2	B	144	LYS	CA-C-N	9.42	137.92	117.20
1	A	127	LYS	CB-CA-C	9.41	129.22	110.40
1	C	96	VAL	CA-CB-CG2	9.40	125.01	110.90
1	C	105	LEU	CD1-CG-CD2	-9.39	82.32	110.50
1	A	24	TYR	CG-CD2-CE2	9.37	128.79	121.30
2	D	48	LEU	CB-CG-CD2	9.37	126.92	111.00
2	D	99	ASP	OD1-CG-OD2	9.36	141.09	123.30
2	B	49	SER	CA-C-N	9.35	137.78	117.20
2	D	89	SER	CA-C-O	9.35	139.74	120.10
2	B	127	GLN	O-C-N	-9.34	107.75	122.70
1	A	19	ALA	CB-CA-C	-9.33	96.10	110.10
1	C	103	HIS	CG-ND1-CE1	-9.33	93.57	105.70
2	D	35	TYR	CB-CG-CD2	9.33	126.60	121.00
1	C	94	ASP	CB-CG-OD2	-9.32	109.91	118.30
2	D	40	ARG	CA-CB-CG	9.32	133.91	113.40
2	D	145	TYR	CG-CD2-CE2	-9.32	113.84	121.30
1	C	5	ALA	N-CA-CB	9.32	123.14	110.10
1	A	56	LYS	CB-CG-CD	-9.32	87.38	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	LEU	N-CA-CB	-9.31	91.78	110.40
2	D	1	VAL	CA-C-O	-9.31	100.55	120.10
1	A	52	SER	O-C-N	-9.31	107.81	122.70
1	C	48	LEU	C-N-CA	9.29	144.94	121.70
2	D	67	VAL	N-CA-CB	-9.28	91.08	111.50
2	D	122	PHE	CD1-CE1-CZ	-9.28	108.96	120.10
2	D	16	GLY	C-N-CA	9.28	144.90	121.70
2	D	116	HIS	ND1-CG-CD2	9.27	121.78	108.80
2	B	81	LEU	CA-CB-CG	9.26	136.59	115.30
1	A	6	ASP	O-C-N	9.25	137.50	122.70
1	C	112	HIS	O-C-N	-9.25	107.91	122.70
2	D	23	VAL	CA-CB-CG2	-9.24	97.03	110.90
2	B	10	ALA	CB-CA-C	-9.22	96.27	110.10
2	D	122	PHE	CG-CD2-CE2	9.20	130.92	120.80
1	A	11	LYS	C-N-CA	-9.17	98.78	121.70
2	D	51	PRO	N-CD-CG	-9.15	89.47	103.20
1	C	72	HIS	O-C-N	-9.15	108.06	122.70
2	D	90	GLU	CB-CG-CD	-9.15	89.49	114.20
1	A	43	PHE	CD1-CE1-CZ	9.15	131.08	120.10
1	A	19	ALA	O-C-N	-9.14	108.07	122.70
2	D	53	ALA	CA-C-O	9.14	139.29	120.10
2	D	41	PHE	CA-C-O	-9.13	100.93	120.10
1	A	7	LYS	CA-C-N	-9.12	97.13	117.20
2	B	118	PHE	CE1-CZ-CE2	-9.12	103.58	120.00
1	C	131	SER	CA-C-O	-9.12	100.95	120.10
1	C	45	HIS	O-C-N	9.11	137.28	122.70
2	B	146	HIS	CB-CG-ND1	-9.10	100.45	123.20
2	D	10	ALA	N-CA-CB	-9.08	97.38	110.10
2	D	95	LYS	CA-C-O	9.07	139.16	120.10
1	A	29	LEU	CB-CG-CD1	-9.07	95.58	111.00
1	A	86	LEU	CB-CG-CD2	9.07	126.42	111.00
2	B	66	LYS	CD-CE-NZ	-9.06	90.85	111.70
1	C	86	LEU	CA-C-O	9.06	139.13	120.10
1	A	14	TRP	C-N-CA	-9.06	103.27	122.30
1	C	38	THR	CA-CB-OG1	-9.05	89.99	109.00
1	C	112	HIS	C-N-CA	9.03	144.28	121.70
1	C	12	ALA	N-CA-C	9.03	135.38	111.00
1	A	118	THR	CA-CB-OG1	9.03	127.95	109.00
2	B	15	TRP	O-C-N	9.00	138.51	123.20
1	C	44	PRO	CA-N-CD	9.00	124.30	111.70
2	B	41	PHE	CG-CD2-CE2	-8.99	110.91	120.80
1	C	117	PHE	CB-CG-CD2	8.98	127.09	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	77	HIS	CA-C-N	-8.98	97.44	117.20
2	B	90	GLU	CA-C-N	-8.98	97.45	117.20
1	A	38	THR	CA-CB-CG2	-8.97	99.84	112.40
2	B	144	LYS	C-N-CA	8.97	144.13	121.70
1	A	134	THR	O-C-N	-8.97	108.35	122.70
2	D	17	LYS	CD-CE-NZ	-8.97	91.08	111.70
2	B	37	TRP	CZ3-CH2-CZ2	8.96	132.35	121.60
1	A	62	VAL	CG1-CB-CG2	-8.95	96.58	110.90
2	D	53	ALA	CB-CA-C	-8.95	96.68	110.10
1	A	78	ASN	CB-CG-ND2	8.94	138.16	116.70
1	A	2	LEU	N-CA-CB	-8.94	92.52	110.40
2	D	52	ASP	CA-C-O	-8.94	101.33	120.10
2	B	2	HIS	CA-C-N	-8.92	97.57	117.20
1	A	112	HIS	CA-C-O	-8.92	101.37	120.10
2	B	5	PRO	O-C-N	8.92	136.97	122.70
2	D	21	ASP	O-C-N	-8.91	108.45	122.70
2	D	120	LYS	CB-CG-CD	8.90	134.75	111.60
1	C	87	HIS	O-C-N	8.90	136.94	122.70
1	A	56	LYS	CA-C-O	8.88	138.74	120.10
1	A	98	PHE	CB-CG-CD2	8.87	127.01	120.80
1	C	77	PRO	O-C-N	-8.88	108.50	122.70
2	B	42	PHE	CE1-CZ-CE2	-8.87	104.04	120.00
2	D	44	SER	CA-C-N	8.87	136.71	117.20
2	D	77	HIS	ND1-CE1-NE2	-8.85	90.44	109.90
2	B	7	GLU	CB-CA-C	8.84	128.08	110.40
2	D	2	HIS	C-N-CA	-8.84	99.60	121.70
2	B	47	ASP	N-CA-CB	-8.84	94.69	110.60
2	D	3	LEU	C-N-CA	8.83	143.78	121.70
1	C	77	PRO	N-CA-C	8.82	135.03	112.10
1	C	128	PHE	CD1-CE1-CZ	8.82	130.68	120.10
2	B	12	THR	CA-CB-CG2	-8.81	100.06	112.40
1	A	62	VAL	CA-C-N	-8.81	97.83	117.20
1	C	82	ALA	CA-C-O	8.79	138.56	120.10
1	C	50	HIS	O-C-N	8.78	138.13	123.20
1	C	53	ALA	CA-C-N	-8.76	97.93	117.20
1	C	112	HIS	CA-C-N	8.76	136.47	117.20
2	D	57	ASN	O-C-N	-8.76	104.46	121.10
2	B	47	ASP	CB-CA-C	-8.73	92.94	110.40
2	B	130	TYR	CZ-CE2-CD2	-8.73	111.94	119.80
2	D	35	TYR	CB-CG-CD1	-8.73	115.76	121.00
2	D	108	ASN	OD1-CG-ND2	8.72	141.97	121.90
2	B	111	VAL	O-C-N	-8.72	108.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	VAL	N-CA-C	-8.72	87.46	111.00
2	B	6	GLU	CG-CD-OE1	-8.71	100.87	118.30
1	A	50	HIS	CG-CD2-NE2	-8.71	92.64	109.20
1	C	84	SER	CB-CA-C	-8.70	93.57	110.10
2	D	122	PHE	CE1-CZ-CE2	8.70	135.66	120.00
1	C	11	LYS	CA-CB-CG	8.70	132.53	113.40
2	D	93	CYS	CA-CB-SG	-8.68	98.37	114.00
1	C	74	ASP	O-C-N	8.68	136.58	122.70
2	D	16	GLY	CA-C-N	8.67	136.28	117.20
1	A	50	HIS	CA-C-N	8.67	133.53	116.20
1	A	106	LEU	CB-CG-CD1	8.66	125.72	111.00
2	B	5	PRO	CA-C-N	-8.64	98.20	117.20
1	A	56	LYS	O-C-N	-8.63	108.52	123.20
2	B	60	VAL	CG1-CB-CG2	8.63	124.71	110.90
2	B	3	LEU	CA-C-N	-8.63	98.22	117.20
1	C	137	THR	OG1-CB-CG2	8.63	129.84	110.00
1	C	18	GLY	CA-C-N	-8.61	98.25	117.20
2	B	48	LEU	C-N-CA	-8.61	100.17	121.70
1	A	128	PHE	CE1-CZ-CE2	8.59	135.46	120.00
2	D	43	GLU	CA-C-N	-8.59	98.31	117.20
2	B	40	ARG	CA-C-N	8.58	136.08	117.20
2	D	55	MET	CA-C-O	-8.57	102.11	120.10
2	D	40	ARG	O-C-N	-8.56	109.00	122.70
2	B	51	PRO	O-C-N	-8.54	109.04	122.70
1	C	36	PHE	CG-CD2-CE2	-8.52	111.42	120.80
2	D	143	HIS	CG-CD2-NE2	-8.52	93.01	109.20
1	A	13	ALA	O-C-N	8.51	136.32	122.70
1	C	114	PRO	N-CD-CG	-8.50	90.45	103.20
1	C	62	VAL	CA-C-N	-8.49	98.51	117.20
2	D	95	LYS	CB-CG-CD	-8.49	89.52	111.60
2	B	80	ASN	CB-CG-ND2	-8.46	96.39	116.70
2	D	119	GLY	CA-C-O	8.46	135.83	120.60
1	C	46	PHE	CD1-CE1-CZ	8.46	130.25	120.10
2	D	122	PHE	CB-CG-CD1	8.46	126.72	120.80
1	A	63	ALA	O-C-N	-8.45	109.18	122.70
2	B	71	PHE	CZ-CE2-CD2	8.45	130.24	120.10
2	D	71	PHE	CZ-CE2-CD2	8.45	130.24	120.10
1	C	124	SER	O-C-N	8.44	136.21	122.70
1	C	50	HIS	CB-CG-CD2	8.44	156.96	130.80
2	D	146	HIS	N-CA-CB	-8.44	95.41	110.60
2	B	36	PRO	N-CD-CG	8.43	115.84	103.20
1	A	60	LYS	CA-C-O	8.43	137.79	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	VAL	C-N-CA	-8.41	100.67	121.70
2	B	88	LEU	CB-CG-CD2	-8.41	96.71	111.00
2	B	9	SER	N-CA-CB	8.40	123.10	110.50
1	C	69	ALA	O-C-N	8.40	136.14	122.70
2	B	115	ALA	N-CA-CB	-8.38	98.36	110.10
1	A	71	ALA	O-C-N	-8.38	109.29	122.70
2	B	50	THR	N-CA-CB	-8.38	94.38	110.30
1	A	77	PRO	CA-CB-CG	-8.37	88.10	104.00
2	D	2	HIS	ND1-CG-CD2	-8.35	94.31	106.00
2	D	59	LYS	CA-C-N	-8.35	98.83	117.20
2	B	114	LEU	CB-CA-C	8.34	126.05	110.20
2	D	7	GLU	OE1-CD-OE2	-8.34	113.30	123.30
2	B	35	TYR	CD1-CG-CD2	-8.33	108.73	117.90
1	A	54	GLN	O-C-N	8.33	136.03	122.70
2	B	85	PHE	CB-CG-CD1	8.32	126.63	120.80
2	B	103	PHE	CB-CG-CD1	-8.31	114.98	120.80
1	A	75	ASP	N-CA-CB	-8.30	95.65	110.60
1	C	81	SER	CA-CB-OG	-8.30	88.78	111.20
1	A	90	LYS	N-CA-C	8.30	133.42	111.00
2	D	60	VAL	CA-CB-CG1	-8.30	98.45	110.90
2	B	73	ASP	CA-C-N	8.30	132.79	116.20
1	C	95	PRO	CA-C-N	8.30	135.45	117.20
2	D	90	GLU	CA-CB-CG	-8.29	95.16	113.40
1	C	50	HIS	ND1-CG-CD2	-8.28	94.40	106.00
2	B	146	HIS	CA-CB-CG	-8.28	99.52	113.60
2	D	55	MET	CB-CG-SD	8.28	137.24	112.40
1	A	126	ASP	CB-CG-OD1	-8.28	110.85	118.30
1	A	58	HIS	C-N-CA	-8.27	104.94	122.30
2	D	52	ASP	O-C-N	8.26	135.91	122.70
1	A	1	VAL	C-N-CA	-8.25	101.07	121.70
2	B	48	LEU	CB-CA-C	8.25	125.87	110.20
2	B	99	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	A	4	PRO	N-CD-CG	-8.24	90.84	103.20
2	D	118	PHE	CG-CD2-CE2	-8.23	111.74	120.80
2	D	6	GLU	CA-C-N	-8.23	99.09	117.20
2	B	41	PHE	CB-CG-CD1	-8.23	115.04	120.80
2	B	89	SER	N-CA-CB	-8.23	98.16	110.50
1	C	83	LEU	CB-CA-C	-8.22	94.58	110.20
1	C	22	GLY	C-N-CA	8.22	142.25	121.70
1	A	16	LYS	N-CA-CB	8.21	125.38	110.60
1	A	117	PHE	CD1-CG-CD2	8.21	128.98	118.30
1	C	7	LYS	CB-CA-C	8.21	126.82	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	GLY	CA-C-N	8.21	135.26	117.20
2	B	2	HIS	N-CA-CB	-8.20	95.83	110.60
1	C	117	PHE	CG-CD2-CE2	8.21	129.82	120.80
2	D	93	CYS	CB-CA-C	8.19	126.78	110.40
2	B	127	GLN	CA-C-O	8.18	137.27	120.10
1	A	117	PHE	CB-CG-CD2	-8.17	115.08	120.80
1	A	7	LYS	N-CA-C	8.17	133.06	111.00
2	D	20	VAL	CB-CA-C	8.17	126.92	111.40
2	B	94	ASP	CA-C-N	8.16	135.16	117.20
1	A	72	HIS	O-C-N	-8.16	109.64	122.70
2	D	9	SER	CA-CB-OG	8.15	133.21	111.20
1	A	114	PRO	N-CA-CB	-8.15	93.52	103.30
2	D	92	HIS	ND1-CE1-NE2	8.15	127.83	109.90
2	B	40	ARG	CA-C-O	-8.15	102.99	120.10
1	C	141	ARG	CA-C-O	-8.15	102.99	120.10
1	A	70	VAL	CG1-CB-CG2	-8.14	97.87	110.90
2	B	23	VAL	CG1-CB-CG2	8.14	123.93	110.90
2	D	37	TRP	CE3-CZ3-CH2	-8.14	112.24	121.20
2	D	2	HIS	CB-CA-C	8.14	126.68	110.40
2	D	143	HIS	O-C-N	8.14	135.72	122.70
2	D	85	PHE	O-C-N	-8.13	109.69	122.70
2	B	67	VAL	CG1-CB-CG2	8.12	123.89	110.90
1	C	50	HIS	CE1-NE2-CD2	-8.12	86.30	106.60
1	A	114	PRO	CA-CB-CG	8.11	120.21	104.80
1	C	54	GLN	O-C-N	8.11	135.68	122.70
2	D	93	CYS	N-CA-CB	-8.11	96.00	110.60
1	A	33	PHE	CG-CD1-CE1	8.11	129.72	120.80
1	C	138	SER	CA-C-O	-8.11	103.07	120.10
2	D	86	ALA	CB-CA-C	-8.11	97.94	110.10
1	C	90	LYS	CG-CD-CE	-8.10	87.59	111.90
1	A	6	ASP	C-N-CA	-8.10	101.45	121.70
2	D	92	HIS	CB-CA-C	-8.10	94.21	110.40
1	A	117	PHE	CG-CD1-CE1	-8.09	111.90	120.80
2	D	146	HIS	CB-CG-CD2	8.09	155.89	130.80
2	D	68	LEU	CB-CG-CD1	8.09	124.75	111.00
2	D	47	ASP	CA-CB-CG	-8.07	95.64	113.40
2	B	118	PHE	CD1-CG-CD2	-8.06	107.82	118.30
2	D	16	GLY	O-C-N	-8.06	109.81	122.70
2	B	19	ASN	CB-CG-ND2	-8.05	97.37	116.70
2	D	110	LEU	CA-C-O	8.05	137.01	120.10
1	C	74	ASP	CA-CB-CG	8.05	131.11	113.40
1	C	117	PHE	CZ-CE2-CD2	-8.05	110.44	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	SER	CA-C-O	8.04	136.98	120.10
1	C	17	VAL	C-N-CA	-8.04	105.42	122.30
2	D	121	GLU	O-C-N	8.02	135.54	122.70
1	A	70	VAL	CA-CB-CG1	8.02	122.92	110.90
2	B	134	VAL	O-C-N	-8.00	109.90	122.70
2	B	54	VAL	CG1-CB-CG2	8.00	123.69	110.90
2	D	92	HIS	CG-CD2-NE2	8.00	124.39	109.20
2	D	63	HIS	O-C-N	7.97	136.76	123.20
1	A	52	SER	CB-CA-C	7.97	125.24	110.10
1	A	59	GLY	O-C-N	-7.97	109.95	122.70
2	D	108	ASN	CB-CG-ND2	-7.97	97.57	116.70
1	A	42	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	C	26	ALA	CA-C-O	7.96	136.83	120.10
2	D	6	GLU	N-CA-CB	7.96	124.93	110.60
1	C	43	PHE	CD1-CE1-CZ	7.96	129.65	120.10
2	D	144	LYS	CG-CD-CE	7.96	135.78	111.90
2	B	64	GLY	O-C-N	-7.96	109.97	122.70
1	C	49	SER	N-CA-CB	7.95	122.42	110.50
2	B	38	THR	N-CA-CB	7.94	125.38	110.30
1	A	1	VAL	O-C-N	7.93	135.39	122.70
1	A	24	TYR	CG-CD1-CE1	-7.92	114.96	121.30
1	A	110	ALA	CA-C-O	7.92	136.73	120.10
1	A	81	SER	O-C-N	-7.91	110.04	122.70
2	B	12	THR	O-C-N	-7.91	110.04	122.70
2	D	17	LYS	CG-CD-CE	7.89	135.58	111.90
1	C	98	PHE	CE1-CZ-CE2	-7.89	105.80	120.00
2	B	79	ASP	N-CA-CB	-7.88	96.41	110.60
1	C	114	PRO	N-CA-C	-7.88	91.61	112.10
1	C	12	ALA	CB-CA-C	-7.88	98.28	110.10
1	A	63	ALA	N-CA-CB	-7.88	99.07	110.10
1	A	110	ALA	C-N-CA	7.87	141.36	121.70
1	A	4	PRO	CA-CB-CG	-7.86	89.06	104.00
2	D	15	TRP	NE1-CE2-CZ2	7.86	139.04	130.40
1	A	106	LEU	O-C-N	-7.86	110.13	122.70
2	B	78	LEU	CA-CB-CG	-7.85	97.24	115.30
1	C	14	TRP	CE2-CD2-CG	-7.85	101.02	107.30
2	D	72	SER	CA-CB-OG	-7.85	90.01	111.20
2	B	26	GLU	O-C-N	7.83	135.23	122.70
1	C	110	ALA	O-C-N	-7.83	110.17	122.70
2	B	87	THR	CB-CA-C	-7.83	90.46	111.60
2	B	57	ASN	O-C-N	-7.82	106.24	121.10
2	D	92	HIS	N-CA-CB	-7.82	96.53	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	PHE	CB-CG-CD1	-7.82	115.33	120.80
2	D	40	ARG	CA-C-N	7.82	134.39	117.20
1	A	19	ALA	N-CA-C	-7.81	89.91	111.00
1	A	27	GLU	OE1-CD-OE2	7.81	132.67	123.30
2	D	9	SER	C-N-CA	-7.79	102.22	121.70
1	A	21	ALA	N-CA-CB	7.78	120.99	110.10
2	B	99	ASP	CB-CG-OD1	-7.78	111.30	118.30
1	C	43	PHE	CG-CD1-CE1	-7.78	112.24	120.80
1	A	16	LYS	CD-CE-NZ	7.78	129.59	111.70
2	B	66	LYS	CG-CD-CE	-7.77	88.60	111.90
2	D	66	LYS	CG-CD-CE	-7.76	88.63	111.90
1	C	115	ALA	N-CA-CB	7.75	120.95	110.10
2	D	99	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	A	93	VAL	O-C-N	-7.73	110.33	122.70
1	A	98	PHE	CZ-CE2-CD2	-7.73	110.82	120.10
2	D	78	LEU	C-N-CA	-7.73	102.37	121.70
1	A	132	VAL	CG1-CB-CG2	-7.71	98.56	110.90
1	A	20	HIS	CG-CD2-NE2	-7.71	94.56	109.20
1	A	92	ARG	O-C-N	-7.70	110.38	122.70
1	C	42	TYR	CD1-CE1-CZ	7.70	126.73	119.80
2	D	50	THR	CA-CB-OG1	7.70	125.17	109.00
2	D	146	HIS	CA-C-O	7.70	136.26	120.10
1	A	3	SER	O-C-N	-7.69	106.49	121.10
1	A	75	ASP	CA-C-N	-7.69	100.29	117.20
2	B	79	ASP	OD1-CG-OD2	-7.69	108.70	123.30
1	C	17	VAL	CB-CA-C	7.68	126.00	111.40
1	A	51	GLY	O-C-N	7.68	134.98	122.70
1	A	56	LYS	CD-CE-NZ	-7.68	94.05	111.70
2	D	141	LEU	CB-CG-CD2	-7.68	97.95	111.00
2	D	122	PHE	CD1-CG-CD2	-7.67	108.32	118.30
1	A	69	ALA	N-CA-CB	-7.67	99.36	110.10
1	C	23	GLU	CB-CG-CD	-7.67	93.49	114.20
1	A	8	THR	CA-CB-CG2	-7.67	101.67	112.40
2	B	80	ASN	CA-C-O	-7.67	104.00	120.10
2	B	122	PHE	CD1-CE1-CZ	-7.67	110.90	120.10
2	D	3	LEU	CD1-CG-CD2	-7.66	87.51	110.50
1	A	48	LEU	CB-CG-CD1	-7.64	98.01	111.00
2	B	45	PHE	O-C-N	-7.63	110.23	123.20
2	B	55	MET	O-C-N	7.63	136.17	123.20
1	A	2	LEU	CB-CG-CD1	7.63	123.96	111.00
1	A	108	THR	CA-CB-CG2	-7.62	101.73	112.40
1	C	3	SER	CB-CA-C	7.61	124.56	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	ASP	OD1-CG-OD2	7.61	137.76	123.30
1	A	17	VAL	C-N-CA	-7.60	106.33	122.30
1	C	63	ALA	CA-C-O	7.60	136.07	120.10
1	A	3	SER	CA-C-O	7.58	136.03	120.10
2	B	130	TYR	CD1-CE1-CZ	7.58	126.62	119.80
1	C	3	SER	O-C-N	-7.58	106.71	121.10
2	D	89	SER	O-C-N	-7.57	110.59	122.70
1	A	101	LEU	O-C-N	-7.56	110.60	122.70
2	D	97	HIS	ND1-CG-CD2	7.56	119.38	108.80
1	C	49	SER	O-C-N	-7.55	110.61	122.70
2	D	131	GLN	CG-CD-OE1	-7.55	106.50	121.60
2	D	94	ASP	N-CA-CB	-7.55	97.01	110.60
1	C	99	LYS	CG-CD-CE	-7.55	89.25	111.90
2	D	72	SER	CA-C-N	-7.54	100.60	117.20
1	C	74	ASP	CB-CG-OD1	7.54	125.08	118.30
1	C	72	HIS	CA-C-O	7.53	135.91	120.10
2	B	13	ALA	O-C-N	-7.53	110.66	122.70
1	C	106	LEU	C-N-CA	7.53	140.52	121.70
2	D	48	LEU	CA-CB-CG	-7.52	98.00	115.30
1	A	7	LYS	N-CA-CB	-7.51	97.08	110.60
1	C	67	THR	CA-CB-CG2	-7.51	101.88	112.40
1	C	42	TYR	CA-CB-CG	-7.51	99.12	113.40
2	D	92	HIS	CG-ND1-CE1	-7.51	95.94	105.70
2	D	50	THR	CA-CB-CG2	-7.50	101.90	112.40
2	D	117	HIS	O-C-N	-7.50	110.71	122.70
1	C	137	THR	CA-CB-CG2	-7.49	101.91	112.40
1	A	61	LYS	CB-CA-C	-7.49	95.42	110.40
1	A	84	SER	O-C-N	7.48	134.67	122.70
1	C	17	VAL	CA-C-N	-7.48	101.24	116.20
1	C	75	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	C	110	ALA	CB-CA-C	7.48	121.32	110.10
1	A	85	ASP	OD1-CG-OD2	-7.48	109.09	123.30
2	B	3	LEU	O-C-N	7.45	134.62	122.70
2	B	140	ALA	O-C-N	-7.44	110.79	122.70
1	C	95	PRO	O-C-N	-7.44	110.80	122.70
1	C	51	GLY	CA-C-O	7.43	133.98	120.60
1	C	40	LYS	CD-CE-NZ	-7.43	94.61	111.70
2	D	98	VAL	CA-CB-CG2	-7.43	99.76	110.90
2	D	17	LYS	CB-CG-CD	-7.42	92.30	111.60
2	D	2	HIS	N-CA-C	7.41	131.02	111.00
1	A	77	PRO	O-C-N	-7.41	110.84	122.70
2	B	46	GLY	O-C-N	7.40	134.55	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	17	LYS	CA-C-N	7.38	133.42	117.20
1	C	56	LYS	CA-C-O	7.37	135.58	120.10
1	C	107	VAL	O-C-N	-7.37	110.90	122.70
2	D	47	ASP	C-N-CA	-7.37	103.27	121.70
1	A	28	ALA	CA-C-N	-7.37	100.99	117.20
2	B	71	PHE	CG-CD2-CE2	-7.37	112.69	120.80
1	C	141	ARG	NH1-CZ-NH2	7.36	127.50	119.40
1	A	87	HIS	CA-CB-CG	-7.36	101.09	113.60
1	C	24	TYR	OH-CZ-CE2	-7.36	100.24	120.10
2	D	110	LEU	O-C-N	-7.35	110.93	122.70
1	C	99	LYS	CA-C-N	-7.35	101.03	117.20
2	B	77	HIS	ND1-CE1-NE2	7.35	126.07	109.90
1	A	105	LEU	O-C-N	7.34	134.45	122.70
1	A	61	LYS	CD-CE-NZ	7.33	128.55	111.70
1	A	65	ALA	C-N-CA	-7.32	103.39	121.70
2	B	38	THR	CA-CB-CG2	-7.32	102.15	112.40
2	D	130	TYR	CZ-CE2-CD2	7.32	126.39	119.80
1	A	127	LYS	CG-CD-CE	-7.31	89.96	111.90
2	D	6	GLU	C-N-CA	-7.31	103.42	121.70
2	D	131	GLN	OE1-CD-NE2	7.31	138.72	121.90
1	C	44	PRO	N-CD-CG	-7.31	92.24	103.20
1	A	89	HIS	CG-CD2-NE2	-7.29	95.36	109.20
2	D	5	PRO	O-C-N	-7.29	111.04	122.70
1	C	24	TYR	CG-CD2-CE2	-7.28	115.47	121.30
2	D	57	ASN	C-N-CD	7.27	143.66	128.40
2	D	126	VAL	O-C-N	7.27	134.33	122.70
1	A	136	LEU	CD1-CG-CD2	7.26	132.29	110.50
1	C	15	GLY	O-C-N	-7.26	111.09	122.70
2	D	35	TYR	CG-CD1-CE1	7.25	127.10	121.30
2	D	36	PRO	N-CD-CG	7.24	114.06	103.20
1	A	6	ASP	CB-CG-OD1	7.24	124.81	118.30
2	D	65	LYS	N-CA-CB	-7.23	97.58	110.60
2	D	144	LYS	O-C-N	-7.23	111.13	122.70
2	D	7	GLU	CA-C-O	-7.23	104.92	120.10
2	B	95	LYS	N-CA-CB	-7.22	97.60	110.60
1	C	74	ASP	CA-C-N	-7.22	101.31	117.20
2	B	35	TYR	CZ-CE2-CD2	7.21	126.29	119.80
2	D	112	CYS	CA-C-N	-7.21	101.34	117.20
2	D	141	LEU	CB-CG-CD1	-7.20	98.75	111.00
1	A	5	ALA	CB-CA-C	-7.20	99.31	110.10
2	B	84	THR	CA-C-O	7.19	135.19	120.10
2	D	143	HIS	ND1-CG-CD2	7.18	118.85	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	LYS	CA-CB-CG	-7.17	97.62	113.40
2	D	38	THR	CA-CB-CG2	-7.17	102.37	112.40
2	B	20	VAL	CA-C-N	7.16	132.96	117.20
2	B	36	PRO	CA-N-CD	-7.16	101.48	111.50
2	B	61	LYS	O-C-N	-7.16	111.25	122.70
1	C	117	PHE	CE1-CZ-CE2	7.16	132.88	120.00
1	A	23	GLU	N-CA-CB	-7.16	97.72	110.60
2	D	43	GLU	CB-CG-CD	-7.16	94.88	114.20
2	D	144	LYS	CB-CA-C	7.15	124.70	110.40
2	B	126	VAL	O-C-N	-7.15	111.26	122.70
1	A	103	HIS	CA-C-O	7.15	135.11	120.10
2	D	122	PHE	CG-CD1-CE1	7.14	128.66	120.80
1	C	37	PRO	N-CD-CG	7.13	113.90	103.20
2	B	77	HIS	CB-CG-CD2	-7.13	108.70	130.80
1	A	134	THR	N-CA-CB	-7.13	96.76	110.30
2	D	45	PHE	CG-CD1-CE1	-7.13	112.96	120.80
1	A	83	LEU	CD1-CG-CD2	-7.13	89.12	110.50
2	D	93	CYS	CA-C-N	-7.12	101.54	117.20
2	B	9	SER	CA-C-N	-7.12	101.54	117.20
1	A	10	VAL	O-C-N	7.11	134.08	122.70
1	A	42	TYR	CA-CB-CG	-7.11	99.89	113.40
1	A	17	VAL	CA-CB-CG2	7.10	121.54	110.90
1	C	49	SER	N-CA-C	-7.09	91.86	111.00
2	D	3	LEU	CB-CG-CD1	-7.09	98.95	111.00
2	B	6	GLU	CG-CD-OE2	7.08	132.46	118.30
1	A	49	SER	CA-C-O	7.08	134.96	120.10
1	C	118	THR	N-CA-CB	-7.07	96.87	110.30
1	C	94	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	50	HIS	O-C-N	-7.06	111.19	123.20
2	B	12	THR	CA-CB-OG1	-7.06	94.17	109.00
1	C	47	ASP	N-CA-CB	-7.06	97.90	110.60
2	B	31	LEU	CB-CG-CD1	-7.05	99.02	111.00
2	B	130	TYR	CB-CG-CD2	-7.05	116.77	121.00
2	D	80	ASN	CB-CA-C	-7.05	96.31	110.40
2	D	92	HIS	CA-C-O	-7.05	105.30	120.10
1	C	17	VAL	CA-C-O	7.04	134.88	120.10
2	D	1	VAL	CB-CA-C	-7.04	98.03	111.40
1	C	78	ASN	N-CA-C	7.03	129.98	111.00
2	D	13	ALA	CA-C-O	7.03	134.86	120.10
2	B	50	THR	CA-CB-OG1	7.01	123.72	109.00
1	C	86	LEU	CA-C-N	-7.00	101.81	117.20
2	D	137	VAL	CB-CA-C	-7.00	98.10	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	LEU	O-C-N	-7.00	111.51	122.70
1	C	112	HIS	CG-CD2-NE2	6.99	122.48	109.20
1	A	58	HIS	CA-CB-CG	-6.98	101.73	113.60
1	C	14	TRP	CD2-CE3-CZ3	6.98	127.87	118.80
1	C	99	LYS	CB-CG-CD	6.97	129.72	111.60
1	A	39	THR	O-C-N	6.96	133.84	122.70
2	B	65	LYS	CB-CG-CD	-6.96	93.49	111.60
1	A	17	VAL	N-CA-CB	6.95	126.78	111.50
1	A	81	SER	CA-C-N	6.94	132.47	117.20
2	B	15	TRP	CG-CD1-NE1	6.94	117.04	110.10
2	B	28	LEU	CA-C-O	6.94	134.67	120.10
2	D	45	PHE	C-N-CA	-6.94	107.73	122.30
2	B	82	LYS	O-C-N	-6.92	111.43	123.20
2	D	85	PHE	CB-CG-CD2	6.92	125.65	120.80
2	D	19	ASN	CB-CG-ND2	-6.91	100.11	116.70
1	A	61	LYS	CA-C-N	-6.91	102.01	117.20
1	A	138	SER	CB-CA-C	-6.90	96.98	110.10
2	B	112	CYS	N-CA-CB	6.90	123.02	110.60
1	C	99	LYS	CA-CB-CG	6.89	128.57	113.40
1	C	107	VAL	CA-C-O	6.89	134.58	120.10
1	A	60	LYS	CA-C-N	-6.89	102.04	117.20
1	A	105	LEU	N-CA-CB	-6.88	96.63	110.40
2	D	14	LEU	O-C-N	6.88	133.70	122.70
2	D	71	PHE	CD1-CE1-CZ	6.87	128.34	120.10
1	C	52	SER	CA-C-N	6.87	132.31	117.20
2	B	126	VAL	CA-C-N	6.87	132.31	117.20
2	D	56	GLY	CA-C-O	6.86	132.95	120.60
1	C	76	MET	N-CA-CB	-6.86	98.25	110.60
1	A	43	PHE	CG-CD1-CE1	-6.86	113.25	120.80
2	B	76	ALA	CA-C-O	6.86	134.50	120.10
2	B	69	GLY	CA-C-N	-6.86	102.11	117.20
2	B	77	HIS	CB-CG-ND1	6.86	140.34	123.20
1	A	18	GLY	CA-C-O	-6.86	108.26	120.60
2	D	39	GLN	O-C-N	-6.86	111.73	122.70
2	D	52	ASP	CA-CB-CG	6.85	128.48	113.40
1	C	43	PHE	CE1-CZ-CE2	-6.85	107.67	120.00
2	B	15	TRP	NE1-CE2-CD2	-6.84	100.46	107.30
2	B	20	VAL	CA-CB-CG1	-6.84	100.64	110.90
2	B	84	THR	N-CA-CB	6.83	123.29	110.30
1	C	128	PHE	O-C-N	6.83	133.64	122.70
2	D	76	ALA	N-CA-C	-6.83	92.55	111.00
1	C	33	PHE	CZ-CE2-CD2	6.83	128.29	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	VAL	CA-CB-CG1	6.82	121.14	110.90
2	B	66	LYS	O-C-N	6.81	133.60	122.70
1	A	31	ARG	O-C-N	6.81	133.59	122.70
2	B	80	ASN	N-CA-C	-6.80	92.63	111.00
2	D	4	THR	OG1-CB-CG2	6.79	125.62	110.00
2	D	42	PHE	C-N-CA	-6.79	104.73	121.70
2	B	52	ASP	OD1-CG-OD2	-6.79	110.41	123.30
1	C	141	ARG	CG-CD-NE	-6.79	97.55	111.80
1	A	113	LEU	CB-CG-CD1	6.78	122.53	111.00
1	C	131	SER	CB-CA-C	-6.77	97.23	110.10
2	D	76	ALA	CA-C-O	-6.77	105.88	120.10
1	A	68	ASN	O-C-N	-6.76	111.88	122.70
1	A	129	LEU	CB-CG-CD2	-6.76	99.51	111.00
2	B	49	SER	N-CA-C	-6.76	92.75	111.00
2	B	2	HIS	ND1-CG-CD2	6.76	118.26	108.80
2	B	41	PHE	CA-C-O	-6.76	105.91	120.10
2	B	84	THR	O-C-N	-6.76	111.89	122.70
2	B	142	ALA	CA-C-O	-6.75	105.93	120.10
2	D	60	VAL	O-C-N	-6.75	111.90	122.70
2	B	58	PRO	O-C-N	6.75	133.50	122.70
2	D	81	LEU	CB-CG-CD2	6.75	122.47	111.00
2	B	113	VAL	CA-C-N	6.75	132.04	117.20
1	C	45	HIS	CB-CG-ND1	-6.74	106.34	123.20
2	D	84	THR	CA-C-N	-6.74	102.38	117.20
2	D	48	LEU	C-N-CA	-6.73	104.88	121.70
2	D	85	PHE	CE1-CZ-CE2	-6.72	107.89	120.00
2	D	126	VAL	CA-CB-CG1	-6.72	100.81	110.90
1	C	21	ALA	N-CA-CB	-6.72	100.69	110.10
1	C	55	VAL	CA-CB-CG1	-6.72	100.82	110.90
1	C	31	ARG	NH1-CZ-NH2	6.72	126.79	119.40
1	C	58	HIS	O-C-N	6.71	134.62	123.20
1	C	29	LEU	CA-C-O	6.71	134.19	120.10
1	A	61	LYS	C-N-CA	-6.70	104.94	121.70
1	C	4	PRO	CA-C-N	-6.70	102.46	117.20
2	D	40	ARG	NH1-CZ-NH2	6.70	126.77	119.40
2	D	92	HIS	CE1-NE2-CD2	-6.70	89.85	106.60
2	D	100	PRO	O-C-N	6.70	133.41	122.70
1	C	83	LEU	N-CA-CB	-6.69	97.01	110.40
2	D	41	PHE	C-N-CA	-6.69	104.97	121.70
2	D	26	GLU	O-C-N	6.69	133.41	122.70
2	B	139	ASN	CA-CB-CG	-6.68	98.70	113.40
2	D	19	ASN	CB-CA-C	6.67	123.74	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	75	LEU	CB-CA-C	6.67	122.87	110.20
1	A	96	VAL	CA-CB-CG1	6.67	120.90	110.90
2	B	66	LYS	CB-CA-C	-6.67	97.07	110.40
2	B	90	GLU	CG-CD-OE2	-6.67	104.97	118.30
2	B	90	GLU	CA-CB-CG	-6.65	98.76	113.40
2	D	80	ASN	C-N-CA	-6.65	105.07	121.70
2	D	91	LEU	CA-C-O	6.65	134.06	120.10
1	A	33	PHE	CD1-CE1-CZ	-6.64	112.13	120.10
2	B	44	SER	CA-C-O	-6.64	106.15	120.10
1	C	7	LYS	CA-C-N	-6.64	102.59	117.20
1	C	10	VAL	CG1-CB-CG2	-6.64	100.28	110.90
1	C	38	THR	CB-CA-C	6.63	129.49	111.60
1	C	130	ALA	N-CA-CB	6.62	119.37	110.10
2	B	141	LEU	CB-CA-C	6.62	122.78	110.20
1	A	24	TYR	CA-CB-CG	-6.62	100.83	113.40
2	B	88	LEU	CB-CG-CD1	-6.62	99.75	111.00
1	A	78	ASN	O-C-N	-6.59	112.15	122.70
1	C	64	ASP	CA-CB-CG	6.59	127.89	113.40
1	C	140	TYR	CD1-CG-CD2	-6.59	110.65	117.90
2	D	13	ALA	CA-C-N	-6.59	102.71	117.20
2	D	23	VAL	CG1-CB-CG2	6.58	121.43	110.90
2	D	1	VAL	CG1-CB-CG2	-6.58	100.37	110.90
1	A	84	SER	CB-CA-C	-6.57	97.62	110.10
2	D	103	PHE	N-CA-CB	6.57	122.42	110.60
1	A	77	PRO	N-CA-CB	6.56	111.17	103.30
2	B	28	LEU	O-C-N	-6.56	112.05	123.20
2	D	137	VAL	CG1-CB-CG2	6.56	121.39	110.90
2	B	74	GLY	N-CA-C	6.56	129.49	113.10
1	C	139	LYS	CA-CB-CG	-6.56	98.97	113.40
1	A	81	SER	C-N-CA	6.55	138.09	121.70
2	B	141	LEU	O-C-N	-6.55	112.22	122.70
1	A	126	ASP	CA-C-O	6.55	133.86	120.10
1	A	140	TYR	CD1-CG-CD2	-6.55	110.69	117.90
2	B	101	GLU	O-C-N	-6.55	112.22	122.70
2	D	8	LYS	CA-C-O	6.55	133.85	120.10
2	D	51	PRO	CA-C-O	6.54	135.90	120.20
1	A	50	HIS	ND1-CG-CD2	-6.54	96.84	106.00
2	B	101	GLU	CG-CD-OE1	-6.54	105.22	118.30
2	B	17	LYS	C-N-CA	6.54	138.04	121.70
2	B	103	PHE	N-CA-CB	6.54	122.36	110.60
1	C	140	TYR	O-C-N	6.53	133.15	122.70
2	D	144	LYS	N-CA-CB	6.53	122.36	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	LYS	O-C-N	-6.53	112.25	122.70
1	C	6	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	83	LEU	CB-CA-C	-6.52	97.81	110.20
1	A	46	PHE	CD1-CE1-CZ	6.52	127.92	120.10
2	D	92	HIS	CB-CG-CD2	6.51	150.99	130.80
1	C	42	TYR	CB-CG-CD2	6.51	124.91	121.00
2	D	66	LYS	CB-CA-C	6.51	123.42	110.40
2	B	27	ALA	N-CA-CB	-6.51	100.99	110.10
