Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2023 – 01:17 AM EST

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

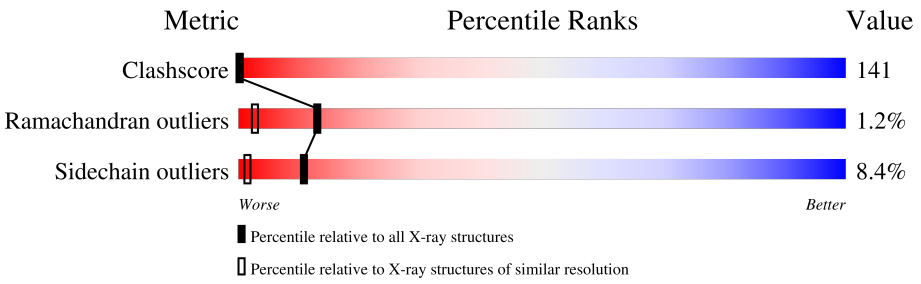
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	• 43% 30% 25%
1	C	141	6% 37% 40% 17%
2	B	146	• 46% 30% 22%
2	D	146	8% 32% 28% 32%

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.

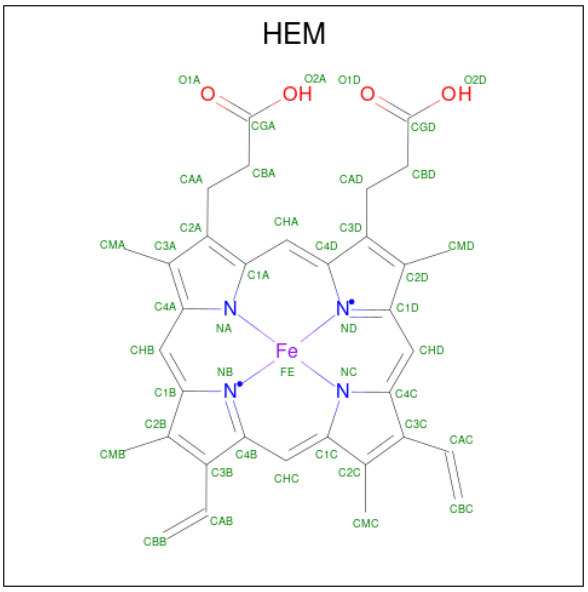
- Molecule 1 is a protein called Hemoglobin subunit alpha.

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

- Molecule 2 is a protein called Hemoglobin subunit beta.

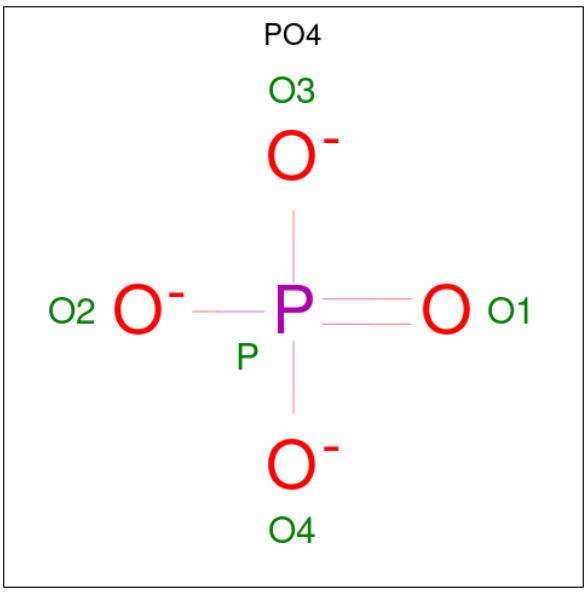
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1123	724	195	201	3	0	0	0
2	D	146	1123	724	195	201	3	0	0	0

- 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
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
3	B	1	43	34	1	4	4	0	0
3	C	1	43	34	1	4	4	0	0
3	D	1	43	34	1	4	4	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

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

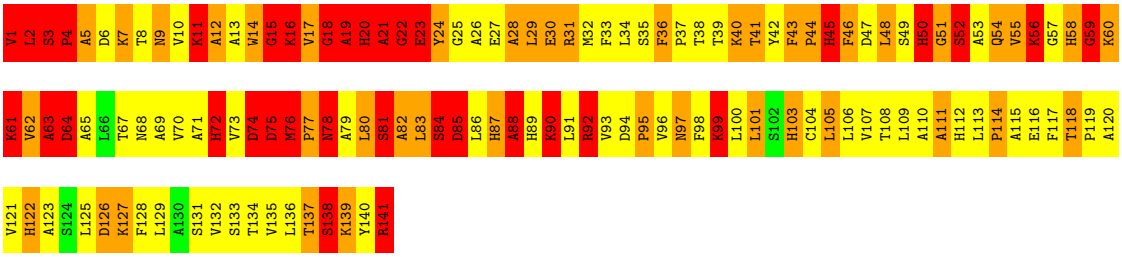
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

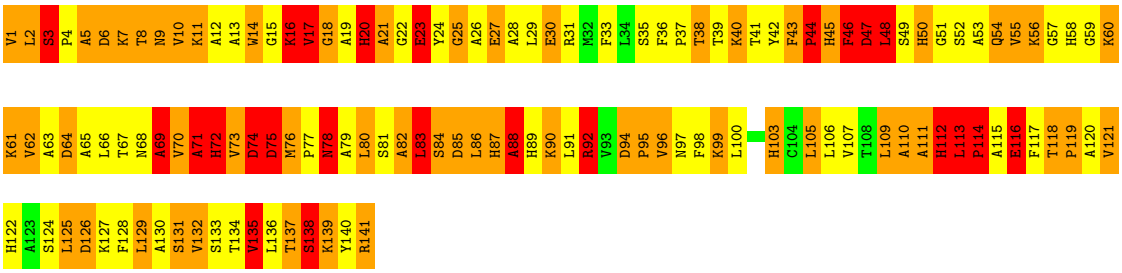
• Molecule 1: Hemoglobin subunit alpha

Chain A:



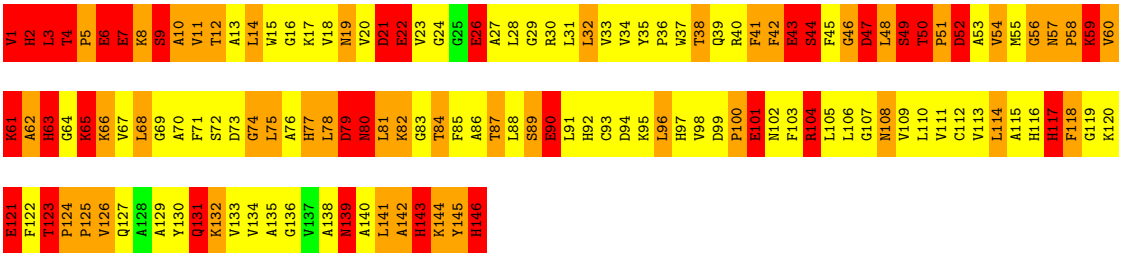
• Molecule 1: Hemoglobin subunit alpha

Chain C:



• Molecule 2: Hemoglobin subunit beta

Chain B:



• Molecule 2: Hemoglobin subunit beta

Chain D: 8% 32% 28% 32%

V1 H2 L3 T4 P5 E6 E7 K8 S9 A10 V11 T12 A13 L14 W15 G16 K17 V18 N19 V20 D21 E22 V23 G24 G25 E26 A27 L28 G29 R30 L31 L32 V33 V34 Y35 P36 W37 T38 Q39 R40 F41 F42 E43 S44 F45 G46 D47 L48 S49 T50 P51 D52 A53 V54 M55 G56 N57 P58 K59 V60

K61 A62 H63 G64 K65 K66 V67 L68 G69 A70 F71 S72 D73 G74 L75 A76 H77 L78 D79 N80 L81 K82 G83 T84 F85 A86 T87 L88 S89 E90 L91 H92 C93 D94 K95 L96 H97 V98 D99 P100 E101 N102 F103 R104 L105 L106 G107 N108 V109 L110 V111 C112 V113 L114 A115 H116 H117 F118 G119 K120

E121 F122 T123 P124 P125 V126 Q127 Y130 Q131 K132 V133 V134 A135 G136 V137 A138 N139 A140 L141 A142 H143 K144 Y145 H146

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.15Å 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	8.18	372/1097 (33.9%)	6.34	444/1491 (29.8%)
1	C	8.79	358/1097 (32.6%)	7.51	407/1491 (27.3%)
2	B	10.83	418/1153 (36.3%)	6.61	445/1566 (28.4%)
2	D	10.56	437/1153 (37.9%)	7.84	527/1566 (33.7%)
All	All	9.69	1585/4500 (35.2%)	7.11	1823/6114 (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	50
1	C	2	45
2	B	2	49
2	D	5	62
All	All	10	206

All (1585) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	GLU	CD-OE1	143.10	2.83	1.25
1	C	92	ARG	NE-CZ	126.09	2.96	1.33
2	D	6	GLU	CD-OE2	121.76	2.59	1.25
2	B	26	GLU	CD-OE2	106.91	2.43	1.25
1	C	23	GLU	CD-OE1	101.98	2.37	1.25
2	D	104	ARG	NE-CZ	96.16	2.58	1.33
1	A	92	ARG	NE-CZ	95.64	2.57	1.33
2	B	22	GLU	CD-OE2	78.68	2.12	1.25
2	B	104	ARG	NE-CZ	61.71	2.13	1.33
2	D	90	GLU	CG-CD	60.84	2.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	43	GLU	CG-CD	60.68	2.42	1.51
2	D	22	GLU	CG-CD	58.05	2.39	1.51
2	B	121	GLU	CD-OE1	56.02	1.87	1.25
2	D	52	ASP	CG-OD2	51.93	2.44	1.25
2	D	2	HIS	CG-ND1	49.82	2.48	1.38
2	B	104	ARG	CZ-NH2	49.78	1.97	1.33
2	D	26	GLU	CD-OE1	48.95	1.79	1.25
1	A	60	LYS	CE-NZ	47.97	2.69	1.49
1	A	90	LYS	CE-NZ	47.25	2.67	1.49
2	B	22	GLU	CD-OE1	46.76	1.77	1.25
1	C	1	VAL	CB-CG2	45.67	2.48	1.52
2	B	65	LYS	CE-NZ	44.01	2.59	1.49
2	D	73	ASP	CG-OD2	43.86	2.26	1.25
1	C	1	VAL	N-CA	43.63	2.33	1.46
1	C	116	GLU	CB-CG	42.96	2.33	1.52
1	C	23	GLU	CG-CD	42.52	2.15	1.51
1	A	23	GLU	CD-OE1	42.43	1.72	1.25
2	B	104	ARG	CZ-NH1	42.08	1.87	1.33
1	C	92	ARG	CZ-NH1	41.74	1.87	1.33
2	D	26	GLU	CD-OE2	41.30	1.71	1.25
2	B	2	HIS	CG-CD2	41.16	2.05	1.35
1	C	30	GLU	CD-OE2	-41.16	0.80	1.25
1	C	138	SER	CA-CB	40.99	2.14	1.52
2	D	22	GLU	CB-CG	-40.05	0.76	1.52
2	D	132	LYS	CE-NZ	39.96	2.48	1.49
1	A	75	ASP	CB-CG	-39.78	0.68	1.51
1	A	138	SER	CA-CB	39.63	2.12	1.52
2	D	43	GLU	CB-CG	-38.92	0.78	1.52
2	D	5	PRO	CA-CB	38.88	2.31	1.53
1	A	23	GLU	CG-CD	38.87	2.10	1.51
2	D	58	PRO	CG-CD	-38.66	0.23	1.50
2	B	117	HIS	CD2-NE2	37.98	2.21	1.42
1	A	78	ASN	CG-OD1	37.89	2.07	1.24
2	B	6	GLU	CD-OE1	37.89	1.67	1.25
2	B	6	GLU	CG-CD	36.91	2.07	1.51
2	B	121	GLU	CG-CD	36.89	2.07	1.51
2	B	139	ASN	CB-CG	-36.83	0.66	1.51
2	B	2	HIS	CB-CG	-36.80	0.83	1.50
2	B	43	GLU	CD-OE1	-36.70	0.85	1.25
2	D	101	GLU	CG-CD	36.67	2.06	1.51
2	B	90	GLU	CG-CD	36.67	2.06	1.51
1	A	92	ARG	CZ-NH2	-36.38	0.85	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	82	LYS	CD-CE	36.27	2.42	1.51
1	C	56	LYS	CD-CE	35.42	2.39	1.51
2	D	90	GLU	CD-OE1	35.19	1.64	1.25
2	B	65	LYS	CB-CG	-34.95	0.58	1.52
2	D	26	GLU	CB-CG	34.85	2.18	1.52
2	D	47	ASP	CA-C	34.66	2.43	1.52
1	C	23	GLU	CD-OE2	-34.48	0.87	1.25
2	B	82	LYS	CE-NZ	34.39	2.35	1.49
2	B	66	LYS	CD-CE	34.35	2.37	1.51
1	A	75	ASP	CG-OD2	34.24	2.04	1.25
2	B	59	LYS	CD-CE	34.19	2.36	1.51
2	B	101	GLU	CG-CD	33.86	2.02	1.51
2	B	65	LYS	CD-CE	33.62	2.35	1.51
2	B	2	HIS	ND1-CE1	33.35	2.18	1.34
1	C	1	VAL	CB-CG1	33.06	2.22	1.52
2	D	121	GLU	CG-CD	32.86	2.01	1.51
1	A	30	GLU	CG-CD	32.45	2.00	1.51
2	B	82	LYS	CD-CE	-32.41	0.70	1.51
2	D	120	LYS	CE-NZ	32.26	2.29	1.49
2	D	79	ASP	CG-OD1	32.23	1.99	1.25
2	B	2	HIS	CD2-NE2	31.98	2.09	1.42
1	A	81	SER	CA-CB	31.87	2.00	1.52
2	D	43	GLU	CD-OE1	31.86	1.60	1.25
2	D	79	ASP	CG-OD2	31.84	1.98	1.25
2	B	8	LYS	CE-NZ	31.47	2.27	1.49
2	D	47	ASP	N-CA	31.45	2.09	1.46
2	D	2	HIS	CA-CB	30.85	2.21	1.53
2	B	146	HIS	CB-CG	30.52	2.04	1.50
2	D	6	GLU	CB-CG	-30.43	0.94	1.52
2	D	66	LYS	CD-CE	30.42	2.27	1.51
2	D	43	GLU	CD-OE2	30.34	1.59	1.25
2	D	6	GLU	CG-CD	30.33	1.97	1.51
2	B	90	GLU	CD-OE1	-30.21	0.92	1.25
1	C	99	LYS	CD-CE	30.13	2.26	1.51
2	D	6	GLU	CA-C	30.02	2.31	1.52
1	A	127	LYS	CB-CG	-29.96	0.71	1.52
1	C	30	GLU	CG-CD	29.51	1.96	1.51
2	D	2	HIS	CG-CD2	29.47	1.85	1.35
2	B	49	SER	C-O	29.47	1.79	1.23
1	A	92	ARG	CG-CD	29.46	2.25	1.51
2	D	143	HIS	CG-CD2	29.11	1.85	1.35
1	C	99	LYS	CB-CG	-29.00	0.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	LYS	CD-CE	28.73	2.23	1.51
1	A	99	LYS	CE-NZ	28.58	2.20	1.49
2	B	65	LYS	CG-CD	28.58	2.49	1.52
2	D	6	GLU	CD-OE1	-28.58	0.94	1.25
2	B	12	THR	CB-CG2	-28.55	0.58	1.52
2	B	77	HIS	CG-CD2	28.35	1.83	1.35
2	D	3	LEU	C-O	28.21	1.76	1.23
2	D	65	LYS	CD-CE	27.82	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	-27.44	0.95	1.25
1	A	15	GLY	C-O	27.24	1.67	1.23
2	D	144	LYS	CE-NZ	27.12	2.16	1.49
1	A	78	ASN	CB-CG	-27.11	0.88	1.51
2	D	146	HIS	ND1-CE1	-26.98	0.67	1.34
2	D	43	GLU	CG-CD	26.85	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	-26.29	0.85	1.51
2	D	26	GLU	CG-CD	25.80	1.90	1.51
2	B	143	HIS	ND1-CE1	25.76	1.99	1.34
2	D	45	PHE	C-N	-25.48	0.87	1.33
2	B	117	HIS	CG-ND1	25.41	1.94	1.38
1	A	17	VAL	C-O	-25.41	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	-25.10	0.98	1.53
2	B	1	VAL	C-O	24.89	1.70	1.23
2	D	2	HIS	CB-CG	-24.73	1.05	1.50
1	A	75	ASP	CG-OD1	24.71	1.82	1.25
1	A	49	SER	CB-OG	-24.44	1.10	1.42
2	B	5	PRO	N-CD	24.24	1.81	1.47
2	B	8	LYS	CB-CG	-24.20	0.87	1.52
2	D	121	GLU	CD-OE1	24.18	1.52	1.25
1	C	49	SER	CB-OG	-24.16	1.10	1.42
1	A	96	VAL	CB-CG2	-24.09	1.02	1.52
2	D	76	ALA	N-CA	24.03	1.94	1.46
2	B	1	VAL	CB-CG1	24.00	2.03	1.52
2	B	1	VAL	C-N	-23.87	0.79	1.34
1	C	46	PHE	CD2-CE2	-23.55	0.92	1.39
2	B	43	GLU	CD-OE2	23.54	1.51	1.25
2	B	47	ASP	CG-OD2	23.24	1.78	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	LYS	CE-NZ	23.09	2.06	1.49
2	B	121	GLU	CB-CG	-22.88	1.08	1.52
2	B	2	HIS	CG-ND1	22.78	1.88	1.38
2	D	121	GLU	CB-CG	-22.66	1.09	1.52
2	B	22	GLU	CG-CD	22.61	1.85	1.51
2	D	77	HIS	ND1-CE1	22.61	1.91	1.34
1	C	92	ARG	CD-NE	-22.58	1.08	1.46
2	B	45	PHE	CG-CD2	-22.50	1.04	1.38
2	D	2	HIS	ND1-CE1	22.26	1.90	1.34
2	D	50	THR	CA-CB	22.25	2.11	1.53
2	B	49	SER	CB-OG	22.23	1.71	1.42
2	D	104	ARG	CD-NE	22.21	1.84	1.46
2	D	77	HIS	CD2-NE2	22.14	1.88	1.42
1	C	56	LYS	CG-CD	21.99	2.27	1.52
2	D	65	LYS	CG-CD	21.95	2.27	1.52
2	B	58	PRO	N-CD	21.91	1.78	1.47
1	A	14	TRP	CG-CD1	21.87	1.67	1.36
1	A	50	HIS	CA-CB	21.84	2.02	1.53
2	D	5	PRO	N-CA	21.75	1.84	1.47
2	B	2	HIS	CA-CB	21.69	2.01	1.53
1	A	18	GLY	CA-C	21.68	1.86	1.51
1	A	85	ASP	CG-OD1	-21.67	0.75	1.25
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	-21.45	0.97	1.52
1	C	15	GLY	C-O	21.34	1.57	1.23
2	D	146	HIS	CG-ND1	21.17	1.85	1.38
1	C	60	LYS	CE-NZ	21.17	2.02	1.49
1	A	72	HIS	CG-ND1	21.10	1.85	1.38
1	A	64	ASP	CB-CG	21.03	1.96	1.51
2	D	8	LYS	CD-CE	20.92	2.03	1.51
1	A	85	ASP	CG-OD2	20.92	1.73	1.25
2	B	49	SER	CA-CB	20.57	1.83	1.52
1	C	14	TRP	CZ3-CH2	20.54	1.73	1.40
1	A	50	HIS	C-N	-20.39	0.96	1.33
2	B	144	LYS	CE-NZ	20.27	1.99	1.49
2	B	42	PHE	CG-CD1	20.18	1.69	1.38
2	D	139	ASN	CG-OD1	20.14	1.68	1.24
2	D	42	PHE	CG-CD1	20.05	1.68	1.38
2	D	95	LYS	CE-NZ	19.98	1.99	1.49
2	B	144	LYS	CD-CE	19.94	2.01	1.51
1	A	75	ASP	CA-CB	19.92	1.97	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	146	HIS	ND1-CE1	19.87	1.84	1.34
2	D	17	LYS	CE-NZ	19.82	1.98	1.49
2	D	9	SER	CB-OG	-19.80	1.16	1.42
1	A	22	GLY	CA-C	-19.74	1.20	1.51
1	A	96	VAL	CB-CG1	-19.71	1.11	1.52
1	A	74	ASP	CG-OD1	-19.66	0.80	1.25
1	C	61	LYS	CE-NZ	19.62	1.98	1.49
1	A	84	SER	CA-CB	19.62	1.82	1.52
2	D	13	ALA	CA-CB	-19.61	1.11	1.52
1	C	22	GLY	CA-C	-19.51	1.20	1.51
2	D	4	THR	C-N	-19.45	0.97	1.34
1	A	24	TYR	CE1-CZ	-19.35	1.13	1.38
2	D	80	ASN	CG-OD1	19.29	1.66	1.24
2	D	7	GLU	CD-OE1	19.28	1.46	1.25
2	D	46	GLY	CA-C	19.22	1.82	1.51
1	C	114	PRO	CA-C	19.04	1.91	1.52
2	D	1	VAL	CA-C	19.04	2.02	1.52
2	D	95	LYS	CG-CD	18.95	2.16	1.52
2	D	7	GLU	CB-CG	18.90	1.88	1.52
2	B	45	PHE	CE1-CZ	-18.82	1.01	1.37
1	A	139	LYS	CE-NZ	18.78	1.96	1.49
1	C	72	HIS	CG-ND1	18.77	1.80	1.38
2	B	44	SER	CB-OG	-18.59	1.18	1.42
2	D	66	LYS	CE-NZ	18.55	1.95	1.49
2	D	47	ASP	CA-CB	18.51	1.94	1.53
1	A	14	TRP	CD2-CE2	18.43	1.63	1.41
2	B	79	ASP	CG-OD2	18.34	1.67	1.25
2	B	146	HIS	CG-ND1	-18.30	0.98	1.38
2	D	82	LYS	CE-NZ	18.28	1.94	1.49
1	C	84	SER	CB-OG	-18.23	1.18	1.42
1	A	15	GLY	C-N	-18.16	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
2	B	9	SER	N-CA	-18.12	1.10	1.46
1	C	112	HIS	CG-ND1	18.09	1.78	1.38
1	A	14	TRP	NE1-CE2	-18.05	1.14	1.37
2	D	8	LYS	CE-NZ	18.03	1.94	1.49
2	D	101	GLU	CD-OE2	17.98	1.45	1.25
1	A	74	ASP	C-N	-17.88	0.93	1.34
2	B	40	ARG	CZ-NH2	17.86	1.56	1.33
2	B	117	HIS	CG-CD2	17.86	1.66	1.35
2	D	20	VAL	CB-CG1	-17.81	1.15	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	LYS	CD-CE	17.80	1.95	1.51
1	C	84	SER	CA-CB	17.77	1.79	1.52
2	D	53	ALA	C-O	-17.76	0.89	1.23
1	C	20	HIS	ND1-CE1	17.70	1.79	1.34
2	B	9	SER	CA-CB	17.56	1.79	1.52
1	A	99	LYS	CD-CE	17.54	1.95	1.51
2	D	76	ALA	CA-C	-17.41	1.07	1.52
2	B	59	LYS	CE-NZ	17.33	1.92	1.49
1	A	46	PHE	CG-CD2	-17.27	1.12	1.38
2	D	22	GLU	CD-OE1	17.20	1.44	1.25
2	D	78	LEU	CG-CD2	-17.12	0.88	1.51
1	C	11	LYS	CE-NZ	17.10	1.91	1.49
1	A	60	LYS	CD-CE	17.01	1.93	1.51
1	A	67	THR	CB-OG1	-16.95	1.09	1.43
1	C	74	ASP	C-O	-16.95	0.91	1.23
1	A	37	PRO	N-CD	-16.93	1.24	1.47
2	D	58	PRO	N-CD	16.83	1.71	1.47
2	D	1	VAL	CB-CG2	-16.77	1.17	1.52
2	D	83	GLY	C-O	16.70	1.50	1.23
2	B	76	ALA	C-O	-16.66	0.91	1.23
2	B	5	PRO	N-CA	-16.65	1.19	1.47
1	A	17	VAL	CA-C	16.63	1.96	1.52
2	D	20	VAL	CB-CG2	-16.63	1.18	1.52
1	A	116	GLU	CD-OE2	16.62	1.44	1.25
2	D	19	ASN	CG-OD1	16.48	1.60	1.24
1	A	16	LYS	CD-CE	16.41	1.92	1.51
2	D	2	HIS	C-O	16.36	1.54	1.23
1	C	105	LEU	CG-CD2	16.35	2.12	1.51
2	D	144	LYS	CD-CE	-16.26	1.10	1.51
2	B	117	HIS	ND1-CE1	16.22	1.75	1.34
2	D	117	HIS	CG-ND1	16.13	1.74	1.38
2	B	87	THR	CA-CB	16.12	1.95	1.53
2	B	124	PRO	N-CD	16.09	1.70	1.47
2	B	146	HIS	CG-CD2	16.07	1.63	1.35
2	D	59	LYS	CG-CD	-16.06	0.97	1.52
2	D	43	GLU	CA-CB	-16.04	1.18	1.53
2	B	79	ASP	CB-CG	-16.03	1.18	1.51
1	C	90	LYS	CD-CE	16.00	1.91	1.51
2	D	66	LYS	CG-CD	15.98	2.06	1.52
1	A	99	LYS	CB-CG	-15.94	1.09	1.52
2	B	145	TYR	C-N	-15.93	0.97	1.34
2	D	73	ASP	C-N	15.92	1.61	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	74	GLY	C-N	15.90	1.70	1.34
2	B	139	ASN	CG-OD1	15.89	1.58	1.24
2	D	43	GLU	CA-C	15.87	1.94	1.52
2	B	132	LYS	CE-NZ	15.84	1.88	1.49
1	A	56	LYS	CG-CD	15.82	2.06	1.52
1	C	72	HIS	CG-CD2	15.71	1.62	1.35
2	B	40	ARG	NE-CZ	15.66	1.53	1.33
1	C	72	HIS	CB-CG	-15.58	1.22	1.50
2	D	1	VAL	N-CA	15.53	1.77	1.46
2	D	66	LYS	CB-CG	-15.53	1.10	1.52
1	A	131	SER	CB-OG	-15.52	1.22	1.42
1	A	137	THR	CB-CG2	-15.51	1.01	1.52
2	B	145	TYR	CD2-CE2	15.50	1.62	1.39
2	D	19	ASN	CG-ND2	15.47	1.71	1.32
2	B	21	ASP	CB-CG	15.43	1.84	1.51
1	A	99	LYS	CG-CD	-15.38	1.00	1.52
2	D	12	THR	CA-CB	15.37	1.93	1.53
2	D	130	TYR	CE1-CZ	15.37	1.58	1.38
1	C	16	LYS	CB-CG	15.32	1.94	1.52
1	C	82	ALA	C-N	15.31	1.69	1.34
2	D	117	HIS	CE1-NE2	-15.31	0.97	1.32
2	D	41	PHE	CE1-CZ	-15.26	1.08	1.37
2	D	52	ASP	N-CA	15.26	1.76	1.46
2	B	87	THR	CB-CG2	15.26	2.02	1.52
1	A	84	SER	CB-OG	-15.24	1.22	1.42
1	A	14	TRP	CB-CG	-15.22	1.22	1.50
2	B	59	LYS	CG-CD	-15.21	1.00	1.52
1	C	70	VAL	C-N	-15.11	0.99	1.34
1	A	44	PRO	CA-C	15.09	1.83	1.52
2	B	1	VAL	CA-CB	15.07	1.86	1.54
1	A	50	HIS	CG-CD2	15.04	1.61	1.35
1	A	17	VAL	C-N	14.97	1.59	1.33
1	C	14	TRP	CG-CD1	14.88	1.57	1.36
2	D	59	LYS	CD-CE	14.88	1.88	1.51
1	A	23	GLU	CD-OE2	14.85	1.42	1.25
1	A	3	SER	C-N	14.85	1.62	1.34
1	C	114	PRO	N-CA	14.84	1.72	1.47
1	C	25	GLY	C-O	14.82	1.47	1.23
2	D	80	ASN	N-CA	14.80	1.75	1.46
1	A	1	VAL	N-CA	-14.76	1.16	1.46
2	D	73	ASP	CA-CB	14.72	1.86	1.53
1	C	78	ASN	CA-C	-14.69	1.14	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	THR	CA-CB	14.64	1.91	1.53
2	D	21	ASP	CG-OD1	14.62	1.58	1.25
1	A	20	HIS	CG-ND1	14.62	1.71	1.38
2	D	117	HIS	CG-CD2	14.56	1.60	1.35
1	C	72	HIS	CA-CB	14.55	1.85	1.53
2	B	108	ASN	CB-CG	14.53	1.84	1.51
1	C	7	LYS	N-CA	14.53	1.75	1.46
2	B	143	HIS	CG-ND1	14.50	1.70	1.38
1	C	68	ASN	CG-OD1	-14.49	0.92	1.24
2	D	21	ASP	C-O	14.42	1.50	1.23
2	D	73	ASP	CG-OD1	14.40	1.58	1.25
1	A	52	SER	N-CA	14.38	1.75	1.46
2	D	8	LYS	CA-CB	14.37	1.85	1.53
1	A	16	LYS	CG-CD	14.35	2.01	1.52
2	B	44	SER	C-O	14.32	1.50	1.23
2	D	55	MET	CA-C	14.32	1.90	1.52
1	A	1	VAL	CA-CB	14.28	1.84	1.54
2	B	145	TYR	CE1-CZ	14.28	1.57	1.38
1	A	14	TRP	CE2-CZ2	-14.26	1.15	1.39
1	C	118	THR	C-N	-14.22	1.07	1.34
2	B	125	PRO	N-CD	14.18	1.67	1.47
1	C	139	LYS	CE-NZ	14.15	1.84	1.49
1	C	37	PRO	N-CD	-14.14	1.28	1.47
2	D	15	TRP	CD2-CE2	14.13	1.58	1.41
1	A	74	ASP	CG-OD2	14.06	1.57	1.25
2	D	125	PRO	N-CD	14.03	1.67	1.47
2	B	90	GLU	CA-CB	14.03	1.84	1.53
2	D	108	ASN	CB-CG	14.01	1.83	1.51
2	D	117	HIS	CB-CG	-14.01	1.24	1.50
1	C	1	VAL	CA-CB	-13.96	1.25	1.54
2	D	80	ASN	CA-CB	-13.96	1.16	1.53
1	A	2	LEU	C-N	-13.95	1.01	1.34
2	B	81	LEU	C-N	13.91	1.66	1.34
2	D	40	ARG	CZ-NH1	-13.88	1.15	1.33
2	B	66	LYS	N-CA	-13.85	1.18	1.46
1	C	14	TRP	CD2-CE2	13.73	1.57	1.41
2	D	79	ASP	CB-CG	-13.72	1.23	1.51
2	D	30	ARG	CD-NE	-13.72	1.23	1.46
2	D	76	ALA	C-O	13.67	1.49	1.23
2	B	102	ASN	CG-OD1	-13.66	0.94	1.24
2	B	130	TYR	CD2-CE2	13.64	1.59	1.39
2	D	18	VAL	CA-CB	-13.64	1.26	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	ASP	CB-CG	13.57	1.80	1.51
2	B	143	HIS	CB-CG	13.53	1.74	1.50
1	A	1	VAL	CB-CG2	-13.47	1.24	1.52
1	C	131	SER	CA-CB	13.44	1.73	1.52
2	B	1	VAL	CB-CG2	-13.43	1.24	1.52
2	B	80	ASN	N-CA	13.41	1.73	1.46
1	A	50	HIS	C-O	13.38	1.48	1.23
1	A	56	LYS	CD-CE	13.36	1.84	1.51
1	A	127	LYS	CG-CD	13.35	1.97	1.52
2	B	7	GLU	CB-CG	13.31	1.77	1.52
1	A	90	LYS	CD-CE	13.25	1.84	1.51
1	A	14	TRP	CA-CB	13.24	1.83	1.53
1	A	92	ARG	CZ-NH1	13.19	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	D	20	VAL	CA-C	-13.01	1.19	1.52
2	B	40	ARG	CZ-NH1	-13.00	1.16	1.33
2	D	49	SER	CA-C	12.98	1.86	1.52
1	C	50	HIS	CG-ND1	12.98	1.67	1.38
2	D	18	VAL	CB-CG2	12.95	1.80	1.52
1	C	68	ASN	C-O	12.95	1.48	1.23
2	B	5	PRO	CA-C	12.93	1.78	1.52
1	A	26	ALA	N-CA	-12.92	1.20	1.46
1	A	106	LEU	CB-CG	-12.92	1.15	1.52
2	D	48	LEU	N-CA	12.91	1.72	1.46
1	C	14	TRP	CD2-CE3	-12.90	1.21	1.40
2	B	40	ARG	CD-NE	-12.89	1.24	1.46
2	D	126	VAL	CA-CB	12.87	1.81	1.54
1	A	20	HIS	CE1-NE2	-12.86	1.03	1.32
2	B	46	GLY	C-O	12.83	1.44	1.23
2	B	66	LYS	CE-NZ	12.81	1.81	1.49
1	A	33	PHE	CE2-CZ	-12.80	1.13	1.37
1	C	72	HIS	CA-C	-12.77	1.19	1.52
1	A	71	ALA	CA-C	-12.76	1.19	1.52
1	A	24	TYR	CE2-CZ	12.75	1.55	1.38
1	C	140	TYR	CG-CD1	-12.73	1.22	1.39
1	A	134	THR	CB-OG1	-12.69	1.17	1.43
2	B	6	GLU	C-O	12.69	1.47	1.23
2	D	21	ASP	CB-CG	12.68	1.78	1.51
2	B	89	SER	CB-OG	12.67	1.58	1.42