1	A	71	ALA	CB-CA-C	6.50	119.86	110.10
2	B	7	GLU	N-CA-C	-6.50	93.45	111.00
2	B	132	LYS	CG-CD-CE	-6.50	92.40	111.90
1	A	23	GLU	CG-CD-OE2	-6.50	105.30	118.30
2	D	51	PRO	O-C-N	-6.50	112.30	122.70
1	A	3	SER	N-CA-CB	-6.49	100.76	110.50
2	B	138	ALA	CA-C-O	6.49	133.73	120.10
1	A	84	SER	N-CA-CB	6.48	120.22	110.50
2	B	24	GLY	CA-C-O	6.48	132.26	120.60
1	A	36	PHE	O-C-N	6.47	133.40	121.10
1	A	51	GLY	C-N-CA	-6.47	105.52	121.70
2	B	90	GLU	CA-C-O	6.47	133.69	120.10
2	B	91	LEU	C-N-CA	-6.47	105.53	121.70
2	D	100	PRO	CA-N-CD	-6.46	102.45	111.50
2	D	135	ALA	N-CA-CB	6.45	119.14	110.10
2	D	145	TYR	CD1-CE1-CZ	-6.45	113.99	119.80
2	B	2	HIS	CA-C-O	6.45	133.65	120.10
2	D	49	SER	CA-C-N	-6.45	103.01	117.20
2	B	99	ASP	N-CA-C	-6.45	93.59	111.00
2	B	65	LYS	CA-CB-CG	-6.45	99.22	113.40
2	B	3	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	C	1	VAL	CA-C-O	6.44	133.62	120.10
1	C	96	VAL	CA-CB-CG1	-6.44	101.25	110.90
2	D	15	TRP	CZ3-CH2-CZ2	6.44	129.32	121.60
1	C	36	PHE	C-N-CD	6.43	141.89	128.40
1	A	76	MET	N-CA-CB	-6.42	99.03	110.60
2	B	37	TRP	CD2-CE3-CZ3	-6.42	110.45	118.80
2	B	81	LEU	CB-CG-CD1	6.42	121.92	111.00
2	D	105	LEU	CA-CB-CG	6.42	130.07	115.30
2	D	100	PRO	CB-CA-C	6.42	128.05	112.00
1	C	61	LYS	O-C-N	6.42	132.97	122.70
1	A	72	HIS	ND1-CE1-NE2	-6.42	95.79	109.90
2	B	59	LYS	CG-CD-CE	-6.41	92.66	111.90
1	C	58	HIS	CE1-NE2-CD2	-6.41	90.57	106.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	VAL	N-CA-CB	6.41	125.61	111.50
2	B	118	PHE	CZ-CE2-CD2	6.40	127.78	120.10
1	C	11	LYS	CB-CA-C	6.39	123.19	110.40
2	D	59	LYS	CD-CE-NZ	-6.39	97.00	111.70
2	D	122	PHE	N-CA-CB	-6.39	99.10	110.60
2	D	90	GLU	C-N-CA	-6.39	105.73	121.70
2	B	142	ALA	N-CA-CB	6.38	119.04	110.10
1	C	18	GLY	C-N-CA	-6.38	105.75	121.70
1	A	125	LEU	O-C-N	-6.38	112.50	122.70
1	C	16	LYS	N-CA-C	-6.38	93.78	111.00
1	C	112	HIS	CA-CB-CG	-6.38	102.76	113.60
2	D	24	GLY	CA-C-N	6.37	128.94	116.20
1	A	86	LEU	C-N-CA	-6.37	105.78	121.70
1	C	91	LEU	N-CA-CB	-6.37	97.67	110.40
1	C	133	SER	N-CA-CB	6.37	120.05	110.50
2	B	80	ASN	C-N-CA	-6.36	105.79	121.70
1	C	2	LEU	CB-CG-CD2	6.36	121.81	111.00
1	C	80	LEU	CB-CG-CD2	-6.36	100.19	111.00
2	D	18	VAL	CG1-CB-CG2	-6.36	100.73	110.90
1	C	13	ALA	CB-CA-C	6.36	119.63	110.10
2	B	79	ASP	CB-CG-OD2	6.35	124.02	118.30
2	D	60	VAL	CA-CB-CG2	6.35	120.42	110.90
2	B	13	ALA	N-CA-C	6.34	128.12	111.00
1	C	47	ASP	CA-CB-CG	-6.34	99.45	113.40
1	A	33	PHE	CA-C-O	6.34	133.41	120.10
2	D	45	PHE	CE1-CZ-CE2	-6.34	108.59	120.00
2	B	14	LEU	CD1-CG-CD2	6.34	129.51	110.50
1	A	74	ASP	OD1-CG-OD2	-6.33	111.27	123.30
2	B	36	PRO	N-CA-CB	6.32	110.89	103.30
2	B	5	PRO	N-CD-CG	-6.32	93.72	103.20
2	D	74	GLY	CA-C-O	6.32	131.97	120.60
2	B	37	TRP	CD1-CG-CD2	-6.31	101.25	106.30
2	B	103	PHE	CG-CD2-CE2	-6.31	113.86	120.80
2	D	64	GLY	CA-C-O	6.31	131.96	120.60
1	C	109	LEU	CD1-CG-CD2	6.31	129.43	110.50
1	A	99	LYS	CB-CG-CD	6.31	128.00	111.60
2	B	66	LYS	CA-CB-CG	6.31	127.27	113.40
1	A	64	ASP	CB-CA-C	-6.30	97.79	110.40
2	B	6	GLU	CB-CA-C	-6.30	97.80	110.40
1	C	98	PHE	CB-CG-CD1	-6.30	116.39	120.80
1	C	103	HIS	O-C-N	-6.30	112.62	122.70
1	C	118	THR	O-C-N	6.30	133.07	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	PHE	CG-CD1-CE1	6.30	127.72	120.80
1	A	22	GLY	N-CA-C	6.29	128.83	113.10
1	A	30	GLU	CG-CD-OE2	-6.29	105.72	118.30
1	A	56	LYS	CA-C-N	-6.29	103.63	116.20
1	A	112	HIS	CB-CG-ND1	-6.28	107.49	123.20
1	C	50	HIS	CA-C-O	-6.28	106.91	120.10
2	D	139	ASN	CA-C-O	6.27	133.28	120.10
1	C	69	ALA	CB-CA-C	6.27	119.51	110.10
2	B	78	LEU	CA-C-O	-6.27	106.93	120.10
1	C	65	ALA	CB-CA-C	-6.27	100.69	110.10
1	A	7	LYS	C-N-CA	-6.26	106.04	121.70
1	C	47	ASP	CA-C-N	-6.25	103.44	117.20
2	D	4	THR	CA-C-N	6.25	134.61	117.10
2	D	96	LEU	O-C-N	6.25	132.71	122.70
1	A	86	LEU	CD1-CG-CD2	-6.25	91.75	110.50
1	A	64	ASP	N-CA-C	6.25	127.87	111.00
1	A	132	VAL	CA-CB-CG1	6.24	120.26	110.90
1	C	58	HIS	CG-CD2-NE2	6.24	121.05	109.20
1	A	99	LYS	CD-CE-NZ	-6.24	97.36	111.70
2	D	6	GLU	N-CA-C	-6.24	94.16	111.00
2	B	61	LYS	CG-CD-CE	-6.23	93.21	111.90
2	D	85	PHE	CA-CB-CG	-6.23	98.96	113.90
1	A	83	LEU	O-C-N	-6.22	112.74	122.70
1	A	128	PHE	CG-CD1-CE1	-6.22	113.95	120.80
1	A	15	GLY	O-C-N	-6.22	112.75	122.70
2	D	39	GLN	N-CA-CB	-6.21	99.42	110.60
2	B	95	LYS	N-CA-C	6.21	127.77	111.00
1	A	138	SER	O-C-N	6.20	132.62	122.70
2	D	141	LEU	CD1-CG-CD2	-6.20	91.89	110.50
1	C	1	VAL	CB-CA-C	-6.20	99.62	111.40
1	C	5	ALA	CA-C-N	-6.20	103.56	117.20
2	B	145	TYR	O-C-N	6.20	132.62	122.70
2	D	77	HIS	CG-ND1-CE1	-6.20	97.65	105.70
1	C	54	GLN	CA-C-N	-6.19	103.57	117.20
2	D	80	ASN	CB-CG-OD1	-6.19	109.21	121.60
1	C	74	ASP	N-CA-CB	-6.19	99.46	110.60
1	A	75	ASP	C-N-CA	-6.19	106.23	121.70
1	A	4	PRO	O-C-N	-6.18	112.81	122.70
2	D	41	PHE	CB-CG-CD1	-6.18	116.47	120.80
2	D	131	GLN	CA-C-O	6.18	133.09	120.10
2	B	63	HIS	CA-CB-CG	6.18	124.11	113.60
1	A	24	TYR	CB-CG-CD1	-6.18	117.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	PHE	CZ-CE2-CD2	-6.18	112.69	120.10
1	A	28	ALA	C-N-CA	-6.18	106.26	121.70
1	C	50	HIS	CA-CB-CG	-6.18	103.10	113.60
2	B	81	LEU	C-N-CA	-6.17	106.27	121.70
1	C	141	ARG	CB-CG-CD	-6.17	95.55	111.60
2	D	31	LEU	CA-C-N	-6.17	103.62	117.20
2	B	21	ASP	OD1-CG-OD2	6.17	135.02	123.30
2	B	8	LYS	CG-CD-CE	6.17	130.40	111.90
2	B	93	CYS	O-C-N	6.17	132.57	122.70
2	B	61	LYS	CB-CA-C	-6.16	98.08	110.40
2	D	15	TRP	NE1-CE2-CD2	-6.16	101.14	107.30
2	B	103	PHE	CD1-CG-CD2	6.16	126.30	118.30
2	D	7	GLU	CB-CG-CD	-6.15	97.58	114.20
2	B	14	LEU	N-CA-CB	-6.15	98.09	110.40
2	B	19	ASN	CB-CG-OD1	6.15	133.91	121.60
2	B	37	TRP	N-CA-CB	-6.15	99.53	110.60
2	D	24	GLY	C-N-CA	6.15	135.21	122.30
2	B	44	SER	C-N-CA	6.15	137.07	121.70
1	C	100	LEU	CB-CA-C	6.14	121.86	110.20
2	D	1	VAL	C-N-CA	-6.14	106.36	121.70
2	D	19	ASN	CA-C-O	-6.14	107.21	120.10
2	B	120	LYS	CG-CD-CE	-6.13	93.51	111.90
2	B	120	LYS	CB-CA-C	-6.13	98.14	110.40
2	B	35	TYR	O-C-N	6.12	132.74	121.10
1	C	122	HIS	CB-CA-C	6.12	122.65	110.40
1	A	79	ALA	O-C-N	6.11	132.48	122.70
2	B	76	ALA	N-CA-C	6.11	127.50	111.00
1	A	58	HIS	CG-ND1-CE1	-6.11	97.76	105.70
1	A	96	VAL	CA-C-O	6.11	132.93	120.10
1	C	38	THR	N-CA-CB	-6.11	98.69	110.30
1	C	21	ALA	CA-C-N	6.11	128.42	116.20
1	C	11	LYS	O-C-N	-6.11	112.93	122.70
2	D	48	LEU	CB-CG-CD1	-6.10	100.63	111.00
2	D	93	CYS	C-N-CA	-6.10	106.45	121.70
2	B	90	GLU	OE1-CD-OE2	6.09	130.61	123.30
2	B	73	ASP	C-N-CA	6.09	135.10	122.30
1	C	77	PRO	CA-C-O	6.09	134.81	120.20
2	B	41	PHE	CG-CD1-CE1	-6.09	114.10	120.80
1	A	58	HIS	CA-C-N	-6.07	104.06	116.20
1	C	43	PHE	CD1-CG-CD2	6.07	126.19	118.30
2	B	50	THR	N-CA-C	6.06	127.37	111.00
2	B	12	THR	CA-C-O	6.06	132.82	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	GLU	CA-CB-CG	-6.06	100.08	113.40
1	A	1	VAL	CA-C-N	-6.05	103.88	117.20
1	A	83	LEU	CB-CG-CD2	6.05	121.29	111.00
1	C	25	GLY	C-N-CA	6.05	136.83	121.70
1	C	72	HIS	CE1-NE2-CD2	-6.05	91.47	106.60
1	C	103	HIS	ND1-CE1-NE2	6.05	123.21	109.90
1	A	89	HIS	C-N-CA	6.05	136.82	121.70
2	B	36	PRO	O-C-N	-6.05	113.03	122.70
2	D	12	THR	N-CA-CB	-6.04	98.82	110.30
2	D	102	ASN	CA-C-N	6.04	130.50	117.20
2	B	104	ARG	CG-CD-NE	-6.04	99.11	111.80
1	C	47	ASP	O-C-N	6.03	132.35	122.70
1	A	18	GLY	CA-C-N	-6.03	103.93	117.20
1	C	138	SER	CB-CA-C	-6.03	98.64	110.10
2	B	97	HIS	CG-CD2-NE2	-6.03	97.75	109.20
1	A	15	GLY	C-N-CA	6.02	136.76	121.70
1	A	45	HIS	CB-CG-ND1	-6.02	108.14	123.20
2	D	92	HIS	CA-CB-CG	-6.02	103.37	113.60
1	A	56	LYS	CB-CA-C	6.02	122.43	110.40
2	B	30	ARG	CD-NE-CZ	6.02	132.02	123.60
1	A	85	ASP	CA-CB-CG	-6.01	100.18	113.40
1	A	109	LEU	CD1-CG-CD2	6.01	128.53	110.50
1	A	99	LYS	CA-CB-CG	6.01	126.62	113.40
1	C	39	THR	CA-CB-CG2	-6.00	103.99	112.40
2	D	125	PRO	CA-C-N	-6.00	104.01	117.20
1	A	40	LYS	CB-CA-C	-5.99	98.41	110.40
1	C	75	ASP	N-CA-CB	-5.99	99.81	110.60
2	D	17	LYS	N-CA-CB	5.99	121.38	110.60
1	A	26	ALA	O-C-N	-5.98	113.13	122.70
2	B	108	ASN	CB-CG-OD1	-5.96	109.68	121.60
1	A	27	GLU	N-CA-CB	-5.96	99.87	110.60
1	A	117	PHE	O-C-N	5.95	132.22	122.70
2	B	46	GLY	CA-C-O	-5.95	109.89	120.60
2	D	103	PHE	CG-CD2-CE2	-5.95	114.25	120.80
1	A	46	PHE	CG-CD1-CE1	5.95	127.34	120.80
2	B	140	ALA	CA-C-N	5.95	130.28	117.20
1	A	84	SER	CA-CB-OG	-5.95	95.14	111.20
1	A	49	SER	N-CA-C	-5.94	94.96	111.00
1	C	45	HIS	CA-C-O	-5.94	107.63	120.10
2	B	91	LEU	N-CA-CB	-5.94	98.53	110.40
1	C	77	PRO	CA-CB-CG	5.94	116.08	104.80
1	C	124	SER	CA-C-O	-5.93	107.64	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	126	VAL	CA-C-N	-5.93	104.14	117.20
2	D	78	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	14	TRP	CB-CG-CD1	-5.93	119.29	127.00
2	D	21	ASP	C-N-CA	5.93	136.52	121.70
2	D	19	ASN	O-C-N	-5.93	113.22	122.70
2	D	88	LEU	CB-CG-CD1	-5.93	100.93	111.00
1	A	54	GLN	OE1-CD-NE2	-5.92	108.29	121.90
2	B	28	LEU	CB-CA-C	5.92	121.44	110.20
1	A	89	HIS	CA-C-O	5.92	132.52	120.10
2	B	33	VAL	O-C-N	5.92	132.16	122.70
1	A	126	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	134	THR	CA-C-N	5.91	130.20	117.20
2	D	57	ASN	CB-CG-OD1	5.91	133.42	121.60
1	A	134	THR	CA-CB-OG1	5.91	121.40	109.00
2	B	69	GLY	CA-C-O	5.91	131.23	120.60
2	D	103	PHE	CZ-CE2-CD2	5.90	127.18	120.10
1	A	28	ALA	CA-C-O	5.90	132.49	120.10
1	A	131	SER	CA-C-O	-5.89	107.72	120.10
1	C	37	PRO	CA-N-CD	-5.89	103.25	111.50
1	C	14	TRP	CA-CB-CG	-5.89	102.51	113.70
2	B	24	GLY	O-C-N	-5.89	113.19	123.20
2	D	91	LEU	CB-CG-CD2	5.89	121.01	111.00
1	A	67	THR	CA-CB-OG1	5.89	121.36	109.00
2	D	95	LYS	CG-CD-CE	5.89	129.56	111.90
2	B	50	THR	CA-C-O	-5.89	107.74	120.10
1	A	135	VAL	CA-C-N	5.88	130.14	117.20
2	B	11	VAL	O-C-N	5.88	132.11	122.70
1	C	50	HIS	CB-CG-ND1	-5.88	108.51	123.20
1	C	77	PRO	N-CA-CB	-5.87	96.14	102.60
2	B	123	THR	O-C-N	5.87	132.25	121.10
1	C	89	HIS	CB-CA-C	5.87	122.14	110.40
2	D	130	TYR	CD1-CG-CD2	-5.87	111.44	117.90
1	A	7	LYS	O-C-N	5.87	132.09	122.70
1	A	8	THR	N-CA-CB	-5.86	99.16	110.30
1	C	92	ARG	CG-CD-NE	-5.86	99.50	111.80
1	C	90	LYS	CA-CB-CG	-5.85	100.53	113.40
1	A	81	SER	CB-CA-C	-5.85	98.99	110.10
2	D	141	LEU	O-C-N	-5.84	113.35	122.70
2	B	79	ASP	CA-CB-CG	-5.84	100.55	113.40
1	A	64	ASP	N-CA-CB	-5.84	100.09	110.60
2	B	132	LYS	O-C-N	-5.83	113.37	122.70
2	D	137	VAL	CA-CB-CG2	-5.83	102.15	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	PHE	N-CA-CB	5.83	121.09	110.60
1	C	136	LEU	CB-CG-CD1	-5.83	101.10	111.00
1	A	73	VAL	CB-CA-C	5.82	122.46	111.40
2	B	17	LYS	CA-CB-CG	-5.82	100.60	113.40
2	D	60	VAL	CA-C-O	5.81	132.31	120.10
1	A	44	PRO	CA-N-CD	5.81	119.83	111.70
1	A	103	HIS	CG-ND1-CE1	-5.81	98.15	105.70
1	A	11	LYS	CD-CE-NZ	-5.80	98.36	111.70
2	D	53	ALA	CA-C-N	-5.80	104.44	117.20
2	D	12	THR	C-N-CA	5.80	136.20	121.70
1	A	132	VAL	CA-C-N	5.79	129.95	117.20
1	A	54	GLN	CA-C-O	-5.79	107.94	120.10
1	C	11	LYS	CA-C-O	5.79	132.25	120.10
2	D	97	HIS	N-CA-CB	5.79	121.01	110.60
1	A	16	LYS	CA-C-N	-5.78	104.48	117.20
1	A	21	ALA	N-CA-C	-5.78	95.41	111.00
2	B	37	TRP	CE3-CZ3-CH2	5.78	127.55	121.20
1	C	46	PHE	CA-C-O	5.77	132.21	120.10
2	D	82	LYS	CA-C-N	5.76	127.72	116.20
1	C	89	HIS	ND1-CG-CD2	5.76	116.86	108.80
2	D	68	LEU	CB-CA-C	-5.76	99.26	110.20
1	C	83	LEU	CB-CG-CD1	-5.76	101.21	111.00
1	C	15	GLY	CA-C-N	5.75	129.86	117.20
2	D	22	GLU	CB-CA-C	5.75	121.91	110.40
1	C	12	ALA	N-CA-CB	5.75	118.16	110.10
1	C	118	THR	CB-CA-C	-5.75	96.08	111.60
2	B	9	SER	C-N-CA	-5.74	107.35	121.70
2	B	36	PRO	CA-C-N	5.74	129.83	117.20
2	B	8	LYS	CA-C-N	5.74	129.82	117.20
2	B	75	LEU	CD1-CG-CD2	-5.74	93.29	110.50
2	D	112	CYS	CA-C-O	5.74	132.15	120.10
1	A	4	PRO	CA-C-N	-5.73	104.59	117.20
2	B	96	LEU	N-CA-C	5.73	126.48	111.00
1	A	103	HIS	N-CA-CB	5.73	120.92	110.60
1	A	14	TRP	NE1-CE2-CD2	-5.73	101.57	107.30
1	C	47	ASP	CB-CA-C	-5.73	98.94	110.40
2	D	56	GLY	C-N-CA	5.72	136.01	121.70
1	C	78	ASN	CB-CA-C	5.72	121.85	110.40
2	B	17	LYS	CB-CA-C	-5.72	98.96	110.40
1	A	32	MET	CA-CB-CG	5.72	123.02	113.30
2	B	13	ALA	CB-CA-C	-5.71	101.53	110.10
1	A	137	THR	CA-C-N	5.71	129.76	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	CYS	CA-C-O	-5.71	108.12	120.10
1	C	27	GLU	OE1-CD-OE2	-5.71	116.45	123.30
2	D	108	ASN	CB-CG-OD1	-5.71	110.19	121.60
2	B	39	GLN	OE1-CD-NE2	5.70	135.01	121.90
2	B	97	HIS	ND1-CG-CD2	5.70	116.78	108.80
1	C	41	THR	C-N-CA	5.70	135.95	121.70
1	C	36	PHE	CZ-CE2-CD2	5.70	126.94	120.10
2	D	28	LEU	O-C-N	-5.70	113.51	123.20
1	C	116	GLU	CA-C-O	-5.70	108.14	120.10
2	B	62	ALA	C-N-CA	-5.70	107.46	121.70
2	B	110	LEU	CB-CA-C	5.69	121.01	110.20
2	D	13	ALA	CB-CA-C	-5.69	101.57	110.10
2	D	20	VAL	CA-C-N	-5.68	104.69	117.20
2	D	92	HIS	ND1-CG-CD2	-5.68	98.04	106.00
2	D	54	VAL	CA-C-N	5.68	129.69	117.20
2	D	143	HIS	CB-CG-CD2	-5.68	113.20	130.80
1	A	52	SER	N-CA-CB	-5.67	102.00	110.50
2	B	50	THR	O-C-N	5.67	131.87	121.10
2	D	15	TRP	CE3-CZ3-CH2	-5.67	114.96	121.20
1	A	2	LEU	C-N-CA	-5.67	107.53	121.70
1	A	88	ALA	N-CA-CB	5.67	118.03	110.10
2	B	131	GLN	CG-CD-NE2	5.67	130.30	116.70
1	A	35	SER	CB-CA-C	-5.67	99.34	110.10
2	B	91	LEU	CB-CA-C	5.66	120.96	110.20
1	A	33	PHE	O-C-N	-5.66	113.64	122.70
2	D	54	VAL	CA-CB-CG2	5.66	119.39	110.90
2	B	131	GLN	CG-CD-OE1	-5.66	110.29	121.60
2	D	121	GLU	CA-C-N	-5.65	104.76	117.20
2	B	39	GLN	CG-CD-OE1	-5.65	110.30	121.60
1	A	8	THR	O-C-N	-5.65	113.67	122.70
2	D	33	VAL	CA-CB-CG1	-5.64	102.44	110.90
1	A	77	PRO	N-CA-C	5.64	126.75	112.10
1	C	47	ASP	C-N-CA	-5.63	107.61	121.70
2	D	143	HIS	CA-C-O	-5.63	108.27	120.10
1	A	98	PHE	CE1-CZ-CE2	5.63	130.14	120.00
2	B	11	VAL	CB-CA-C	5.63	122.10	111.40
1	C	125	LEU	O-C-N	-5.63	113.69	122.70
2	D	39	GLN	C-N-CA	5.63	135.77	121.70
1	C	88	ALA	CA-C-N	-5.63	104.82	117.20
1	A	55	VAL	CA-C-O	5.62	131.91	120.10
1	A	71	ALA	CA-C-O	-5.62	108.29	120.10
1	C	83	LEU	CA-CB-CG	-5.62	102.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASP	C-N-CA	-5.62	107.65	121.70
1	A	13	ALA	C-N-CA	-5.62	107.66	121.70
2	D	6	GLU	CB-CG-CD	5.62	129.37	114.20
1	A	13	ALA	CA-C-N	-5.61	104.85	117.20
2	D	63	HIS	CB-CG-ND1	-5.61	109.17	123.20
2	B	4	THR	O-C-N	-5.61	110.44	121.10
2	B	92	HIS	CB-CA-C	-5.61	99.18	110.40
1	C	3	SER	N-CA-CB	-5.61	102.09	110.50
1	C	69	ALA	CA-C-O	-5.61	108.33	120.10
2	D	58	PRO	CA-C-O	-5.61	106.75	120.20
1	A	48	LEU	CA-C-N	-5.60	104.87	117.20
1	A	113	LEU	CB-CA-C	-5.60	99.57	110.20
2	B	143	HIS	CB-CG-CD2	-5.60	113.45	130.80
1	C	72	HIS	CG-CD2-NE2	5.59	119.82	109.20
1	A	8	THR	CA-C-N	-5.59	104.91	117.20
1	C	131	SER	CA-CB-OG	-5.58	96.12	111.20
2	B	33	VAL	CA-CB-CG2	-5.58	102.53	110.90
1	C	35	SER	N-CA-C	5.57	126.05	111.00
1	C	106	LEU	CA-CB-CG	5.57	128.12	115.30
2	B	91	LEU	CB-CG-CD2	5.57	120.47	111.00
2	B	79	ASP	N-CA-C	-5.57	95.96	111.00
2	B	124	PRO	CA-C-N	5.57	132.69	117.10
2	D	139	ASN	O-C-N	-5.56	113.80	122.70
2	B	3	LEU	CB-CA-C	-5.56	99.64	110.20
2	B	80	ASN	O-C-N	5.56	131.59	122.70
2	B	117	HIS	C-N-CA	5.56	135.60	121.70
1	C	44	PRO	CA-C-O	-5.56	106.86	120.20
2	B	80	ASN	CB-CA-C	5.55	121.50	110.40
1	A	131	SER	C-N-CA	-5.55	107.83	121.70
2	B	135	ALA	CB-CA-C	5.53	118.40	110.10
1	A	26	ALA	CA-C-N	-5.53	105.04	117.20
2	B	13	ALA	CA-C-O	5.53	131.70	120.10
1	A	94	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	98	PHE	N-CA-CB	5.52	120.53	110.60
2	D	72	SER	O-C-N	-5.52	113.87	122.70
1	C	99	LYS	CA-C-O	5.51	131.66	120.10
2	D	44	SER	CA-CB-OG	5.50	126.06	111.20
1	A	116	GLU	CB-CG-CD	-5.50	99.34	114.20
2	D	44	SER	N-CA-CB	5.50	118.75	110.50
2	D	45	PHE	CD1-CG-CD2	-5.50	111.15	118.30
2	D	11	VAL	CA-CB-CG1	-5.49	102.66	110.90
2	D	118	PHE	CA-C-N	5.49	127.18	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	LEU	O-C-N	5.49	131.48	122.70
2	B	68	LEU	CB-CG-CD2	5.48	120.32	111.00
1	C	19	ALA	CA-C-O	5.48	131.61	120.10
2	D	62	ALA	CA-C-N	-5.48	105.14	117.20
1	A	57	GLY	CA-C-O	-5.48	110.74	120.60
2	D	64	GLY	CA-C-N	-5.48	105.14	117.20
1	C	89	HIS	CB-CG-CD2	-5.47	113.83	130.80
1	A	16	LYS	CB-CG-CD	-5.47	97.38	111.60
1	C	24	TYR	CA-C-O	5.47	131.58	120.10
1	C	29	LEU	C-N-CA	5.46	135.35	121.70
1	A	20	HIS	ND1-CG-CD2	-5.46	98.36	106.00
1	C	121	VAL	CB-CA-C	5.46	121.77	111.40
2	D	59	LYS	C-N-CA	-5.46	108.05	121.70
1	C	113	LEU	CD1-CG-CD2	5.45	126.86	110.50
1	A	139	LYS	CA-C-N	5.45	129.18	117.20
1	C	65	ALA	O-C-N	-5.44	113.99	122.70
1	C	133	SER	CA-CB-OG	-5.44	96.51	111.20
1	C	58	HIS	ND1-CE1-NE2	5.44	121.87	109.90
2	B	124	PRO	N-CD-CG	-5.43	95.05	103.20
2	B	143	HIS	ND1-CE1-NE2	5.43	121.86	109.90
1	C	14	TRP	CB-CA-C	-5.43	99.53	110.40
2	D	73	ASP	CB-CA-C	-5.43	99.54	110.40
1	A	5	ALA	N-CA-CB	-5.42	102.51	110.10
2	B	92	HIS	CG-ND1-CE1	-5.42	98.65	105.70
2	B	91	LEU	CA-CB-CG	-5.42	102.83	115.30
1	C	14	TRP	CE2-CD2-CE3	5.42	125.20	118.70
2	D	85	PHE	CG-CD2-CE2	-5.42	114.84	120.80
1	A	84	SER	C-N-CA	-5.42	108.16	121.70
2	D	66	LYS	N-CA-C	-5.41	96.38	111.00
1	C	53	ALA	C-N-CA	-5.41	108.18	121.70
1	C	98	PHE	CG-CD1-CE1	5.40	126.74	120.80
1	A	12	ALA	CA-C-N	5.40	129.08	117.20
2	D	3	LEU	CB-CA-C	5.40	120.46	110.20
1	C	111	ALA	CA-C-O	-5.39	108.78	120.10
1	A	85	ASP	O-C-N	-5.39	114.08	122.70
1	C	12	ALA	CA-C-N	-5.38	105.36	117.20
1	A	4	PRO	C-N-CA	-5.38	108.26	121.70
1	A	61	LYS	CA-C-O	-5.37	108.81	120.10
2	D	91	LEU	N-CA-C	5.37	125.51	111.00
2	D	74	GLY	CA-C-N	-5.37	105.39	117.20
1	A	112	HIS	O-C-N	5.36	131.28	122.70
1	A	60	LYS	N-CA-C	5.36	125.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	84	THR	CA-CB-OG1	-5.36	97.74	109.00
1	A	88	ALA	CA-C-O	-5.36	108.85	120.10
1	C	119	PRO	N-CA-CB	5.36	109.73	103.30
1	C	79	ALA	O-C-N	5.36	131.27	122.70
1	A	10	VAL	CA-CB-CG2	5.35	118.92	110.90
1	C	92	ARG	CA-C-O	5.35	131.34	120.10
1	A	67	THR	CA-CB-CG2	-5.35	104.91	112.40
2	D	119	GLY	CA-C-N	-5.35	105.44	117.20
2	B	41	PHE	CD1-CE1-CZ	5.34	126.51	120.10
2	D	75	LEU	N-CA-CB	-5.34	99.72	110.40
2	B	77	HIS	N-CA-C	-5.34	96.58	111.00
2	D	5	PRO	CB-CG-CD	5.34	127.31	106.50
2	D	68	LEU	CA-C-O	5.33	131.30	120.10
1	C	48	LEU	N-CA-CB	-5.33	99.74	110.40
1	C	35	SER	CA-C-O	5.33	131.29	120.10
2	B	71	PHE	N-CA-CB	-5.32	101.02	110.60
1	A	64	ASP	CA-C-N	-5.32	105.50	117.20
2	B	124	PRO	N-CA-CB	5.32	109.68	103.30
1	C	78	ASN	CA-C-N	-5.32	105.50	117.20
2	B	118	PHE	CB-CA-C	5.30	121.01	110.40
2	D	78	LEU	O-C-N	-5.30	114.22	122.70
1	A	89	HIS	ND1-CG-CD2	-5.30	98.58	106.00
2	D	54	VAL	N-CA-CB	-5.30	99.84	111.50
1	C	139	LYS	CB-CG-CD	-5.29	97.84	111.60
1	C	50	HIS	ND1-CE1-NE2	5.29	121.54	109.90
1	A	89	HIS	N-CA-C	5.29	125.28	111.00
2	D	92	HIS	N-CA-C	-5.28	96.73	111.00
1	A	71	ALA	N-CA-CB	-5.28	102.71	110.10
1	A	24	TYR	CB-CA-C	-5.27	99.86	110.40
2	D	66	LYS	CB-CG-CD	5.27	125.30	111.60
2	D	117	HIS	ND1-CE1-NE2	5.27	121.49	109.90
2	D	83	GLY	CA-C-N	5.27	128.79	117.20
2	B	101	GLU	CA-C-O	5.27	131.16	120.10
1	C	20	HIS	ND1-CG-CD2	5.26	116.17	108.80
2	D	117	HIS	CB-CG-CD2	5.26	147.11	130.80
2	B	77	HIS	CE1-NE2-CD2	5.26	119.75	106.60
1	A	62	VAL	CA-CB-CG2	-5.25	103.02	110.90
1	A	83	LEU	CA-C-N	5.25	128.76	117.20
2	B	89	SER	CB-CA-C	5.25	120.08	110.10
2	B	122	PHE	CZ-CE2-CD2	-5.25	113.80	120.10
1	C	20	HIS	ND1-CE1-NE2	-5.25	98.36	109.90
2	D	75	LEU	CA-CB-CG	5.25	127.36	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	VAL	C-N-CA	5.24	134.81	121.70
2	D	74	GLY	C-N-CA	-5.24	108.60	121.70
1	A	140	TYR	N-CA-CB	5.24	120.03	110.60
1	A	141	ARG	CB-CG-CD	-5.24	97.98	111.60
1	A	2	LEU	CA-C-N	-5.24	105.68	117.20
1	C	7	LYS	N-CA-CB	-5.24	101.18	110.60
1	A	95	PRO	CA-C-N	5.23	128.72	117.20
2	D	63	HIS	C-N-CA	-5.23	111.32	122.30
1	A	50	HIS	CA-CB-CG	-5.23	104.71	113.60
1	A	90	LYS	CG-CD-CE	-5.23	96.21	111.90
2	D	139	ASN	CB-CG-ND2	-5.23	104.15	116.70
2	D	77	HIS	CB-CG-ND1	-5.23	110.13	123.20
2	D	41	PHE	CD1-CG-CD2	5.22	125.09	118.30
1	A	71	ALA	C-N-CA	5.22	134.75	121.70
1	C	140	TYR	CD1-CE1-CZ	5.22	124.50	119.80
1	A	82	ALA	O-C-N	-5.22	114.35	122.70
1	C	28	ALA	O-C-N	5.21	131.04	122.70
1	A	112	HIS	CE1-NE2-CD2	-5.21	93.57	106.60
2	B	54	VAL	O-C-N	-5.21	114.37	122.70
2	D	102	ASN	C-N-CA	5.21	134.72	121.70
2	D	127	GLN	CB-CA-C	5.21	120.82	110.40
1	A	24	TYR	CA-C-N	5.21	126.61	116.20
1	A	41	THR	CA-C-N	5.21	128.65	117.20
1	C	137	THR	O-C-N	5.21	131.03	122.70
2	B	54	VAL	CA-CB-CG1	-5.21	103.09	110.90
1	A	11	LYS	O-C-N	-5.20	114.38	122.70
1	A	23	GLU	CB-CG-CD	-5.20	100.16	114.20
1	A	72	HIS	CB-CA-C	-5.20	100.00	110.40
2	B	7	GLU	CA-CB-CG	5.20	124.83	113.40
2	D	91	LEU	CA-C-N	-5.19	105.77	117.20
2	B	119	GLY	O-C-N	-5.19	114.39	122.70
1	A	73	VAL	CG1-CB-CG2	5.19	119.20	110.90
2	B	17	LYS	N-CA-CB	5.19	119.94	110.60
1	C	75	ASP	CA-C-N	-5.19	105.78	117.20
2	D	100	PRO	N-CA-CB	5.19	109.53	103.30
1	C	76	MET	CB-CG-SD	-5.18	96.86	112.40
2	B	85	PHE	CB-CA-C	5.18	120.76	110.40
2	B	22	GLU	N-CA-CB	-5.17	101.29	110.60
1	A	139	LYS	CD-CE-NZ	-5.17	99.81	111.70
2	B	15	TRP	CZ3-CH2-CZ2	5.16	127.80	121.60
2	B	82	LYS	CG-CD-CE	-5.16	96.42	111.90
2	D	90	GLU	N-CA-CB	-5.16	101.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	143	HIS	CB-CA-C	5.16	120.72	110.40
1	A	101	LEU	CB-CG-CD1	5.16	119.77	111.00
2	B	45	PHE	CD1-CG-CD2	-5.16	111.60	118.30
1	C	75	ASP	N-CA-C	-5.16	97.08	111.00
1	A	19	ALA	CA-C-N	5.15	128.53	117.20
2	B	95	LYS	CA-C-O	5.15	130.92	120.10
2	B	89	SER	CA-CB-OG	-5.15	97.29	111.20
2	D	106	LEU	CB-CG-CD2	-5.15	102.25	111.00
1	C	58	HIS	C-N-CA	-5.15	111.49	122.30
1	C	40	LYS	CB-CG-CD	-5.14	98.23	111.60
2	D	58	PRO	N-CA-CB	5.14	109.47	103.30
2	B	75	LEU	CB-CA-C	-5.14	100.44	110.20
1	C	17	VAL	N-CA-CB	5.14	122.81	111.50
2	D	44	SER	C-N-CA	5.14	134.55	121.70
1	A	74	ASP	C-N-CA	5.14	134.54	121.70
2	B	66	LYS	C-N-CA	-5.14	108.86	121.70
1	C	36	PHE	O-C-N	5.14	130.86	121.10
1	A	106	LEU	CB-CG-CD2	5.13	119.73	111.00
1	A	30	GLU	CA-CB-CG	-5.13	102.11	113.40
1	A	39	THR	C-N-CA	-5.12	108.89	121.70
1	C	65	ALA	CA-C-O	5.12	130.86	120.10
2	B	26	GLU	C-N-CA	-5.12	108.89	121.70
1	A	14	TRP	O-C-N	5.12	131.91	123.20
2	B	55	MET	C-N-CA	-5.12	111.55	122.30
2	B	145	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	16	LYS	CA-C-O	5.12	130.85	120.10
2	B	106	LEU	O-C-N	-5.11	114.51	123.20
2	D	9	SER	CA-C-O	-5.11	109.37	120.10
2	D	83	GLY	N-CA-C	-5.11	100.33	113.10
1	C	62	VAL	CA-C-O	5.11	130.82	120.10
1	C	3	SER	CA-C-O	5.10	130.81	120.10
2	B	62	ALA	O-C-N	5.09	130.85	122.70
2	D	132	LYS	CG-CD-CE	-5.09	96.62	111.90
2	B	93	CYS	N-CA-CB	-5.09	101.43	110.60
1	C	75	ASP	CA-CB-CG	5.09	124.60	113.40
2	B	145	TYR	C-N-CA	5.09	134.42	121.70
1	A	25	GLY	CA-C-O	5.08	129.75	120.60
1	A	59	GLY	CA-C-O	5.08	129.75	120.60
2	B	116	HIS	CG-CD2-NE2	5.08	118.86	109.20
2	D	77	HIS	O-C-N	-5.08	114.57	122.70
1	C	117	PHE	CD1-CE1-CZ	-5.08	114.01	120.10
1	A	44	PRO	CB-CA-C	-5.08	99.31	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	TYR	CB-CG-CD1	5.07	124.04	121.00
2	B	111	VAL	CA-CB-CG1	-5.07	103.29	110.90
2	B	145	TYR	CA-CB-CG	5.07	123.04	113.40
1	A	83	LEU	N-CA-CB	-5.07	100.26	110.40
1	A	92	ARG	C-N-CA	5.07	134.38	121.70
1	C	35	SER	O-C-N	-5.07	114.59	122.70
1	A	58	HIS	CA-C-O	-5.07	109.46	120.10
1	A	103	HIS	ND1-CE1-NE2	5.06	121.04	109.90
2	D	73	ASP	N-CA-CB	5.06	119.71	110.60
2	B	1	VAL	O-C-N	5.06	130.79	122.70
2	B	76	ALA	CA-C-N	-5.06	106.07	117.20
2	D	9	SER	N-CA-CB	-5.06	102.91	110.50
1	A	47	ASP	CA-C-N	-5.05	106.08	117.20
1	A	14	TRP	CD1-CG-CD2	-5.05	102.26	106.30
1	C	36	PHE	CA-C-N	-5.04	102.98	117.10
2	D	42	PHE	CD1-CG-CD2	5.04	124.85	118.30
1	A	88	ALA	CA-C-N	-5.04	106.12	117.20
1	A	119	PRO	O-C-N	-5.04	114.64	122.70
2	B	103	PHE	CG-CD1-CE1	-5.04	115.26	120.80
2	D	40	ARG	N-CA-C	-5.04	97.40	111.00
1	A	136	LEU	CB-CG-CD2	5.04	119.56	111.00
1	A	82	ALA	CA-C-O	5.04	130.68	120.10
1	A	109	LEU	C-N-CA	-5.03	109.11	121.70
2	B	8	LYS	C-N-CA	5.03	134.28	121.70
2	B	27	ALA	O-C-N	-5.03	114.65	122.70
2	B	15	TRP	CB-CG-CD2	-5.03	120.06	126.60
1	A	90	LYS	CB-CG-CD	5.03	124.67	111.60
2	B	3	LEU	CD1-CG-CD2	-5.03	95.42	110.50
1	A	34	LEU	CA-CB-CG	5.03	126.86	115.30
2	D	88	LEU	CD1-CG-CD2	5.03	125.58	110.50
1	C	26	ALA	O-C-N	-5.02	114.67	122.70
2	D	48	LEU	CA-C-N	-5.02	106.16	117.20
1	A	100	LEU	CD1-CG-CD2	-5.01	95.47	110.50
2	D	137	VAL	N-CA-C	5.01	124.53	111.00
2	B	2	HIS	CE1-NE2-CD2	-5.01	94.08	106.60
2	B	37	TRP	O-C-N	-5.00	114.70	122.70
2	D	12	THR	CA-C-N	5.00	128.21	117.20