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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	-12.62	1.25	1.42
2	B	73	ASP	CA-C	-12.62	1.20	1.52
2	B	71	PHE	C-N	-12.61	1.05	1.34
1	C	7	LYS	CG-CD	12.55	1.95	1.52
1	A	140	TYR	CE1-CZ	-12.50	1.22	1.38
2	B	2	HIS	CE1-NE2	12.48	1.61	1.32
1	A	56	LYS	C-N	12.47	1.55	1.33
2	D	139	ASN	CA-CB	-12.45	1.20	1.53
2	B	43	GLU	CA-CB	-12.44	1.26	1.53
2	B	8	LYS	C-O	12.43	1.47	1.23
2	D	50	THR	N-CA	12.43	1.71	1.46
1	C	75	ASP	N-CA	12.42	1.71	1.46
1	A	19	ALA	C-O	12.42	1.47	1.23
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	-12.35	1.11	1.52
2	B	80	ASN	CG-OD1	12.34	1.51	1.24
2	D	40	ARG	C-O	12.34	1.46	1.23
1	A	77	PRO	CA-C	-12.32	1.28	1.52
1	A	76	MET	CB-CG	-12.25	1.12	1.51
1	A	46	PHE	CB-CG	-12.24	1.30	1.51
1	A	45	HIS	C-N	12.23	1.62	1.34
1	C	4	PRO	N-CA	-12.21	1.26	1.47
2	B	74	GLY	N-CA	-12.21	1.27	1.46
1	C	73	VAL	CA-CB	12.20	1.80	1.54
2	D	36	PRO	N-CD	-12.19	1.30	1.47
1	A	59	GLY	CA-C	-12.19	1.32	1.51
2	D	77	HIS	CE1-NE2	-12.19	1.04	1.32
1	C	140	TYR	CE2-CZ	-12.16	1.22	1.38
1	A	24	TYR	CB-CG	12.15	1.69	1.51
2	B	2	HIS	CA-C	12.14	1.84	1.52
2	D	73	ASP	CA-C	-12.14	1.21	1.52
1	A	73	VAL	CA-C	-12.13	1.21	1.52
2	B	74	GLY	CA-C	-12.12	1.32	1.51
2	D	94	ASP	CG-OD2	12.11	1.53	1.25
2	D	117	HIS	ND1-CE1	12.09	1.65	1.34
2	D	44	SER	CA-CB	-12.07	1.34	1.52
2	D	63	HIS	CA-CB	-12.04	1.27	1.53
1	A	27	GLU	CG-CD	12.03	1.70	1.51
2	D	18	VAL	N-CA	12.03	1.70	1.46
2	B	61	LYS	CG-CD	12.01	1.93	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	SER	CA-C	-11.99	1.21	1.52
2	B	65	LYS	CA-CB	11.99	1.80	1.53
1	C	61	LYS	CD-CE	11.97	1.81	1.51
1	C	115	ALA	CA-C	-11.97	1.21	1.52
2	D	104	ARG	CZ-NH1	11.96	1.48	1.33
2	B	94	ASP	CG-OD2	-11.95	0.97	1.25
1	C	8	THR	CA-CB	11.93	1.84	1.53
2	B	63	HIS	CG-ND1	11.91	1.65	1.38
2	D	146	HIS	CE1-NE2	11.91	1.60	1.32
1	C	7	LYS	CD-CE	-11.88	1.21	1.51
1	C	20	HIS	CG-ND1	11.87	1.64	1.38
2	D	7	GLU	CD-OE2	11.86	1.38	1.25
1	A	12	ALA	C-O	11.84	1.45	1.23
2	D	79	ASP	CA-C	11.83	1.83	1.52
2	D	145	TYR	CE2-CZ	-11.82	1.23	1.38
1	C	1	VAL	CA-C	11.81	1.83	1.52
1	C	18	GLY	C-O	11.80	1.42	1.23
2	B	45	PHE	CD1-CE1	11.79	1.62	1.39
1	A	137	THR	CB-OG1	11.77	1.66	1.43
1	A	5	ALA	CA-CB	11.76	1.77	1.52
2	D	17	LYS	C-N	11.76	1.61	1.34
1	C	72	HIS	C-O	11.75	1.45	1.23
1	C	20	HIS	CB-CG	11.71	1.71	1.50
1	C	7	LYS	CE-NZ	-11.69	1.19	1.49
2	D	121	GLU	CA-CB	11.69	1.79	1.53
2	D	35	TYR	CG-CD2	-11.68	1.24	1.39
1	C	74	ASP	CG-OD1	11.66	1.52	1.25
2	D	11	VAL	CB-CG1	-11.65	1.28	1.52
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	11.55	1.63	1.34
2	D	40	ARG	CB-CG	-11.50	1.21	1.52
1	A	14	TRP	CZ2-CH2	-11.46	1.15	1.37
2	D	82	LYS	C-N	11.44	1.53	1.33
2	B	118	PHE	CD2-CE2	-11.43	1.16	1.39
2	D	52	ASP	CB-CG	11.41	1.75	1.51
2	D	131	GLN	CG-CD	11.41	1.77	1.51
2	B	104	ARG	CD-NE	11.40	1.65	1.46
1	C	133	SER	C-O	11.40	1.45	1.23
1	C	116	GLU	CD-OE1	-11.39	1.13	1.25
2	B	46	GLY	C-N	-11.38	1.07	1.34
2	B	142	ALA	CA-C	11.38	1.82	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	71	ALA	CA-CB	-11.36	1.28	1.52
2	B	90	GLU	CB-CG	-11.36	1.30	1.52
1	A	15	GLY	CA-C	11.34	1.70	1.51
1	A	64	ASP	CG-OD1	11.34	1.51	1.25
2	D	130	TYR	CD1-CE1	11.33	1.56	1.39
1	C	87	HIS	CA-C	11.32	1.82	1.52
1	C	119	PRO	N-CD	11.31	1.63	1.47
1	A	71	ALA	C-O	11.29	1.44	1.23
2	D	78	LEU	CA-CB	11.29	1.79	1.53
2	B	1	VAL	N-CA	11.28	1.69	1.46
1	C	78	ASN	CB-CG	11.27	1.76	1.51
2	D	78	LEU	C-O	-11.26	1.01	1.23
1	C	16	LYS	CA-C	11.23	1.82	1.52
2	D	12	THR	N-CA	11.23	1.68	1.46
1	C	72	HIS	ND1-CE1	-11.23	1.06	1.34
2	B	145	TYR	CA-CB	-11.23	1.29	1.53
2	B	69	GLY	N-CA	-11.23	1.29	1.46
1	A	4	PRO	C-N	11.21	1.59	1.34
1	A	7	LYS	C-N	11.19	1.59	1.34
1	A	29	LEU	CA-CB	11.19	1.79	1.53
1	C	24	TYR	CD2-CE2	11.18	1.56	1.39
2	D	19	ASN	C-O	11.18	1.44	1.23
2	B	121	GLU	CD-OE2	-11.17	1.13	1.25
1	C	24	TYR	CG-CD1	11.15	1.53	1.39
1	C	11	LYS	CA-C	-11.13	1.24	1.52
2	B	81	LEU	N-CA	11.11	1.68	1.46
1	A	72	HIS	CA-CB	11.10	1.78	1.53
2	B	79	ASP	C-O	-11.09	1.02	1.23
2	D	7	GLU	CG-CD	-11.08	1.35	1.51
1	C	90	LYS	CG-CD	11.07	1.90	1.52
2	D	143	HIS	ND1-CE1	11.07	1.62	1.34
2	D	4	THR	CA-CB	11.06	1.82	1.53
2	D	6	GLU	C-O	-11.06	1.02	1.23
1	C	10	VAL	CA-C	11.05	1.81	1.52
2	D	8	LYS	N-CA	11.03	1.68	1.46
1	A	128	PHE	CG-CD2	-11.01	1.22	1.38
2	D	73	ASP	CB-CG	-11.00	1.28	1.51
2	B	26	GLU	CB-CG	10.99	1.73	1.52
2	B	118	PHE	CG-CD2	10.99	1.55	1.38
2	D	102	ASN	C-O	10.99	1.44	1.23
1	C	128	PHE	CG-CD2	-10.97	1.22	1.38
2	D	18	VAL	CB-CG1	-10.97	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	19	ALA	C-O	10.94	1.44	1.23
1	C	75	ASP	C-N	10.94	1.59	1.34
1	A	33	PHE	CG-CD2	10.92	1.55	1.38
2	D	94	ASP	N-CA	10.91	1.68	1.46
1	C	70	VAL	N-CA	10.88	1.68	1.46
2	D	82	LYS	CG-CD	10.87	1.89	1.52
2	D	45	PHE	CD1-CE1	10.85	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	D	40	ARG	NE-CZ	10.81	1.47	1.33
2	B	49	SER	N-CA	10.77	1.67	1.46
1	A	112	HIS	ND1-CE1	10.77	1.61	1.34
1	A	141	ARG	NE-CZ	10.76	1.47	1.33
2	B	7	GLU	CD-OE2	10.73	1.37	1.25
1	C	20	HIS	CE1-NE2	10.73	1.57	1.32
2	B	2	HIS	C-O	10.72	1.43	1.23
1	A	58	HIS	CB-CG	10.70	1.69	1.50
1	C	49	SER	C-N	10.68	1.58	1.34
1	A	49	SER	C-N	10.67	1.58	1.34
2	B	80	ASN	CB-CG	10.66	1.75	1.51
1	C	15	GLY	C-N	-10.66	1.09	1.34
2	D	144	LYS	CA-CB	-10.66	1.30	1.53
1	C	38	THR	CA-CB	10.65	1.81	1.53
2	B	22	GLU	CB-CG	-10.64	1.31	1.52
2	D	93	CYS	CB-SG	10.61	2.00	1.82
2	D	101	GLU	CB-CG	10.61	1.72	1.52
2	B	47	ASP	N-CA	10.59	1.67	1.46
1	C	24	TYR	CE1-CZ	-10.58	1.24	1.38
2	D	40	ARG	CZ-NH2	10.57	1.46	1.33
2	D	40	ARG	CD-NE	-10.56	1.28	1.46
2	D	80	ASN	CB-CG	-10.55	1.26	1.51
1	C	114	PRO	CA-CB	-10.55	1.32	1.53
2	D	46	GLY	C-O	10.54	1.40	1.23
2	B	143	HIS	CG-CD2	-10.54	1.17	1.35
1	C	117	PHE	CD1-CE1	10.53	1.60	1.39
2	D	45	PHE	CG-CD2	-10.53	1.23	1.38
1	A	49	SER	CA-CB	-10.53	1.37	1.52
1	A	89	HIS	CG-CD2	10.52	1.53	1.35
1	C	46	PHE	CE2-CZ	10.49	1.57	1.37
2	B	61	LYS	CB-CG	-10.49	1.24	1.52
2	D	63	HIS	CB-CG	10.47	1.69	1.50
2	B	73	ASP	CG-OD2	-10.47	1.01	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	THR	CB-OG1	-10.46	1.22	1.43
2	B	80	ASN	CA-C	10.45	1.80	1.52
2	B	61	LYS	CE-NZ	10.42	1.75	1.49
1	C	71	ALA	N-CA	10.42	1.67	1.46
2	B	143	HIS	CE1-NE2	10.41	1.56	1.32
2	D	113	VAL	CB-CG2	10.38	1.74	1.52
1	A	20	HIS	CG-CD2	10.35	1.53	1.35
2	B	3	LEU	CA-CB	10.33	1.77	1.53
2	D	67	VAL	CA-CB	10.33	1.76	1.54
1	A	83	LEU	CB-CG	-10.30	1.22	1.52
1	C	112	HIS	CB-CG	-10.30	1.31	1.50
2	D	78	LEU	N-CA	-10.29	1.25	1.46
1	C	50	HIS	CB-CG	-10.29	1.31	1.50
2	D	60	VAL	N-CA	10.28	1.67	1.46
2	D	136	GLY	N-CA	-10.28	1.30	1.46
1	A	36	PHE	CG-CD2	10.27	1.54	1.38
1	A	61	LYS	CE-NZ	10.26	1.74	1.49
2	D	19	ASN	CA-C	-10.26	1.26	1.52
2	B	12	THR	CB-OG1	-10.23	1.22	1.43
2	B	41	PHE	CG-CD2	10.23	1.54	1.38
1	C	2	LEU	CA-C	10.23	1.79	1.52
1	A	77	PRO	C-O	10.19	1.43	1.23
2	D	58	PRO	C-O	10.18	1.43	1.23
2	B	46	GLY	CA-C	10.16	1.68	1.51
1	A	3	SER	CB-OG	-10.16	1.29	1.42
1	C	24	TYR	CZ-OH	10.15	1.55	1.37
2	D	84	THR	CB-OG1	-10.14	1.23	1.43
1	A	4	PRO	CA-CB	10.13	1.73	1.53
1	C	92	ARG	C-O	-10.12	1.04	1.23
1	C	127	LYS	C-O	10.11	1.42	1.23
2	B	51	PRO	N-CD	10.10	1.61	1.47
2	D	58	PRO	CB-CG	10.09	2.00	1.50
1	A	72	HIS	CD2-NE2	10.07	1.63	1.42
2	D	61	LYS	CE-NZ	-10.07	1.23	1.49
1	C	14	TRP	NE1-CE2	-10.04	1.24	1.37
1	C	41	THR	C-O	10.04	1.42	1.23
1	A	141	ARG	CB-CG	10.02	1.79	1.52
2	B	4	THR	CA-C	-9.98	1.27	1.52
1	C	17	VAL	C-N	9.98	1.51	1.33
1	C	128	PHE	CB-CG	9.96	1.68	1.51
2	B	113	VAL	C-O	9.95	1.42	1.23
1	C	17	VAL	CB-CG1	-9.94	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	42	PHE	CE2-CZ	9.94	1.56	1.37
2	D	77	HIS	CA-CB	9.93	1.75	1.53
2	D	8	LYS	CB-CG	9.91	1.79	1.52
1	C	47	ASP	CB-CG	9.91	1.72	1.51
1	A	33	PHE	CG-CD1	-9.90	1.24	1.38
2	D	37	TRP	CE2-CZ2	9.90	1.56	1.39
1	A	122	HIS	N-CA	9.89	1.66	1.46
1	A	140	TYR	CG-CD1	9.89	1.52	1.39
1	C	50	HIS	CE1-NE2	9.87	1.55	1.32
1	C	51	GLY	N-CA	-9.86	1.31	1.46
1	C	44	PRO	C-N	-9.86	1.11	1.34
1	A	40	LYS	CA-CB	9.85	1.75	1.53
1	A	140	TYR	CZ-OH	-9.85	1.21	1.37
1	A	1	VAL	CB-CG1	-9.84	1.32	1.52
2	B	17	LYS	C-O	9.83	1.42	1.23
2	B	103	PHE	CE1-CZ	-9.83	1.18	1.37
2	B	132	LYS	CA-CB	-9.80	1.32	1.53
1	C	36	PHE	CG-CD2	9.79	1.53	1.38
1	C	46	PHE	CE1-CZ	-9.79	1.18	1.37
2	D	1	VAL	CB-CG1	9.77	1.73	1.52
2	B	10	ALA	CA-C	9.76	1.78	1.52
1	A	44	PRO	N-CD	-9.75	1.34	1.47
1	A	90	LYS	CG-CD	-9.74	1.19	1.52
2	B	126	VAL	C-O	9.74	1.41	1.23
2	D	139	ASN	CG-ND2	9.71	1.57	1.32
2	B	50	THR	CA-CB	-9.69	1.28	1.53
2	B	104	ARG	CG-CD	9.68	1.76	1.51
1	C	138	SER	CB-OG	-9.66	1.29	1.42
1	A	72	HIS	CB-CG	-9.63	1.32	1.50
1	A	33	PHE	CD2-CE2	9.62	1.58	1.39
2	D	4	THR	C-O	9.62	1.41	1.23
1	C	18	GLY	CA-C	-9.62	1.36	1.51
2	D	53	ALA	C-N	9.61	1.56	1.34
2	B	73	ASP	CB-CG	9.60	1.72	1.51
2	B	118	PHE	CB-CG	-9.60	1.35	1.51
1	C	44	PRO	CA-CB	9.60	1.72	1.53
1	A	17	VAL	N-CA	-9.60	1.27	1.46
1	A	2	LEU	CA-C	9.57	1.77	1.52
2	B	42	PHE	CE1-CZ	-9.56	1.19	1.37
2	B	41	PHE	CA-C	9.55	1.77	1.52
2	B	82	LYS	CA-C	-9.54	1.28	1.52
1	C	56	LYS	CE-NZ	9.52	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
2	B	73	ASP	CG-OD1	9.50	1.47	1.25
2	B	2	HIS	C-N	-9.49	1.12	1.34
1	C	46	PHE	CB-CG	-9.48	1.35	1.51
1	C	20	HIS	CD2-NE2	-9.47	1.17	1.38
1	A	77	PRO	CA-CB	9.47	1.72	1.53
2	D	46	GLY	N-CA	-9.45	1.31	1.46
2	D	72	SER	CA-CB	9.45	1.67	1.52
2	B	6	GLU	CA-C	9.44	1.77	1.52
1	C	76	MET	CG-SD	9.41	2.05	1.81
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	B	44	SER	C-N	9.38	1.55	1.34
1	C	132	VAL	CB-CG2	9.36	1.72	1.52
1	C	128	PHE	CD2-CE2	9.35	1.57	1.39
2	D	15	TRP	CZ3-CH2	9.34	1.54	1.40
2	D	83	GLY	C-N	9.34	1.55	1.34
2	B	83	GLY	N-CA	9.30	1.59	1.46
1	A	14	TRP	CD1-NE1	9.29	1.53	1.38
1	C	71	ALA	CA-C	-9.28	1.28	1.52
2	D	36	PRO	N-CA	9.28	1.63	1.47
2	B	146	HIS	N-CA	9.27	1.64	1.46
1	A	46	PHE	CE1-CZ	9.26	1.54	1.37
2	D	77	HIS	C-N	9.26	1.55	1.34
1	C	81	SER	CB-OG	9.25	1.54	1.42
1	C	47	ASP	CG-OD1	-9.24	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
1	C	22	GLY	C-O	9.22	1.38	1.23
1	A	50	HIS	CB-CG	-9.20	1.33	1.50
2	B	143	HIS	CA-C	9.20	1.76	1.52
1	C	61	LYS	CA-C	9.20	1.76	1.52
2	D	93	CYS	C-O	-9.19	1.05	1.23
1	A	104	CYS	N-CA	9.19	1.64	1.46
1	C	38	THR	CB-OG1	9.19	1.61	1.43
2	B	63	HIS	ND1-CE1	9.18	1.57	1.34
1	C	12	ALA	C-N	9.17	1.55	1.34
2	B	51	PRO	C-O	9.16	1.41	1.23
1	C	103	HIS	CG-ND1	9.16	1.58	1.38
1	C	43	PHE	CG-CD2	9.14	1.52	1.38
2	B	21	ASP	CG-OD2	9.13	1.46	1.25
1	C	81	SER	CA-CB	9.13	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	HIS	CA-C	9.12	1.76	1.52
1	C	42	TYR	CG-CD1	9.11	1.50	1.39
2	D	53	ALA	CA-C	9.11	1.76	1.52
2	D	42	PHE	CE1-CZ	-9.10	1.20	1.37
1	C	69	ALA	N-CA	9.09	1.64	1.46
1	A	86	LEU	CB-CG	-9.08	1.26	1.52
2	D	137	VAL	CA-CB	9.08	1.73	1.54
2	D	15	TRP	NE1-CE2	9.07	1.49	1.37
1	C	95	PRO	CA-C	-9.06	1.34	1.52
2	B	37	TRP	NE1-CE2	-9.06	1.25	1.37
1	C	72	HIS	N-CA	-9.03	1.28	1.46
1	A	88	ALA	C-O	-9.01	1.06	1.23
2	B	40	ARG	C-N	-9.01	1.13	1.34
2	B	77	HIS	CB-CG	9.01	1.66	1.50
2	B	18	VAL	CB-CG2	9.00	1.71	1.52
1	C	14	TRP	CZ2-CH2	-8.99	1.20	1.37
2	B	117	HIS	CE1-NE2	8.99	1.53	1.32
1	A	67	THR	C-O	8.99	1.40	1.23
2	D	49	SER	C-O	8.98	1.40	1.23
2	B	7	GLU	CG-CD	-8.97	1.38	1.51
2	D	79	ASP	CA-CB	8.95	1.73	1.53
2	D	59	LYS	CA-C	8.94	1.76	1.52
1	C	16	LYS	CE-NZ	8.93	1.71	1.49
2	B	26	GLU	CG-CD	-8.91	1.38	1.51
1	C	48	LEU	C-O	8.91	1.40	1.23
2	D	92	HIS	CA-C	8.90	1.76	1.52
1	C	131	SER	CA-C	8.88	1.76	1.52
2	D	146	HIS	C-OXT	8.87	1.40	1.23
1	C	56	LYS	CA-C	-8.87	1.29	1.52
1	C	99	LYS	CG-CD	8.87	1.82	1.52
1	C	21	ALA	C-N	-8.86	1.17	1.33
1	C	141	ARG	CZ-NH2	8.86	1.44	1.33
2	D	5	PRO	CB-CG	-8.85	1.05	1.50
2	B	94	ASP	CB-CG	8.84	1.70	1.51
1	C	57	GLY	C-O	8.84	1.37	1.23
1	C	113	LEU	CA-CB	-8.83	1.33	1.53
1	C	42	TYR	CE2-CZ	8.83	1.50	1.38
1	C	77	PRO	CA-C	-8.83	1.35	1.52
1	C	126	ASP	CB-CG	8.83	1.70	1.51
1	A	87	HIS	CA-C	8.82	1.75	1.52
2	D	10	ALA	CA-C	8.81	1.75	1.52
1	C	115	ALA	CA-CB	8.80	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	97	HIS	CB-CG	8.80	1.65	1.50
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	4	PRO	N-CA	-8.77	1.32	1.47
1	A	57	GLY	CA-C	8.77	1.65	1.51
1	A	138	SER	CB-OG	-8.77	1.30	1.42
1	A	33	PHE	CA-C	-8.74	1.30	1.52
1	C	68	ASN	CG-ND2	8.74	1.54	1.32
2	D	143	HIS	CB-CG	-8.74	1.34	1.50
2	B	73	ASP	C-O	8.72	1.40	1.23
2	D	61	LYS	CD-CE	8.72	1.73	1.51
1	A	45	HIS	CE1-NE2	8.71	1.52	1.32
1	A	78	ASN	C-O	8.70	1.39	1.23
2	D	12	THR	C-O	8.70	1.39	1.23
2	D	82	LYS	CB-CG	-8.70	1.29	1.52
1	A	68	ASN	C-O	8.69	1.39	1.23
2	D	4	THR	CB-CG2	-8.69	1.23	1.52
2	D	71	PHE	N-CA	8.68	1.63	1.46
1	C	46	PHE	C-N	8.68	1.54	1.34
2	B	50	THR	N-CA	-8.67	1.29	1.46
2	D	20	VAL	N-CA	8.67	1.63	1.46
2	D	121	GLU	N-CA	-8.67	1.29	1.46
2	D	8	LYS	CG-CD	-8.67	1.23	1.52
1	A	29	LEU	N-CA	8.66	1.63	1.46
1	C	85	ASP	CG-OD1	-8.66	1.05	1.25
1	A	105	LEU	CG-CD2	-8.65	1.19	1.51
1	A	27	GLU	CD-OE1	-8.65	1.16	1.25
1	A	8	THR	CB-OG1	-8.64	1.25	1.43
1	C	115	ALA	N-CA	-8.62	1.29	1.46
2	B	44	SER	CA-CB	-8.62	1.40	1.52
2	B	145	TYR	CA-C	8.62	1.75	1.52
2	D	146	HIS	CA-CB	8.60	1.72	1.53
2	D	6	GLU	CA-CB	8.58	1.72	1.53
1	A	37	PRO	N-CA	8.58	1.61	1.47
2	B	69	GLY	C-N	8.58	1.53	1.34
1	C	16	LYS	CG-CD	8.56	1.81	1.52
1	C	118	THR	CA-CB	8.55	1.75	1.53
2	D	80	ASN	C-O	-8.54	1.07	1.23
2	D	23	VAL	CB-CG1	-8.54	1.34	1.52
2	D	85	PHE	N-CA	8.53	1.63	1.46
1	A	42	TYR	CE1-CZ	-8.52	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	47	ASP	CA-C	8.52	1.75	1.52
1	C	54	GLN	CA-C	8.52	1.75	1.52
2	B	20	VAL	CA-C	-8.51	1.30	1.52
1	A	62	VAL	CA-C	8.51	1.75	1.52
2	B	42	PHE	CB-CG	-8.51	1.36	1.51
1	A	10	VAL	CB-CG2	-8.50	1.35	1.52
2	B	10	ALA	N-CA	-8.49	1.29	1.46
2	D	7	GLU	CA-C	8.49	1.75	1.52
2	D	43	GLU	C-O	-8.49	1.07	1.23
1	A	30	GLU	CB-CG	-8.47	1.36	1.52
2	D	145	TYR	CD2-CE2	8.46	1.52	1.39
1	C	95	PRO	N-CA	8.46	1.61	1.47
2	B	95	LYS	CA-CB	8.45	1.72	1.53
1	A	46	PHE	CD2-CE2	8.44	1.56	1.39
2	B	75	LEU	CB-CG	-8.44	1.28	1.52
1	C	26	ALA	C-N	8.43	1.53	1.34
1	C	47	ASP	CA-CB	8.42	1.72	1.53
1	C	59	GLY	N-CA	-8.42	1.33	1.46
2	B	134	VAL	N-CA	-8.41	1.29	1.46
2	D	125	PRO	N-CA	-8.41	1.32	1.47
1	A	3	SER	N-CA	8.40	1.63	1.46
2	D	123	THR	CB-CG2	8.40	1.80	1.52
1	C	131	SER	N-CA	8.37	1.63	1.46
1	C	137	THR	CA-C	8.36	1.74	1.52
2	D	146	HIS	N-CA	8.36	1.63	1.46
1	A	141	ARG	CA-CB	-8.34	1.35	1.53
2	B	54	VAL	CA-C	-8.32	1.31	1.52
1	C	70	VAL	CA-C	8.32	1.74	1.52
1	C	114	PRO	N-CD	8.31	1.59	1.47
2	B	37	TRP	CG-CD1	8.30	1.48	1.36
2	D	30	ARG	CZ-NH2	8.30	1.43	1.33
1	A	21	ALA	C-O	-8.29	1.07	1.23
2	D	41	PHE	CG-CD2	-8.27	1.26	1.38
2	D	70	ALA	C-O	8.27	1.39	1.23
1	C	140	TYR	CG-CD2	8.27	1.49	1.39
2	D	110	LEU	C-N	8.27	1.53	1.34
2	B	41	PHE	C-O	-8.26	1.07	1.23
2	B	49	SER	CA-C	-8.25	1.31	1.52
2	B	52	ASP	CG-OD1	-8.25	1.06	1.25
2	B	69	GLY	CA-C	8.25	1.65	1.51
1	C	40	LYS	CE-NZ	8.24	1.69	1.49
1	C	50	HIS	CA-CB	8.24	1.72	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	95	LYS	CA-C	-8.23	1.31	1.52
1	A	47	ASP	CA-C	8.22	1.74	1.52
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	A	134	THR	CA-C	-8.21	1.31	1.52
2	B	20	VAL	C-O	8.19	1.39	1.23
2	D	14	LEU	CA-CB	8.19	1.72	1.53
2	B	94	ASP	C-O	8.19	1.39	1.23
2	B	93	CYS	CB-SG	8.18	1.96	1.82
1	C	14	TRP	C-O	8.18	1.38	1.23
2	B	84	THR	CB-OG1	8.17	1.59	1.43
2	D	94	ASP	CG-OD1	-8.17	1.06	1.25
2	B	84	THR	CB-CG2	-8.16	1.25	1.52
2	D	11	VAL	CB-CG2	8.15	1.70	1.52
1	C	96	VAL	CB-CG2	-8.13	1.35	1.52
2	D	13	ALA	C-N	8.13	1.52	1.34
2	B	77	HIS	ND1-CE1	-8.12	1.14	1.34
2	B	142	ALA	C-N	-8.11	1.15	1.34
2	B	69	GLY	C-O	-8.11	1.10	1.23
2	D	19	ASN	C-N	-8.10	1.15	1.34
2	D	55	MET	CB-CG	-8.10	1.25	1.51
1	A	78	ASN	CG-ND2	-8.09	1.12	1.32
1	C	25	GLY	N-CA	-8.08	1.33	1.46
1	C	113	LEU	CG-CD2	-8.08	1.22	1.51
2	D	58	PRO	CA-C	8.08	1.69	1.52
1	A	76	MET	CG-SD	8.07	2.02	1.81
2	D	104	ARG	CZ-NH2	-8.05	1.22	1.33
2	D	130	TYR	CE2-CZ	-8.04	1.28	1.38
2	B	59	LYS	CA-CB	-8.04	1.36	1.53
2	B	16	GLY	N-CA	8.04	1.58	1.46
2	B	118	PHE	CE1-CZ	8.03	1.52	1.37
1	A	105	LEU	CB-CG	-8.03	1.29	1.52
2	D	51	PRO	N-CD	8.03	1.59	1.47
2	D	54	VAL	C-O	8.02	1.38	1.23
2	D	80	ASN	CA-C	8.01	1.73	1.52
1	A	17	VAL	CA-CB	-8.01	1.38	1.54
1	A	88	ALA	CA-C	8.01	1.73	1.52
2	D	3	LEU	C-N	8.01	1.52	1.34
1	C	3	SER	CA-CB	-8.00	1.41	1.52
2	D	76	ALA	CA-CB	-8.00	1.35	1.52
2	B	7	GLU	N-CA	7.99	1.62	1.46
2	D	41	PHE	CA-C	7.98	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	41	PHE	CB-CG	7.97	1.64	1.51
2	D	132	LYS	CD-CE	7.97	1.71	1.51
1	C	17	VAL	C-O	7.97	1.38	1.23
1	C	58	HIS	CG-CD2	-7.96	1.22	1.35
1	A	114	PRO	N-CA	7.96	1.60	1.47
2	B	101	GLU	C-N	7.96	1.52	1.34
1	C	45	HIS	ND1-CE1	-7.96	1.14	1.34
2	D	122	PHE	CG-CD2	7.94	1.50	1.38
2	D	122	PHE	CG-CD1	-7.93	1.26	1.38
2	B	80	ASN	C-O	-7.92	1.08	1.23
2	B	45	PHE	CB-CG	7.91	1.64	1.51
1	A	141	ARG	N-CA	7.88	1.62	1.46
1	A	132	VAL	C-O	7.87	1.38	1.23
2	B	81	LEU	CA-C	-7.87	1.32	1.52
1	A	16	LYS	C-O	-7.85	1.08	1.23
2	B	121	GLU	N-CA	-7.85	1.30	1.46
1	A	7	LYS	N-CA	7.85	1.62	1.46
2	D	39	GLN	CD-OE1	7.85	1.41	1.24
2	D	116	HIS	CE1-NE2	7.84	1.50	1.32
1	C	48	LEU	CA-C	-7.84	1.32	1.52
1	C	11	LYS	CD-CE	-7.84	1.31	1.51
1	A	44	PRO	CA-CB	-7.83	1.37	1.53
2	B	143	HIS	CA-CB	-7.82	1.36	1.53
1	A	8	THR	C-N	7.82	1.52	1.34
2	B	22	GLU	N-CA	7.82	1.61	1.46
2	D	54	VAL	N-CA	7.82	1.61	1.46
1	A	16	LYS	C-N	7.81	1.52	1.34
2	B	117	HIS	CB-CG	-7.81	1.35	1.50
2	D	18	VAL	CA-C	7.81	1.73	1.52
2	D	135	ALA	CA-C	7.80	1.73	1.52
1	C	74	ASP	CB-CG	-7.80	1.35	1.51
1	C	64	ASP	CG-OD2	-7.79	1.07	1.25
2	B	19	ASN	CG-OD1	-7.78	1.06	1.24
2	B	15	TRP	CG-CD1	-7.77	1.25	1.36
1	A	49	SER	N-CA	7.77	1.61	1.46
2	B	8	LYS	CG-CD	7.76	1.78	1.52
2	D	146	HIS	CD2-NE2	7.76	1.58	1.42
1	C	128	PHE	CA-C	7.74	1.73	1.52
2	D	8	LYS	CA-C	-7.74	1.32	1.52
2	D	16	GLY	CA-C	-7.74	1.39	1.51
1	A	13	ALA	CA-C	7.73	1.73	1.52
2	B	123	THR	C-N	-7.73	1.19	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	16	GLY	C-O	7.73	1.36	1.23
2	B	95	LYS	C-N	7.73	1.51	1.34
2	B	64	GLY	C-O	-7.71	1.11	1.23
2	B	42	PHE	CE2-CZ	7.71	1.51	1.37
1	A	132	VAL	CA-CB	-7.71	1.38	1.54
2	B	35	TYR	CE2-CZ	-7.70	1.28	1.38
1	C	23	GLU	N-CA	-7.69	1.30	1.46
1	C	114	PRO	C-O	7.68	1.38	1.23
1	C	49	SER	CA-C	-7.68	1.32	1.52
1	C	52	SER	N-CA	7.67	1.61	1.46
2	D	97	HIS	ND1-CE1	7.67	1.53	1.34
1	C	8	THR	CA-C	-7.66	1.33	1.52
1	C	31	ARG	CD-NE	7.66	1.59	1.46
2	D	118	PHE	CD2-CE2	7.65	1.54	1.39
1	A	20	HIS	CA-CB	-7.65	1.37	1.53
1	A	43	PHE	CG-CD2	-7.64	1.27	1.38
2	B	101	GLU	CD-OE1	-7.64	1.17	1.25
2	D	45	PHE	CA-C	7.63	1.72	1.52
1	A	53	ALA	CA-CB	7.63	1.68	1.52
2	D	48	LEU	C-N	7.63	1.51	1.34
2	B	15	TRP	NE1-CE2	7.62	1.47	1.37
1	A	60	LYS	C-N	7.61	1.51	1.34
2	D	25	GLY	CA-C	-7.61	1.39	1.51
2	D	92	HIS	CG-ND1	7.61	1.55	1.38
2	D	2	HIS	CD2-NE2	7.61	1.57	1.42
1	A	99	LYS	CA-C	-7.60	1.33	1.52
2	B	112	CYS	CA-CB	-7.60	1.37	1.53
2	B	66	LYS	CA-C	7.58	1.72	1.52
2	D	58	PRO	C-N	-7.57	1.16	1.34
2	B	134	VAL	C-O	7.57	1.37	1.23
1	C	55	VAL	N-CA	7.56	1.61	1.46
1	A	42	TYR	CA-C	7.56	1.72	1.52
1	A	127	LYS	C-N	-7.55	1.16	1.34
2	B	97	HIS	CB-CG	7.55	1.63	1.50
2	D	17	LYS	CB-CG	-7.54	1.32	1.52
1	C	83	LEU	C-O	7.53	1.37	1.23
2	B	61	LYS	CD-CE	7.53	1.70	1.51
2	D	60	VAL	CA-C	-7.53	1.33	1.52
1	C	18	GLY	N-CA	7.52	1.57	1.46
1	C	24	TYR	CD1-CE1	7.52	1.50	1.39
1	C	76	MET	CA-C	-7.51	1.33	1.52
2	B	71	PHE	CG-CD2	7.51	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	LYS	N-CA	-7.51	1.31	1.46
2	B	120	LYS	CB-CG	-7.50	1.32	1.52
2	D	15	TRP	CZ2-CH2	-7.50	1.23	1.37
1	A	122	HIS	ND1-CE1	7.49	1.53	1.34
2	D	45	PHE	C-O	7.48	1.37	1.23
2	D	75	LEU	CG-CD2	-7.47	1.24	1.51
2	D	68	LEU	CG-CD1	-7.46	1.24	1.51
1	C	94	ASP	CG-OD1	-7.46	1.08	1.25
1	C	7	LYS	C-N	7.45	1.51	1.34
2	D	104	ARG	CG-CD	7.44	1.70	1.51
2	B	16	GLY	CA-C	-7.44	1.40	1.51
2	B	53	ALA	CA-CB	-7.44	1.36	1.52
1	A	106	LEU	C-O	7.43	1.37	1.23
1	A	8	THR	CB-CG2	-7.43	1.27	1.52
1	C	105	LEU	CG-CD1	7.43	1.79	1.51
2	D	86	ALA	CA-CB	7.42	1.68	1.52
1	A	90	LYS	CB-CG	7.41	1.72	1.52
1	C	106	LEU	CA-C	-7.41	1.33	1.52
1	C	12	ALA	C-O	7.39	1.37	1.23
2	D	5	PRO	N-CD	7.39	1.58	1.47
2	D	43	GLU	N-CA	7.39	1.61	1.46
2	D	130	TYR	CD2-CE2	7.37	1.50	1.39
2	B	136	GLY	N-CA	7.36	1.57	1.46
1	A	131	SER	CA-CB	7.36	1.64	1.52
1	A	24	TYR	CG-CD1	-7.35	1.29	1.39
2	B	17	LYS	CD-CE	7.35	1.69	1.51
1	C	2	LEU	CG-CD2	-7.35	1.24	1.51
2	B	28	LEU	CB-CG	7.34	1.73	1.52
2	B	57	ASN	CG-OD1	-7.34	1.07	1.24
2	B	72	SER	N-CA	7.34	1.61	1.46
2	B	124	PRO	C-N	-7.34	1.20	1.34
2	B	145	TYR	CB-CG	7.34	1.62	1.51
1	A	72	HIS	CG-CD2	7.33	1.48	1.35
2	B	13	ALA	CA-CB	7.33	1.67	1.52
1	C	12	ALA	N-CA	-7.32	1.31	1.46
1	A	76	MET	N-CA	7.32	1.60	1.46
2	B	144	LYS	C-O	7.31	1.37	1.23
1	A	106	LEU	CA-C	-7.31	1.33	1.52
2	D	10	ALA	N-CA	7.31	1.60	1.46
1	C	112	HIS	C-N	-7.30	1.17	1.34
2	B	112	CYS	CB-SG	7.29	1.94	1.82
1	A	120	ALA	C-N	-7.29	1.17	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	61	LYS	CG-CD	-7.28	1.27	1.52
1	A	11	LYS	CB-CG	-7.28	1.32	1.52
1	A	74	ASP	N-CA	7.27	1.60	1.46
1	C	59	GLY	C-O	7.27	1.35	1.23
2	D	1	VAL	CA-CB	7.27	1.70	1.54
2	D	50	THR	CA-C	7.26	1.71	1.52
2	D	6	GLU	N-CA	-7.24	1.31	1.46
1	C	2	LEU	CA-CB	-7.24	1.37	1.53