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	137	THR	CB

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

All (207) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Mainchain
1	A	101	LEU	Mainchain
1	A	106	LEU	Mainchain
1	A	11	LYS	Mainchain
1	A	111	ALA	Mainchain
1	A	114	PRO	Mainchain
1	A	118	THR	Mainchain
1	A	12	ALA	Mainchain
1	A	122	HIS	Mainchain
1	A	126	ASP	Sidechain
1	A	141	ARG	Sidechain
1	A	15	GLY	Mainchain
1	A	18	GLY	Peptide
1	A	19	ALA	Mainchain
1	A	20	HIS	Sidechain
1	A	21	ALA	Mainchain
1	A	22	GLY	Mainchain
1	A	23	GLU	Sidechain
1	A	24	TYR	Sidechain
1	A	3	SER	Mainchain
1	A	36	PHE	Sidechain
1	A	4	PRO	Mainchain
1	A	41	THR	Mainchain
1	A	45	HIS	Sidechain
1	A	46	PHE	Mainchain
1	A	48	LEU	Mainchain
1	A	50	HIS	Sidechain
1	A	52	SER	Mainchain
1	A	54	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	A	56	LYS	Mainchain
1	A	59	GLY	Mainchain
1	A	61	LYS	Mainchain
1	A	63	ALA	Mainchain
1	A	64	ASP	Sidechain
1	A	72	HIS	Sidechain
1	A	74	ASP	Mainchain
1	A	75	ASP	Mainchain
1	A	76	MET	Mainchain
1	A	78	ASN	Mainchain,Sidechain
1	A	81	SER	Mainchain
1	A	82	ALA	Mainchain
1	A	83	LEU	Mainchain
1	A	85	ASP	Mainchain,Sidechain
1	A	88	ALA	Mainchain
1	A	9	ASN	Mainchain
1	A	90	LYS	Mainchain
1	A	92	ARG	Sidechain
1	A	97	ASN	Mainchain
1	A	99	LYS	Mainchain
2	B	1	VAL	Mainchain
2	B	100	PRO	Mainchain
2	B	101	GLU	Mainchain
2	B	104	ARG	Sidechain
2	B	114	LEU	Mainchain
2	B	117	HIS	Sidechain
2	B	118	PHE	Sidechain
2	B	121	GLU	Sidechain
2	B	123	THR	Mainchain
2	B	126	VAL	Mainchain
2	B	131	GLN	Mainchain
2	B	139	ASN	Mainchain
2	B	14	LEU	Mainchain
2	B	141	LEU	Mainchain
2	B	143	HIS	Sidechain
2	B	146	HIS	Sidechain
2	B	19	ASN	Sidechain
2	B	2	HIS	Sidechain
2	B	21	ASP	Mainchain,Sidechain
2	B	22	GLU	Sidechain
2	B	26	GLU	Sidechain
2	B	3	LEU	Mainchain