1	C	2	LEU	CG-CD1	-7.24	1.25	1.51
2	D	119	GLY	CA-C	7.24	1.63	1.51
1	A	48	LEU	CA-CB	7.23	1.70	1.53
2	D	81	LEU	CG-CD1	-7.23	1.25	1.51
2	D	44	SER	CA-C	-7.20	1.34	1.52
2	B	72	SER	CB-OG	-7.18	1.32	1.42
1	C	29	LEU	CA-C	-7.18	1.34	1.52
1	C	78	ASN	C-N	7.18	1.50	1.34
1	A	64	ASP	C-N	7.18	1.50	1.34
1	A	20	HIS	CB-CG	-7.17	1.37	1.50
1	A	69	ALA	C-O	-7.16	1.09	1.23
2	B	46	GLY	N-CA	-7.16	1.35	1.46
2	D	67	VAL	CA-C	-7.16	1.34	1.52
2	B	73	ASP	CA-CB	7.14	1.69	1.53
1	A	109	LEU	CG-CD2	-7.14	1.25	1.51
2	D	51	PRO	C-O	7.14	1.37	1.23
1	C	122	HIS	CG-CD2	7.13	1.47	1.35
2	B	85	PHE	CB-CG	-7.12	1.39	1.51
1	A	90	LYS	CA-CB	7.12	1.69	1.53
2	B	54	VAL	CA-CB	7.12	1.69	1.54
2	B	11	VAL	CA-CB	-7.12	1.39	1.54
1	A	43	PHE	CG-CD1	7.12	1.49	1.38
2	B	15	TRP	CD2-CE2	7.11	1.49	1.41
1	C	50	HIS	CA-C	7.11	1.71	1.52
2	D	145	TYR	CE1-CZ	7.10	1.47	1.38
2	D	126	VAL	C-N	7.10	1.50	1.34
2	D	141	LEU	CG-CD2	7.08	1.78	1.51
1	C	117	PHE	CG-CD1	7.08	1.49	1.38
1	A	79	ALA	CA-CB	-7.08	1.37	1.52
2	D	64	GLY	C-N	7.08	1.50	1.34
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	B	37	TRP	CZ3-CH2	-7.05	1.28	1.40
2	D	72	SER	CB-OG	-7.05	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLY	N-CA	7.04	1.56	1.46
1	A	71	ALA	CA-CB	-7.03	1.37	1.52
1	A	96	VAL	CA-CB	7.03	1.69	1.54
1	A	98	PHE	CD1-CE1	-7.03	1.25	1.39
1	C	64	ASP	CB-CG	7.03	1.66	1.51
1	A	48	LEU	CG-CD2	-7.02	1.25	1.51
2	B	95	LYS	C-O	-7.02	1.10	1.23
1	C	61	LYS	CB-CG	-7.01	1.33	1.52
2	D	103	PHE	CG-CD1	7.01	1.49	1.38
2	D	26	GLU	CA-C	7.01	1.71	1.52
2	D	78	LEU	C-N	7.01	1.50	1.34
2	D	146	HIS	CG-CD2	-7.00	1.23	1.35
2	D	126	VAL	C-O	-7.00	1.10	1.23
2	D	98	VAL	CB-CG2	7.00	1.67	1.52
1	A	114	PRO	CA-C	6.99	1.66	1.52
1	A	62	VAL	N-CA	6.98	1.60	1.46
1	C	23	GLU	CA-C	6.97	1.71	1.52
1	A	77	PRO	N-CA	-6.97	1.35	1.47
2	B	50	THR	CB-CG2	6.96	1.75	1.52
1	C	74	ASP	N-CA	6.95	1.60	1.46
2	D	143	HIS	CG-ND1	-6.95	1.23	1.38
1	A	92	ARG	CD-NE	-6.93	1.34	1.46
1	A	56	LYS	CA-C	-6.93	1.34	1.52
1	C	52	SER	C-O	6.92	1.36	1.23
2	B	145	TYR	CD1-CE1	-6.91	1.28	1.39
2	D	10	ALA	CA-CB	-6.90	1.38	1.52
2	B	41	PHE	CE1-CZ	-6.90	1.24	1.37
1	A	60	LYS	C-O	-6.90	1.10	1.23
1	C	133	SER	C-N	-6.90	1.18	1.34
1	A	98	PHE	CE2-CZ	-6.89	1.24	1.37
1	C	130	ALA	C-O	6.89	1.36	1.23
1	C	65	ALA	C-N	6.88	1.49	1.34
1	A	26	ALA	C-N	6.88	1.49	1.34
2	D	105	LEU	CA-CB	-6.88	1.38	1.53
2	D	122	PHE	CD1-CE1	6.88	1.53	1.39
2	B	142	ALA	C-O	6.87	1.36	1.23
2	D	75	LEU	CA-CB	6.87	1.69	1.53
1	A	76	MET	C-N	-6.86	1.21	1.34
1	C	110	ALA	C-O	6.86	1.36	1.23
1	A	8	THR	CA-CB	6.85	1.71	1.53
2	D	86	ALA	N-CA	6.85	1.60	1.46
1	C	40	LYS	N-CA	6.85	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	PRO	CA-C	-6.84	1.39	1.52
1	C	131	SER	CB-OG	6.84	1.51	1.42
1	C	87	HIS	CE1-NE2	-6.83	1.17	1.32
2	D	7	GLU	C-N	-6.83	1.18	1.34
2	D	77	HIS	N-CA	-6.83	1.32	1.46
2	D	28	LEU	C-N	6.82	1.45	1.33
2	D	51	PRO	CA-C	-6.82	1.39	1.52
2	B	32	LEU	CG-CD1	-6.80	1.26	1.51
2	B	34	VAL	N-CA	6.80	1.59	1.46
2	B	123	THR	CB-OG1	-6.80	1.29	1.43
1	C	132	VAL	CA-CB	-6.80	1.40	1.54
2	B	79	ASP	N-CA	6.79	1.59	1.46
1	A	41	THR	CA-C	-6.79	1.35	1.52
1	A	80	LEU	N-CA	6.78	1.59	1.46
2	B	120	LYS	CE-NZ	-6.78	1.32	1.49
2	B	121	GLU	CA-CB	6.77	1.68	1.53
1	C	14	TRP	C-N	-6.77	1.20	1.33
2	B	54	VAL	C-O	6.76	1.36	1.23
2	D	131	GLN	C-O	-6.76	1.10	1.23
1	A	79	ALA	CA-C	6.75	1.70	1.52
2	D	13	ALA	C-O	-6.74	1.10	1.23
2	B	12	THR	CA-CB	6.74	1.70	1.53
2	B	67	VAL	N-CA	6.74	1.59	1.46
1	C	48	LEU	N-CA	6.74	1.59	1.46
2	B	35	TYR	CD2-CE2	-6.73	1.29	1.39
2	B	13	ALA	N-CA	-6.72	1.32	1.46
1	C	98	PHE	CG-CD2	-6.72	1.28	1.38
2	D	95	LYS	N-CA	6.72	1.59	1.46
2	D	32	LEU	C-O	6.72	1.36	1.23
2	D	91	LEU	C-N	6.72	1.49	1.34
2	D	18	VAL	C-N	-6.72	1.18	1.34
1	A	117	PHE	CD2-CE2	6.71	1.52	1.39
1	C	38	THR	CA-C	-6.71	1.35	1.52
2	B	39	GLN	N-CA	6.71	1.59	1.46
1	C	124	SER	CA-CB	6.71	1.63	1.52
2	B	13	ALA	C-N	6.71	1.49	1.34
2	D	15	TRP	CG-CD2	6.70	1.55	1.43
2	D	94	ASP	CB-CG	6.70	1.65	1.51
1	A	12	ALA	N-CA	-6.70	1.32	1.46
1	C	139	LYS	CG-CD	-6.70	1.29	1.52
2	D	1	VAL	C-N	-6.70	1.18	1.34
1	A	8	THR	CA-C	-6.69	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	SER	C-O	6.68	1.36	1.23
2	D	110	LEU	CA-CB	-6.67	1.38	1.53
1	A	73	VAL	CB-CG2	-6.67	1.38	1.52
1	A	139	LYS	N-CA	6.67	1.59	1.46
2	B	73	ASP	N-CA	6.67	1.59	1.46
2	B	19	ASN	CG-ND2	6.66	1.49	1.32
2	B	83	GLY	CA-C	-6.66	1.41	1.51
2	B	124	PRO	C-O	6.65	1.36	1.23
2	B	37	TRP	CD2-CE2	6.64	1.49	1.41
1	C	60	LYS	CD-CE	-6.64	1.34	1.51
1	A	120	ALA	N-CA	-6.64	1.33	1.46
2	D	68	LEU	CB-CG	-6.63	1.33	1.52
2	D	84	THR	N-CA	-6.62	1.33	1.46
1	A	42	TYR	CG-CD2	6.62	1.47	1.39
2	B	119	GLY	C-O	6.62	1.34	1.23
2	D	54	VAL	CB-CG1	6.61	1.66	1.52
2	B	63	HIS	CA-CB	-6.60	1.39	1.53
2	B	120	LYS	CA-CB	6.60	1.68	1.53
2	B	144	LYS	CA-C	-6.59	1.35	1.52
1	A	41	THR	C-O	6.59	1.35	1.23
1	C	43	PHE	N-CA	6.59	1.59	1.46
2	D	44	SER	C-N	6.59	1.49	1.34
1	A	33	PHE	C-N	6.59	1.49	1.34
2	B	63	HIS	C-N	-6.59	1.21	1.33
1	A	22	GLY	C-N	6.59	1.49	1.34
1	C	109	LEU	C-N	6.59	1.49	1.34
1	A	11	LYS	N-CA	6.58	1.59	1.46
2	B	76	ALA	N-CA	-6.58	1.33	1.46
2	D	93	CYS	N-CA	6.57	1.59	1.46
2	B	3	LEU	N-CA	6.57	1.59	1.46
1	A	20	HIS	CD2-NE2	6.57	1.55	1.42
1	C	87	HIS	CG-CD2	6.56	1.46	1.35
2	B	47	ASP	C-N	6.55	1.49	1.34
1	C	78	ASN	CA-CB	6.55	1.70	1.53
1	C	52	SER	CA-CB	-6.55	1.43	1.52
1	C	68	ASN	N-CA	-6.55	1.33	1.46
2	B	8	LYS	N-CA	-6.54	1.33	1.46
1	A	5	ALA	N-CA	-6.54	1.33	1.46
2	B	58	PRO	CB-CG	-6.54	1.17	1.50
2	B	123	THR	CA-C	6.54	1.70	1.52
1	A	113	LEU	CB-CG	6.54	1.71	1.52
2	B	93	CYS	C-O	-6.53	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	68	LEU	CG-CD2	-6.51	1.27	1.51
1	A	92	ARG	CB-CG	-6.51	1.34	1.52
1	A	40	LYS	C-O	-6.51	1.10	1.23
2	D	117	HIS	CD2-NE2	-6.50	1.23	1.38
2	D	47	ASP	C-N	-6.50	1.19	1.34
2	D	126	VAL	CB-CG1	-6.50	1.39	1.52
2	B	102	ASN	CG-ND2	6.50	1.49	1.32
1	C	27	GLU	CD-OE2	6.49	1.32	1.25
2	D	14	LEU	N-CA	-6.49	1.33	1.46
2	D	32	LEU	CG-CD2	-6.49	1.27	1.51
2	B	123	THR	C-O	-6.49	1.11	1.23
1	C	36	PHE	CD2-CE2	-6.48	1.26	1.39
1	A	18	GLY	C-O	6.48	1.34	1.23
2	B	77	HIS	CA-CB	-6.48	1.39	1.53
1	A	113	LEU	CA-CB	-6.46	1.38	1.53
1	C	95	PRO	C-O	6.46	1.36	1.23
2	D	48	LEU	CG-CD1	6.44	1.75	1.51
2	D	83	GLY	CA-C	-6.44	1.41	1.51
1	C	46	PHE	CA-CB	6.44	1.68	1.53
2	B	48	LEU	N-CA	6.44	1.59	1.46
1	A	74	ASP	C-O	6.43	1.35	1.23
2	B	90	GLU	C-N	6.43	1.48	1.34
1	A	60	LYS	CA-CB	6.42	1.68	1.53
2	B	53	ALA	C-N	6.42	1.48	1.34
1	C	58	HIS	CA-C	6.42	1.69	1.52
2	B	35	TYR	CG-CD1	6.42	1.47	1.39
1	A	68	ASN	C-N	6.42	1.48	1.34
1	A	35	SER	N-CA	-6.39	1.33	1.46
1	C	120	ALA	C-O	6.38	1.35	1.23
1	A	45	HIS	CA-CB	-6.38	1.40	1.53
2	D	66	LYS	C-N	6.38	1.48	1.34
1	A	72	HIS	CA-C	-6.38	1.36	1.52
2	B	8	LYS	CD-CE	-6.38	1.35	1.51
1	C	113	LEU	CG-CD1	6.37	1.75	1.51
1	A	94	ASP	CA-C	6.37	1.69	1.52
1	A	95	PRO	C-O	6.36	1.35	1.23
2	D	71	PHE	CE1-CZ	-6.36	1.25	1.37
2	B	104	ARG	CA-CB	6.36	1.68	1.53
1	A	63	ALA	CA-C	-6.35	1.36	1.52
1	C	130	ALA	CA-CB	-6.34	1.39	1.52
1	A	70	VAL	N-CA	6.33	1.59	1.46
1	C	45	HIS	CB-CG	6.33	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	PRO	C-N	-6.33	1.19	1.34
1	C	50	HIS	CG-CD2	-6.33	1.25	1.35
1	A	61	LYS	CA-C	6.33	1.69	1.52
2	D	55	MET	CA-CB	6.33	1.67	1.53
2	B	140	ALA	CA-CB	6.32	1.65	1.52
2	B	120	LYS	CD-CE	6.32	1.67	1.51
1	C	63	ALA	CA-C	-6.32	1.36	1.52
1	C	122	HIS	CA-CB	-6.31	1.40	1.53
2	B	133	VAL	CB-CG1	-6.30	1.39	1.52
2	B	109	VAL	CB-CG2	6.30	1.66	1.52
2	B	145	TYR	C-O	6.29	1.35	1.23
2	B	98	VAL	CA-C	6.29	1.69	1.52
1	C	128	PHE	CE2-CZ	-6.29	1.25	1.37
2	B	98	VAL	CB-CG2	6.28	1.66	1.52
1	A	60	LYS	CA-C	-6.28	1.36	1.52
1	A	108	THR	CA-CB	6.28	1.69	1.53
1	A	11	LYS	CA-CB	-6.27	1.40	1.53
2	B	15	TRP	CB-CG	6.26	1.61	1.50
2	B	80	ASN	CA-CB	-6.26	1.36	1.53
1	C	73	VAL	CA-C	6.26	1.69	1.52
1	C	17	VAL	CB-CG2	6.24	1.66	1.52
1	A	60	LYS	CB-CG	-6.23	1.35	1.52
2	B	92	HIS	CD2-NE2	-6.23	1.24	1.38
2	D	112	CYS	C-O	-6.23	1.11	1.23
1	C	99	LYS	C-O	-6.23	1.11	1.23
2	D	30	ARG	C-N	-6.23	1.19	1.34
2	D	85	PHE	CE1-CZ	6.22	1.49	1.37
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	D	120	LYS	CB-CG	-6.21	1.35	1.52
2	B	48	LEU	CA-CB	-6.20	1.39	1.53
1	C	41	THR	N-CA	6.20	1.58	1.46
2	B	106	LEU	CG-CD2	-6.20	1.28	1.51
1	C	128	PHE	CE1-CZ	-6.18	1.25	1.37
2	D	47	ASP	C-O	6.18	1.35	1.23
2	B	118	PHE	CD1-CE1	6.18	1.51	1.39
2	D	48	LEU	CA-C	6.17	1.69	1.52
1	C	10	VAL	CB-CG1	6.17	1.65	1.52
1	A	128	PHE	CG-CD1	6.17	1.48	1.38
1	A	30	GLU	CD-OE2	6.17	1.32	1.25
2	B	103	PHE	CG-CD2	-6.16	1.29	1.38
1	C	48	LEU	CG-CD2	6.16	1.74	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	37	TRP	CD2-CE2	-6.16	1.33	1.41
1	C	106	LEU	N-CA	6.16	1.58	1.46
2	D	118	PHE	CG-CD2	6.15	1.48	1.38
1	A	10	VAL	CA-C	6.15	1.69	1.52
1	A	25	GLY	CA-C	-6.15	1.42	1.51
2	D	59	LYS	N-CA	-6.14	1.34	1.46
2	B	35	TYR	C-N	-6.14	1.22	1.34
1	A	97	ASN	CG-ND2	6.13	1.48	1.32
2	B	91	LEU	CG-CD2	-6.13	1.29	1.51
1	A	16	LYS	CB-CG	6.13	1.69	1.52
2	D	116	HIS	CG-ND1	-6.13	1.25	1.38
1	A	52	SER	CB-OG	-6.12	1.34	1.42
2	B	44	SER	N-CA	6.12	1.58	1.46
2	D	95	LYS	CA-C	-6.12	1.37	1.52
2	B	90	GLU	N-CA	-6.12	1.34	1.46
1	C	2	LEU	C-N	-6.12	1.20	1.34
2	B	132	LYS	CD-CE	6.10	1.66	1.51
2	B	6	GLU	C-N	-6.10	1.20	1.34
1	C	19	ALA	N-CA	-6.10	1.34	1.46
2	D	140	ALA	C-N	-6.10	1.20	1.34
2	D	60	VAL	C-N	6.09	1.48	1.34
1	C	50	HIS	C-N	-6.08	1.22	1.33
2	D	118	PHE	CE1-CZ	6.08	1.48	1.37
2	B	130	TYR	CE1-CZ	-6.08	1.30	1.38
2	D	84	THR	CA-C	6.07	1.68	1.52
2	D	144	LYS	CB-CG	6.06	1.69	1.52
2	D	23	VAL	C-N	-6.06	1.22	1.33
1	C	73	VAL	CB-CG1	-6.06	1.40	1.52
1	A	87	HIS	CB-CG	6.06	1.60	1.50
1	C	128	PHE	C-O	6.05	1.34	1.23
2	D	12	THR	CA-C	-6.05	1.37	1.52
1	A	11	LYS	CG-CD	-6.05	1.31	1.52
1	C	4	PRO	CA-C	6.04	1.65	1.52
1	A	92	ARG	CA-C	-6.03	1.37	1.52
2	D	74	GLY	N-CA	-6.03	1.37	1.46
1	A	46	PHE	CG-CD1	6.03	1.47	1.38
1	A	40	LYS	CD-CE	-6.02	1.36	1.51
1	C	88	ALA	CA-C	6.02	1.68	1.52
2	D	51	PRO	C-N	6.02	1.47	1.34
2	D	145	TYR	N-CA	-6.01	1.34	1.46
2	B	82	LYS	CG-CD	6.00	1.72	1.52
2	B	118	PHE	CA-CB	-6.00	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	MET	SD-CE	-5.99	1.44	1.77
2	B	52	ASP	CG-OD2	5.99	1.39	1.25
1	A	64	ASP	C-O	-5.97	1.12	1.23
2	B	40	ARG	CG-CD	5.97	1.66	1.51
1	C	3	SER	C-N	5.97	1.45	1.34
1	A	12	ALA	CA-CB	5.96	1.65	1.52
1	C	2	LEU	C-O	5.96	1.34	1.23
2	D	78	LEU	CA-C	-5.96	1.37	1.52
2	B	145	TYR	CE2-CZ	5.96	1.46	1.38
2	B	34	VAL	CB-CG2	-5.96	1.40	1.52
2	B	129	ALA	C-O	5.96	1.34	1.23
1	A	86	LEU	C-N	5.94	1.47	1.34
1	C	17	VAL	CA-CB	5.94	1.67	1.54
2	D	125	PRO	CG-CD	-5.94	1.31	1.50
1	A	34	LEU	CB-CG	-5.93	1.35	1.52