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Mol	Chain	Res	Type	Group
2	B	38	THR	Mainchain
2	B	4	THR	Mainchain
2	B	43	GLU	Mainchain
2	B	44	SER	Mainchain
2	B	47	ASP	Mainchain,Sidechain
2	B	49	SER	Mainchain,Peptide
2	B	52	ASP	Sidechain
2	B	56	GLY	Mainchain
2	B	59	LYS	Mainchain
2	B	6	GLU	Sidechain
2	B	60	VAL	Mainchain
2	B	61	LYS	Mainchain
2	B	62	ALA	Mainchain
2	B	63	HIS	Mainchain,Sidechain
2	B	7	GLU	Mainchain
2	B	78	LEU	Mainchain
2	B	79	ASP	Mainchain,Sidechain
2	B	80	ASN	Mainchain,Sidechain
2	B	84	THR	Mainchain
2	B	90	GLU	Mainchain,Sidechain
1	C	109	LEU	Mainchain
1	C	110	ALA	Mainchain
1	C	111	ALA	Mainchain
1	C	112	HIS	Mainchain
1	C	113	LEU	Mainchain
1	C	114	PRO	Mainchain
1	C	116	GLU	Mainchain,Sidechain
1	C	119	PRO	Mainchain
1	C	125	LEU	Mainchain
1	C	126	ASP	Sidechain
1	C	135	VAL	Mainchain
1	C	138	SER	Mainchain
1	C	14	TRP	Mainchain
1	C	141	ARG	Sidechain
1	C	17	VAL	Mainchain
1	C	18	GLY	Mainchain
1	C	20	HIS	Sidechain
1	C	21	ALA	Mainchain
1	C	23	GLU	Sidechain
1	C	25	GLY	Mainchain
1	C	3	SER	Mainchain
1	C	44	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	C	45	HIS	Mainchain,Sidechain
1	C	46	PHE	Mainchain,Sidechain
1	C	47	ASP	Mainchain,Sidechain
1	C	48	LEU	Mainchain
1	C	5	ALA	Mainchain
1	C	64	ASP	Sidechain
1	C	69	ALA	Mainchain
1	C	71	ALA	Mainchain
1	C	72	HIS	Mainchain
1	C	74	ASP	Mainchain
1	C	75	ASP	Mainchain,Sidechain
1	C	78	ASN	Sidechain
1	C	80	LEU	Mainchain
1	C	83	LEU	Mainchain
1	C	88	ALA	Mainchain
1	C	9	ASN	Sidechain
1	C	92	ARG	Sidechain
1	C	95	PRO	Mainchain
2	D	1	VAL	Mainchain
2	D	101	GLU	Sidechain
2	D	104	ARG	Sidechain
2	D	108	ASN	Sidechain
2	D	117	HIS	Mainchain,Sidechain
2	D	118	PHE	Sidechain
2	D	120	LYS	Mainchain
2	D	121	GLU	Sidechain
2	D	127	GLN	Sidechain
2	D	137	VAL	Mainchain
2	D	139	ASN	Sidechain
2	D	143	HIS	Sidechain
2	D	144	LYS	Mainchain
2	D	146	HIS	Sidechain
2	D	17	LYS	Mainchain
2	D	18	VAL	Peptide
2	D	19	ASN	Sidechain
2	D	2	HIS	Mainchain,Sidechain
2	D	21	ASP	Mainchain,Sidechain
2	D	22	GLU	Mainchain,Sidechain
2	D	26	GLU	Sidechain
2	D	3	LEU	Mainchain,Peptide
2	D	33	VAL	Mainchain
2	D	34	VAL	Mainchain

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Mol	Chain	Res	Type	Group
2	D	40	ARG	Sidechain
2	D	42	PHE	Mainchain
2	D	43	GLU	Sidechain
2	D	46	GLY	Mainchain
2	D	48	LEU	Mainchain,Peptide
2	D	49	SER	Mainchain,Peptide
2	D	5	PRO	Mainchain
2	D	52	ASP	Mainchain,Sidechain
2	D	56	GLY	Mainchain
2	D	6	GLU	Sidechain
2	D	60	VAL	Mainchain
2	D	63	HIS	Sidechain
2	D	64	GLY	Mainchain
2	D	66	LYS	Mainchain
2	D	7	GLU	Sidechain
2	D	73	ASP	Mainchain
2	D	75	LEU	Mainchain
2	D	76	ALA	Mainchain
2	D	77	HIS	Sidechain
2	D	79	ASP	Mainchain,Sidechain
2	D	8	LYS	Mainchain
2	D	80	ASN	Mainchain
2	D	83	GLY	Mainchain
2	D	84	THR	Mainchain
2	D	90	GLU	Sidechain
2	D	92	HIS	Mainchain,Sidechain
2	D	94	ASP	Sidechain
2	D	96	LEU	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1061	239	0
1	C	1069	0	1063	255	1
2	B	1123	0	1104	323	0
2	D	1123	0	1108	422	0
3	A	43	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	30	10	0
3	C	43	0	30	14	0
3	D	43	0	30	11	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	56	0	0	1	0
5	B	57	0	0	1	2
5	C	59	0	0	0	1
5	D	49	0	0	1	0
All	All	4779	0	4456	1271	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 141.

All (1271) 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:3:LEU:CA	2:B:3:LEU:CB	1.77	1.63
2:B:104:ARG:CD	2:B:104:ARG:CG	1.76	1.62
2:D:77:HIS:CB	2:D:77:HIS:CA	1.75	1.62
1:A:5:ALA:CB	1:A:5:ALA:CA	1.77	1.62
1:C:48:LEU:CD2	1:C:48:LEU:CG	1.74	1.62
2:B:7:GLU:CG	2:B:7:GLU:CB	1.77	1.61
1:A:40:LYS:CA	1:A:40:LYS:CB	1.75	1.60
2:D:8:LYS:CG	2:D:8:LYS:CB	1.79	1.60
2:D:18:VAL:CB	2:D:18:VAL:CG2	1.80	1.60
1:C:113:LEU:CD1	1:C:113:LEU:CG	1.75	1.60
2:B:8:LYS:CB	2:B:8:LYS:CA	1.74	1.60
2:D:113:VAL:CG2	2:D:113:VAL:CB	1.74	1.59
1:A:72:HIS:CA	1:A:72:HIS:CB	1.78	1.59
1:C:118:THR:CA	1:C:118:THR:CB	1.75	1.59
2:D:48:LEU:CG	2:D:48:LEU:CD1	1.75	1.59
2:D:123:THR:CG2	2:D:123:THR:CB	1.80	1.59
2:D:2:HIS:CD2	2:D:2:HIS:CG	1.85	1.59
2:D:141:LEU:CG	2:D:141:LEU:CD2	1.78	1.59
1:A:84:SER:CB	1:A:84:SER:CA	1.82	1.58
2:D:126:VAL:CB	2:D:126:VAL:CA	1.81	1.58
2:B:50:THR:CG2	2:B:50:THR:CB	1.75	1.58
1:A:141:ARG:CB	1:A:141:ARG:CG	1.79	1.57
2:B:65:LYS:CB	2:B:65:LYS:CA	1.80	1.57
2:D:78:LEU:CA	2:D:78:LEU:CB	1.79	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TRP:CA	1:A:14:TRP:CB	1.83	1.57
2:D:4:THR:CB	2:D:4:THR:CA	1.82	1.57
2:D:121:GLU:CB	2:D:121:GLU:CA	1.79	1.57
2:B:77:HIS:CG	2:B:77:HIS:CD2	1.84	1.56
1:C:99:LYS:CD	1:C:99:LYS:CG	1.82	1.56
2:D:8:LYS:N	2:D:8:LYS:CA	1.68	1.56
2:D:67:VAL:CA	2:D:67:VAL:CB	1.76	1.56
2:B:143:HIS:ND1	2:B:143:HIS:CG	1.70	1.56
1:C:70:VAL:C	1:C:70:VAL:CA	1.74	1.56
1:C:73:VAL:CB	1:C:73:VAL:CA	1.80	1.56
1:A:1:VAL:CB	1:A:1:VAL:CA	1.84	1.56
1:A:56:LYS:CE	1:A:56:LYS:CD	1.84	1.56
2:B:47:ASP:CA	2:B:47:ASP:N	1.67	1.56
1:C:105:LEU:CD1	1:C:105:LEU:CG	1.79	1.56
1:A:31:ARG:NE	1:A:31:ARG:CD	1.68	1.55
2:D:18:VAL:N	2:D:18:VAL:CA	1.70	1.55
1:A:29:LEU:CB	1:A:29:LEU:CA	1.79	1.55
2:D:94:ASP:N	2:D:94:ASP:CA	1.68	1.55
2:B:8:LYS:CD	2:B:8:LYS:CG	1.78	1.55
1:C:40:LYS:CE	1:C:40:LYS:NZ	1.69	1.54
2:B:9:SER:CB	2:B:9:SER:CA	1.79	1.54
1:C:61:LYS:CE	1:C:61:LYS:CD	1.81	1.54
1:C:84:SER:CB	1:C:84:SER:CA	1.79	1.54
2:B:49:SER:N	2:B:49:SER:CA	1.67	1.54
2:B:80:ASN:CG	2:B:80:ASN:CB	1.75	1.54
2:B:90:GLU:CB	2:B:90:GLU:CA	1.84	1.54
2:D:53:ALA:C	2:D:53:ALA:CA	1.76	1.54
2:B:1:VAL:N	2:B:1:VAL:CA	1.69	1.54
1:C:16:LYS:CE	1:C:16:LYS:NZ	1.71	1.54
2:D:7:GLU:C	2:D:7:GLU:CA	1.75	1.54
2:B:49:SER:CA	2:B:49:SER:CB	1.83	1.53
2:B:81:LEU:N	2:B:81:LEU:CA	1.68	1.53
3:B:148:HEM:CBD	3:B:148:HEM:CGD	1.85	1.53
1:A:62:VAL:C	1:A:62:VAL:CA	1.75	1.53
1:C:38:THR:CB	1:C:38:THR:CA	1.81	1.53
1:C:75:ASP:N	1:C:75:ASP:CA	1.71	1.53
1:C:78:ASN:CB	1:C:78:ASN:CG	1.76	1.53
2:D:12:THR:N	2:D:12:THR:CA	1.68	1.53
1:A:58:HIS:C	1:A:58:HIS:CA	1.76	1.53
1:C:54:GLN:CA	1:C:54:GLN:C	1.75	1.53
1:A:87:HIS:C	1:A:87:HIS:CA	1.75	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ASP:CA	2:B:47:ASP:C	1.75	1.52
1:A:90:LYS:CE	1:A:90:LYS:CD	1.84	1.52
2:B:145:TYR:C	2:B:145:TYR:CA	1.75	1.52
2:B:1:VAL:CA	2:B:1:VAL:CB	1.86	1.52
1:C:137:THR:C	1:C:137:THR:CA	1.74	1.52
2:D:22:GLU:CG	2:D:22:GLU:CA	1.85	1.52
2:D:92:HIS:C	2:D:92:HIS:CA	1.76	1.52
2:B:10:ALA:C	2:B:10:ALA:CA	1.78	1.52
2:B:52:ASP:CG	2:B:52:ASP:CB	1.77	1.52
2:B:117:HIS:CE1	2:B:117:HIS:ND1	1.75	1.52
2:D:52:ASP:CG	2:D:52:ASP:CB	1.75	1.51
2:D:10:ALA:C	2:D:10:ALA:CA	1.75	1.51
2:B:6:GLU:C	2:B:6:GLU:CA	1.77	1.51
2:D:45:PHE:C	2:D:46:GLY:CA	1.78	1.51
2:D:59:LYS:C	2:D:59:LYS:CA	1.76	1.51
2:D:131:GLN:CD	2:D:131:GLN:CG	1.77	1.51
1:C:16:LYS:CD	1:C:16:LYS:CG	1.81	1.51
1:C:8:THR:CB	1:C:8:THR:CA	1.84	1.50
1:C:70:VAL:CA	1:C:70:VAL:N	1.68	1.50
2:B:61:LYS:NZ	2:B:61:LYS:CE	1.75	1.50
1:C:131:SER:C	1:C:131:SER:CA	1.76	1.50
2:D:8:LYS:CB	2:D:8:LYS:CA	1.85	1.50
1:C:61:LYS:C	1:C:61:LYS:CA	1.76	1.50
1:C:72:HIS:CB	1:C:72:HIS:CA	1.85	1.50
2:D:47:ASP:CG	2:D:47:ASP:CB	1.76	1.50
2:D:73:ASP:CA	2:D:73:ASP:CB	1.86	1.50
1:C:56:LYS:NZ	1:C:56:LYS:CE	1.72	1.50
2:D:48:LEU:CA	2:D:48:LEU:N	1.72	1.50
2:D:59:LYS:CE	2:D:59:LYS:CD	1.88	1.50
2:B:143:HIS:C	2:B:143:HIS:CA	1.76	1.49
2:D:21:ASP:CG	2:D:21:ASP:CB	1.78	1.49
2:D:50:THR:N	2:D:50:THR:CA	1.71	1.49
2:B:12:THR:CG2	2:B:12:THR:CA	1.89	1.49
1:C:10:VAL:C	1:C:10:VAL:CA	1.81	1.49
2:D:117:HIS:CG	2:D:117:HIS:ND1	1.74	1.49
2:B:124:PRO:CD	2:B:124:PRO:N	1.70	1.48
2:D:80:ASN:N	2:D:80:ASN:CA	1.75	1.48
2:B:5:PRO:C	2:B:5:PRO:CA	1.78	1.48
1:C:7:LYS:N	1:C:7:LYS:CA	1.75	1.48
2:D:1:VAL:N	2:D:1:VAL:CA	1.77	1.48
1:C:2:LEU:C	1:C:2:LEU:CA	1.79	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:LYS:CD	2:D:82:LYS:CG	1.89	1.48
1:A:2:LEU:C	1:A:2:LEU:CA	1.77	1.48
2:B:80:ASN:C	2:B:80:ASN:CA	1.80	1.48
1:C:16:LYS:C	1:C:16:LYS:CA	1.82	1.48
1:C:87:HIS:C	1:C:87:HIS:CA	1.82	1.48
2:D:52:ASP:N	2:D:52:ASP:CA	1.76	1.48
2:B:80:ASN:CA	2:B:80:ASN:N	1.73	1.47
1:A:61:LYS:CE	1:A:61:LYS:NZ	1.74	1.47
1:C:90:LYS:CE	1:C:90:LYS:CD	1.91	1.47
2:D:7:GLU:CG	2:D:7:GLU:CB	1.88	1.47
2:D:108:ASN:CG	2:D:108:ASN:CB	1.83	1.47
2:B:41:PHE:C	2:B:41:PHE:CA	1.77	1.47
3:B:148:HEM:CBA	3:B:148:HEM:CGA	1.91	1.47
2:B:82:LYS:CG	2:B:82:LYS:CE	1.93	1.47
1:A:52:SER:N	1:A:52:SER:CA	1.75	1.47
2:B:21:ASP:CG	2:B:21:ASP:CB	1.84	1.46
1:A:16:LYS:CD	1:A:16:LYS:CE	1.92	1.46
1:A:60:LYS:CE	1:A:60:LYS:CD	1.93	1.46
1:A:74:ASP:CG	1:A:74:ASP:CB	1.80	1.46
2:B:142:ALA:C	2:B:142:ALA:CA	1.82	1.46
1:A:137:THR:CB	1:A:137:THR:CA	1.91	1.46
2:D:47:ASP:CB	2:D:47:ASP:CA	1.94	1.45
1:C:90:LYS:CD	1:C:90:LYS:CG	1.90	1.45
1:A:76:MET:CG	1:A:76:MET:SD	2.02	1.45
2:B:74:GLY:C	2:B:75:LEU:N	1.70	1.45
1:C:16:LYS:CG	1:C:16:LYS:CB	1.93	1.45
2:D:46:GLY:CA	2:D:46:GLY:C	1.82	1.45
1:A:44:PRO:C	1:A:44:PRO:CA	1.83	1.45
2:B:22:GLU:CD	2:B:22:GLU:CG	1.85	1.45
2:D:43:GLU:CG	2:D:43:GLU:CA	1.95	1.45
2:B:2:HIS:CG	2:B:2:HIS:CD2	2.05	1.44
2:B:87:THR:CB	2:B:87:THR:CA	1.95	1.44
3:C:142:HEM:CGD	3:C:142:HEM:CBD	1.93	1.44
2:B:108:ASN:CB	2:B:108:ASN:CG	1.84	1.44
1:C:1:VAL:C	1:C:1:VAL:CA	1.83	1.44
1:C:20:HIS:CE1	1:C:20:HIS:ND1	1.79	1.44
2:B:61:LYS:CD	2:B:61:LYS:CG	1.93	1.44
2:D:22:GLU:CA	2:D:22:GLU:C	1.83	1.44
1:A:99:LYS:CE	1:A:99:LYS:CD	1.95	1.44
2:B:2:HIS:C	2:B:2:HIS:CA	1.84	1.44
2:D:79:ASP:C	2:D:79:ASP:CA	1.83	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:MET:CG	1:C:76:MET:SD	2.05	1.43
2:D:12:THR:CA	2:D:12:THR:CB	1.93	1.43
2:B:139:ASN:CG	2:B:139:ASN:CA	1.87	1.43
1:C:82:ALA:C	1:C:83:LEU:N	1.69	1.43
2:D:49:SER:C	2:D:49:SER:CA	1.86	1.43
2:B:9:SER:CA	2:B:9:SER:C	1.87	1.43
1:C:7:LYS:CD	1:C:7:LYS:CG	1.95	1.43
1:A:11:LYS:CE	1:A:11:LYS:CD	1.96	1.42
2:D:143:HIS:CD2	2:D:143:HIS:CG	1.85	1.42
1:A:20:HIS:ND1	1:A:20:HIS:CG	1.71	1.42
2:B:65:LYS:CA	2:B:65:LYS:CG	1.98	1.42
1:A:137:THR:CB	1:A:137:THR:OG1	1.66	1.42
2:D:19:ASN:ND2	2:D:19:ASN:CG	1.71	1.42
1:A:18:GLY:C	1:A:18:GLY:CA	1.86	1.42
2:D:146:HIS:CG	2:D:146:HIS:ND1	1.85	1.41
1:C:139:LYS:CE	1:C:139:LYS:CD	1.95	1.41
1:C:139:LYS:CE	1:C:139:LYS:NZ	1.84	1.41
1:C:72:HIS:CG	1:C:72:HIS:ND1	1.80	1.41
1:A:75:ASP:CG	1:A:75:ASP:CA	1.88	1.40
1:A:75:ASP:CA	1:A:75:ASP:CB	1.97	1.40
1:A:138:SER:CA	1:A:138:SER:OG	1.68	1.40
2:D:5:PRO:N	2:D:5:PRO:CA	1.84	1.40
2:D:26:GLU:CD	2:D:26:GLU:CG	1.90	1.40
1:A:127:LYS:CD	1:A:127:LYS:CG	1.97	1.40
2:B:66:LYS:CE	2:B:66:LYS:NZ	1.81	1.40
2:D:2:HIS:CE1	2:D:2:HIS:NE2	1.90	1.40
2:B:2:HIS:CG	2:B:2:HIS:ND1	1.89	1.39
2:D:77:HIS:CD2	2:D:77:HIS:NE2	1.88	1.39
1:A:16:LYS:CD	1:A:16:LYS:CG	2.01	1.39
2:D:2:HIS:CE1	2:D:2:HIS:ND1	1.90	1.39
2:D:55:MET:C	2:D:55:MET:CA	1.90	1.39
2:D:58:PRO:CD	2:D:58:PRO:N	1.71	1.39
2:B:125:PRO:N	2:B:125:PRO:CD	1.67	1.39
2:B:144:LYS:CE	2:B:144:LYS:CD	2.01	1.38
1:A:127:LYS:CG	1:A:127:LYS:CA	2.02	1.38
2:B:146:HIS:CB	2:B:146:HIS:CG	2.04	1.38
2:D:43:GLU:CG	2:D:43:GLU:CD	1.92	1.38
2:D:77:HIS:CE1	2:D:77:HIS:ND1	1.91	1.38
1:A:81:SER:CB	1:A:81:SER:CA	2.00	1.37
2:B:2:HIS:CA	2:B:2:HIS:CB	2.01	1.38
1:A:92:ARG:CD	1:A:92:ARG:CZ	2.01	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:PRO:C	1:C:114:PRO:CA	1.91	1.37
1:C:92:ARG:NH1	1:C:92:ARG:CZ	1.87	1.37
2:B:87:THR:CB	2:B:87:THR:CG2	2.02	1.37
1:C:138:SER:CA	1:C:138:SER:OG	1.72	1.37
2:B:49:SER:CB	2:B:49:SER:OG	1.71	1.36
2:B:104:ARG:CZ	2:B:104:ARG:NH1	1.87	1.36
2:D:8:LYS:CD	2:D:8:LYS:CE	2.03	1.36
2:D:104:ARG:CD	2:D:104:ARG:NE	1.84	1.36
2:D:146:HIS:ND1	2:D:146:HIS:CD2	1.91	1.36
1:A:50:HIS:CB	1:A:50:HIS:CA	2.02	1.35
3:D:148:HEM:CGD	3:D:148:HEM:CBD	2.01	1.35
2:D:43:GLU:CA	2:D:43:GLU:C	1.94	1.35
2:B:1:VAL:CB	2:B:1:VAL:CG1	2.03	1.35
2:D:80:ASN:CG	2:D:80:ASN:OD1	1.66	1.34
1:A:17:VAL:C	1:A:17:VAL:CA	1.96	1.34
2:B:132:LYS:NZ	2:B:132:LYS:CE	1.88	1.34
1:C:30:GLU:CD	1:C:30:GLU:CG	1.96	1.34
1:A:16:LYS:CE	1:A:16:LYS:CG	2.06	1.34
1:A:56:LYS:CD	1:A:56:LYS:CG	2.06	1.34
2:D:20:VAL:CA	2:D:20:VAL:CG2	2.05	1.34
2:D:90:GLU:OE1	2:D:90:GLU:CD	1.64	1.33
1:A:64:ASP:CG	1:A:64:ASP:CB	1.95	1.33
2:B:117:HIS:ND1	2:B:117:HIS:CG	1.94	1.33
2:D:6:GLU:CD	2:D:6:GLU:CG	1.97	1.33
2:D:66:LYS:CD	2:D:66:LYS:CG	2.06	1.33
2:B:6:GLU:OE1	2:B:6:GLU:CD	1.67	1.33
2:B:59:LYS:CE	2:B:59:LYS:NZ	1.92	1.33
1:A:78:ASN:CB	1:A:78:ASN:ND2	1.87	1.33
1:A:72:HIS:CA	1:A:72:HIS:CG	2.12	1.32
1:A:61:LYS:CE	1:A:61:LYS:CG	2.06	1.32
1:C:114:PRO:CA	1:C:114:PRO:N	1.72	1.31
2:D:139:ASN:CG	2:D:139:ASN:OD1	1.68	1.31
1:C:11:LYS:CE	1:C:11:LYS:NZ	1.91	1.31
1:C:40:LYS:CE	1:C:40:LYS:CG	2.07	1.30
2:D:8:LYS:CE	2:D:8:LYS:NZ	1.94	1.30
2:D:82:LYS:NZ	2:D:82:LYS:CE	1.94	1.30
2:B:143:HIS:ND1	2:B:143:HIS:CE1	1.99	1.30
2:D:20:VAL:CA	2:D:20:VAL:CB	2.10	1.30
3:D:148:HEM:CGA	3:D:148:HEM:O2A	1.77	1.30
1:A:15:GLY:O	1:A:15:GLY:C	1.67	1.29
1:A:139:LYS:CE	1:A:139:LYS:NZ	1.96	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:VAL:O	2:B:1:VAL:C	1.70	1.29
1:C:112:HIS:CG	1:C:112:HIS:ND1	1.78	1.29
3:A:142:HEM:CGD	3:A:142:HEM:CBD	2.09	1.29
2:D:76:ALA:N	2:D:76:ALA:CA	1.94	1.29
2:B:79:ASP:CG	2:B:79:ASP:OD2	1.67	1.29
2:D:50:THR:CA	2:D:50:THR:CB	2.11	1.29
2:D:66:LYS:NZ	2:D:66:LYS:CE	1.95	1.29
2:D:43:GLU:C	2:D:43:GLU:HB2	1.53	1.29
2:D:1:VAL:CA	2:D:1:VAL:C	2.02	1.28
2:D:26:GLU:CD	2:D:26:GLU:OE2	1.71	1.28
2:D:121:GLU:CD	2:D:121:GLU:CG	2.01	1.28
1:A:30:GLU:CD	1:A:30:GLU:CG	2.00	1.28
2:B:146:HIS:CE1	2:B:146:HIS:ND1	1.84	1.28
1:C:40:LYS:NZ	1:C:40:LYS:CD	1.95	1.28
2:B:101:GLU:CG	2:B:101:GLU:CD	2.02	1.28
1:A:23:GLU:OE1	1:A:23:GLU:CD	1.72	1.27
2:B:12:THR:CG2	2:B:12:THR:OG1	1.78	1.27
2:B:104:ARG:CZ	2:B:104:ARG:NH2	1.97	1.27
1:C:61:LYS:CE	1:C:61:LYS:NZ	1.98	1.27
1:C:105:LEU:CG	1:C:105:LEU:CD2	2.12	1.27
2:D:4:THR:HB	2:D:6:GLU:OE2	1.30	1.27
1:A:138:SER:CA	1:A:138:SER:CB	2.12	1.26
1:C:138:SER:CA	1:C:138:SER:CB	2.14	1.26
1:A:1:VAL:CA	1:A:1:VAL:CG2	2.13	1.26
2:D:95:LYS:NZ	2:D:95:LYS:CE	1.99	1.25
1:C:1:VAL:CG1	1:C:1:VAL:CG2	2.13	1.25
2:B:8:LYS:CA	2:B:8:LYS:CG	2.13	1.25
2:B:144:LYS:CE	2:B:144:LYS:NZ	1.99	1.25
1:C:1:VAL:CG2	1:C:1:VAL:HG13	1.64	1.25
2:D:17:LYS:CE	2:D:17:LYS:NZ	1.98	1.25
1:A:85:ASP:CG	1:A:85:ASP:OD2	1.73	1.24
1:A:72:HIS:CG	1:A:72:HIS:ND1	1.85	1.24
2:B:90:GLU:CD	2:B:90:GLU:CG	2.07	1.24
2:D:125:PRO:CD	2:D:125:PRO:N	1.67	1.24
2:D:95:LYS:CD	2:D:95:LYS:CG	2.17	1.23
2:B:6:GLU:CD	2:B:6:GLU:CG	2.07	1.23
2:B:22:GLU:CD	2:B:22:GLU:OE1	1.77	1.23
2:D:101:GLU:CD	2:D:101:GLU:CG	2.06	1.22
2:B:5:PRO:N	2:B:5:PRO:CD	1.81	1.22
2:B:121:GLU:CD	2:B:121:GLU:CG	2.07	1.22
2:D:26:GLU:CG	2:D:26:GLU:CB	2.18	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:C	1:A:21:ALA:CA	2.09	1.21
2:B:1:VAL:CA	2:B:1:VAL:C	2.09	1.21
1:C:60:LYS:NZ	1:C:60:LYS:CE	2.02	1.21
2:B:49:SER:C	2:B:49:SER:O	1.79	1.21
2:D:3:LEU:O	2:D:3:LEU:C	1.77	1.21
1:A:92:ARG:CD	1:A:92:ARG:NH1	2.03	1.20
2:B:2:HIS:CD2	2:B:2:HIS:NE2	2.09	1.20
1:A:14:TRP:CA	1:A:14:TRP:CG	2.22	1.20
1:C:99:LYS:CG	1:C:99:LYS:CA	2.17	1.20
1:C:1:VAL:CA	1:C:1:VAL:CG1	2.18	1.20
1:A:23:GLU:CD	1:A:23:GLU:CG	2.10	1.19
2:B:47:ASP:CG	2:B:47:ASP:OD2	1.78	1.19
1:A:78:ASN:CG	1:A:78:ASN:CA	2.11	1.19
2:D:65:LYS:CE	2:D:65:LYS:CD	2.20	1.19
2:D:2:HIS:CB	2:D:2:HIS:CA	2.21	1.19
2:D:26:GLU:CD	2:D:26:GLU:OE1	1.79	1.19
1:C:1:VAL:CG1	1:C:1:VAL:CB	2.22	1.18
2:D:58:PRO:CD	2:D:58:PRO:CB	2.20	1.18
2:B:58:PRO:CD	2:B:58:PRO:N	1.78	1.18
1:C:90:LYS:CE	1:C:90:LYS:NZ	2.06	1.18
1:A:75:ASP:CG	1:A:75:ASP:OD1	1.82	1.17
1:C:16:LYS:CE	1:C:16:LYS:CD	2.23	1.17
2:D:43:GLU:CD	2:D:43:GLU:CB	2.13	1.17
1:A:127:LYS:CD	1:A:127:LYS:CB	2.23	1.17
1:A:92:ARG:NH1	1:A:92:ARG:HD3	1.60	1.16
1:C:92:ARG:HH21	1:C:92:ARG:NE	1.42	1.16
2:D:73:ASP:CA	2:D:73:ASP:CG	2.14	1.16
2:B:26:GLU:HG2	2:B:26:GLU:OE2	1.45	1.16
1:C:113:LEU:CD1	1:C:113:LEU:CB	2.22	1.15
2:B:104:ARG:CD	2:B:104:ARG:CZ	2.24	1.15
1:C:23:GLU:CG	1:C:23:GLU:CD	2.15	1.15
2:D:47:ASP:CA	2:D:47:ASP:N	2.09	1.15
1:A:1:VAL:CG2	1:A:1:VAL:N	2.09	1.14
1:C:99:LYS:CD	1:C:99:LYS:CE	2.26	1.14
2:D:77:HIS:NE2	2:D:77:HIS:CG	2.15	1.14
2:B:139:ASN:CG	2:B:139:ASN:ND2	2.01	1.14
2:B:26:GLU:OE2	2:B:26:GLU:CG	1.95	1.13
2:B:121:GLU:CD	2:B:121:GLU:OE1	1.87	1.13
1:C:46:PHE:CE2	1:C:46:PHE:CG	2.02	1.13
1:C:56:LYS:CD	1:C:56:LYS:CG	2.27	1.13
1:C:73:VAL:CA	1:C:73:VAL:CG1	2.26	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:VAL:N	1:A:1:VAL:HG23	1.61	1.13
2:B:108:ASN:CB	2:B:108:ASN:ND2	2.10	1.13
2:D:49:SER:C	2:D:50:THR:CA	2.17	1.13
2:D:6:GLU:CG	2:D:6:GLU:CA	2.28	1.12
2:D:66:LYS:CD	2:D:66:LYS:CE	2.27	1.12
2:B:2:HIS:ND1	2:B:2:HIS:CE1	2.18	1.12
2:B:104:ARG:CZ	2:B:104:ARG:NE	2.13	1.12
1:C:1:VAL:CG1	1:C:1:VAL:HG22	1.77	1.12
2:D:65:LYS:CD	2:D:65:LYS:CG	2.27	1.12
2:D:82:LYS:CD	2:D:82:LYS:NZ	2.12	1.12
2:B:49:SER:CB	2:B:49:SER:C	2.15	1.12
3:C:142:HEM:CGA	3:C:142:HEM:O2A	0.82	1.11
2:D:8:LYS:CG	2:D:8:LYS:CA	2.29	1.10
2:D:46:GLY:C	2:D:47:ASP:CA	2.20	1.10
1:A:16:LYS:CG	1:A:16:LYS:HE2	1.82	1.10
3:C:142:HEM:CGA	3:C:142:HEM:CBA	2.29	1.10
2:D:43:GLU:CD	2:D:43:GLU:HB3	1.71	1.09
1:A:90:LYS:CE	1:A:90:LYS:CG	2.30	1.09
2:B:117:HIS:NE2	2:B:117:HIS:CD2	2.21	1.09
2:D:5:PRO:CA	2:D:5:PRO:CB	2.31	1.09
2:D:4:THR:CB	2:D:6:GLU:OE2	2.00	1.08
2:D:78:LEU:CD2	2:D:78:LEU:CD1	2.30	1.08
3:A:142:HEM:CGA	3:A:142:HEM:CBA	2.32	1.07
2:D:144:LYS:CE	2:D:144:LYS:NZ	2.16	1.07
1:C:16:LYS:CD	1:C:16:LYS:CB	2.33	1.07
2:D:22:GLU:CA	2:D:22:GLU:HG3	1.61	1.07
2:D:43:GLU:C	2:D:43:GLU:CB	2.23	1.07
2:D:8:LYS:CB	2:D:8:LYS:CD	2.33	1.06
2:D:10:ALA:C	2:D:10:ALA:CB	2.23	1.06
2:D:78:LEU:CB	2:D:78:LEU:CD2	2.33	1.06
1:A:75:ASP:CB	1:A:75:ASP:OD2	2.02	1.06
1:A:78:ASN:CG	1:A:78:ASN:HB3	1.50	1.06
2:D:76:ALA:N	2:D:76:ALA:CB	2.17	1.06
1:C:84:SER:CA	1:C:84:SER:OG	2.04	1.05
1:A:99:LYS:CE	1:A:99:LYS:NZ	2.20	1.05
2:D:26:GLU:CG	2:D:26:GLU:OE1	2.05	1.05
1:A:78:ASN:CG	1:A:78:ASN:HB2	1.51	1.04
2:B:65:LYS:CD	2:B:65:LYS:CE	2.35	1.04
1:C:116:GLU:CG	1:C:116:GLU:CB	2.33	1.04
2:D:6:GLU:CG	2:D:6:GLU:HB3	1.55	1.04
2:D:141:LEU:CD2	2:D:141:LEU:CD1	2.34	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:CD	1:A:92:ARG:HH11	1.66	1.04
2:B:59:LYS:CE	2:B:59:LYS:CD	2.36	1.04
1:A:75:ASP:CG	1:A:75:ASP:HB2	1.42	1.03
2:B:8:LYS:CG	2:B:8:LYS:HB2	1.52	1.03
2:B:48:LEU:C	2:B:49:SER:CA	2.27	1.03
1:A:16:LYS:HE2	1:A:16:LYS:HG3	1.38	1.03
1:C:38:THR:H	1:C:38:THR:HG22	1.22	1.03
2:D:4:THR:C	2:D:5:PRO:CA	2.27	1.03
2:D:6:GLU:CB	2:D:6:GLU:HG3	1.51	1.03
2:D:58:PRO:CD	2:D:58:PRO:CA	2.37	1.03
2:B:66:LYS:CE	2:B:66:LYS:CD	2.37	1.02
1:C:92:ARG:HH21	1:C:92:ARG:CD	1.72	1.02
1:A:75:ASP:OD2	1:A:75:ASP:HB3	1.54	1.02
1:C:99:LYS:CD	1:C:99:LYS:CB	2.36	1.02
2:D:6:GLU:CB	2:D:6:GLU:HG2	1.51	1.02
1:A:75:ASP:CG	1:A:75:ASP:HB3	1.42	1.02
2:B:81:LEU:N	2:B:81:LEU:CB	2.23	1.02
1:C:1:VAL:CB	1:C:1:VAL:N	2.22	1.02
1:C:40:LYS:CD	1:C:40:LYS:HE2	1.53	1.02
2:B:139:ASN:ND2	2:B:139:ASN:OD1	1.91	1.02
1:C:40:LYS:CE	1:C:40:LYS:HD2	1.50	1.02
1:C:40:LYS:CD	1:C:40:LYS:HE3	1.53	1.01
2:D:6:GLU:CG	2:D:6:GLU:HB2	1.55	1.01
2:D:79:ASP:CG	2:D:79:ASP:OD1	1.99	1.01
1:C:90:LYS:CD	1:C:90:LYS:CB	2.39	1.01
2:D:79:ASP:CG	2:D:79:ASP:OD2	1.98	1.01
2:B:1:VAL:CA	2:B:2:HIS:N	2.23	1.01
3:D:148:HEM:CGA	3:D:148:HEM:CBA	2.39	1.01
2:D:1:VAL:CA	2:D:2:HIS:N	2.23	1.01
1:C:56:LYS:CE	1:C:56:LYS:CD	2.39	1.00
2:B:46:GLY:C	2:B:47:ASP:CA	2.29	1.00
1:C:40:LYS:CE	1:C:40:LYS:HD3	1.50	1.00
1:A:74:ASP:CG	1:A:74:ASP:OD1	0.80	1.00
2:D:18:VAL:CG2	2:D:18:VAL:CG1	2.40	1.00
1:A:92:ARG:CZ	1:A:92:ARG:NH2	0.85	1.00
1:C:30:GLU:CD	1:C:30:GLU:OE2	0.80	1.00
2:D:77:HIS:CB	2:D:77:HIS:C	2.29	0.99
2:D:47:ASP:C	2:D:48:LEU:CA	2.30	0.99
1:A:1:VAL:HG23	1:A:1:VAL:H3	1.12	0.99
2:B:101:GLU:CG	2:B:101:GLU:OE2	2.09	0.99
2:D:12:THR:CA	2:D:12:THR:CG2	2.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:LYS:CG	2:B:8:LYS:HB3	1.52	0.99
2:D:47:ASP:CB	2:D:47:ASP:N	2.25	0.99
1:A:92:ARG:NH1	1:A:92:ARG:HD2	1.75	0.99
2:D:78:LEU:CG	2:D:78:LEU:HD21	1.51	0.99
2:D:6:GLU:CA	2:D:6:GLU:C	2.31	0.99
2:B:132:LYS:NZ	2:B:132:LYS:CD	2.26	0.99
2:D:79:ASP:C	2:D:79:ASP:CB	2.31	0.99
2:D:146:HIS:ND1	2:D:146:HIS:NE2	2.10	0.98
2:D:53:ALA:C	2:D:53:ALA:CB	2.30	0.98
2:D:104:ARG:CD	2:D:104:ARG:HH11	1.76	0.98
2:D:82:LYS:CD	2:D:82:LYS:CE	2.42	0.98
1:A:78:ASN:CB	1:A:78:ASN:CG	0.88	0.98
2:D:43:GLU:CB	2:D:43:GLU:HG3	1.47	0.98
2:B:2:HIS:CA	2:B:3:LEU:N	2.28	0.97
2:B:82:LYS:CG	2:B:82:LYS:HE2	1.74	0.97
1:A:2:LEU:CA	1:A:3:SER:N	2.27	0.97
2:B:8:LYS:NZ	2:B:8:LYS:CE	2.27	0.97
2:D:52:ASP:CB	2:D:52:ASP:N	2.28	0.97
2:B:139:ASN:CG	2:B:139:ASN:HB3	1.37	0.97
2:D:43:GLU:CB	2:D:43:GLU:HG2	1.47	0.97
2:B:9:SER:CA	2:B:9:SER:OG	2.13	0.96
2:B:49:SER:N	2:B:49:SER:C	2.18	0.96
2:B:90:GLU:CA	2:B:90:GLU:CG	2.41	0.96
2:D:45:PHE:C	2:D:46:GLY:HA3	1.85	0.96
1:C:139:LYS:CD	1:C:139:LYS:NZ	2.27	0.96
3:B:148:HEM:CGA	3:B:148:HEM:O2A	0.66	0.96
1:C:38:THR:CA	1:C:38:THR:CG2	2.44	0.96
2:D:20:VAL:CA	2:D:20:VAL:HG22	1.91	0.96
2:D:45:PHE:CA	2:D:46:GLY:N	2.27	0.96
2:D:78:LEU:HG	2:D:78:LEU:HD22	0.96	0.96
1:C:61:LYS:CD	1:C:61:LYS:NZ	2.29	0.95