2	B	23	VAL	C-O	5.92	1.34	1.23
1	A	58	HIS	CE1-NE2	-5.91	1.19	1.32
2	B	117	HIS	CA-CB	5.91	1.67	1.53
2	B	7	GLU	CD-OE1	5.91	1.32	1.25
1	C	14	TRP	CD1-NE1	5.91	1.48	1.38
2	B	146	HIS	CA-C	-5.91	1.37	1.52
1	A	140	TYR	N-CA	-5.91	1.34	1.46
2	B	94	ASP	CG-OD1	-5.90	1.11	1.25
2	D	68	LEU	C-N	5.90	1.43	1.33
1	A	114	PRO	N-CD	-5.90	1.39	1.47
2	D	11	VAL	N-CA	5.90	1.58	1.46
1	A	26	ALA	CA-C	5.89	1.68	1.52
1	C	25	GLY	CA-C	-5.89	1.42	1.51
1	C	6	ASP	CG-OD1	5.89	1.39	1.25
2	B	58	PRO	CA-CB	5.88	1.65	1.53
2	D	58	PRO	CA-CB	5.88	1.65	1.53
2	D	72	SER	C-O	5.88	1.34	1.23
1	A	71	ALA	N-CA	5.87	1.58	1.46
2	D	121	GLU	CA-C	5.87	1.68	1.52
1	C	26	ALA	C-O	-5.87	1.12	1.23
2	D	126	VAL	CA-C	5.87	1.68	1.52
2	B	29	GLY	N-CA	-5.86	1.37	1.46
2	D	85	PHE	CD2-CE2	5.85	1.50	1.39
2	B	116	HIS	CG-ND1	5.85	1.51	1.38
2	D	71	PHE	CD2-CE2	5.85	1.50	1.39
1	C	24	TYR	C-O	-5.85	1.12	1.23
2	B	92	HIS	CA-C	5.84	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	GLY	CA-C	-5.83	1.42	1.51
2	D	92	HIS	CB-CG	5.83	1.60	1.50
2	B	66	LYS	CA-CB	5.83	1.66	1.53
2	B	63	HIS	CG-CD2	5.83	1.45	1.35
1	C	105	LEU	N-CA	-5.82	1.34	1.46
1	C	89	HIS	CE1-NE2	-5.82	1.19	1.32
1	A	64	ASP	N-CA	-5.82	1.34	1.46
1	A	43	PHE	CE1-CZ	-5.81	1.26	1.37
1	A	24	TYR	CD1-CE1	5.81	1.48	1.39
2	D	63	HIS	CE1-NE2	-5.81	1.19	1.32
2	B	92	HIS	CG-ND1	5.80	1.51	1.38
2	B	35	TYR	CZ-OH	5.80	1.47	1.37
2	B	26	GLU	CA-CB	-5.80	1.41	1.53
2	B	84	THR	C-N	5.80	1.47	1.34
2	B	84	THR	C-O	-5.79	1.12	1.23
1	A	6	ASP	CA-CB	-5.79	1.41	1.53
2	D	37	TRP	N-CA	-5.79	1.34	1.46
1	A	20	HIS	C-N	-5.79	1.20	1.34
1	A	51	GLY	C-O	-5.79	1.14	1.23
1	C	33	PHE	CA-C	-5.78	1.38	1.52
2	B	14	LEU	CG-CD1	-5.78	1.30	1.51
1	C	57	GLY	N-CA	-5.78	1.37	1.46
2	D	60	VAL	CB-CG1	5.78	1.65	1.52
2	D	118	PHE	C-O	5.78	1.34	1.23
2	D	139	ASN	CB-CG	-5.77	1.37	1.51
1	C	29	LEU	CA-CB	5.76	1.67	1.53
1	A	28	ALA	C-O	-5.76	1.12	1.23
2	D	115	ALA	C-O	-5.76	1.12	1.23
1	C	47	ASP	CA-C	5.76	1.68	1.52
1	A	47	ASP	CA-CB	5.75	1.66	1.53
1	C	61	LYS	C-N	5.75	1.47	1.34
2	B	72	SER	C-O	5.75	1.34	1.23
2	D	103	PHE	CB-CG	5.74	1.61	1.51
1	A	92	ARG	N-CA	5.74	1.57	1.46
2	D	21	ASP	N-CA	5.74	1.57	1.46
2	B	33	VAL	CB-CG2	-5.74	1.40	1.52
2	D	97	HIS	C-N	5.73	1.47	1.34
1	C	121	VAL	CA-CB	-5.72	1.42	1.54
1	A	36	PHE	C-O	5.72	1.34	1.23
1	A	112	HIS	CA-CB	5.72	1.66	1.53
2	D	51	PRO	CG-CD	5.71	1.69	1.50
1	A	21	ALA	CA-CB	-5.71	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	PHE	CD1-CE1	5.71	1.50	1.39
2	B	87	THR	CB-OG1	-5.71	1.31	1.43
2	D	145	TYR	CG-CD2	5.70	1.46	1.39
1	C	124	SER	CB-OG	5.70	1.49	1.42
1	A	37	PRO	CA-C	-5.70	1.41	1.52
2	D	90	GLU	C-O	-5.70	1.12	1.23
2	B	71	PHE	CE1-CZ	-5.69	1.26	1.37
1	C	9	ASN	CG-ND2	-5.69	1.18	1.32
1	A	5	ALA	CA-C	5.69	1.67	1.52
1	C	31	ARG	CZ-NH2	-5.68	1.25	1.33
1	C	141	ARG	CZ-NH1	-5.68	1.25	1.33
1	A	78	ASN	N-CA	-5.68	1.34	1.46
1	C	141	ARG	CA-C	5.67	1.67	1.52
1	A	59	GLY	C-O	5.67	1.32	1.23
1	C	84	SER	C-N	5.67	1.47	1.34
1	A	34	LEU	CA-CB	-5.66	1.40	1.53
2	B	126	VAL	C-N	-5.66	1.21	1.34
1	C	46	PHE	CA-C	-5.65	1.38	1.52
2	B	62	ALA	C-O	-5.65	1.12	1.23
1	C	54	GLN	CA-CB	-5.65	1.41	1.53
2	D	30	ARG	CG-CD	-5.65	1.37	1.51
2	B	140	ALA	C-O	5.64	1.34	1.23
1	A	109	LEU	CG-CD1	-5.64	1.30	1.51
1	C	33	PHE	CE1-CZ	-5.64	1.26	1.37
2	D	49	SER	CA-CB	5.64	1.61	1.52
1	C	129	LEU	CA-CB	-5.63	1.40	1.53
1	A	75	ASP	N-CA	5.63	1.57	1.46
1	C	136	LEU	C-O	5.62	1.34	1.23
1	A	46	PHE	N-CA	-5.62	1.35	1.46
1	A	63	ALA	CA-CB	5.62	1.64	1.52
2	D	85	PHE	CG-CD1	5.62	1.47	1.38
1	C	141	ARG	CG-CD	5.62	1.66	1.51
1	C	113	LEU	C-N	-5.61	1.23	1.34
1	C	134	THR	CB-OG1	-5.61	1.32	1.43
1	A	115	ALA	C-O	-5.60	1.12	1.23
2	B	9	SER	CB-OG	5.60	1.49	1.42
1	C	28	ALA	N-CA	5.60	1.57	1.46
1	C	134	THR	C-O	5.60	1.33	1.23
2	D	14	LEU	CG-CD2	-5.60	1.31	1.51
2	B	17	LYS	CB-CG	5.59	1.67	1.52
2	B	71	PHE	CD1-CE1	5.58	1.50	1.39
1	A	2	LEU	N-CA	5.57	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	140	TYR	C-O	5.57	1.33	1.23
1	C	8	THR	CB-CG2	-5.57	1.33	1.52
1	A	105	LEU	CA-CB	5.56	1.66	1.53
2	B	92	HIS	ND1-CE1	5.56	1.48	1.34
1	C	92	ARG	C-N	5.56	1.46	1.34
2	D	51	PRO	N-CA	-5.55	1.37	1.47
2	B	114	LEU	CA-CB	-5.55	1.41	1.53
2	B	47	ASP	CB-CG	-5.54	1.40	1.51
1	C	30	GLU	N-CA	-5.54	1.35	1.46
2	B	43	GLU	C-N	5.54	1.46	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
2	B	119	GLY	CA-C	-5.54	1.43	1.51
1	C	53	ALA	CA-CB	-5.54	1.40	1.52
1	A	9	ASN	C-O	-5.53	1.12	1.23
1	A	54	GLN	CA-C	5.53	1.67	1.52
2	B	37	TRP	CB-CG	-5.53	1.40	1.50
2	B	120	LYS	C-N	-5.52	1.21	1.34
1	A	93	VAL	CA-C	-5.52	1.38	1.52
1	C	13	ALA	C-O	5.52	1.33	1.23
2	B	28	LEU	C-N	5.51	1.43	1.33
1	A	48	LEU	CG-CD1	5.51	1.72	1.51
2	D	102	ASN	CG-OD1	-5.51	1.11	1.24
1	C	141	ARG	NE-CZ	5.50	1.40	1.33
1	C	97	ASN	CA-CB	-5.50	1.38	1.53
1	A	123	ALA	C-O	5.50	1.33	1.23
2	B	116	HIS	ND1-CE1	5.50	1.48	1.34
2	D	99	ASP	C-N	-5.49	1.23	1.34
1	A	112	HIS	C-O	5.49	1.33	1.23
2	B	57	ASN	N-CA	-5.49	1.35	1.46
2	D	31	LEU	C-N	5.49	1.46	1.34
2	B	30	ARG	NE-CZ	-5.47	1.25	1.33
2	B	70	ALA	N-CA	-5.47	1.35	1.46
1	A	3	SER	CA-C	-5.47	1.38	1.52
1	C	135	VAL	C-N	5.47	1.46	1.34
1	C	12	ALA	CA-C	-5.46	1.38	1.52
2	D	50	THR	CB-OG1	5.46	1.54	1.43
1	C	46	PHE	C-O	5.46	1.33	1.23
2	D	17	LYS	N-CA	-5.46	1.35	1.46
2	D	71	PHE	CG-CD2	5.46	1.47	1.38
2	B	17	LYS	CG-CD	-5.46	1.33	1.52
1	A	72	HIS	N-CA	-5.46	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	PHE	C-N	-5.46	1.21	1.34
1	A	87	HIS	CG-ND1	5.45	1.50	1.38
2	D	59	LYS	CE-NZ	5.44	1.62	1.49
1	A	139	LYS	CD-CE	-5.44	1.37	1.51
1	A	43	PHE	CB-CG	5.44	1.60	1.51
2	D	74	GLY	C-N	5.43	1.46	1.34
1	A	129	LEU	CA-C	-5.43	1.38	1.52
2	D	60	VAL	CB-CG2	-5.42	1.41	1.52
1	A	141	ARG	CZ-NH2	5.42	1.40	1.33
2	B	109	VAL	C-O	5.42	1.33	1.23
1	A	140	TYR	C-N	-5.42	1.21	1.34
2	B	23	VAL	C-N	-5.42	1.23	1.33
2	B	144	LYS	CB-CG	5.40	1.67	1.52
2	B	100	PRO	C-O	5.39	1.34	1.23
1	A	85	ASP	C-O	-5.39	1.13	1.23
1	A	39	THR	C-N	-5.39	1.21	1.34
1	C	4	PRO	CA-CB	5.39	1.64	1.53
1	A	61	LYS	CB-CG	5.39	1.67	1.52
1	C	139	LYS	CB-CG	5.38	1.67	1.52
2	B	68	LEU	C-O	5.38	1.33	1.23
2	D	104	ARG	CB-CG	-5.38	1.38	1.52
1	C	37	PRO	CA-C	5.38	1.63	1.52
1	C	109	LEU	CG-CD2	-5.38	1.31	1.51
2	D	42	PHE	CD1-CE1	5.37	1.50	1.39
2	B	23	VAL	CA-C	5.37	1.67	1.52
1	C	38	THR	N-CA	5.37	1.57	1.46
1	A	91	LEU	CG-CD1	-5.37	1.31	1.51
2	B	6	GLU	CA-CB	5.37	1.65	1.53
2	B	33	VAL	CA-C	5.37	1.67	1.52
2	D	92	HIS	N-CA	5.36	1.57	1.46
1	C	46	PHE	N-CA	-5.36	1.35	1.46
1	A	91	LEU	CA-CB	5.36	1.66	1.53
2	D	35	TYR	CD1-CE1	5.36	1.47	1.39
2	B	57	ASN	C-O	5.35	1.33	1.23
1	C	35	SER	C-N	5.34	1.46	1.34
1	C	115	ALA	C-O	5.34	1.33	1.23
1	C	89	HIS	C-N	-5.34	1.21	1.34
1	C	85	ASP	CG-OD2	5.34	1.37	1.25
2	B	17	LYS	CA-C	-5.33	1.39	1.52
2	B	48	LEU	CG-CD2	-5.33	1.32	1.51
1	A	52	SER	C-N	5.32	1.46	1.34
2	B	13	ALA	CA-C	-5.32	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	CYS	C-N	-5.32	1.21	1.34
2	B	15	TRP	CA-CB	-5.32	1.42	1.53
2	D	102	ASN	CG-ND2	5.32	1.46	1.32
2	D	49	SER	N-CA	5.31	1.56	1.46
2	B	43	GLU	N-CA	5.30	1.56	1.46
1	A	21	ALA	N-CA	5.30	1.56	1.46
1	C	12	ALA	CA-CB	-5.30	1.41	1.52
2	D	12	THR	CB-OG1	5.29	1.53	1.43
1	A	107	VAL	CB-CG2	5.29	1.64	1.52
1	C	54	GLN	N-CA	5.28	1.56	1.46
1	C	94	ASP	N-CA	-5.28	1.35	1.46
2	B	101	GLU	CA-CB	-5.28	1.42	1.53
2	D	102	ASN	N-CA	5.27	1.56	1.46
2	B	28	LEU	CA-C	-5.27	1.39	1.52
2	B	108	ASN	CG-OD1	5.27	1.35	1.24
2	B	86	ALA	CA-C	-5.27	1.39	1.52
1	A	14	TRP	CA-C	5.26	1.66	1.52
1	C	5	ALA	CA-C	5.26	1.66	1.52
1	A	114	PRO	C-O	-5.25	1.12	1.23
1	C	54	GLN	CB-CG	-5.25	1.38	1.52
2	B	63	HIS	CE1-NE2	-5.25	1.20	1.32
1	C	116	GLU	C-N	-5.24	1.22	1.34
2	B	3	LEU	CG-CD1	-5.24	1.32	1.51
2	B	79	ASP	C-N	5.24	1.46	1.34
1	A	84	SER	C-O	-5.24	1.13	1.23
2	B	24	GLY	N-CA	-5.24	1.38	1.46
1	C	56	LYS	C-N	5.24	1.42	1.33
1	C	82	ALA	CA-C	-5.24	1.39	1.52
1	C	29	LEU	N-CA	5.23	1.56	1.46
1	C	45	HIS	CG-ND1	5.23	1.50	1.38
1	A	27	GLU	CD-OE2	-5.23	1.19	1.25
2	B	71	PHE	CG-CD1	-5.22	1.30	1.38
2	D	131	GLN	CB-CG	-5.22	1.38	1.52
1	C	27	GLU	C-N	5.22	1.46	1.34
2	D	68	LEU	CG-CD2	-5.21	1.32	1.51
2	B	119	GLY	C-N	-5.21	1.22	1.34
2	B	42	PHE	C-N	-5.21	1.22	1.34
2	B	85	PHE	CD2-CE2	5.21	1.49	1.39
2	B	78	LEU	CB-CG	5.20	1.67	1.52
1	A	46	PHE	C-N	5.19	1.46	1.34
2	D	31	LEU	C-O	-5.19	1.13	1.23
2	D	42	PHE	CB-CG	5.19	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	91	LEU	CG-CD1	5.19	1.71	1.51
2	B	122	PHE	CE2-CZ	5.19	1.47	1.37
1	A	107	VAL	CB-CG1	-5.18	1.42	1.52
1	C	86	LEU	N-CA	-5.18	1.35	1.46
2	D	145	TYR	CD1-CE1	-5.18	1.31	1.39
2	D	102	ASN	CA-CB	-5.17	1.39	1.53
2	D	112	CYS	CA-C	5.17	1.66	1.52
1	A	88	ALA	N-CA	5.15	1.56	1.46
2	D	118	PHE	CB-CG	5.15	1.60	1.51
2	D	119	GLY	C-N	5.15	1.45	1.34
1	A	35	SER	CA-CB	5.15	1.60	1.52
1	A	135	VAL	C-O	5.15	1.33	1.23
2	B	116	HIS	CB-CG	-5.15	1.40	1.50
1	C	55	VAL	CB-CG2	-5.15	1.42	1.52
1	C	114	PRO	CG-CD	5.14	1.67	1.50
2	D	16	GLY	N-CA	5.14	1.53	1.46
1	A	93	VAL	C-O	5.14	1.33	1.23
2	D	144	LYS	CA-C	-5.13	1.39	1.52
1	C	124	SER	C-N	-5.13	1.22	1.34
2	D	77	HIS	CA-C	5.13	1.66	1.52
1	C	43	PHE	CE1-CZ	5.13	1.47	1.37
1	A	117	PHE	CB-CG	5.12	1.60	1.51
1	A	79	ALA	C-N	-5.11	1.22	1.34
2	D	125	PRO	C-N	5.11	1.45	1.34
2	D	111	VAL	C-N	5.11	1.45	1.34
1	A	9	ASN	CA-C	5.11	1.66	1.52
1	A	19	ALA	CA-C	5.11	1.66	1.52
1	A	121	VAL	CB-CG1	5.10	1.63	1.52
2	B	67	VAL	C-O	5.10	1.33	1.23
2	D	63	HIS	CG-CD2	5.10	1.44	1.35
1	A	75	ASP	C-O	5.10	1.33	1.23
1	C	73	VAL	CB-CG2	-5.10	1.42	1.52
1	A	115	ALA	N-CA	5.08	1.56	1.46
2	B	68	LEU	CA-CB	-5.08	1.42	1.53
2	B	105	LEU	CA-CB	-5.08	1.42	1.53
1	C	85	ASP	C-N	5.08	1.45	1.34
2	B	107	GLY	C-O	5.08	1.31	1.23
1	C	66	LEU	CG-CD1	-5.07	1.33	1.51
1	C	86	LEU	C-O	-5.07	1.13	1.23
1	A	63	ALA	C-O	5.07	1.32	1.23
2	B	85	PHE	N-CA	5.07	1.56	1.46
2	D	52	ASP	CG-OD1	-5.07	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	30	ARG	CZ-NH1	5.06	1.39	1.33
1	C	4	PRO	C-N	-5.06	1.22	1.34
1	A	129	LEU	CG-CD2	5.05	1.70	1.51
1	C	58	HIS	CA-CB	-5.05	1.42	1.53
2	D	57	ASN	CG-ND2	-5.05	1.20	1.32
1	A	112	HIS	C-N	-5.04	1.22	1.34
1	A	39	THR	C-O	-5.04	1.13	1.23
1	A	69	ALA	C-N	5.04	1.45	1.34
1	C	43	PHE	CG-CD1	5.04	1.46	1.38
2	B	64	GLY	CA-C	-5.04	1.43	1.51
2	B	103	PHE	CD2-CE2	5.03	1.49	1.39
2	B	132	LYS	C-N	5.03	1.45	1.34
1	A	81	SER	CB-OG	5.03	1.48	1.42
1	A	137	THR	C-N	-5.02	1.22	1.34
1	A	85	ASP	C-N	5.02	1.45	1.34
1	C	113	LEU	CA-C	5.02	1.66	1.52
1	A	68	ASN	CG-OD1	-5.02	1.12	1.24
1	A	54	GLN	CD-NE2	5.02	1.45	1.32
2	B	108	ASN	CG-ND2	-5.02	1.20	1.32
2	D	78	LEU	CG-CD1	5.01	1.70	1.51
2	D	116	HIS	C-O	5.01	1.32	1.23