2:D:120:LYS:NZ	2:D:120:LYS:CE	2.29	0.95
1:A:85:ASP:CG	1:A:85:ASP:OD1	0.75	0.95
1:A:127:LYS:CG	1:A:127:LYS:CE	2.44	0.95
3:C:142:HEM:O2A	3:C:142:HEM:CBA	2.14	0.95
2:B:8:LYS:CB	2:B:8:LYS:HG3	1.44	0.95
2:D:20:VAL:CA	2:D:20:VAL:HG23	1.91	0.95
2:D:121:GLU:CA	2:D:121:GLU:CG	2.45	0.95
2:B:139:ASN:CG	2:B:139:ASN:HB2	1.37	0.94
1:A:17:VAL:C	1:A:17:VAL:O	0.75	0.94
2:B:8:LYS:CB	2:B:8:LYS:HG2	1.44	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:CG	1:A:75:ASP:OD2	2.04	0.94
2:D:77:HIS:CE1	2:D:77:HIS:CG	2.52	0.94
2:D:126:VAL:CA	2:D:126:VAL:CG2	2.46	0.94
2:D:141:LEU:CD2	2:D:141:LEU:CB	2.45	0.94
1:C:1:VAL:HG13	1:C:1:VAL:HG22	0.95	0.94
2:D:79:ASP:C	2:D:80:ASN:CA	2.35	0.94
1:A:61:LYS:CD	1:A:61:LYS:HE2	1.42	0.94
2:D:6:GLU:CG	2:D:6:GLU:CB	0.94	0.94
1:A:61:LYS:CE	1:A:61:LYS:HD3	1.44	0.93
1:A:92:ARG:CZ	1:A:92:ARG:HD2	1.94	0.93
1:C:7:LYS:CG	1:C:7:LYS:CE	2.45	0.93
2:D:20:VAL:CA	2:D:20:VAL:CG1	2.45	0.93
1:A:78:ASN:CG	1:A:78:ASN:OD1	2.07	0.93
1:C:1:VAL:N	1:C:1:VAL:HB	1.81	0.93
1:A:61:LYS:CE	1:A:61:LYS:HD2	1.44	0.93
1:A:137:THR:OG1	1:A:137:THR:CG2	2.14	0.93
2:B:87:THR:CG2	2:B:87:THR:OG1	2.16	0.93
1:A:92:ARG:HD3	1:A:92:ARG:HH11	1.21	0.93
1:A:61:LYS:CD	1:A:61:LYS:HE3	1.42	0.93
3:B:148:HEM:CBA	3:B:148:HEM:O2A	2.15	0.93
2:D:22:GLU:CG	2:D:22:GLU:HB3	1.43	0.93
2:D:7:GLU:C	2:D:8:LYS:CA	2.37	0.92
1:A:85:ASP:OD1	1:A:85:ASP:CB	2.15	0.92
2:B:2:HIS:CD2	2:B:2:HIS:CB	2.52	0.92
2:D:22:GLU:CG	2:D:22:GLU:HB2	1.43	0.92
2:D:52:ASP:CB	2:D:52:ASP:OD1	2.17	0.92
1:A:127:LYS:CB	1:A:127:LYS:HG2	1.40	0.92
2:B:82:LYS:CE	2:B:82:LYS:HD3	1.40	0.92
3:D:148:HEM:CBA	3:D:148:HEM:O1A	2.18	0.92
1:C:1:VAL:C	1:C:1:VAL:CB	2.38	0.92
1:C:46:PHE:CE2	1:C:46:PHE:CD2	0.92	0.92
2:D:92:HIS:C	2:D:92:HIS:CB	2.37	0.92
2:D:67:VAL:CA	2:D:67:VAL:CG1	2.47	0.92
2:D:73:ASP:CB	2:D:73:ASP:C	2.38	0.92
1:C:1:VAL:CA	1:C:1:VAL:N	2.33	0.91
1:A:90:LYS:CE	1:A:90:LYS:HG3	1.98	0.91
2:D:79:ASP:CA	2:D:80:ASN:N	2.33	0.91
2:D:45:PHE:C	2:D:46:GLY:N	0.87	0.91
2:B:82:LYS:CE	2:B:82:LYS:HD2	1.40	0.91
1:C:84:SER:CB	1:C:84:SER:C	2.39	0.91
2:B:82:LYS:CD	2:B:82:LYS:HE3	1.39	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:LYS:CD	2:D:65:LYS:CB	2.49	0.91
2:D:139:ASN:OD1	2:D:139:ASN:CB	2.19	0.91
2:B:2:HIS:C	2:B:2:HIS:CB	2.39	0.90
2:B:104:ARG:CZ	2:B:104:ARG:HD3	1.98	0.90
2:D:108:ASN:CB	2:D:108:ASN:ND2	2.33	0.90
2:B:8:LYS:CB	2:B:8:LYS:CD	2.49	0.90
2:D:22:GLU:CG	2:D:22:GLU:CD	2.39	0.90
1:A:56:LYS:CD	1:A:56:LYS:CB	2.49	0.90
1:A:137:THR:CA	1:A:137:THR:CG2	2.45	0.90
2:B:65:LYS:CA	2:B:65:LYS:HG3	2.01	0.90
1:C:1:VAL:CG2	1:C:1:VAL:CB	2.48	0.90
2:D:126:VAL:CA	2:D:126:VAL:CG1	2.48	0.90
2:B:65:LYS:CG	2:B:65:LYS:CD	2.49	0.90
1:C:72:HIS:CA	1:C:72:HIS:CG	2.54	0.90
2:D:3:LEU:O	2:D:4:THR:N	2.03	0.90
1:A:61:LYS:NZ	1:A:61:LYS:CD	2.34	0.90
1:A:62:VAL:CA	1:A:63:ALA:N	2.33	0.90
2:B:82:LYS:CE	2:B:82:LYS:NZ	2.35	0.90
2:D:22:GLU:CB	2:D:22:GLU:HG2	1.39	0.90
2:B:82:LYS:HE2	2:B:82:LYS:CD	1.39	0.90
1:C:30:GLU:CG	1:C:30:GLU:OE2	2.20	0.90
1:A:127:LYS:CB	1:A:127:LYS:HG3	1.40	0.89
2:D:26:GLU:CG	2:D:26:GLU:OE2	2.20	0.89
2:D:22:GLU:HG3	2:D:22:GLU:CB	1.39	0.89
2:D:67:VAL:CB	2:D:67:VAL:N	2.36	0.89
2:B:12:THR:C	2:B:12:THR:HG23	1.93	0.89
2:B:65:LYS:CA	2:B:65:LYS:HG2	2.01	0.89
2:B:80:ASN:CB	2:B:80:ASN:ND2	2.33	0.89
2:B:80:ASN:C	2:B:81:LEU:CA	2.40	0.89
1:C:46:PHE:CE2	1:C:46:PHE:HD2	1.60	0.89
1:A:127:LYS:CG	1:A:127:LYS:HB2	1.37	0.88
2:B:10:ALA:C	2:B:10:ALA:CB	2.41	0.88
2:B:47:ASP:C	2:B:47:ASP:CB	2.41	0.88
1:A:1:VAL:CA	1:A:1:VAL:CG1	2.50	0.88
2:D:66:LYS:NZ	3:D:148:HEM:O1A	2.06	0.88
1:A:127:LYS:CG	1:A:127:LYS:HB3	1.37	0.88
2:B:2:HIS:CG	2:B:2:HIS:CB	0.83	0.88
2:D:76:ALA:N	2:D:76:ALA:C	2.26	0.88
2:D:78:LEU:CD2	2:D:78:LEU:CG	0.88	0.88
1:C:1:VAL:CA	1:C:1:VAL:CG2	2.51	0.88
2:B:22:GLU:CD	2:B:22:GLU:OE2	2.12	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LYS:CG	1:C:99:LYS:HB3	1.36	0.88
1:C:99:LYS:CB	1:C:99:LYS:HG3	1.36	0.87
1:A:51:GLY:C	1:A:52:SER:CA	2.43	0.87
2:B:117:HIS:ND1	2:B:117:HIS:CB	2.37	0.87
2:D:47:ASP:CA	2:D:47:ASP:C	2.43	0.87
2:D:90:GLU:CD	2:D:90:GLU:CG	2.43	0.87
1:C:72:HIS:CB	1:C:72:HIS:C	2.41	0.87
1:A:72:HIS:CB	1:A:72:HIS:C	2.42	0.87
2:B:43:GLU:CD	2:B:43:GLU:CG	2.42	0.87
2:B:2:HIS:CG	2:B:2:HIS:HB2	1.42	0.87
1:C:16:LYS:CD	1:C:16:LYS:HB3	2.03	0.87
3:C:142:HEM:O2A	3:C:142:HEM:O1A	1.92	0.87
1:A:50:HIS:CB	1:A:50:HIS:N	2.37	0.87
2:D:80:ASN:N	2:D:80:ASN:HB3	1.89	0.87
2:B:8:LYS:CB	2:B:8:LYS:CG	0.87	0.87
2:B:8:LYS:CA	2:B:8:LYS:HG3	2.02	0.87
1:C:38:THR:H	1:C:38:THR:CG2	1.88	0.87
2:B:139:ASN:OD1	2:B:139:ASN:CB	2.20	0.86
2:D:146:HIS:ND1	2:D:146:HIS:CE1	0.67	0.86
1:C:99:LYS:CB	1:C:99:LYS:HG2	1.36	0.86
2:B:2:HIS:CG	2:B:2:HIS:HB3	1.42	0.86
2:D:78:LEU:CG	2:D:78:LEU:HD22	1.51	0.86
1:A:127:LYS:CD	1:A:127:LYS:HB2	2.06	0.86
1:C:38:THR:HG22	1:C:38:THR:N	1.91	0.86
1:A:141:ARG:CG	1:A:141:ARG:CA	2.53	0.86
2:B:47:ASP:N	2:B:47:ASP:CB	2.39	0.86
1:C:99:LYS:CG	1:C:99:LYS:HB2	1.36	0.86
2:D:94:ASP:N	2:D:94:ASP:CB	2.38	0.86
2:D:104:ARG:HH11	2:D:104:ARG:HD2	1.36	0.86
2:D:49:SER:C	2:D:49:SER:CB	2.44	0.86
1:A:31:ARG:CD	1:A:31:ARG:CZ	2.54	0.85
2:B:108:ASN:CB	2:B:108:ASN:HD22	1.88	0.85
1:A:17:VAL:CA	1:A:18:GLY:N	2.38	0.85
1:A:58:HIS:CA	1:A:59:GLY:N	2.39	0.85
1:C:8:THR:CA	1:C:8:THR:CG2	2.55	0.85
1:C:40:LYS:CE	1:C:40:LYS:CD	0.85	0.85
1:A:138:SER:CA	1:A:138:SER:HG	1.85	0.85
1:C:38:THR:CG2	1:C:38:THR:N	2.39	0.85
1:A:141:ARG:CB	1:A:141:ARG:CD	2.55	0.85
2:D:7:GLU:CB	2:D:7:GLU:CD	2.45	0.85
1:A:137:THR:CA	1:A:137:THR:OG1	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:VAL:CG2	2:D:20:VAL:C	2.45	0.84
2:B:12:THR:CG2	2:B:12:THR:C	2.45	0.84
2:D:93:CYS:C	2:D:94:ASP:CA	2.45	0.84
2:D:146:HIS:ND1	2:D:146:HIS:HE1	1.35	0.84
2:B:7:GLU:CG	2:B:7:GLU:CA	2.47	0.84
1:A:75:ASP:CB	1:A:75:ASP:C	2.45	0.84
2:B:5:PRO:C	2:B:5:PRO:N	2.31	0.84
2:B:49:SER:CA	2:B:49:SER:O	2.25	0.84
1:C:56:LYS:CE	1:C:56:LYS:CG	2.55	0.84
2:D:59:LYS:CA	2:D:60:VAL:N	2.40	0.84
2:D:77:HIS:CA	2:D:77:HIS:CG	2.61	0.84
1:C:118:THR:CB	1:C:118:THR:N	2.40	0.84
1:A:44:PRO:C	1:A:44:PRO:CB	2.46	0.83
2:D:19:ASN:ND2	2:D:19:ASN:OD1	2.10	0.83
2:B:65:LYS:CB	2:B:65:LYS:HG3	1.32	0.83
1:C:70:VAL:CA	1:C:71:ALA:N	2.36	0.83
1:C:105:LEU:CD2	1:C:105:LEU:CB	2.56	0.83
2:D:78:LEU:CD2	2:D:78:LEU:HG	0.56	0.83
2:B:5:PRO:CA	2:B:6:GLU:N	2.40	0.83
3:B:148:HEM:CBA	3:B:148:HEM:O1A	2.24	0.83
2:D:77:HIS:NE2	2:D:77:HIS:ND1	2.18	0.83
1:C:48:LEU:CD2	1:C:48:LEU:CD1	2.57	0.83
1:C:40:LYS:NZ	1:C:40:LYS:HD3	1.92	0.83
2:B:47:ASP:CA	2:B:48:LEU:N	2.41	0.83
1:A:60:LYS:CE	1:A:60:LYS:CG	2.57	0.82
2:B:65:LYS:CB	2:B:65:LYS:HG2	1.32	0.82
2:B:61:LYS:NZ	2:B:61:LYS:CD	2.42	0.82
1:A:99:LYS:CE	1:A:99:LYS:CG	2.52	0.82
2:B:65:LYS:CG	2:B:65:LYS:HB2	1.31	0.82
1:C:60:LYS:NZ	1:C:60:LYS:CD	2.41	0.82
1:C:105:LEU:CD1	1:C:105:LEU:CB	2.57	0.82
2:D:4:THR:CA	2:D:4:THR:CG2	2.54	0.82
1:A:84:SER:CA	1:A:84:SER:OG	2.28	0.82
2:D:78:LEU:HG	2:D:78:LEU:HD23	0.83	0.82
2:B:3:LEU:CB	2:B:3:LEU:N	2.42	0.82
2:D:113:VAL:CG2	2:D:113:VAL:CG1	2.58	0.82
2:D:2:HIS:CG	2:D:2:HIS:ND1	2.48	0.81
1:A:61:LYS:CE	1:A:61:LYS:CD	0.81	0.81
2:D:48:LEU:CD1	2:D:48:LEU:CB	2.58	0.81
1:A:5:ALA:CB	1:A:5:ALA:N	2.43	0.81
2:B:121:GLU:CG	2:B:121:GLU:OE2	2.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLU:OE2	1:C:23:GLU:CB	2.29	0.81
1:C:105:LEU:CD1	1:C:105:LEU:CD2	2.58	0.81
2:D:48:LEU:N	2:D:48:LEU:CB	2.42	0.81
2:D:80:ASN:N	2:D:80:ASN:CB	2.40	0.81
1:A:21:ALA:CA	1:A:22:GLY:N	2.43	0.81
1:C:23:GLU:CG	1:C:23:GLU:OE2	2.28	0.81
2:B:65:LYS:CG	2:B:65:LYS:HB3	1.31	0.81
1:C:76:MET:SD	1:C:76:MET:CB	2.68	0.81
1:A:72:HIS:CG	1:A:72:HIS:N	2.48	0.81
1:A:92:ARG:CZ	1:A:92:ARG:HH21	1.48	0.81
2:B:65:LYS:CG	2:B:65:LYS:CE	2.58	0.81
2:D:18:VAL:CG2	2:D:18:VAL:CA	2.58	0.81
1:A:50:HIS:CB	1:A:50:HIS:C	2.50	0.81
2:B:143:HIS:ND1	2:B:143:HIS:CB	2.43	0.81
2:D:20:VAL:HG23	2:D:20:VAL:C	2.01	0.81
1:A:92:ARG:CZ	1:A:92:ARG:HH22	1.48	0.80
1:A:76:MET:SD	1:A:76:MET:CB	2.66	0.80
2:B:12:THR:CB	2:B:12:THR:HG22	1.28	0.80
1:C:139:LYS:CE	1:C:139:LYS:CG	2.56	0.80
2:D:49:SER:O	2:D:50:THR:HA	1.81	0.80
2:B:65:LYS:CB	2:B:65:LYS:CD	2.59	0.80
2:D:43:GLU:CG	2:D:43:GLU:HB2	1.29	0.80
2:B:8:LYS:CA	2:B:8:LYS:HG2	2.09	0.80
2:D:45:PHE:O	2:D:46:GLY:N	2.14	0.80
1:C:73:VAL:CA	1:C:73:VAL:CG2	2.59	0.80
2:D:43:GLU:CG	2:D:43:GLU:HB3	1.29	0.80
2:D:55:MET:CA	2:D:56:GLY:N	2.43	0.80
1:A:1:VAL:CA	1:A:1:VAL:HG22	2.12	0.80
1:C:1:VAL:CG2	1:C:1:VAL:HA	2.12	0.80
1:A:138:SER:OG	1:A:138:SER:HA	1.81	0.79
2:D:59:LYS:CE	2:D:59:LYS:CG	2.52	0.79
3:A:142:HEM:CBA	3:A:142:HEM:O1A	2.31	0.79
1:A:74:ASP:OD1	1:A:74:ASP:OD2	2.00	0.79
1:A:81:SER:CB	1:A:81:SER:N	2.45	0.79
2:B:146:HIS:CB	2:B:146:HIS:CD2	2.66	0.79
2:D:49:SER:O	2:D:50:THR:CA	2.31	0.79
2:D:82:LYS:NZ	2:D:82:LYS:HD2	1.98	0.79
2:B:12:THR:HG23	2:B:12:THR:CB	1.28	0.79
1:C:61:LYS:CE	1:C:61:LYS:CG	2.59	0.79
2:D:17:LYS:NZ	2:D:17:LYS:CD	2.46	0.79
1:C:69:ALA:C	1:C:70:VAL:CA	2.50	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:LYS:CG	2:D:8:LYS:CE	2.59	0.78
2:D:50:THR:CB	2:D:50:THR:C	2.50	0.78
2:B:2:HIS:ND1	2:B:2:HIS:CB	2.44	0.78
2:B:2:HIS:CG	2:B:2:HIS:CA	2.65	0.78
2:B:59:LYS:CE	2:B:59:LYS:CG	2.61	0.78
1:C:70:VAL:CA	1:C:70:VAL:O	2.32	0.78
1:C:74:ASP:C	1:C:75:ASP:CA	2.51	0.78
2:B:65:LYS:HG3	2:B:65:LYS:C	2.03	0.78
2:B:117:HIS:CG	2:B:117:HIS:NE2	2.52	0.78
1:C:46:PHE:CD2	1:C:46:PHE:HE2	1.48	0.78
2:D:6:GLU:OE2	2:D:6:GLU:OE1	2.02	0.78
1:A:75:ASP:CG	1:A:75:ASP:CB	0.68	0.77
2:D:7:GLU:CA	2:D:7:GLU:CG	2.63	0.77
2:D:43:GLU:CG	2:D:43:GLU:CB	0.78	0.77
1:C:118:THR:CB	1:C:118:THR:C	2.52	0.77
2:D:11:VAL:C	2:D:12:THR:CA	2.52	0.77
2:B:87:THR:CB	2:B:87:THR:C	2.52	0.77
2:B:2:HIS:CD2	2:B:2:HIS:CE1	2.72	0.77
2:B:82:LYS:HE2	2:B:82:LYS:CB	2.14	0.77
1:A:133:SER:O	1:A:137:THR:HG22	1.85	0.77
1:C:92:ARG:NE	1:C:92:ARG:NH2	2.27	0.76
2:D:132:LYS:NZ	2:D:132:LYS:CE	2.49	0.76
2:B:41:PHE:CA	2:B:42:PHE:N	2.46	0.76
1:C:90:LYS:CE	1:C:90:LYS:CG	2.63	0.76
2:B:41:PHE:CA	2:B:41:PHE:O	2.31	0.76
1:A:18:GLY:CA	1:A:19:ALA:N	2.49	0.76
3:D:148:HEM:CBD	3:D:148:HEM:O1D	2.34	0.76
2:B:80:ASN:CA	2:B:80:ASN:O	2.31	0.76
2:B:87:THR:CA	2:B:87:THR:OG1	2.32	0.76
1:A:40:LYS:CA	1:A:40:LYS:CG	2.61	0.76
1:C:131:SER:CA	1:C:131:SER:O	2.34	0.76
1:A:2:LEU:CA	1:A:2:LEU:O	2.33	0.76
3:A:142:HEM:CBA	3:A:142:HEM:O2A	2.33	0.76
2:B:139:ASN:ND2	2:B:139:ASN:CB	2.47	0.76
2:B:121:GLU:CD	2:B:121:GLU:CB	2.52	0.76
2:D:12:THR:C	2:D:12:THR:HG22	2.07	0.76
1:A:40:LYS:CB	1:A:40:LYS:C	2.53	0.76
2:D:22:GLU:CG	2:D:22:GLU:CB	0.76	0.76
2:B:61:LYS:CE	2:B:61:LYS:CG	2.64	0.76
2:B:139:ASN:CG	2:B:139:ASN:CB	0.66	0.76
2:D:46:GLY:CA	2:D:46:GLY:O	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:CZ	1:A:92:ARG:HD3	1.95	0.75
3:A:142:HEM:CBD	3:A:142:HEM:O1D	2.35	0.75
2:D:47:ASP:CB	2:D:47:ASP:OD1	2.34	0.75
2:D:101:GLU:CG	2:D:101:GLU:OE2	2.33	0.75
2:D:104:ARG:NE	2:D:104:ARG:CG	2.49	0.75
1:C:70:VAL:N	1:C:70:VAL:CB	2.49	0.75
1:A:17:VAL:CA	1:A:17:VAL:O	2.34	0.75
2:B:8:LYS:CB	2:B:8:LYS:N	2.49	0.75
2:B:43:GLU:O	2:B:44:SER:C	2.23	0.75
2:D:143:HIS:CD2	2:D:143:HIS:CB	2.67	0.75
1:C:7:LYS:N	1:C:7:LYS:CB	2.49	0.74
2:D:2:HIS:CG	2:D:2:HIS:CA	2.70	0.74
3:B:148:HEM:CBD	3:B:148:HEM:O1D	2.35	0.74
1:C:99:LYS:CG	1:C:99:LYS:CB	0.74	0.74
1:C:30:GLU:CG	1:C:30:GLU:OE1	2.35	0.74
2:D:22:GLU:C	2:D:22:GLU:HG3	2.09	0.73
2:D:82:LYS:CD	2:D:82:LYS:HZ2	1.99	0.73
2:B:7:GLU:CB	2:B:7:GLU:CD	2.56	0.73
1:C:2:LEU:CA	1:C:2:LEU:O	2.36	0.73
2:D:113:VAL:CG2	2:D:113:VAL:CA	2.65	0.73
2:B:49:SER:O	2:B:50:THR:N	2.19	0.73
1:C:54:GLN:CA	1:C:55:VAL:N	2.51	0.73
2:D:95:LYS:CD	2:D:95:LYS:CB	2.67	0.73
1:A:11:LYS:CE	1:A:11:LYS:CG	2.64	0.73
1:A:50:HIS:CA	1:A:50:HIS:CG	2.68	0.73
2:D:78:LEU:CB	2:D:78:LEU:N	2.49	0.73
1:A:81:SER:CA	1:A:81:SER:OG	2.35	0.73
2:B:12:THR:HG21	2:B:12:THR:HB	0.75	0.73
2:D:7:GLU:C	2:D:7:GLU:CB	2.57	0.73
2:D:73:ASP:CG	2:D:73:ASP:OD2	2.26	0.73
2:B:43:GLU:CG	2:B:43:GLU:OE2	2.36	0.73
1:A:74:ASP:CB	1:A:74:ASP:OD1	2.37	0.73
2:B:5:PRO:C	2:B:5:PRO:CB	2.54	0.73
2:B:61:LYS:CD	2:B:61:LYS:CB	2.62	0.73
1:C:10:VAL:CA	1:C:11:LYS:N	2.52	0.72
2:D:7:GLU:CA	2:D:7:GLU:O	2.38	0.72
1:A:56:LYS:CD	1:A:56:LYS:NZ	2.52	0.72
1:A:1:VAL:CG2	1:A:1:VAL:H1	1.99	0.72
2:D:47:ASP:N	2:D:47:ASP:HB3	2.04	0.72
2:B:12:THR:CB	2:B:12:THR:HG21	1.28	0.72
2:B:6:GLU:C	2:B:6:GLU:CB	2.58	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:GLU:CG	2:B:7:GLU:HA	2.19	0.72
2:D:82:LYS:CD	2:D:82:LYS:HZ3	1.99	0.72
1:C:75:ASP:N	1:C:75:ASP:C	2.43	0.72
1:A:84:SER:CB	1:A:84:SER:C	2.57	0.72
3:B:148:HEM:CBD	3:B:148:HEM:O2D	2.38	0.72
1:C:16:LYS:C	1:C:16:LYS:N	2.43	0.72
2:D:79:ASP:OD2	2:D:79:ASP:CB	2.37	0.72
2:D:131:GLN:CG	2:D:131:GLN:NE2	2.49	0.72
1:C:16:LYS:HB3	1:C:16:LYS:HD3	1.70	0.71
1:C:116:GLU:CB	1:C:116:GLU:CD	2.57	0.71
2:D:12:THR:CG2	2:D:12:THR:C	2.58	0.71
2:D:22:GLU:CA	2:D:23:VAL:N	2.53	0.71
2:D:50:THR:N	2:D:50:THR:CB	2.53	0.71
2:D:104:ARG:CD	2:D:104:ARG:NH1	2.52	0.71
2:D:132:LYS:NZ	2:D:132:LYS:CD	2.53	0.71
2:B:59:LYS:NZ	2:B:59:LYS:CD	2.53	0.71
2:B:146:HIS:CG	2:B:146:HIS:CA	2.73	0.71
1:A:127:LYS:CG	1:A:127:LYS:CB	0.71	0.71
2:B:145:TYR:CA	2:B:145:TYR:O	2.38	0.71
2:D:7:GLU:CA	2:D:8:LYS:N	2.49	0.71
2:D:45:PHE:O	2:D:46:GLY:HA3	1.90	0.71
2:B:2:HIS:CG	2:B:2:HIS:CE1	2.77	0.71
1:C:92:ARG:CD	1:C:92:ARG:NH2	2.52	0.71
2:D:10:ALA:C	2:D:10:ALA:HB3	2.08	0.71
2:B:146:HIS:CB	2:B:146:HIS:ND1	2.42	0.71
1:C:75:ASP:N	1:C:75:ASP:CB	2.54	0.71
2:B:49:SER:OG	2:B:49:SER:C	2.29	0.71
1:C:2:LEU:C	1:C:2:LEU:CB	2.57	0.71
2:D:1:VAL:HB	2:D:2:HIS:N	2.06	0.71
2:B:74:GLY:CA	2:B:75:LEU:N	2.51	0.71
1:A:50:HIS:C	1:A:50:HIS:CG	2.64	0.70
1:A:87:HIS:C	1:A:87:HIS:CB	2.60	0.70
1:C:1:VAL:C	1:C:1:VAL:CG1	2.59	0.70
1:A:52:SER:N	1:A:52:SER:CB	2.54	0.70
2:D:43:GLU:CA	2:D:44:SER:N	2.53	0.70
1:A:87:HIS:CA	1:A:88:ALA:N	2.50	0.70
2:D:59:LYS:C	2:D:59:LYS:CB	2.57	0.70
1:C:16:LYS:CG	1:C:16:LYS:HA	2.22	0.70
3:C:142:HEM:CBD	3:C:142:HEM:O1D	2.33	0.70
1:C:82:ALA:C	1:C:83:LEU:CA	2.58	0.70
2:B:6:GLU:C	2:B:6:GLU:N	2.43	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LYS:CE	2:B:82:LYS:CD	0.70	0.70
1:A:85:ASP:OD2	1:A:85:ASP:OD1	2.10	0.70
1:C:30:GLU:CD	1:C:50:HIS:HD2	1.94	0.70
2:D:49:SER:CA	2:D:50:THR:N	2.52	0.70
2:B:5:PRO:N	2:B:6:GLU:N	2.40	0.70
2:D:8:LYS:CB	2:D:8:LYS:N	2.55	0.70
2:D:123:THR:CG2	2:D:123:THR:CA	2.70	0.70
2:D:17:LYS:NZ	2:D:17:LYS:HD3	2.07	0.69
1:C:40:LYS:NZ	1:C:40:LYS:HD2	2.01	0.69
2:D:8:LYS:CB	2:D:8:LYS:HD3	2.21	0.69
2:D:12:THR:CA	2:D:12:THR:OG1	2.40	0.69
1:A:137:THR:OG1	1:A:137:THR:HG22	1.93	0.69
2:D:73:ASP:OD2	5:D:174:HOH:O	2.10	0.69
2:B:2:HIS:CG	2:B:2:HIS:C	2.66	0.69
2:B:8:LYS:HG2	2:B:8:LYS:C	2.12	0.69
1:A:92:ARG:CD	1:A:92:ARG:NH2	2.56	0.69
2:B:90:GLU:CG	2:B:90:GLU:OE1	2.38	0.69
2:B:145:TYR:C	2:B:145:TYR:CB	2.55	0.69
1:C:56:LYS:NZ	1:C:56:LYS:CD	2.56	0.69
2:D:47:ASP:CA	2:D:48:LEU:N	2.55	0.69
2:D:139:ASN:OD1	2:D:139:ASN:HB3	1.91	0.69
2:D:141:LEU:CD2	2:D:141:LEU:HD13	2.20	0.69
1:A:127:LYS:CG	1:A:127:LYS:HA	2.15	0.69
2:D:4:THR:O	2:D:5:PRO:CA	2.40	0.69
1:C:1:VAL:CA	1:C:2:LEU:N	2.55	0.68
1:C:56:LYS:CD	1:C:56:LYS:CB	2.70	0.68
1:A:29:LEU:CA	1:A:29:LEU:CG	2.70	0.68
2:D:121:GLU:CG	2:D:121:GLU:OE2	2.42	0.68
1:A:11:LYS:CD	1:A:11:LYS:NZ	2.56	0.68
1:C:1:VAL:C	1:C:1:VAL:HG12	2.12	0.68
1:A:78:ASN:ND2	1:A:78:ASN:OD1	2.27	0.68
2:B:52:ASP:CB	2:B:52:ASP:OD2	2.41	0.68
2:D:78:LEU:CB	2:D:78:LEU:C	2.58	0.68
1:A:74:ASP:CG	1:A:74:ASP:CA	2.60	0.68
2:B:117:HIS:CE1	2:B:117:HIS:CG	2.82	0.68
2:B:143:HIS:C	2:B:143:HIS:CB	2.60	0.68
2:B:3:LEU:CB	2:B:3:LEU:C	2.61	0.68
2:B:65:LYS:CG	2:B:65:LYS:C	2.60	0.68
2:B:49:SER:N	2:B:49:SER:CB	2.57	0.68
1:C:16:LYS:CB	1:C:16:LYS:HD3	2.23	0.68
1:C:131:SER:C	1:C:131:SER:CB	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:SER:CA	1:C:138:SER:HG	2.05	0.68
1:A:5:ALA:CB	1:A:5:ALA:C	2.62	0.67
1:C:118:THR:CA	1:C:118:THR:HB	2.16	0.67
2:B:1:VAL:CA	2:B:1:VAL:CG2	2.64	0.67
1:A:139:LYS:NZ	1:A:139:LYS:CD	2.57	0.67
2:D:24:GLY:CA	2:D:68:LEU:HD22	2.24	0.67
3:C:142:HEM:CBD	3:C:142:HEM:O2D	2.35	0.67
2:B:9:SER:CA	2:B:10:ALA:N	2.56	0.67
2:B:74:GLY:O	2:B:75:LEU:N	2.28	0.67
2:D:1:VAL:CB	2:D:2:HIS:N	2.58	0.67
1:C:113:LEU:CD1	1:C:113:LEU:HB3	2.21	0.67
2:B:65:LYS:CE	2:B:65:LYS:HG3	2.24	0.67
1:C:48:LEU:CD2	1:C:48:LEU:CB	2.66	0.67
1:C:38:THR:CA	1:C:38:THR:OG1	2.42	0.67
2:D:104:ARG:NE	2:D:104:ARG:CZ	2.58	0.67
2:D:123:THR:CG2	2:D:123:THR:OG1	2.42	0.67
1:C:61:LYS:C	1:C:61:LYS:CB	2.60	0.66
1:C:113:LEU:HD22	1:C:116:GLU:HG3	1.77	0.66
2:D:82:LYS:CG	2:D:82:LYS:CE	2.73	0.66
2:D:24:GLY:HA2	2:D:68:LEU:HD22	1.76	0.66
2:D:82:LYS:CD	2:D:82:LYS:CB	2.68	0.66
1:A:127:LYS:HG3	1:A:127:LYS:HA	1.77	0.66
2:D:65:LYS:CD	2:D:65:LYS:NZ	2.59	0.66
2:D:101:GLU:CG	2:D:101:GLU:OE1	2.43	0.66
1:C:54:GLN:C	1:C:54:GLN:CB	2.59	0.66
2:D:43:GLU:HB2	2:D:43:GLU:HG3	1.34	0.66
2:D:55:MET:CA	2:D:55:MET:O	2.42	0.66
2:D:79:ASP:N	2:D:80:ASN:N	2.43	0.66
2:B:6:GLU:CA	2:B:7:GLU:N	2.54	0.66
2:D:43:GLU:HB3	2:D:43:GLU:OE1	1.95	0.66
2:B:50:THR:CG2	2:B:50:THR:OG1	2.43	0.66
2:B:65:LYS:CE	2:B:65:LYS:NZ	2.59	0.66
1:C:10:VAL:C	1:C:10:VAL:CB	2.65	0.66
1:C:6:ASP:C	1:C:7:LYS:CA	2.62	0.66
1:C:135:VAL:O	1:C:138:SER:HB2	1.95	0.66
2:D:26:GLU:OE2	2:D:26:GLU:CB	2.43	0.66
2:D:92:HIS:CA	2:D:92:HIS:O	2.40	0.66
1:A:44:PRO:CA	1:A:45:HIS:N	2.55	0.66
1:A:75:ASP:CB	1:A:75:ASP:OD1	2.44	0.66
1:A:92:ARG:CZ	1:A:92:ARG:NE	2.57	0.66
2:B:12:THR:CA	2:B:12:THR:HG23	1.88	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:CD	1:A:30:GLU:CB	2.63	0.65
2:D:92:HIS:C	2:D:92:HIS:N	2.49	0.65
2:D:8:LYS:CB	2:D:8:LYS:C	2.61	0.65
2:D:48:LEU:CD1	2:D:48:LEU:CD2	2.72	0.65
1:C:38:THR:CB	1:C:38:THR:N	2.56	0.65
1:A:15:GLY:O	1:A:16:LYS:N	2.19	0.65
2:D:1:VAL:CA	2:D:2:HIS:H	2.07	0.65
1:A:62:VAL:C	1:A:62:VAL:CB	2.63	0.65
3:C:142:HEM:HBB2	3:C:142:HEM:CMB	2.25	0.65
1:C:23:GLU:OE2	1:C:23:GLU:HB2	1.96	0.65
2:D:78:LEU:CG	2:D:78:LEU:HD23	1.51	0.65
2:B:82:LYS:CD	2:B:82:LYS:NZ	2.59	0.65
2:B:108:ASN:CG	2:B:108:ASN:CA	2.64	0.65
2:B:21:ASP:CB	2:B:21:ASP:OD1	2.42	0.64
1:C:92:ARG:NH1	1:C:92:ARG:HD2	2.12	0.64
2:D:8:LYS:CG	2:D:8:LYS:C	2.65	0.64
1:C:27:GLU:OE2	1:C:112:HIS:HE1	1.80	0.64
1:A:21:ALA:CA	1:A:21:ALA:O	2.44	0.64
1:A:137:THR:CB	1:A:137:THR:C	2.64	0.64
2:B:57:ASN:C	2:B:58:PRO:CD	2.64	0.64
2:B:104:ARG:CG	2:B:104:ARG:NE	2.60	0.64
2:D:131:GLN:CG	2:D:131:GLN:OE1	2.39	0.64
1:A:127:LYS:CG	1:A:127:LYS:HE2	2.27	0.64
2:D:80:ASN:OD1	2:D:80:ASN:CB	2.39	0.64
1:C:7:LYS:CG	1:C:7:LYS:HE3	2.27	0.64
1:A:1:VAL:CG2	1:A:1:VAL:H3	1.89	0.64
1:C:1:VAL:HB	1:C:1:VAL:H1	1.63	0.64
1:C:105:LEU:CD2	1:C:105:LEU:HD13	2.28	0.63
3:C:142:HEM:HBB2	3:C:142:HEM:HMB1	1.80	0.63
2:D:65:LYS:CE	2:D:65:LYS:CG	2.77	0.63
1:C:1:VAL:CG1	1:C:1:VAL:HA	2.23	0.63
1:C:60:LYS:NZ	1:C:60:LYS:HD3	2.13	0.63
2:D:46:GLY:CA	2:D:47:ASP:N	2.60	0.63
2:D:67:VAL:CG1	2:D:67:VAL:C	2.66	0.63
2:B:80:ASN:CB	2:B:80:ASN:N	2.57	0.63
1:A:90:LYS:CD	1:A:90:LYS:NZ	2.62	0.63
2:B:48:LEU:O	2:B:49:SER:CA	2.47	0.63
2:B:52:ASP:CG	2:B:52:ASP:CA	2.64	0.63
2:B:82:LYS:CE	2:B:82:LYS:HG2	2.20	0.63
1:C:87:HIS:C	1:C:87:HIS:CB	2.66	0.63
2:D:52:ASP:N	2:D:52:ASP:HB2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:HIS:CG	2:D:2:HIS:NE2	2.67	0.63
2:B:90:GLU:CB	2:B:90:GLU:C	2.67	0.62
2:B:142:ALA:CA	2:B:143:HIS:N	2.54	0.62
1:C:87:HIS:CA	1:C:88:ALA:N	2.61	0.62
2:D:58:PRO:CG	2:D:58:PRO:HD3	1.11	0.62
2:D:104:ARG:HD2	2:D:104:ARG:NH1	2.10	0.62
2:D:5:PRO:CB	2:D:5:PRO:C	2.68	0.62
2:D:12:THR:N	2:D:12:THR:C	2.49	0.62
2:B:80:ASN:CG	2:B:80:ASN:CA	2.62	0.62
1:C:73:VAL:H	1:C:73:VAL:HG12	1.64	0.62
1:C:61:LYS:CA	1:C:62:VAL:N	2.62	0.62
2:D:4:THR:CA	2:D:4:THR:OG1	2.46	0.62
2:D:76:ALA:N	2:D:76:ALA:HB2	2.13	0.62
1:A:40:LYS:CB	1:A:40:LYS:N	2.59	0.62
2:B:65:LYS:HG3	2:B:65:LYS:HE2	1.82	0.62
2:D:58:PRO:CG	2:D:58:PRO:HD2	1.11	0.62
2:D:6:GLU:CD	2:D:6:GLU:CB	2.67	0.62
2:D:53:ALA:CA	2:D:54:VAL:N	2.63	0.62
1:A:81:SER:CB	1:A:81:SER:C	2.66	0.61
1:C:23:GLU:CD	1:C:23:GLU:OE1	2.37	0.61
1:C:137:THR:CA	1:C:137:THR:O	2.42	0.61
1:A:58:HIS:CA	1:A:58:HIS:O	2.45	0.61
1:C:113:LEU:CD1	1:C:113:LEU:HB2	2.28	0.61
2:B:12:THR:CA	2:B:12:THR:HG22	1.88	0.61
2:B:80:ASN:OD1	2:B:80:ASN:HA	2.00	0.61
2:D:76:ALA:N	2:D:76:ALA:HB3	2.13	0.61
2:D:141:LEU:HD13	2:D:141:LEU:HD22	1.82	0.61
3:C:142:HEM:CBA	3:C:142:HEM:O1A	2.48	0.61
2:D:19:ASN:ND2	2:D:19:ASN:CB	2.63	0.61
2:D:59:LYS:CD	2:D:59:LYS:NZ	2.63	0.61
2:D:94:ASP:N	2:D:94:ASP:C	2.50	0.61
1:A:99:LYS:CE	1:A:99:LYS:HG3	2.29	0.61
2:D:121:GLU:CB	2:D:121:GLU:C	2.68	0.61
1:A:16:LYS:CD	1:A:16:LYS:CB	2.78	0.61
2:B:41:PHE:C	2:B:41:PHE:CB	2.67	0.61
1:C:105:LEU:CD2	1:C:105:LEU:HB2	2.29	0.61
2:D:21:ASP:CB	2:D:21:ASP:OD2	2.42	0.60
2:B:82:LYS:HE2	2:B:82:LYS:HB3	1.82	0.60
1:A:17:VAL:N	1:A:18:GLY:N	2.48	0.60
2:D:8:LYS:CA	2:D:8:LYS:HG3	2.26	0.60
2:B:66:LYS:CE	2:B:66:LYS:HG3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ASN:C	2:B:80:ASN:N	2.55	0.60
3:C:142:HEM:CGD	3:C:142:HEM:CAD	2.73	0.60
2:D:12:THR:CB	2:D:12:THR:C	2.66	0.60
2:B:6:GLU:OE1	2:B:6:GLU:OE2	2.09	0.60
1:C:82:ALA:CA	1:C:83:LEU:N	2.58	0.60
2:D:77:HIS:CD2	2:D:77:HIS:CE1	2.70	0.60
1:A:75:ASP:CB	1:A:75:ASP:N	2.64	0.60
1:C:73:VAL:CA	1:C:73:VAL:HG12	2.30	0.60
1:C:92:ARG:HD2	1:C:92:ARG:HH11	1.65	0.60
1:C:56:LYS:CD	1:C:56:LYS:HB3	2.32	0.59
2:B:63:HIS:HE1	3:B:148:HEM:C4D	2.20	0.59
2:B:65:LYS:CB	2:B:65:LYS:C	2.66	0.59
2:B:66:LYS:CE	2:B:66:LYS:CG	2.80	0.59
1:A:127:LYS:CD	1:A:127:LYS:HB3	2.28	0.59
2:B:80:ASN:CB	2:B:80:ASN:OD1	2.50	0.59
2:D:4:THR:OG1	2:D:6:GLU:OE2	2.19	0.59
1:C:8:THR:CA	1:C:8:THR:OG1	2.46	0.59
1:A:137:THR:CB	1:A:137:THR:HG1	2.10	0.58
1:A:16:LYS:CE	1:A:16:LYS:HG2	2.22	0.58
2:D:132:LYS:NZ	2:D:132:LYS:HD3	2.18	0.58
2:D:1:VAL:HB	2:D:2:HIS:H	1.67	0.58
1:A:52:SER:N	1:A:52:SER:C	2.46	0.58
1:C:138:SER:OG	1:C:138:SER:HA	1.96	0.58
1:A:90:LYS:CE	1:A:90:LYS:NZ	2.67	0.58
2:D:7:GLU:C	2:D:7:GLU:N	2.55	0.58
2:D:76:ALA:CB	2:D:76:ALA:H	2.12	0.58
2:B:12:THR:CG2	2:B:12:THR:CB	0.58	0.58
2:B:65:LYS:CB	2:B:65:LYS:CG	0.58	0.58
1:A:62:VAL:CA	1:A:62:VAL:O	2.44	0.58
2:B:26:GLU:OE2	2:B:26:GLU:CB	2.52	0.58
2:D:10:ALA:C	2:D:10:ALA:N	2.57	0.57
1:C:137:THR:CA	1:C:138:SER:N	2.58	0.57
2:D:52:ASP:N	2:D:52:ASP:C	2.56	0.57
1:A:75:ASP:CB	1:A:75:ASP:O	2.53	0.57
2:B:9:SER:C	2:B:9:SER:OG	2.43	0.57
1:C:73:VAL:HG12	1:C:73:VAL:N	2.19	0.57
2:D:79:ASP:O	2:D:80:ASN:CA	2.51	0.57
1:C:73:VAL:CA	1:C:73:VAL:HG13	2.30	0.57
2:D:79:ASP:C	2:D:79:ASP:HB2	2.25	0.57
2:B:77:HIS:CD2	2:B:77:HIS:CB	2.84	0.57
2:B:90:GLU:CB	2:B:90:GLU:CD	2.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ALA:C	2:B:142:ALA:N	2.54	0.57
2:B:2:HIS:CB	2:B:2:HIS:N	2.66	0.57
2:B:146:HIS:CG	2:B:146:HIS:C	2.79	0.56
1:C:2:LEU:C	1:C:2:LEU:N	2.54	0.56
1:C:16:LYS:NZ	1:C:16:LYS:CD	2.68	0.56
2:D:78:LEU:CD1	2:D:78:LEU:HD21	2.19	0.56
2:D:90:GLU:OE1	2:D:90:GLU:CG	2.53	0.56
2:B:143:HIS:CA	2:B:144:LYS:N	2.62	0.56
2:D:21:ASP:OD1	2:D:65:LYS:HG3	2.06	0.56
1:A:60:LYS:CE	1:A:60:LYS:NZ	2.68	0.56
1:A:87:HIS:CA	1:A:87:HIS:O	2.44	0.56
2:B:90:GLU:CG	2:B:90:GLU:N	2.68	0.56
1:C:92:ARG:HH21	1:C:92:ARG:HD2	1.68	0.56
2:D:51:PRO:C	2:D:52:ASP:CA	2.71	0.56
2:D:52:ASP:CG	2:D:52:ASP:OD2	2.44	0.56
1:A:14:TRP:CB	1:A:14:TRP:N	2.63	0.56
2:D:22:GLU:C	2:D:22:GLU:N	2.53	0.55
2:D:82:LYS:HD2	2:D:82:LYS:HZ2	1.62	0.55
1:A:75:ASP:CG	1:A:75:ASP:C	2.65	0.55
1:C:47:ASP:C	1:C:47:ASP:OD1	2.44	0.55
1:C:118:THR:HG23	1:C:121:VAL:H	1.71	0.55
2:D:50:THR:CA	2:D:50:THR:CG2	2.81	0.55
1:C:7:LYS:CG	1:C:7:LYS:HE2	2.34	0.55
1:C:78:ASN:CB	1:C:78:ASN:OD1	2.48	0.55
2:D:47:ASP:CG	2:D:47:ASP:CA	2.74	0.55
1:C:114:PRO:C	1:C:114:PRO:N	2.60	0.55
1:C:118:THR:CA	1:C:118:THR:CG2	2.59	0.55
2:D:43:GLU:HB2	2:D:44:SER:N	2.16	0.55
2:B:4:THR:C	2:B:5:PRO:CD	2.73	0.55
2:B:12:THR:CG2	2:B:12:THR:HB	1.04	0.55
2:B:143:HIS:ND1	2:B:143:HIS:HB3	2.21	0.55
2:D:20:VAL:HG22	2:D:20:VAL:C	2.18	0.55
1:C:131:SER:CA	1:C:132:VAL:N	2.60	0.54
2:D:47:ASP:N	2:D:47:ASP:C	2.60	0.54
2:D:79:ASP:N	2:D:80:ASN:H	2.04	0.54
2:B:26:GLU:OE2	2:B:26:GLU:CD	2.43	0.54
1:A:15:GLY:O	1:A:15:GLY:CA	2.56	0.54
1:A:75:ASP:HB3	1:A:75:ASP:O	2.07	0.54
1:C:84:SER:HB2	1:C:139:LYS:HD2	1.90	0.54
2:D:58:PRO:CD	2:D:58:PRO:HG2	1.03	0.54
2:B:21:ASP:CB	2:B:21:ASP:OD2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LEU:N	2:B:81:LEU:HB2	2.18	0.54
2:D:104:ARG:NE	2:D:104:ARG:HH21	2.06	0.54
3:A:142:HEM:CGA	3:A:142:HEM:CAA	2.82	0.54
1:C:40:LYS:HD3	1:C:40:LYS:HZ3	1.72	0.54
2:D:18:VAL:CB	2:D:18:VAL:N	2.54	0.54
2:D:121:GLU:CB	2:D:121:GLU:N	2.60	0.54
1:A:64:ASP:CB	1:A:64:ASP:OD2	2.51	0.54
2:B:2:HIS:ND1	2:B:2:HIS:HB3	2.20	0.54
1:A:20:HIS:O	1:A:21:ALA:C	2.46	0.54
2:B:41:PHE:C	2:B:41:PHE:N	2.57	0.54
2:B:108:ASN:HD22	2:B:108:ASN:HB2	1.70	0.54
2:D:18:VAL:CG2	2:D:18:VAL:HG11	2.37	0.54
1:C:8:THR:CB	1:C:8:THR:C	2.67	0.53
1:C:61:LYS:NZ	1:C:61:LYS:HD2	2.19	0.53
1:C:8:THR:CB	1:C:8:THR:N	2.67	0.53
1:C:90:LYS:CD	1:C:90:LYS:NZ	2.71	0.53
2:D:3:LEU:O	2:D:4:THR:CA	2.55	0.53
1:A:1:VAL:HG22	1:A:1:VAL:H1	1.70	0.53
1:C:76:MET:CG	1:C:76:MET:CE	2.81	0.53
2:D:59:LYS:CE	2:D:59:LYS:HG2	2.38	0.53
2:B:3:LEU:CA	2:B:3:LEU:CG	2.81	0.53
2:B:124:PRO:C	2:B:125:PRO:CD	2.60	0.53
2:D:126:VAL:CB	2:D:126:VAL:N	2.65	0.53
2:B:90:GLU:HG3	2:B:90:GLU:H	1.72	0.53
2:B:142:ALA:CA	2:B:142:ALA:O	2.55	0.53
1:C:73:VAL:CG1	1:C:73:VAL:N	2.68	0.53
2:D:73:ASP:O	2:D:76:ALA:HB3	2.08	0.53
2:B:101:GLU:CD	2:B:101:GLU:CB	2.75	0.53
2:B:47:ASP:C	2:B:47:ASP:HB3	2.29	0.53
2:D:121:GLU:CA	2:D:121:GLU:HG3	2.37	0.53
1:C:139:LYS:CD	1:C:139:LYS:HZ3	2.15	0.53
2:D:2:HIS:NE2	2:D:2:HIS:ND1	2.57	0.53
2:D:102:ASN:HB3	3:D:148:HEM:HMC1	1.90	0.53
1:A:23:GLU:OE1	1:A:23:GLU:CG	2.57	0.52
2:B:79:ASP:OD2	2:B:79:ASP:CA	2.56	0.52
1:A:81:SER:CB	1:A:81:SER:H	2.22	0.52
2:B:41:PHE:N	2:B:42:PHE:N	2.57	0.52
2:D:79:ASP:O	2:D:80:ASN:HA	2.10	0.52
2:D:92:HIS:C	2:D:92:HIS:HB3	2.29	0.52
1:A:14:TRP:CG	1:A:14:TRP:HA	2.34	0.52
2:D:58:PRO:CD	2:D:58:PRO:HG3	1.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:VAL:C	2:D:67:VAL:HG12	2.29	0.52
2:B:8:LYS:CG	2:B:8:LYS:C	2.70	0.52
1:C:92:ARG:CZ	1:C:92:ARG:HD2	2.40	0.52
2:D:90:GLU:CB	2:D:90:GLU:OE2	2.58	0.52
2:D:95:LYS:HA	2:D:95:LYS:HD3	1.91	0.52
1:A:61:LYS:CG	1:A:61:LYS:HE2	2.11	0.52
3:D:148:HEM:O1A	3:D:148:HEM:CAA	2.56	0.52
2:B:1:VAL:CA	2:B:1:VAL:CG1	2.88	0.52
2:B:22:GLU:OE1	2:B:22:GLU:OE2	2.28	0.52
2:D:65:LYS:CD	2:D:65:LYS:HB3	2.36	0.52
2:B:80:ASN:CA	2:B:80:ASN:OD1	2.57	0.52
2:D:10:ALA:HB3	2:D:11:VAL:N	2.24	0.51
2:D:20:VAL:HG13	2:D:20:VAL:N	2.26	0.51
2:D:3:LEU:O	2:D:3:LEU:CA	2.58	0.51
1:A:133:SER:O	1:A:137:THR:CG2	2.57	0.51
1:C:138:SER:CB	1:C:138:SER:N	2.72	0.51
2:D:58:PRO:HD3	2:D:58:PRO:HG2	1.04	0.51
2:B:22:GLU:CG	2:B:22:GLU:OE1	2.59	0.51
1:C:99:LYS:CG	1:C:99:LYS:CE	2.88	0.51
1:C:139:LYS:NZ	1:C:139:LYS:HD2	2.20	0.51
2:D:5:PRO:CA	2:D:5:PRO:CG	2.81	0.51
1:A:50:HIS:CB	1:A:50:HIS:H	2.23	0.50
2:D:73:ASP:CB	2:D:73:ASP:OD2	2.59	0.50
1:C:72:HIS:CB	1:C:72:HIS:N	2.63	0.50
1:C:82:ALA:O	1:C:83:LEU:CA	2.59	0.50
2:D:26:GLU:OE2	2:D:26:GLU:OE1	2.30	0.50
2:D:104:ARG:NE	2:D:104:ARG:NH2	2.59	0.50
1:A:2:LEU:HA	1:A:3:SER:N	2.21	0.50
1:C:78:ASN:CB	1:C:78:ASN:ND2	2.66	0.50
1:C:137:THR:C	1:C:137:THR:N	2.59	0.50
1:C:40:LYS:HG2	1:C:48:LEU:HD13	1.94	0.50
2:B:142:ALA:C	2:B:142:ALA:CB	2.72	0.50
2:D:67:VAL:CB	2:D:67:VAL:C	2.64	0.50
2:D:82:LYS:CE	2:D:82:LYS:HG3	2.41	0.50
1:C:92:ARG:CZ	1:C:92:ARG:CD	2.89	0.50
2:B:10:ALA:CA	2:B:11:VAL:N	2.66	0.50
1:A:78:ASN:CG	1:A:78:ASN:HA	2.20	0.50
2:B:143:HIS:C	2:B:143:HIS:N	2.60	0.50
1:C:90:LYS:CD	1:C:90:LYS:HB3	2.38	0.50
1:C:103:HIS:HE1	2:D:131:GLN:OE1	1.94	0.50
2:D:67:VAL:CA	2:D:67:VAL:CG2	2.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:VAL:O	2:B:2:HIS:HA	2.11	0.50
2:B:50:THR:O	2:B:54:VAL:HG23	2.11	0.50
2:D:1:VAL:CB	2:D:2:HIS:H	2.23	0.50
2:D:8:LYS:CG	2:D:8:LYS:HA	2.38	0.50
2:D:12:THR:N	2:D:12:THR:CB	2.75	0.50
2:B:8:LYS:CB	2:B:8:LYS:C	2.69	0.49
2:D:73:ASP:OD2	2:D:73:ASP:OD1	2.30	0.49
1:C:7:LYS:CD	1:C:7:LYS:CB	2.80	0.49
2:D:10:ALA:CA	2:D:10:ALA:O	2.52	0.49
1:C:105:LEU:HD13	1:C:105:LEU:HD22	1.92	0.49
2:B:145:TYR:CA	2:B:146:HIS:N	2.46	0.49
2:D:22:GLU:CG	2:D:22:GLU:C	2.80	0.49
2:D:55:MET:N	2:D:56:GLY:N	2.59	0.49
2:B:8:LYS:CD	2:B:8:LYS:HG2	2.21	0.49
1:C:82:ALA:O	1:C:83:LEU:N	2.36	0.49
2:B:80:ASN:ND2	2:B:80:ASN:HB3	2.27	0.49
1:C:7:LYS:N	1:C:7:LYS:CG	2.76	0.49
2:D:108:ASN:CG	2:D:108:ASN:CA	2.73	0.49
1:A:2:LEU:C	1:A:2:LEU:CB	2.75	0.49
1:A:51:GLY:C	1:A:52:SER:C	2.71	0.49
2:B:5:PRO:N	2:B:6:GLU:H	2.10	0.49
1:C:16:LYS:N	1:C:17:VAL:N	2.61	0.49
2:D:18:VAL:N	2:D:18:VAL:C	2.63	0.49
2:D:73:ASP:CG	2:D:73:ASP:N	2.65	0.49
1:A:44:PRO:C	1:A:44:PRO:HB2	2.33	0.49
1:A:50:HIS:HA	5:A:173:HOH:O	2.13	0.48
2:B:65:LYS:CB	2:B:65:LYS:CE	2.91	0.48
2:D:123:THR:HB	2:D:124:PRO:CD	2.43	0.48
2:B:22:GLU:CG	2:B:22:GLU:OE2	2.61	0.48
1:C:10:VAL:CA	1:C:10:VAL:O	2.47	0.48
2:D:121:GLU:CG	2:D:121:GLU:OE1	2.60	0.48
2:B:96:LEU:HD13	3:B:148:HEM:C3D	2.48	0.48
1:C:60:LYS:HD3	1:C:60:LYS:HZ2	1.79	0.48
1:A:16:LYS:CG	1:A:16:LYS:NZ	2.71	0.48
1:A:17:VAL:C	1:A:17:VAL:CG1	2.81	0.48
2:B:87:THR:CA	2:B:87:THR:CG2	2.92	0.48
2:D:8:LYS:HG3	2:D:8:LYS:HA	1.95	0.48
2:D:47:ASP:CA	2:D:47:ASP:OD2	2.62	0.48
2:D:67:VAL:CB	2:D:67:VAL:H	2.24	0.48
1:A:72:HIS:CB	1:A:72:HIS:O	2.62	0.48
2:D:6:GLU:CB	2:D:6:GLU:C	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HH11	1:A:92:ARG:HD2	1.47	0.48
2:D:1:VAL:CA	2:D:1:VAL:O	2.61	0.48
3:C:142:HEM:HMB1	3:C:142:HEM:CBB	2.44	0.47
2:D:4:THR:CB	2:D:4:THR:C	2.76	0.47
1:C:118:THR:CA	1:C:118:THR:OG1	2.54	0.47
2:D:8:LYS:C	2:D:8:LYS:HG2	2.33	0.47
1:A:75:ASP:OD1	1:A:75:ASP:OD2	2.33	0.47
1:A:137:THR:CG2	1:A:137:THR:N	2.78	0.47
2:B:90:GLU:CB	2:B:90:GLU:OE1	2.63	0.47
2:B:4:THR:HA	2:B:5:PRO:CD	2.44	0.47
1:C:16:LYS:C	1:C:16:LYS:CB	2.71	0.47
1:A:84:SER:HB2	1:A:139:LYS:HD2	1.97	0.47
2:B:49:SER:CB	2:B:49:SER:HG	2.14	0.47
1:A:138:SER:CB	1:A:138:SER:C	2.81	0.47
2:D:20:VAL:HG22	2:D:21:ASP:N	2.30	0.47
2:D:49:SER:N	2:D:50:THR:N	2.63	0.47
1:C:113:LEU:HB3	1:C:113:LEU:HD13	1.96	0.47
1:C:56:LYS:CG	1:C:56:LYS:HE3	2.42	0.47
1:C:61:LYS:CD	1:C:61:LYS:HZ3	2.25	0.47
2:D:45:PHE:O	2:D:46:GLY:CA	2.44	0.46
1:A:76:MET:O	1:A:77:PRO:C	2.49	0.46
1:C:56:LYS:HE3	1:C:56:LYS:HG3	1.98	0.46
2:D:47:ASP:CB	2:D:47:ASP:C	2.84	0.46
2:B:12:THR:CG2	2:B:12:THR:HG1	2.16	0.46
2:D:5:PRO:HA	2:D:8:LYS:HB3	1.96	0.46
2:D:15:TRP:HE1	2:D:72:SER:HB3	1.80	0.46
1:A:23:GLU:CD	1:A:23:GLU:CB	2.80	0.46
1:C:70:VAL:C	1:C:70:VAL:CB	2.70	0.46
1:C:116:GLU:CB	1:C:116:GLU:OE1	2.63	0.46
2:B:2:HIS:ND1	2:B:2:HIS:O	2.48	0.46
2:B:2:HIS:CG	2:B:2:HIS:O	2.69	0.46
2:B:6:GLU:C	2:B:6:GLU:HB2	2.36	0.46
2:D:82:LYS:HD3	2:D:143:HIS:NE2	2.31	0.46
1:A:64:ASP:CB	1:A:64:ASP:OD1	2.62	0.46
1:A:87:HIS:C	1:A:87:HIS:N	2.62	0.46
2:B:74:GLY:C	2:B:75:LEU:CA	2.73	0.46
1:C:3:SER:O	1:C:7:LYS:HG3	2.16	0.45
1:A:1:VAL:HG23	1:A:1:VAL:H1	1.64	0.45
1:A:85:ASP:OD2	1:A:85:ASP:CB	2.62	0.45
2:B:1:VAL:O	2:B:2:HIS:CA	2.63	0.45
1:C:76:MET:SD	1:C:76:MET:HB3	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:LEU:N	2:D:49:SER:N	2.63	0.45
3:D:148:HEM:CGD	3:D:148:HEM:CAD	2.85	0.45
1:C:92:ARG:NH2	1:C:92:ARG:HD2	2.28	0.45
2:B:6:GLU:CD	2:B:6:GLU:CB	2.69	0.45
2:D:2:HIS:ND1	2:D:2:HIS:CB	2.77	0.45
1:A:16:LYS:HG2	1:A:16:LYS:NZ	2.31	0.45
2:B:52:ASP:CB	2:B:52:ASP:OD1	2.44	0.45
2:D:90:GLU:CD	2:D:90:GLU:CB	2.85	0.45
2:B:57:ASN:CA	2:B:58:PRO:CD	2.95	0.45
2:D:20:VAL:HG23	2:D:20:VAL:HA	1.93	0.45
1:A:103:HIS:HE1	2:B:131:GLN:OE1	2.00	0.45
2:B:1:VAL:N	5:B:197:HOH:O	2.50	0.45
2:B:139:ASN:CA	2:B:139:ASN:OD1	2.61	0.45
1:C:137:THR:C	1:C:137:THR:CB	2.76	0.45
2:D:1:VAL:C	2:D:1:VAL:CB	2.81	0.45
2:D:121:GLU:CB	2:D:121:GLU:OE2	2.65	0.45
1:A:29:LEU:CB	1:A:29:LEU:C	2.74	0.45
2:B:89:SER:OG	2:B:144:LYS:HB2	2.17	0.45
1:A:17:VAL:C	1:A:18:GLY:C	2.74	0.44
1:A:55:VAL:O	1:A:56:LYS:C	2.53	0.44
2:D:10:ALA:CA	2:D:11:VAL:N	2.65	0.44
1:A:18:GLY:C	1:A:18:GLY:N	2.61	0.44
2:B:82:LYS:CE	2:B:82:LYS:CB	2.78	0.44
1:C:30:GLU:OE2	1:C:50:HIS:HD2	1.99	0.44
2:D:12:THR:CA	2:D:12:THR:HG23	2.41	0.44
2:D:124:PRO:C	2:D:125:PRO:CD	2.67	0.44
1:A:28:ALA:CB	1:A:105:LEU:HD23	2.48	0.44
2:B:79:ASP:OD2	2:B:79:ASP:HA	2.16	0.44
2:B:80:ASN:O	2:B:81:LEU:CA	2.63	0.44
2:D:20:VAL:CA	2:D:20:VAL:HG12	2.41	0.44
1:C:105:LEU:HD23	1:C:129:LEU:HD22	2.00	0.44
2:D:94:ASP:N	2:D:94:ASP:HB2	2.29	0.44
1:A:29:LEU:CB	1:A:29:LEU:N	2.74	0.44
2:D:20:VAL:CA	2:D:20:VAL:HG13	2.41	0.44
2:D:43:GLU:CG	2:D:43:GLU:N	2.78	0.44
1:A:43:PHE:N	1:A:44:PRO:CD	2.80	0.43
2:B:65:LYS:CG	2:B:65:LYS:HE2	2.39	0.43
2:D:6:GLU:HB2	2:D:6:GLU:C	2.38	0.43
2:B:6:GLU:N	2:B:7:GLU:N	2.65	0.43
2:B:90:GLU:CB	2:B:90:GLU:N	2.64	0.43
2:D:47:ASP:CA	2:D:48:LEU:H	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LYS:CE	2:B:144:LYS:HD3	2.29	0.43
2:D:17:LYS:HE3	2:D:121:GLU:OE1	2.17	0.43
2:B:2:HIS:CB	2:B:2:HIS:O	2.66	0.43
2:B:79:ASP:O	2:B:80:ASN:CA	2.65	0.43
2:D:63:HIS:CE1	3:D:148:HEM:C4D	3.06	0.43
1:C:113:LEU:HD13	1:C:116:GLU:HB2	1.99	0.43
2:B:41:PHE:N	2:B:42:PHE:H	2.16	0.43
3:C:142:HEM:CGA	3:C:142:HEM:CAA	2.95	0.43
2:D:47:ASP:HB3	2:D:47:ASP:O	2.19	0.43
2:B:63:HIS:CE1	3:B:148:HEM:C4D	3.05	0.43
1:C:86:LEU:CD2	3:C:142:HEM:HBA2	2.49	0.43
2:B:74:GLY:O	2:B:75:LEU:CA	2.67	0.42
1:C:94:ASP:OD2	1:C:96:VAL:HG13	2.18	0.42
2:D:17:LYS:HD3	2:D:17:LYS:HZ2	1.81	0.42
1:A:78:ASN:ND2	1:A:78:ASN:HA	2.30	0.42
2:B:123:THR:CA	2:B:124:PRO:CD	2.97	0.42
2:D:53:ALA:C	2:D:53:ALA:HB1	2.33	0.42
2:D:80:ASN:OD1	2:D:80:ASN:HB2	2.18	0.42
2:D:6:GLU:N	2:D:7:GLU:N	2.67	0.42
1:C:30:GLU:OE1	1:C:30:GLU:CB	2.66	0.42
2:D:79:ASP:C	2:D:80:ASN:HB3	2.39	0.42
1:A:56:LYS:CD	1:A:56:LYS:HB3	2.44	0.42
2:D:59:LYS:N	2:D:60:VAL:N	2.67	0.42
1:A:7:LYS:O	1:A:11:LYS:HG3	2.19	0.42
2:B:10:ALA:C	2:B:10:ALA:N	2.54	0.42
2:D:6:GLU:CA	2:D:7:GLU:N	2.77	0.42
2:D:47:ASP:HB3	2:D:47:ASP:H	1.80	0.42
1:A:87:HIS:N	1:A:88:ALA:N	2.67	0.42
1:C:56:LYS:CE	1:C:56:LYS:HG3	2.46	0.42
1:A:16:LYS:HG3	1:A:16:LYS:O	2.20	0.42
1:A:56:LYS:CE	1:A:56:LYS:CG	2.98	0.42
2:B:101:GLU:CG	2:B:101:GLU:OE1	2.59	0.42
2:D:123:THR:HB	2:D:124:PRO:HD2	2.02	0.42
2:B:65:LYS:CD	2:B:65:LYS:HB2	2.46	0.41
2:D:52:ASP:HB2	2:D:52:ASP:H	1.84	0.41
1:C:43:PHE:N	1:C:44:PRO:CD	2.84	0.41
2:D:121:GLU:CB	2:D:121:GLU:CD	2.68	0.41
2:D:141:LEU:HD23	2:D:141:LEU:HA	2.03	0.41
2:D:22:GLU:CD	2:D:22:GLU:CB	2.87	0.41
1:C:2:LEU:O	1:C:2:LEU:CB	2.69	0.41
1:A:60:LYS:CD	1:A:60:LYS:NZ	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:CB	2:B:65:LYS:N	2.65	0.41
2:B:117:HIS:ND1	2:B:117:HIS:NE2	2.57	0.41
1:C:138:SER:CB	1:C:138:SER:C	2.89	0.41
2:D:88:LEU:HA	2:D:88:LEU:HD23	1.92	0.41
2:D:79:ASP:CA	2:D:79:ASP:OD2	2.69	0.41
2:D:92:HIS:HA	2:D:96:LEU:HB2	2.02	0.41
1:A:85:ASP:OD1	1:A:85:ASP:CA	2.67	0.40
1:C:105:LEU:CD1	1:C:105:LEU:HB2	2.49	0.40
2:D:52:ASP:CB	2:D:52:ASP:H	2.28	0.40
2:D:17:LYS:O	2:D:18:VAL:CA	2.68	0.40
2:B:101:GLU:CB	2:B:101:GLU:OE1	2.70	0.40
2:B:142:ALA:N	2:B:143:HIS:N	2.69	0.40
2:B:145:TYR:C	2:B:145:TYR:N	2.61	0.40
2:B:77:HIS:CD2	2:B:77:HIS:HA	2.56	0.40
1:A:21:ALA:C	1:A:21:ALA:N	2.72	0.40
1:C:2:LEU:HD23	1:C:2:LEU:HA	1.95	0.40
3:D:148:HEM:O1D	3:D:148:HEM:HBD1	2.17	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASP:OD2	5:B:204:HOH:O[2_657]	1.41	0.79
5:B:204:HOH:O	5:C:161:HOH:O[2_647]	2.02	0.18