All (1823) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	92	ARG	NE-CZ-NH2	-165.74	37.43	120.30
2	D	104	ARG	NE-CZ-NH2	-86.93	76.84	120.30
2	D	6	GLU	OE1-CD-OE2	-66.30	43.74	123.30
2	D	104	ARG	NE-CZ-NH1	-58.45	91.08	120.30
1	A	92	ARG	NE-CZ-NH2	-57.17	91.72	120.30
1	C	92	ARG	NE-CZ-NH1	-56.23	92.19	120.30
1	A	92	ARG	CD-NE-CZ	-51.90	50.94	123.60
2	B	26	GLU	OE1-CD-OE2	-50.92	62.20	123.30
2	B	101	GLU	OE1-CD-OE2	46.01	178.51	123.30
1	A	75	ASP	CB-CG-OD2	-43.84	78.85	118.30
2	B	22	GLU	OE1-CD-OE2	-43.42	71.20	123.30
2	D	73	ASP	CB-CG-OD1	43.27	157.24	118.30
1	A	92	ARG	NE-CZ-NH1	-40.89	99.86	120.30
2	D	40	ARG	NE-CZ-NH2	-38.48	101.06	120.30
1	A	75	ASP	CB-CG-OD1	38.30	152.77	118.30
2	B	104	ARG	CD-NE-CZ	-37.19	71.54	123.60
1	C	1	VAL	CG1-CB-CG2	-35.83	53.57	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	40	ARG	NE-CZ-NH2	-35.57	102.52	120.30
2	B	143	HIS	CG-ND1-CE1	-34.67	59.66	108.20
2	B	104	ARG	NE-CZ-NH2	-34.65	102.98	120.30
1	C	141	ARG	NE-CZ-NH2	-34.60	103.00	120.30
1	C	92	ARG	CD-NE-CZ	-34.44	75.38	123.60
2	D	26	GLU	OE1-CD-OE2	-34.43	81.99	123.30
2	B	143	HIS	ND1-CG-CD2	32.84	154.78	108.80
2	B	26	GLU	CG-CD-OE2	-32.51	53.28	118.30
2	D	20	VAL	CG1-CB-CG2	32.46	162.83	110.90
1	C	75	ASP	CB-CG-OD2	-32.37	89.17	118.30
1	C	30	GLU	OE1-CD-OE2	32.29	162.05	123.30
2	D	73	ASP	CB-CG-OD2	-31.95	89.55	118.30
2	D	52	ASP	CB-CG-OD2	-31.77	89.71	118.30
2	B	30	ARG	NE-CZ-NH2	31.77	136.18	120.30
2	B	43	GLU	OE1-CD-OE2	31.65	161.28	123.30
1	A	92	ARG	CG-CD-NE	-31.16	46.37	111.80
2	D	58	PRO	N-CD-CG	-30.98	56.72	103.20
2	B	5	PRO	N-CA-CB	29.95	139.23	103.30
2	D	30	ARG	NE-CZ-NH1	29.92	135.26	120.30
1	A	92	ARG	NH1-CZ-NH2	29.49	151.84	119.40
2	D	43	GLU	OE1-CD-OE2	-29.31	88.12	123.30
2	D	3	LEU	O-C-N	-29.18	76.00	122.70
2	D	79	ASP	CB-CG-OD2	-29.16	92.06	118.30
1	C	23	GLU	OE1-CD-OE2	-28.53	89.06	123.30
2	D	80	ASN	CA-CB-CG	28.38	175.84	113.40
2	D	101	GLU	OE1-CD-OE2	28.04	156.95	123.30
2	B	42	PHE	CB-CG-CD2	27.92	140.34	120.80
2	D	73	ASP	OD1-CG-OD2	-27.46	71.12	123.30
2	B	45	PHE	CG-CD2-CE2	27.03	150.53	120.80
2	D	104	ARG	CD-NE-CZ	-26.60	86.37	123.60
2	D	20	VAL	CA-CB-CG2	-26.24	71.55	110.90
1	C	74	ASP	CB-CG-OD2	26.05	141.74	118.30
1	A	75	ASP	OD1-CG-OD2	-25.95	73.99	123.30
1	C	1	VAL	CA-CB-CG1	-25.92	72.03	110.90
2	B	44	SER	O-C-N	-25.84	81.36	122.70
2	D	52	ASP	CB-CG-OD1	-25.82	95.06	118.30
2	D	47	ASP	O-C-N	25.77	163.93	122.70
2	B	139	ASN	OD1-CG-ND2	-25.64	62.94	121.90
2	D	26	GLU	CG-CD-OE1	-25.55	67.20	118.30
1	A	31	ARG	NE-CZ-NH2	-25.29	107.66	120.30
1	A	141	ARG	NE-CZ-NH1	25.26	132.93	120.30
2	D	26	GLU	CB-CG-CD	-25.24	46.05	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	46	PHE	CB-CG-CD2	25.12	138.39	120.80
1	A	47	ASP	CB-CG-OD2	-24.54	96.21	118.30
2	B	43	GLU	CG-CD-OE2	-24.54	69.22	118.30
2	D	94	ASP	CB-CG-OD1	-24.47	96.27	118.30
1	A	72	HIS	ND1-CG-CD2	-24.24	72.06	106.00
2	D	43	GLU	CA-CB-CG	23.85	165.87	113.40
2	D	82	LYS	CD-CE-NZ	-23.77	57.02	111.70
2	D	47	ASP	N-CA-CB	-23.75	67.84	110.60
2	B	45	PHE	CZ-CE2-CD2	-23.48	91.92	120.10
1	A	141	ARG	NE-CZ-NH2	-23.44	108.58	120.30
1	C	38	THR	OG1-CB-CG2	-23.40	56.18	110.00
2	B	12	THR	OG1-CB-CG2	23.40	163.82	110.00
2	B	94	ASP	CB-CG-OD1	-23.20	97.42	118.30
1	A	64	ASP	CB-CG-OD1	-23.18	97.44	118.30
2	D	146	HIS	ND1-CG-CD2	-23.11	73.64	106.00
2	D	145	TYR	CB-CG-CD1	23.03	134.82	121.00
2	D	47	ASP	CB-CG-OD1	-22.91	97.68	118.30
1	C	46	PHE	CZ-CE2-CD2	22.87	147.54	120.10
1	C	1	VAL	CA-CB-CG2	-22.77	76.74	110.90
2	B	145	TYR	CB-CG-CD2	-22.56	107.46	121.00
1	A	46	PHE	CB-CG-CD2	22.49	136.54	120.80
2	D	6	GLU	O-C-N	22.47	158.66	122.70
2	D	5	PRO	N-CA-CB	-22.34	76.49	103.30
1	C	24	TYR	CG-CD1-CE1	-22.24	103.50	121.30
2	B	40	ARG	NH1-CZ-NH2	22.24	143.86	119.40
2	D	90	GLU	CG-CD-OE1	-22.03	74.24	118.30
1	A	14	TRP	CD1-NE1-CE2	22.02	128.82	109.00
2	D	71	PHE	CG-CD2-CE2	-21.99	96.61	120.80
2	D	42	PHE	CB-CG-CD1	-21.90	105.47	120.80
2	D	55	MET	O-C-N	21.86	160.37	123.20
2	B	40	ARG	NE-CZ-NH1	-21.85	109.38	120.30
2	D	26	GLU	CG-CD-OE2	-21.77	74.76	118.30
2	B	52	ASP	CB-CG-OD2	-21.75	98.72	118.30
2	D	79	ASP	OD1-CG-OD2	-21.70	82.07	123.30
2	D	17	LYS	O-C-N	-21.69	88.00	122.70
1	A	138	SER	CA-CB-OG	-21.68	52.65	111.20
1	C	73	VAL	CG1-CB-CG2	21.66	145.55	110.90
2	B	1	VAL	CG1-CB-CG2	21.59	145.45	110.90
2	B	49	SER	O-C-N	-21.41	88.45	122.70
2	D	76	ALA	N-CA-CB	-21.34	80.22	110.10
1	C	138	SER	CA-CB-OG	-21.28	53.75	111.20
2	B	101	GLU	CG-CD-OE2	-21.24	75.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	14	TRP	CD1-NE1-CE2	20.99	127.89	109.00
2	D	45	PHE	CB-CG-CD2	20.97	135.48	120.80
2	D	55	MET	C-N-CA	-20.94	78.33	122.30
1	A	64	ASP	CB-CG-OD2	-20.90	99.49	118.30
2	B	26	GLU	CB-CG-CD	20.78	170.31	114.20
2	B	42	PHE	CD1-CE1-CZ	20.70	144.95	120.10
2	D	41	PHE	CG-CD1-CE1	-20.59	98.15	120.80
2	D	118	PHE	CB-CG-CD1	20.51	135.16	120.80
1	C	128	PHE	CB-CG-CD2	-20.20	106.66	120.80
1	C	14	TRP	CG-CD1-NE1	-20.12	89.98	110.10
1	C	23	GLU	CG-CD-OE1	-20.05	78.20	118.30
2	D	72	SER	N-CA-CB	19.95	140.43	110.50
1	A	12	ALA	CB-CA-C	-19.63	80.66	110.10
1	C	47	ASP	CB-CG-OD2	-19.43	100.82	118.30
1	C	1	VAL	N-CA-CB	-19.31	69.02	111.50
1	C	24	TYR	CZ-CE2-CD2	-19.09	102.62	119.80
2	B	21	ASP	CB-CG-OD2	-18.96	101.24	118.30
1	A	90	LYS	CD-CE-NZ	-18.87	68.30	111.70
1	A	2	LEU	O-C-N	18.87	152.89	122.70
2	D	118	PHE	CG-CD1-CE1	18.82	141.50	120.80
1	C	128	PHE	CD1-CG-CD2	18.78	142.71	118.30
2	D	19	ASN	OD1-CG-ND2	-18.78	78.71	121.90
2	D	94	ASP	CB-CG-OD2	-18.72	101.45	118.30
2	D	101	GLU	CG-CD-OE2	-18.71	80.88	118.30
2	D	78	LEU	CB-CG-CD2	18.60	142.62	111.00
1	A	75	ASP	CA-CB-CG	-18.58	72.53	113.40
2	D	42	PHE	CG-CD1-CE1	-18.54	100.41	120.80
2	D	41	PHE	CD1-CE1-CZ	18.49	142.29	120.10
2	D	145	TYR	CB-CG-CD2	-18.42	109.95	121.00
2	B	108	ASN	OD1-CG-ND2	18.42	164.26	121.90
2	D	56	GLY	O-C-N	-18.38	93.29	122.70
1	C	128	PHE	CG-CD1-CE1	-18.19	100.79	120.80
2	B	22	GLU	CG-CD-OE2	-18.13	82.03	118.30
1	C	47	ASP	CB-CG-OD1	-18.12	101.99	118.30
2	D	46	GLY	C-N-CA	-18.05	76.58	121.70
1	A	17	VAL	O-C-N	17.97	153.75	123.20
1	A	85	ASP	CB-CG-OD1	17.96	134.46	118.30
2	B	144	LYS	CG-CD-CE	17.89	165.57	111.90
2	B	45	PHE	CB-CG-CD2	17.84	133.29	120.80
1	A	49	SER	CB-CA-C	17.82	143.95	110.10
1	C	74	ASP	OD1-CG-OD2	-17.76	89.55	123.30
1	C	116	GLU	CG-CD-OE2	-17.76	82.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	16	LYS	N-CA-CB	17.67	142.40	110.60
2	B	65	LYS	CD-CE-NZ	-17.59	71.25	111.70
2	B	6	GLU	OE1-CD-OE2	-17.58	102.21	123.30
2	B	50	THR	CA-CB-CG2	17.57	137.00	112.40
1	A	22	GLY	O-C-N	-17.55	94.63	122.70
1	A	30	GLU	OE1-CD-OE2	17.47	144.27	123.30
2	D	44	SER	O-C-N	-17.47	94.75	122.70
2	D	132	LYS	CD-CE-NZ	-17.44	71.58	111.70
2	B	59	LYS	CD-CE-NZ	-17.43	71.60	111.70
1	A	128	PHE	CZ-CE2-CD2	-17.39	99.23	120.10
2	D	17	LYS	CA-C-O	17.33	156.50	120.10
1	A	1	VAL	CA-CB-CG2	-17.31	84.94	110.90
1	A	31	ARG	NE-CZ-NH1	17.30	128.95	120.30
2	B	21	ASP	CB-CG-OD1	-17.17	102.85	118.30
1	A	1	VAL	CG1-CB-CG2	17.15	138.34	110.90
2	D	130	TYR	CG-CD1-CE1	17.15	135.02	121.30
1	A	23	GLU	CG-CD-OE1	-17.06	84.19	118.30
1	A	33	PHE	CB-CG-CD1	17.04	132.73	120.80
2	D	58	PRO	CA-CB-CG	-16.99	71.72	104.00
2	B	139	ASN	CB-CG-OD1	16.97	155.55	121.60
2	B	2	HIS	CB-CA-C	-16.85	76.70	110.40
1	A	72	HIS	CA-CB-CG	-16.82	85.01	113.60
2	D	18	VAL	O-C-N	16.79	149.56	122.70
2	B	4	THR	CA-CB-CG2	16.73	135.83	112.40
1	C	22	GLY	O-C-N	-16.72	95.95	122.70
2	D	130	TYR	CD1-CE1-CZ	-16.67	104.80	119.80
1	C	14	TRP	CE3-CZ3-CH2	-16.61	102.92	121.20
2	B	74	GLY	CA-C-O	16.60	150.49	120.60
1	C	139	LYS	CD-CE-NZ	-16.57	73.58	111.70
2	B	94	ASP	OD1-CG-OD2	16.57	154.79	123.30
2	B	121	GLU	CG-CD-OE2	-16.56	85.18	118.30
1	A	60	LYS	CD-CE-NZ	-16.50	73.74	111.70
1	C	64	ASP	CB-CG-OD2	-16.50	103.45	118.30
2	B	20	VAL	O-C-N	-16.41	96.44	122.70
1	C	14	TRP	C-N-CA	16.33	156.60	122.30
1	C	61	LYS	CD-CE-NZ	-16.32	74.17	111.70
1	C	46	PHE	CE1-CZ-CE2	-16.30	90.65	120.00
1	A	17	VAL	CA-C-N	-16.29	83.62	116.20
1	A	16	LYS	CG-CD-CE	-16.19	63.33	111.90
1	A	12	ALA	O-C-N	-16.17	96.83	122.70
2	D	8	LYS	CA-CB-CG	-16.14	77.90	113.40
2	B	118	PHE	CB-CG-CD2	16.12	132.09	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	ASN	OD1-CG-ND2	-16.06	84.96	121.90
1	C	14	TRP	O-C-N	-16.06	95.90	123.20
1	C	128	PHE	CG-CD2-CE2	-16.05	103.14	120.80
2	D	78	LEU	CA-C-O	16.03	153.76	120.10
1	C	56	LYS	CD-CE-NZ	-16.02	74.85	111.70
2	B	85	PHE	CZ-CE2-CD2	16.01	139.32	120.10
2	B	1	VAL	C-N-CA	-16.00	81.69	121.70
2	D	47	ASP	CA-C-N	-15.99	82.02	117.20
2	D	46	GLY	CA-C-O	-15.98	91.84	120.60
2	D	13	ALA	N-CA-CB	15.97	132.46	110.10
2	D	94	ASP	OD1-CG-OD2	15.88	153.47	123.30
2	B	65	LYS	CG-CD-CE	-15.84	64.38	111.90
2	D	12	THR	CA-CB-CG2	-15.75	90.35	112.40
1	A	18	GLY	O-C-N	15.69	147.81	122.70
1	C	24	TYR	CE1-CZ-CE2	15.66	144.85	119.80
2	B	32	LEU	CB-CG-CD1	15.65	137.61	111.00
1	A	43	PHE	CB-CG-CD2	15.65	131.75	120.80
2	D	76	ALA	O-C-N	-15.58	97.77	122.70
2	D	76	ALA	CA-C-N	15.57	151.45	117.20
1	C	23	GLU	CG-CD-OE2	-15.56	87.19	118.30
2	B	73	ASP	O-C-N	-15.53	96.80	123.20
1	C	71	ALA	CB-CA-C	15.50	133.35	110.10
2	B	117	HIS	CG-CD2-NE2	-15.47	79.80	109.20
2	D	2	HIS	CE1-NE2-CD2	15.45	145.24	106.60
1	C	85	ASP	CB-CG-OD1	15.45	132.20	118.30
1	C	75	ASP	OD1-CG-OD2	15.44	152.64	123.30
2	D	71	PHE	CD1-CG-CD2	15.44	138.37	118.30
2	B	74	GLY	O-C-N	-15.43	98.02	122.70
1	C	7	LYS	CD-CE-NZ	15.43	147.18	111.70
2	D	77	HIS	CG-CD2-NE2	-15.43	79.89	109.20
2	D	43	GLU	O-C-N	15.42	147.38	122.70
1	A	98	PHE	CB-CG-CD1	-15.39	110.02	120.80
2	D	6	GLU	CG-CD-OE2	-15.39	87.51	118.30
2	D	71	PHE	CB-CG-CD2	-15.39	110.03	120.80
1	A	33	PHE	CB-CG-CD2	-15.30	110.09	120.80
2	D	146	HIS	CG-CD2-NE2	15.28	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	-15.18	91.23	121.60
1	C	56	LYS	CG-CD-CE	-15.18	66.36	111.90
1	A	81	SER	N-CA-CB	-15.14	87.80	110.50
1	C	45	HIS	CG-ND1-CE1	-15.09	86.09	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	VAL	CA-C-N	-15.06	84.06	117.20
2	B	37	TRP	CD1-NE1-CE2	15.06	122.56	109.00
2	D	47	ASP	CB-CA-C	-15.06	80.28	110.40
2	D	121	GLU	OE1-CD-OE2	-14.86	105.47	123.30
2	D	1	VAL	O-C-N	14.85	146.46	122.70
1	A	137	THR	CA-CB-OG1	-14.82	77.88	109.00
2	D	41	PHE	O-C-N	14.82	146.41	122.70
2	D	79	ASP	CB-CA-C	-14.73	80.94	110.40
2	D	90	GLU	OE1-CD-OE2	-14.71	105.65	123.30
2	B	56	GLY	O-C-N	-14.69	99.20	122.70
1	C	73	VAL	CA-CB-CG1	-14.67	88.89	110.90
2	D	50	THR	N-CA-CB	-14.66	82.45	110.30
2	B	58	PRO	N-CD-CG	-14.65	81.22	103.20
1	C	128	PHE	CB-CG-CD1	-14.64	110.55	120.80
1	C	98	PHE	CZ-CE2-CD2	14.63	137.66	120.10
1	C	72	HIS	ND1-CG-CD2	-14.61	85.54	106.00
2	B	145	TYR	CG-CD2-CE2	-14.52	109.69	121.30
1	C	12	ALA	CA-C-O	14.50	150.55	120.10
2	D	59	LYS	O-C-N	14.49	145.89	122.70
1	A	46	PHE	CG-CD2-CE2	14.45	136.70	120.80
2	D	30	ARG	NH1-CZ-NH2	-14.41	103.55	119.40
2	D	101	GLU	CG-CD-OE1	-14.37	89.57	118.30
2	D	71	PHE	CB-CG-CD1	-14.35	110.75	120.80
1	A	116	GLU	OE1-CD-OE2	-14.35	106.08	123.30
1	C	71	ALA	O-C-N	-14.31	99.80	122.70
1	A	85	ASP	CB-CG-OD2	-14.28	105.45	118.30
2	B	132	LYS	CD-CE-NZ	-14.19	79.06	111.70
2	D	77	HIS	ND1-CG-CD2	14.18	128.65	108.80
2	B	49	SER	C-N-CA	14.16	157.11	121.70
2	D	80	ASN	OD1-CG-ND2	14.13	154.40	121.90
2	B	87	THR	OG1-CB-CG2	-14.11	77.55	110.00
1	A	47	ASP	CB-CG-OD1	14.10	130.99	118.30
2	B	26	GLU	CG-CD-OE1	-14.09	90.12	118.30
1	A	50	HIS	N-CA-CB	-14.06	85.29	110.60
2	B	146	HIS	CG-CD2-NE2	-14.03	82.55	109.20
1	A	62	VAL	O-C-N	14.02	145.12	122.70
2	B	146	HIS	ND1-CE1-NE2	-14.01	79.07	109.90
1	C	43	PHE	CG-CD2-CE2	-14.01	105.39	120.80
2	B	94	ASP	CB-CG-OD2	-13.94	105.76	118.30
2	D	73	ASP	O-C-N	-13.94	99.51	123.20
1	A	21	ALA	CA-C-N	-13.90	88.39	116.20
1	C	43	PHE	CZ-CE2-CD2	13.87	136.74	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	77	HIS	CG-CD2-NE2	-13.84	82.91	109.20
2	B	145	TYR	CD1-CG-CD2	13.79	133.06	117.90
2	D	20	VAL	CA-C-O	13.78	149.04	120.10
1	C	14	TRP	NE1-CE2-CZ2	13.76	145.54	130.40
1	C	78	ASN	CA-C-O	13.76	149.00	120.10
2	D	43	GLU	CG-CD-OE2	13.75	145.80	118.30
1	A	21	ALA	C-N-CA	-13.73	93.47	122.30
2	B	28	LEU	CB-CG-CD2	-13.70	87.71	111.00
1	A	33	PHE	CG-CD2-CE2	-13.69	105.74	120.80
2	D	66	LYS	CA-CB-CG	13.69	143.51	113.40
1	C	25	GLY	O-C-N	-13.68	100.81	122.70
2	B	121	GLU	CG-CD-OE1	-13.68	90.94	118.30
1	A	58	HIS	O-C-N	13.65	146.41	123.20
2	D	73	ASP	CA-CB-CG	-13.59	83.50	113.40
1	C	48	LEU	O-C-N	-13.58	100.97	122.70
1	A	14	TRP	CG-CD1-NE1	-13.55	96.55	110.10
2	B	22	GLU	CG-CD-OE1	-13.54	91.22	118.30
1	C	33	PHE	CB-CG-CD1	-13.49	111.35	120.80
2	B	41	PHE	O-C-N	13.49	144.28	122.70
2	B	44	SER	CA-CB-OG	13.45	147.51	111.20
2	D	32	LEU	CB-CG-CD2	13.44	133.85	111.00
1	A	50	HIS	C-N-CA	13.44	150.51	122.30
2	D	46	GLY	O-C-N	13.42	144.17	122.70
2	B	143	HIS	CB-CG-ND1	-13.41	89.67	123.20
2	B	108	ASN	CB-CG-ND2	-13.41	84.52	116.70
2	D	8	LYS	O-C-N	-13.40	101.25	122.70
2	D	2	HIS	O-C-N	13.40	144.14	122.70
2	D	118	PHE	CD1-CE1-CZ	-13.40	104.02	120.10
2	D	146	HIS	CE1-NE2-CD2	-13.40	73.11	106.60
1	C	16	LYS	CB-CG-CD	-13.38	76.80	111.60
2	B	45	PHE	CB-CG-CD1	-13.37	111.44	120.80
1	C	46	PHE	CD1-CG-CD2	-13.37	100.92	118.30
2	D	67	VAL	CG1-CB-CG2	13.36	132.28	110.90
1	A	21	ALA	CB-CA-C	13.35	130.13	110.10
1	C	24	TYR	CD1-CG-CD2	13.35	132.59	117.90
2	B	49	SER	CA-C-O	-13.35	92.07	120.10
2	B	49	SER	CB-CA-C	-13.32	84.79	110.10
2	D	10	ALA	CB-CA-C	-13.32	90.12	110.10
2	D	22	GLU	CG-CD-OE2	-13.29	91.72	118.30
1	A	140	TYR	CB-CG-CD2	13.23	128.94	121.00
1	A	14	TRP	CH2-CZ2-CE2	13.23	130.63	117.40
2	B	117	HIS	CB-CG-ND1	-13.23	90.13	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	ALA	O-C-N	-13.15	101.65	122.70
2	B	5	PRO	CA-N-CD	-13.12	93.13	111.50
2	D	37	TRP	CZ3-CH2-CZ2	13.10	137.32	121.60
2	B	125	PRO	N-CA-CB	13.07	118.99	103.30
2	D	76	ALA	CB-CA-C	13.06	129.70	110.10
2	D	121	GLU	CG-CD-OE2	-13.06	92.17	118.30
2	D	77	HIS	CB-CA-C	-13.01	84.39	110.40
2	D	73	ASP	CA-C-O	12.94	147.28	120.10