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	139/141 (99%)	122 (88%)	14 (10%)	3 (2%)	6 1
1	C	139/141 (99%)	126 (91%)	13 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	144/146 (99%)	129 (90%)	14 (10%)	1 (1%)	22	8
2	D	144/146 (99%)	128 (89%)	13 (9%)	3 (2%)	7	1
All	All	566/574 (99%)	505 (89%)	54 (10%)	7 (1%)	13	3

All (7) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	105 (93%)	8 (7%)	14	2
1	C	113/113 (100%)	110 (97%)	3 (3%)	44	21
2	B	118/118 (100%)	106 (90%)	12 (10%)	7	1
2	D	118/118 (100%)	101 (86%)	17 (14%)	3	0
All	All	462/462 (100%)	422 (91%)	40 (9%)	10	1

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	4	PRO
1	A	45	HIS
1	A	52	SER
1	A	75	ASP

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Mol	Chain	Res	Type
1	A	84	SER
1	A	95	PRO
1	A	138	SER
2	B	1	VAL
2	B	6	GLU
2	B	9	SER
2	B	26	GLU
2	B	32	LEU
2	B	36	PRO
2	B	50	THR
2	B	51	PRO
2	B	65	LYS
2	B	68	LEU
2	B	117	HIS
2	B	146	HIS
1	C	16	LYS
1	C	114	PRO
1	C	138	SER
2	D	1	VAL
2	D	6	GLU
2	D	9	SER
2	D	21	ASP
2	D	22	GLU
2	D	26	GLU
2	D	43	GLU
2	D	47	ASP
2	D	66	LYS
2	D	68	LEU
2	D	72	SER
2	D	75	LEU
2	D	79	ASP
2	D	80	ASN
2	D	92	HIS
2	D	139	ASN
2	D	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	103	HIS
2	B	63	HIS

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Mol	Chain	Res	Type
1	C	50	HIS
1	C	68	ASN
1	C	72	HIS
1	C	103	HIS
1	C	112	HIS
2	D	63	HIS
2	D	80	ASN
2	D	139	ASN

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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEM	D	148	2	27,50,50	4.87	18 (66%)	17,82,82	4.06	9 (52%)
3	HEM	A	142	1	27,50,50	2.75	13 (48%)	17,82,82	3.16	11 (64%)
3	HEM	C	142	1	27,50,50	3.20	15 (55%)	17,82,82	5.10	14 (82%)
3	HEM	B	148	2	27,50,50	3.77	13 (48%)	17,82,82	8.81	13 (76%)

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	D	148	2	-	0/6/54/54	-
3	HEM	A	142	1	-	0/6/54/54	-
3	HEM	C	142	1	-	0/6/54/54	-
3	HEM	B	148	2	-	1/6/54/54	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	148	HEM	CAA-C2A	11.26	1.68	1.52
3	D	148	HEM	C1C-C2C	9.72	1.64	1.42
3	B	148	HEM	C3C-C2C	9.31	1.53	1.40
3	D	148	HEM	C3B-C2B	-8.55	1.28	1.40
3	B	148	HEM	C3B-C2B	-8.31	1.28	1.40
3	C	142	HEM	C3B-CAB	7.36	1.62	1.47
3	D	148	HEM	C1D-CHD	7.09	1.60	1.41
3	D	148	HEM	C4A-NA	-7.03	1.21	1.36
3	B	148	HEM	C3B-CAB	6.58	1.61	1.47
3	B	148	HEM	CMB-C2B	-6.38	1.36	1.51
3	D	148	HEM	C3B-CAB	6.27	1.60	1.47
3	C	142	HEM	C3B-C2B	-6.01	1.32	1.40
3	B	148	HEM	C1B-C2B	5.94	1.56	1.42
3	B	148	HEM	CAD-C3D	5.87	1.62	1.52
3	D	148	HEM	C3C-CAC	-5.70	1.36	1.47
3	C	142	HEM	C1B-C2B	5.64	1.55	1.42
3	A	142	HEM	C4D-C3D	-5.57	1.30	1.42
3	D	148	HEM	C3D-C2D	5.52	1.54	1.37
3	C	142	HEM	CMB-C2B	-5.45	1.38	1.51
3	A	142	HEM	C4B-NB	5.24	1.47	1.36
3	A	142	HEM	C1A-CHA	-5.17	1.26	1.41
3	C	142	HEM	C1C-C2C	5.00	1.53	1.42
3	C	142	HEM	CAD-C3D	4.62	1.60	1.52
3	D	148	HEM	CBB-CAB	-4.60	0.98	1.29
3	B	148	HEM	CMA-C3A	-4.48	1.42	1.51
3	C	142	HEM	C3C-CAC	-4.46	1.38	1.47
3	D	148	HEM	CMB-C2B	-4.39	1.41	1.51
3	A	142	HEM	C3B-C2B	4.35	1.46	1.40
3	D	148	HEM	CBA-CAA	-4.25	1.23	1.53
3	D	148	HEM	CMA-C3A	-4.09	1.43	1.51
3	D	148	HEM	C1B-C2B	-3.97	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	148	HEM	CMC-C2C	3.93	1.60	1.51
3	A	142	HEM	CMD-C2D	3.89	1.59	1.51
3	A	142	HEM	CBD-CAD	-3.89	1.26	1.53
3	A	142	HEM	C1D-ND	-3.62	1.28	1.36
3	A	142	HEM	CBA-CAA	-3.47	1.29	1.53
3	B	148	HEM	CAA-C2A	3.25	1.56	1.52
3	D	148	HEM	C2A-C3A	-3.13	1.28	1.37
3	B	148	HEM	C3C-CAC	-2.91	1.41	1.47
3	C	142	HEM	C4B-NB	-2.76	1.30	1.36
3	C	142	HEM	CBC-CAC	2.76	1.47	1.29
3	B	148	HEM	C1A-NA	2.70	1.41	1.36
3	C	142	HEM	CMA-C3A	-2.69	1.46	1.51
3	A	142	HEM	C3B-CAB	-2.64	1.42	1.47
3	D	148	HEM	C1D-ND	2.61	1.41	1.36
3	A	142	HEM	C1B-C2B	-2.46	1.37	1.42
3	A	142	HEM	C3C-CAC	-2.39	1.42	1.47
3	C	142	HEM	C1D-CHD	2.36	1.47	1.41
3	B	148	HEM	C4D-C3D	2.35	1.47	1.42
3	C	142	HEM	CMD-C2D	-2.29	1.46	1.51
3	A	142	HEM	CMC-C2C	-2.29	1.46	1.51
3	C	142	HEM	C3C-C2C	2.29	1.43	1.40
3	C	142	HEM	C4D-C3D	-2.26	1.37	1.42
3	A	142	HEM	CMA-C3A	-2.21	1.47	1.51
3	D	148	HEM	C4B-CHC	-2.19	1.34	1.41
3	B	148	HEM	C1A-CHA	-2.18	1.34	1.41
3	D	148	HEM	CAD-C3D	2.16	1.56	1.52
3	B	148	HEM	C4A-NA	2.16	1.40	1.36
3	C	142	HEM	C2A-C3A	-2.03	1.31	1.37

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	148	HEM	C4C-C3C-C2C	-21.01	92.22	106.90
3	B	148	HEM	C4A-C3A-C2A	-15.50	96.21	107.00
3	B	148	HEM	C1D-C2D-C3D	-13.79	97.40	107.00
3	B	148	HEM	C3C-C4C-NC	10.33	130.44	110.94
3	B	148	HEM	CMB-C2B-C3B	10.30	143.95	124.68
3	D	148	HEM	C1D-C2D-C3D	-9.84	100.15	107.00
3	C	142	HEM	C1D-C2D-C3D	-8.95	100.77	107.00
3	B	148	HEM	CAA-CBA-CGA	8.51	126.96	112.67
3	A	142	HEM	CAA-CBA-CGA	-8.42	98.55	112.67
3	C	142	HEM	CAA-CBA-CGA	-8.15	98.99	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	148	HEM	C4C-C3C-C2C	-7.86	101.41	106.90
3	C	142	HEM	CMA-C3A-C2A	7.49	139.07	124.94
3	B	148	HEM	CMD-C2D-C3D	7.23	138.58	124.94
3	C	142	HEM	C4A-C3A-C2A	-7.09	102.06	107.00
3	C	142	HEM	CMB-C2B-C3B	6.51	136.86	124.68
3	C	142	HEM	CMA-C3A-C4A	-6.47	118.52	128.46
3	B	148	HEM	CAD-C3D-C2D	-5.84	110.47	127.25
3	C	142	HEM	CMD-C2D-C3D	5.39	135.11	124.94
3	B	148	HEM	CMA-C3A-C2A	5.38	135.08	124.94
3	D	148	HEM	CAA-CBA-CGA	5.03	121.12	112.67
3	D	148	HEM	C4A-C3A-C2A	-4.92	103.57	107.00
3	C	142	HEM	CAA-C2A-C3A	-4.51	114.29	127.25
3	D	148	HEM	CBA-CAA-C2A	-4.29	104.57	112.49
3	B	148	HEM	CBD-CAD-C3D	4.04	119.92	112.48
3	A	142	HEM	CAD-CBD-CGD	3.78	119.01	112.67
3	A	142	HEM	C4C-C3C-C2C	-3.77	104.26	106.90
3	A	142	HEM	C3C-C4C-NC	-3.70	103.97	110.94
3	C	142	HEM	C4C-C3C-C2C	3.66	109.45	106.90
3	D	148	HEM	CMA-C3A-C2A	3.58	131.70	124.94
3	D	148	HEM	CAD-C3D-C2D	-3.44	117.36	127.25
3	B	148	HEM	CAD-CBD-CGD	3.13	117.93	112.67
3	A	142	HEM	C3B-C4B-NB	-3.09	105.21	109.21
3	B	148	HEM	CAA-C2A-C3A	-2.99	118.65	127.25
3	B	148	HEM	CMD-C2D-C1D	-2.99	123.88	128.46
3	C	142	HEM	CMD-C2D-C1D	-2.98	123.89	128.46
3	A	142	HEM	CMB-C2B-C3B	2.94	130.18	124.68
3	C	142	HEM	C3C-C4C-NC	-2.91	105.46	110.94
3	C	142	HEM	CAD-C3D-C2D	-2.83	119.10	127.25
3	D	148	HEM	CMB-C2B-C3B	2.67	129.68	124.68
3	D	148	HEM	CMA-C3A-C4A	-2.60	124.47	128.46
3	A	142	HEM	CMC-C2C-C3C	-2.56	119.89	124.68
3	A	142	HEM	C1D-C2D-C3D	-2.41	105.32	107.00
3	C	142	HEM	CBD-CAD-C3D	-2.36	108.14	112.48
3	A	142	HEM	CBA-CAA-C2A	-2.33	108.20	112.49
3	A	142	HEM	CAD-C3D-C2D	-2.08	121.26	127.25
3	A	142	HEM	CMD-C2D-C1D	-2.06	125.30	128.46
3	C	142	HEM	CAD-CBD-CGD	-2.05	109.22	112.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	148	HEM	C4D-C3D-CAD-CBD

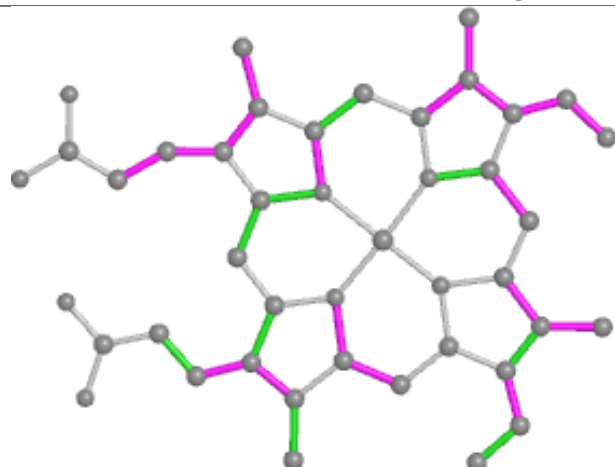
There are no ring outliers.

4 monomers are involved in 41 short contacts:

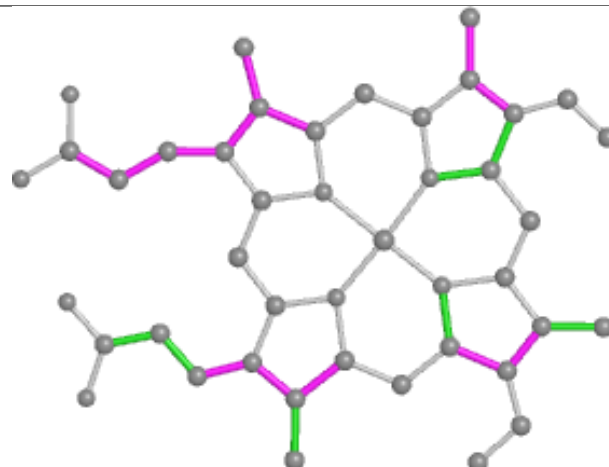
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	148	HEM	11	0
3	A	142	HEM	6	0
3	C	142	HEM	14	0
3	B	148	HEM	10	0

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

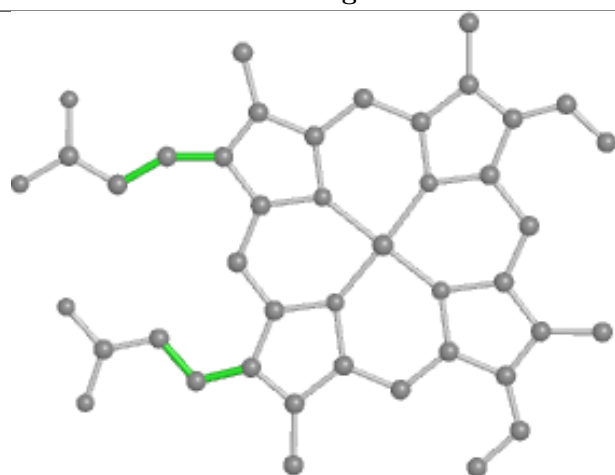
Ligand HEM D 148



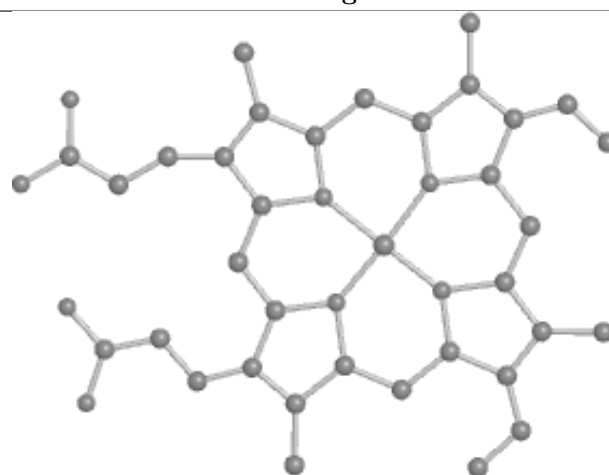
Bond lengths



Bond angles

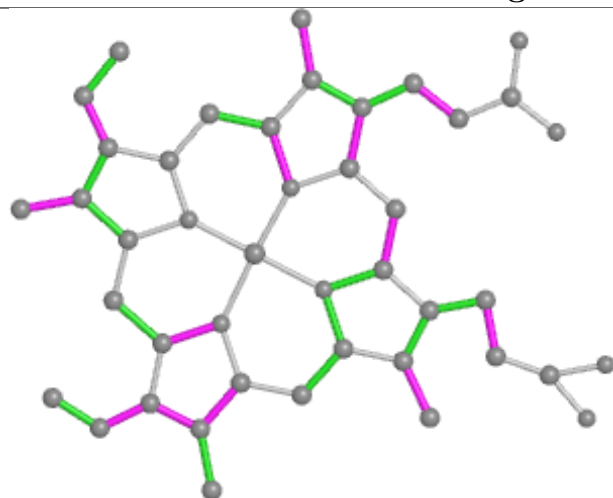


Torsions

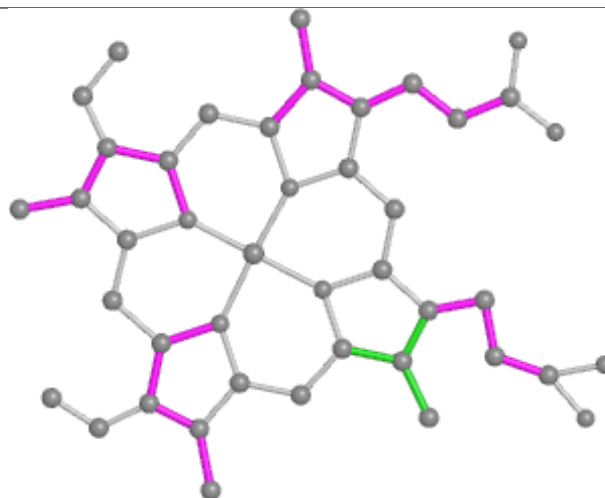


Rings

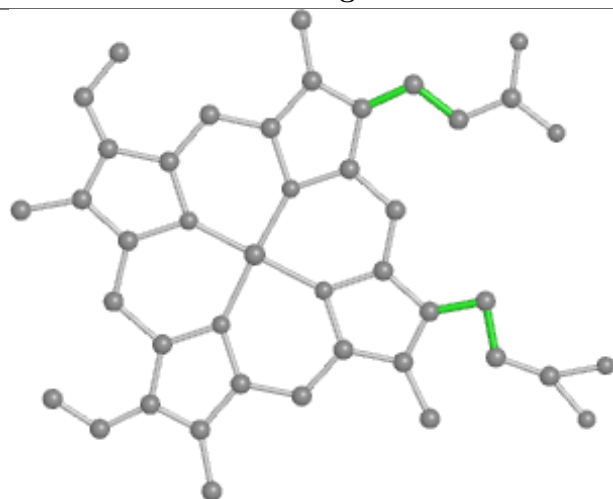
Ligand HEM A 142



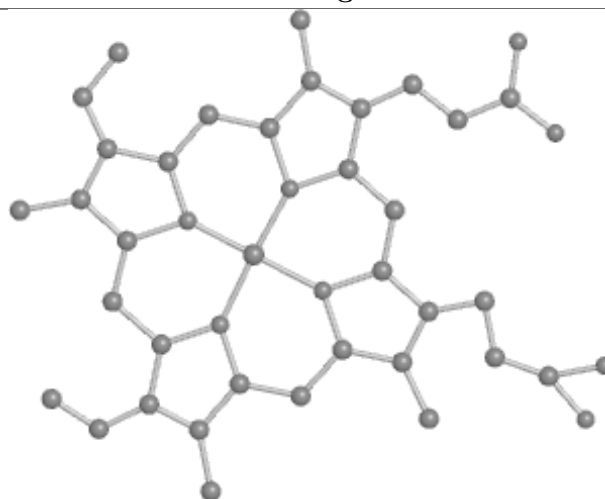
Bond lengths



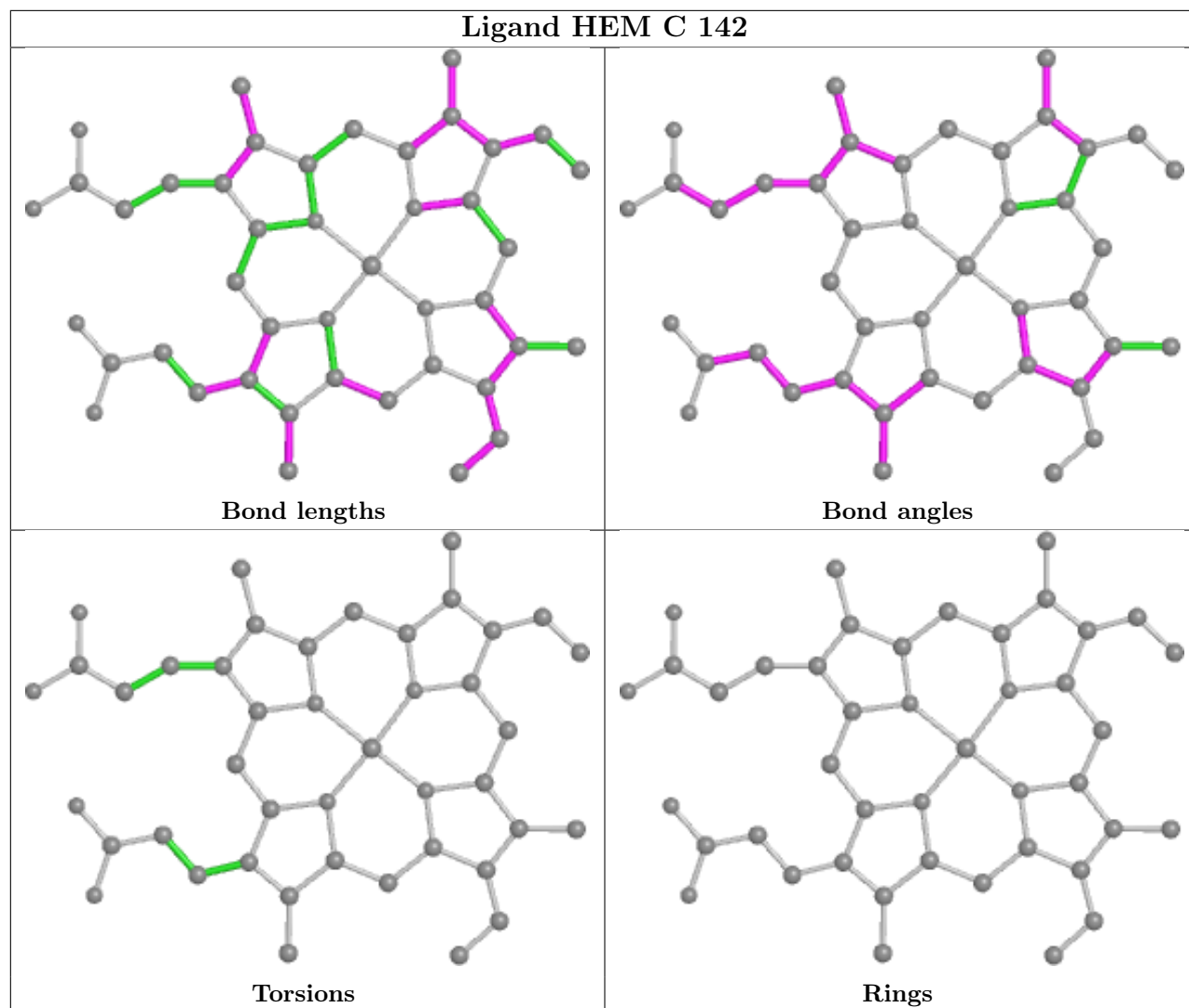
Bond angles

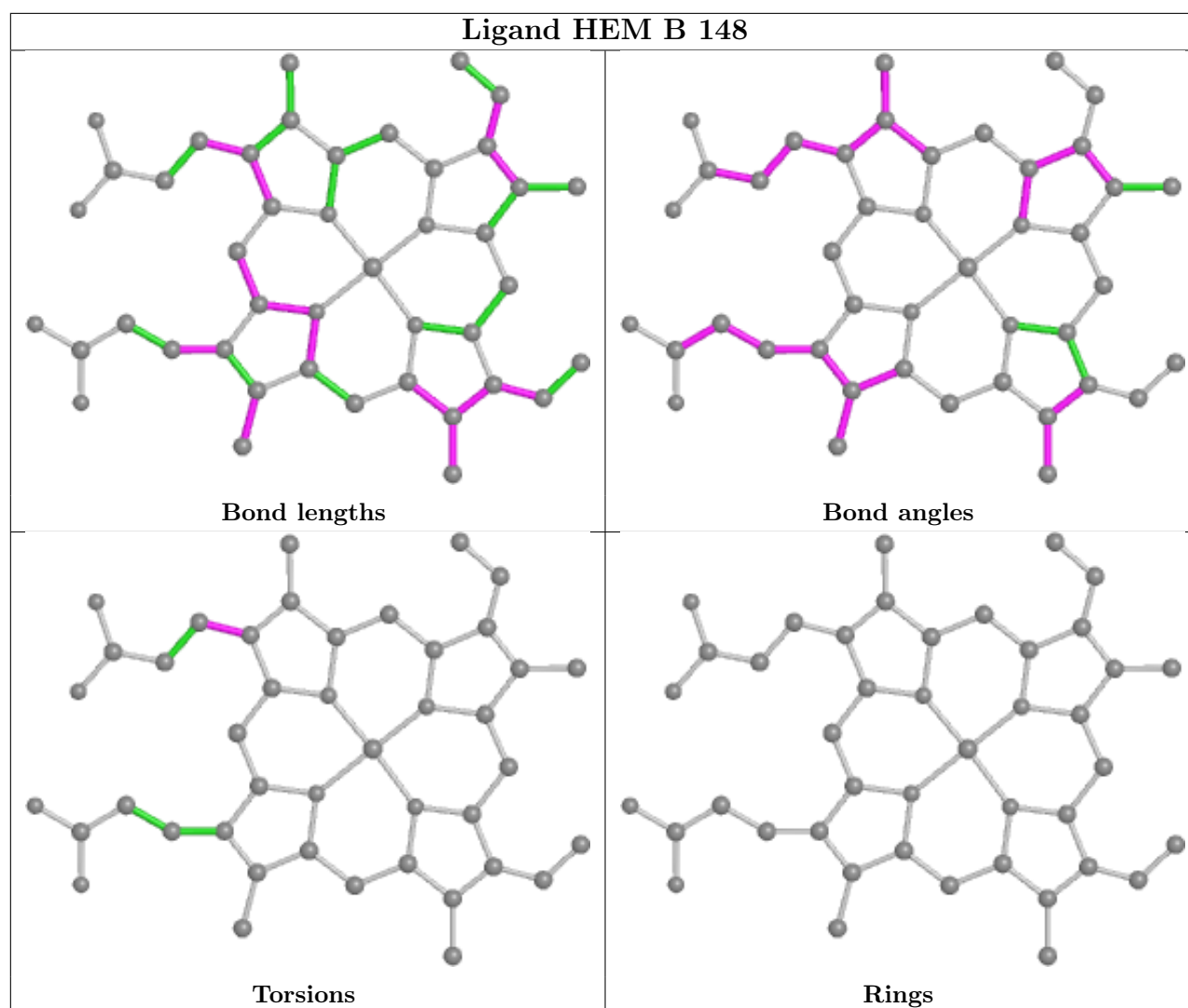


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	74:GLY	C	75:LEU	N	1.70
1	C	82:ALA	C	83:LEU	N	1.69
1	B	81:LEU	C	82:LYS	N	1.66
1	B	76:ALA	C	77:HIS	N	1.64
1	D	95:LYS	C	96:LEU	N	1.64
1	A	3:SER	C	4:PRO	N	1.62
1	A	45:HIS	C	46:PHE	N	1.62
1	D	17:LYS	C	18:VAL	N	1.61
1	D	73:ASP	C	74:GLY	N	1.61
1	B	6:GLU	C	7:GLU	N	1.20
1	B	124:PRO	C	125:PRO	N	1.20
1	C	2:LEU	C	3:SER	N	1.20
1	D	140:ALA	C	141:LEU	N	1.20
1	A	44:PRO	C	45:HIS	N	1.19
1	B	123:THR	C	124:PRO	N	1.19
1	D	30:ARG	C	31:LEU	N	1.19
1	D	47:ASP	C	48:LEU	N	1.19
1	C	133:SER	C	134:THR	N	1.18
1	D	1:VAL	C	2:HIS	N	1.18
1	D	7:GLU	C	8:LYS	N	1.18
1	D	18:VAL	C	19:ASN	N	1.18
1	A	120:ALA	C	121:VAL	N	1.17
1	C	21:ALA	C	22:GLY	N	1.17
1	C	112:HIS	C	113:LEU	N	1.17
1	A	127:LYS	C	128:PHE	N	1.16
1	D	58:PRO	C	59:LYS	N	1.16
1	B	142:ALA	C	143:HIS	N	1.15
1	D	19:ASN	C	20:VAL	N	1.15
1	A	47:ASP	C	48:LEU	N	1.13
1	B	40:ARG	C	41:PHE	N	1.13
1	B	2:HIS	C	3:LEU	N	1.12
1	C	44:PRO	C	45:HIS	N	1.11
1	C	15:GLY	C	16:LYS	N	1.09
1	B	46:GLY	C	47:ASP	N	1.07
1	C	118:THR	C	119:PRO	N	1.07
1	B	71:PHE	C	72:SER	N	1.05
1	A	2:LEU	C	3:SER	N	1.02
1	C	70:VAL	C	71:ALA	N	0.99
1	B	145:TYR	C	146:HIS	N	0.97
1	D	4:THR	C	5:PRO	N	0.97
1	A	50:HIS	C	51:GLY	N	0.96
1	A	74:ASP	C	75:ASP	N	0.93
1	A	15:GLY	C	16:LYS	N	0.92

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

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.