2	B	146	HIS	ND1-CG-CD2	-12.93	87.90	106.00
1	C	140	TYR	CB-CG-CD1	12.92	128.75	121.00
2	D	45	PHE	CG-CD2-CE2	12.90	134.99	120.80
2	B	8	LYS	O-C-N	-12.89	102.07	122.70
1	C	46	PHE	O-C-N	-12.89	102.07	122.70
2	D	79	ASP	N-CA-CB	-12.89	87.40	110.60
1	C	85	ASP	CB-CG-OD2	-12.88	106.71	118.30
2	D	99	ASP	CB-CG-OD1	-12.85	106.74	118.30
1	C	15	GLY	C-N-CA	12.84	153.81	121.70
1	C	19	ALA	O-C-N	-12.84	102.16	122.70
1	A	61	LYS	O-C-N	12.81	143.19	122.70
2	B	76	ALA	CB-CA-C	-12.81	90.89	110.10
2	B	37	TRP	CH2-CZ2-CE2	-12.79	104.61	117.40
1	A	48	LEU	CB-CG-CD2	12.72	132.62	111.00
1	A	74	ASP	CA-C-N	12.71	145.16	117.20
1	C	31	ARG	NE-CZ-NH2	-12.70	113.95	120.30
2	B	87	THR	CA-CB-CG2	-12.69	94.64	112.40
1	C	113	LEU	CB-CG-CD1	-12.68	89.44	111.00
1	C	30	GLU	CG-CD-OE1	-12.68	92.94	118.30
1	C	64	ASP	CB-CG-OD1	-12.68	106.89	118.30
2	D	7	GLU	CG-CD-OE1	-12.67	92.96	118.30
1	C	70	VAL	O-C-N	12.66	142.96	122.70
1	A	46	PHE	CD1-CG-CD2	-12.63	101.88	118.30
2	D	118	PHE	CB-CG-CD2	-12.62	111.97	120.80
2	D	20	VAL	O-C-N	-12.62	102.51	122.70
1	C	50	HIS	CG-CD2-NE2	12.60	133.13	109.20
2	D	49	SER	C-N-CA	-12.58	90.25	121.70
2	D	71	PHE	CG-CD1-CE1	-12.56	106.98	120.80
1	A	24	TYR	CZ-CE2-CD2	-12.53	108.52	119.80
1	C	14	TRP	CB-CG-CD1	-12.53	110.72	127.00
1	C	84	SER	N-CA-CB	12.52	129.28	110.50
2	D	37	TRP	CH2-CZ2-CE2	-12.52	104.88	117.40
2	D	7	GLU	CG-CD-OE2	12.51	143.31	118.30
2	D	63	HIS	CG-CD2-NE2	-12.50	85.44	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	145	TYR	CG-CD1-CE1	12.50	131.30	121.30
2	B	146	HIS	CB-CG-CD2	-12.49	92.07	130.80
1	C	33	PHE	CG-CD2-CE2	-12.49	107.06	120.80
2	B	1	VAL	CA-C-N	-12.49	89.73	117.20
2	D	97	HIS	CG-CD2-NE2	-12.46	85.52	109.20
1	A	36	PHE	CB-CG-CD2	-12.45	112.08	120.80
1	C	126	ASP	CB-CG-OD1	-12.44	107.11	118.30
1	C	14	TRP	CD1-CG-CD2	12.43	116.24	106.30
2	D	65	LYS	CB-CG-CD	-12.41	79.34	111.60
1	A	4	PRO	CB-CA-C	-12.40	80.99	112.00
2	B	68	LEU	CB-CG-CD1	-12.40	89.92	111.00
2	D	45	PHE	O-C-N	12.39	144.26	123.20
1	C	20	HIS	CG-ND1-CE1	-12.37	89.62	105.70
1	A	111	ALA	N-CA-CB	12.37	127.41	110.10
1	C	24	TYR	CB-CG-CD1	-12.34	113.59	121.00
1	A	65	ALA	O-C-N	12.34	142.44	122.70
1	C	24	TYR	CB-CG-CD2	-12.31	113.61	121.00
2	D	53	ALA	N-CA-CB	12.31	127.34	110.10
1	A	89	HIS	CE1-NE2-CD2	12.31	137.38	106.60
2	D	75	LEU	CB-CG-CD2	12.31	131.93	111.00
1	A	89	HIS	ND1-CE1-NE2	-12.30	82.84	109.90
2	D	24	GLY	O-C-N	-12.29	102.30	123.20
1	C	105	LEU	CB-CG-CD2	-12.28	90.12	111.00
2	B	64	GLY	CA-C-O	12.27	142.69	120.60
1	A	34	LEU	CB-CG-CD1	12.26	131.84	111.00
1	A	75	ASP	CB-CA-C	-12.26	85.88	110.40
1	C	52	SER	O-C-N	-12.26	103.09	122.70
2	D	77	HIS	CA-C-O	12.23	145.78	120.10
2	D	130	TYR	CB-CG-CD2	12.22	128.33	121.00
2	D	42	PHE	CB-CG-CD2	12.19	129.33	120.80
2	B	22	GLU	CB-CG-CD	12.15	147.02	114.20
2	B	53	ALA	CA-C-O	12.15	145.63	120.10
1	C	113	LEU	CB-CG-CD2	12.15	131.66	111.00
2	B	4	THR	N-CA-CB	-12.15	87.22	110.30
2	D	93	CYS	O-C-N	12.13	142.12	122.70
1	A	141	ARG	CD-NE-CZ	-12.09	106.67	123.60
1	C	14	TRP	CH2-CZ2-CE2	12.08	129.48	117.40
2	D	65	LYS	CD-CE-NZ	-12.07	83.93	111.70
2	D	121	GLU	CG-CD-OE1	-12.07	94.16	118.30
2	D	79	ASP	CA-C-N	-12.06	90.66	117.20
2	B	85	PHE	CG-CD2-CE2	-12.05	107.55	120.80
2	D	52	ASP	OD1-CG-OD2	-12.03	100.44	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	78	LEU	N-CA-C	12.01	143.43	111.00
2	B	43	GLU	O-C-N	-12.01	103.49	122.70
1	A	42	TYR	CD1-CE1-CZ	12.00	130.60	119.80
2	D	2	HIS	CB-CG-CD2	11.99	167.99	130.80
1	A	15	GLY	CA-C-O	-11.98	99.03	120.60
1	A	20	HIS	CG-ND1-CE1	-11.98	90.13	105.70
2	B	18	VAL	CA-CB-CG2	-11.98	92.94	110.90
1	C	48	LEU	CB-CG-CD1	11.98	131.36	111.00
1	C	116	GLU	CB-CG-CD	-11.98	81.86	114.20
1	A	24	TYR	CD1-CE1-CZ	11.94	130.55	119.80
2	D	80	ASN	CA-C-N	-11.94	90.94	117.20
1	C	53	ALA	CB-CA-C	11.93	128.00	110.10
1	A	7	LYS	CD-CE-NZ	-11.92	84.29	111.70
2	D	83	GLY	O-C-N	-11.92	103.63	122.70
2	B	82	LYS	N-CA-CB	-11.89	89.19	110.60
2	D	52	ASP	N-CA-CB	-11.89	89.20	110.60
1	C	116	GLU	CG-CD-OE1	11.89	142.07	118.30
2	B	44	SER	CB-CA-C	11.86	132.63	110.10
1	C	114	PRO	O-C-N	-11.84	103.75	122.70
2	D	42	PHE	CD1-CE1-CZ	11.84	134.31	120.10
2	D	120	LYS	O-C-N	-11.84	103.76	122.70
1	A	26	ALA	N-CA-CB	11.83	126.67	110.10
2	D	65	LYS	CG-CD-CE	-11.82	76.43	111.90
2	B	1	VAL	CA-C-O	-11.80	95.31	120.10
2	D	20	VAL	CA-CB-CG1	-11.79	93.21	110.90
2	D	21	ASP	N-CA-C	11.78	142.79	111.00
1	A	47	ASP	O-C-N	11.77	141.53	122.70
1	A	14	TRP	CA-CB-CG	-11.77	91.35	113.70
2	D	41	PHE	CZ-CE2-CD2	-11.76	105.99	120.10
2	D	58	PRO	CB-CG-CD	11.76	152.35	106.50
1	C	41	THR	O-C-N	-11.76	103.89	122.70
2	B	79	ASP	O-C-N	-11.75	103.90	122.70
1	C	12	ALA	O-C-N	-11.74	103.92	122.70
2	D	2	HIS	CA-C-O	-11.73	95.47	120.10
2	D	4	THR	CA-C-O	-11.73	95.47	120.10
1	A	21	ALA	CA-C-O	-11.71	95.52	120.10
2	B	42	PHE	CG-CD2-CE2	11.70	133.67	120.80
1	A	112	HIS	CG-ND1-CE1	-11.69	90.50	105.70
2	D	78	LEU	CA-C-N	-11.69	91.47	117.20
2	D	63	HIS	CA-CB-CG	11.68	133.46	113.60
1	A	141	ARG	CG-CD-NE	-11.67	87.28	111.80
1	C	112	HIS	ND1-CG-CD2	-11.67	89.66	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	PHE	CG-CD2-CE2	-11.67	107.97	120.80
1	A	19	ALA	N-CA-CB	11.66	126.43	110.10
1	C	89	HIS	CG-ND1-CE1	-11.65	90.55	105.70
2	D	21	ASP	CB-CG-OD2	-11.65	107.81	118.30
2	D	47	ASP	OD1-CG-OD2	11.64	145.42	123.30
1	A	73	VAL	O-C-N	-11.63	104.09	122.70
1	C	16	LYS	CD-CE-NZ	-11.63	84.96	111.70
1	A	15	GLY	CA-C-N	11.62	142.77	117.20
2	B	2	HIS	CA-CB-CG	11.61	133.33	113.60
1	A	89	HIS	CG-ND1-CE1	11.57	124.40	108.20
2	B	78	LEU	CB-CG-CD2	11.56	130.65	111.00
2	D	2	HIS	CB-CG-ND1	-11.55	94.33	123.20
1	A	140	TYR	CD1-CE1-CZ	11.54	130.19	119.80
2	D	6	GLU	CB-CA-C	-11.54	87.32	110.40
1	C	53	ALA	O-C-N	11.52	141.13	122.70
2	D	45	PHE	CA-C-O	-11.47	96.02	120.10
1	A	64	ASP	OD1-CG-OD2	11.43	145.02	123.30
2	B	43	GLU	N-CA-CB	-11.43	90.03	110.60
2	B	42	PHE	CG-CD1-CE1	-11.41	108.25	120.80
2	D	40	ARG	NE-CZ-NH1	-11.38	114.61	120.30
1	C	114	PRO	CB-CA-C	11.38	140.45	112.00
2	B	9	SER	CA-CB-OG	-11.37	80.51	111.20
2	D	82	LYS	CG-CD-CE	-11.37	77.80	111.90
2	B	145	TYR	N-CA-CB	11.36	131.06	110.60
2	D	58	PRO	CA-N-CD	-11.36	95.59	111.50
1	C	72	HIS	ND1-CE1-NE2	11.36	134.89	109.90
2	B	73	ASP	CB-CG-OD2	-11.33	108.10	118.30
2	D	2	HIS	ND1-CE1-NE2	-11.30	85.03	109.90
2	B	117	HIS	ND1-CG-CD2	11.29	124.61	108.80
2	D	43	GLU	CB-CA-C	-11.28	87.83	110.40
2	B	96	LEU	CB-CG-CD2	-11.28	91.83	111.00
1	A	74	ASP	CA-C-O	-11.26	96.46	120.10
2	D	50	THR	CB-CA-C	-11.25	81.22	111.60
2	D	97	HIS	CE1-NE2-CD2	11.24	134.71	106.60
1	C	118	THR	CA-CB-CG2	11.23	128.13	112.40
1	C	45	HIS	ND1-CE1-NE2	11.23	134.60	109.90
2	D	57	ASN	CA-C-O	11.17	143.56	120.10
1	A	57	GLY	O-C-N	11.16	140.56	122.70
1	C	49	SER	CB-CA-C	11.15	131.29	110.10
2	D	63	HIS	CG-ND1-CE1	-11.15	91.20	105.70
1	A	25	GLY	O-C-N	-11.14	104.87	122.70
1	C	90	LYS	CD-CE-NZ	-11.14	86.07	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	43	GLU	CA-CB-CG	11.12	137.87	113.40
1	C	2	LEU	CA-C-O	-11.12	96.74	120.10
1	A	120	ALA	N-CA-CB	11.12	125.66	110.10
2	B	17	LYS	CD-CE-NZ	-11.12	86.13	111.70
1	C	81	SER	N-CA-CB	-11.11	93.84	110.50
1	C	20	HIS	CB-CG-ND1	-11.10	95.46	123.20
1	A	73	VAL	CA-C-O	11.09	143.39	120.10
2	D	49	SER	CB-CA-C	-11.09	89.03	110.10
2	D	122	PHE	CZ-CE2-CD2	-11.07	106.81	120.10
2	B	144	LYS	O-C-N	-11.06	105.00	122.70
2	D	117	HIS	ND1-CG-CD2	-11.05	90.52	106.00
1	A	46	PHE	CE1-CZ-CE2	-11.04	100.12	120.00
2	D	105	LEU	CB-CG-CD1	11.04	129.77	111.00
1	A	71	ALA	CA-C-N	11.03	141.47	117.20
2	B	5	PRO	CA-CB-CG	-11.04	83.03	104.00
2	D	18	VAL	CA-CB-CG1	11.02	127.43	110.90
1	C	41	THR	CA-C-N	11.01	141.42	117.20
2	D	55	MET	CA-C-N	-11.01	94.18	116.20
1	A	128	PHE	CG-CD2-CE2	10.99	132.89	120.80
2	B	17	LYS	O-C-N	-10.98	105.12	122.70
2	B	85	PHE	CB-CG-CD2	-10.98	113.11	120.80
2	D	85	PHE	CB-CG-CD1	-10.97	113.12	120.80
2	D	45	PHE	CB-CG-CD1	-10.97	113.12	120.80
1	A	45	HIS	CA-CB-CG	10.96	132.23	113.60
1	C	29	LEU	O-C-N	-10.96	105.17	122.70
2	D	21	ASP	OD1-CG-OD2	-10.95	102.49	123.30
2	B	104	ARG	NH1-CZ-NH2	10.95	131.45	119.40
2	D	12	THR	O-C-N	-10.95	105.18	122.70
2	D	126	VAL	CA-CB-CG2	-10.93	94.50	110.90
1	C	115	ALA	O-C-N	-10.92	105.22	122.70
2	B	6	GLU	CA-CB-CG	10.91	137.40	113.40
1	C	89	HIS	ND1-CE1-NE2	10.91	133.91	109.90
2	B	80	ASN	CB-CG-OD1	-10.90	99.80	121.60
1	A	26	ALA	CB-CA-C	-10.90	93.76	110.10
2	D	67	VAL	CA-CB-CG1	-10.86	94.61	110.90
2	B	60	VAL	O-C-N	-10.84	105.35	122.70
1	C	45	HIS	CA-CB-CG	10.82	131.99	113.60
2	B	23	VAL	CA-CB-CG2	-10.80	94.69	110.90
2	B	43	GLU	CG-CD-OE1	-10.81	96.69	118.30
2	B	49	SER	N-CA-CB	-10.80	94.30	110.50
1	C	14	TRP	CA-C-N	10.78	137.76	116.20
1	C	30	GLU	CG-CD-OE2	-10.78	96.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	42	TYR	CB-CG-CD1	10.77	127.46	121.00
1	A	122	HIS	CB-CA-C	10.76	131.92	110.40
1	C	44	PRO	N-CA-CB	-10.76	90.38	103.30
2	B	134	VAL	N-CA-CB	10.75	135.16	111.50
2	D	90	GLU	CG-CD-OE2	-10.75	96.79	118.30
1	A	49	SER	C-N-CA	-10.75	94.82	121.70
1	C	78	ASN	O-C-N	-10.74	105.51	122.70
1	A	116	GLU	CG-CD-OE1	10.73	139.76	118.30
1	C	63	ALA	O-C-N	-10.73	105.53	122.70
1	C	10	VAL	O-C-N	10.73	139.86	122.70
2	D	104	ARG	CG-CD-NE	-10.71	89.31	111.80
2	B	48	LEU	CB-CG-CD2	10.68	129.15	111.00
2	D	79	ASP	C-N-CA	-10.67	95.03	121.70
2	D	9	SER	O-C-N	10.66	139.76	122.70
2	B	3	LEU	C-N-CA	-10.63	95.13	121.70
2	B	45	PHE	CA-C-N	10.63	137.46	116.20
2	D	7	GLU	O-C-N	10.61	139.67	122.70
2	B	78	LEU	CB-CA-C	-10.60	90.05	110.20
2	B	45	PHE	CG-CD1-CE1	-10.59	109.15	120.80
1	C	72	HIS	N-CA-C	10.59	139.60	111.00
2	B	81	LEU	CB-CA-C	10.58	130.30	110.20
1	C	73	VAL	O-C-N	10.57	139.62	122.70
1	C	17	VAL	CG1-CB-CG2	10.55	127.78	110.90
1	A	20	HIS	ND1-CE1-NE2	10.54	133.08	109.90
2	D	77	HIS	CE1-NE2-CD2	10.52	132.89	106.60
2	D	80	ASN	CB-CG-ND2	-10.51	91.49	116.70
2	D	3	LEU	CA-C-O	-10.50	98.05	120.10
1	A	41	THR	O-C-N	-10.49	105.91	122.70
1	C	113	LEU	CA-C-O	-10.49	98.07	120.10
2	B	72	SER	CB-CA-C	10.48	130.02	110.10
2	D	3	LEU	N-CA-C	-10.48	82.71	111.00
2	D	54	VAL	CA-CB-CG1	-10.46	95.21	110.90
2	D	72	SER	CA-C-O	10.44	142.02	120.10
2	B	85	PHE	CD1-CE1-CZ	10.43	132.61	120.10
1	C	116	GLU	CB-CA-C	-10.42	89.56	110.40
1	A	43	PHE	CG-CD2-CE2	10.41	132.25	120.80
1	C	22	GLY	CA-C-N	10.41	140.09	117.20
2	D	12	THR	CA-CB-OG1	-10.41	87.15	109.00
1	A	131	SER	O-C-N	10.40	139.35	122.70
2	D	3	LEU	N-CA-CB	10.40	131.21	110.40
2	D	63	HIS	ND1-CG-CD2	10.40	123.36	108.80
1	A	22	GLY	CA-C-O	10.39	139.31	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	LEU	CA-C-O	-10.38	98.31	120.10
2	D	21	ASP	CB-CG-OD1	10.35	127.62	118.30
1	A	26	ALA	CA-C-O	10.35	141.83	120.10
2	B	35	TYR	CB-CG-CD2	10.35	127.21	121.00
1	A	12	ALA	N-CA-CB	-10.34	95.62	110.10
1	A	72	HIS	CG-CD2-NE2	10.33	128.83	109.20
1	A	141	ARG	CB-CA-C	10.30	131.01	110.40
1	C	56	LYS	O-C-N	-10.30	105.68	123.20
2	B	1	VAL	CA-CB-CG1	-10.30	95.45	110.90
1	A	43	PHE	CZ-CE2-CD2	-10.29	107.75	120.10
1	A	81	SER	CA-CB-OG	-10.29	83.40	111.20
2	D	60	VAL	CG1-CB-CG2	10.25	127.31	110.90
2	B	2	HIS	ND1-CE1-NE2	10.24	132.43	109.90
2	B	85	PHE	CE1-CZ-CE2	-10.23	101.58	120.00
1	C	7	LYS	CA-C-O	10.22	141.55	120.10
2	D	35	TYR	CD1-CE1-CZ	-10.21	110.61	119.80
2	B	90	GLU	N-CA-C	10.21	138.56	111.00
1	C	84	SER	CA-CB-OG	-10.18	83.72	111.20
1	A	106	LEU	CA-CB-CG	10.17	138.70	115.30
1	A	14	TRP	NE1-CE2-CZ2	10.17	141.59	130.40
2	D	19	ASN	CA-C-N	10.16	139.55	117.20
2	D	73	ASP	N-CA-C	10.16	138.43	111.00
1	A	8	THR	CA-C-O	10.15	141.42	120.10
2	B	47	ASP	OD1-CG-OD2	-10.13	104.05	123.30
2	D	3	LEU	CA-CB-CG	-10.11	92.04	115.30
2	B	68	LEU	CD1-CG-CD2	10.11	140.82	110.50
1	A	74	ASP	CB-CG-OD1	10.09	127.38	118.30
1	C	2	LEU	O-C-N	10.09	138.85	122.70
1	A	87	HIS	O-C-N	10.09	138.84	122.70
2	D	5	PRO	CB-CA-C	-10.09	86.78	112.00
2	D	8	LYS	N-CA-CB	-10.09	92.44	110.60
2	B	42	PHE	CD1-CG-CD2	-10.07	105.20	118.30
2	D	146	HIS	ND1-CE1-NE2	10.05	132.02	109.90
2	D	84	THR	CA-CB-CG2	10.05	126.47	112.40
2	D	117	HIS	CG-ND1-CE1	-10.05	92.64	105.70
1	C	131	SER	O-C-N	10.02	138.74	122.70
2	B	30	ARG	NH1-CZ-NH2	-10.01	108.39	119.40
2	D	82	LYS	O-C-N	-10.01	106.18	123.20
1	A	53	ALA	CB-CA-C	-10.00	95.09	110.10
2	D	14	LEU	CB-CG-CD1	-9.99	94.01	111.00
2	B	94	ASP	O-C-N	-9.98	106.73	122.70
1	A	126	ASP	O-C-N	-9.97	106.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	58	PRO	CB-CG-CD	9.95	145.32	106.50
2	D	133	VAL	CG1-CB-CG2	9.95	126.81	110.90
1	C	43	PHE	CB-CG-CD2	-9.94	113.84	120.80
2	B	30	ARG	NE-CZ-NH1	-9.93	115.33	120.30
2	D	6	GLU	CA-C-O	-9.93	99.25	120.10
1	C	79	ALA	CB-CA-C	-9.90	95.24	110.10
1	A	76	MET	CG-SD-CE	9.90	116.04	100.20
2	B	142	ALA	O-C-N	9.89	138.52	122.70
2	D	11	VAL	O-C-N	9.87	138.50	122.70
1	A	50	HIS	CB-CA-C	-9.87	90.66	110.40
2	D	95	LYS	O-C-N	-9.86	106.92	122.70
1	A	105	LEU	CB-CG-CD2	9.84	127.73	111.00
2	B	81	LEU	N-CA-CB	-9.84	90.71	110.40
2	D	60	VAL	CB-CA-C	9.84	130.09	111.40
1	A	88	ALA	O-C-N	9.83	138.43	122.70
2	B	90	GLU	CG-CD-OE1	-9.82	98.66	118.30
2	B	125	PRO	CA-N-CD	-9.81	97.77	111.50
2	B	42	PHE	CB-CG-CD1	-9.81	113.94	120.80
1	A	82	ALA	N-CA-CB	9.79	123.81	110.10
2	B	61	LYS	CD-CE-NZ	-9.80	89.17	111.70
1	C	4	PRO	O-C-N	9.79	138.37	122.70
2	B	87	THR	CA-CB-OG1	-9.78	88.47	109.00
2	D	97	HIS	ND1-CE1-NE2	-9.77	88.40	109.90
1	A	6	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	C	71	ALA	C-N-CA	9.77	146.12	121.70
2	D	30	ARG	CD-NE-CZ	9.77	137.27	123.60
2	B	8	LYS	CB-CG-CD	9.75	136.95	111.60
2	B	45	PHE	CE1-CZ-CE2	9.75	137.54	120.00
1	A	43	PHE	CB-CG-CD1	-9.73	113.99	120.80
1	A	15	GLY	N-CA-C	-9.72	88.81	113.10
2	B	145	TYR	CA-C-O	-9.69	99.75	120.10
2	D	78	LEU	CB-CG-CD1	-9.69	94.53	111.00
1	C	90	LYS	CB-CG-CD	-9.69	86.42	111.60
1	C	58	HIS	CG-ND1-CE1	-9.68	93.11	105.70
1	A	33	PHE	CZ-CE2-CD2	9.68	131.72	120.10
1	C	90	LYS	N-CA-CB	9.67	128.00	110.60
1	C	60	LYS	CD-CE-NZ	-9.65	89.51	111.70
2	D	144	LYS	CD-CE-NZ	9.65	133.89	111.70
1	C	82	ALA	O-C-N	-9.64	107.27	122.70
1	C	14	TRP	CD2-CE2-CZ2	-9.64	110.73	122.30
2	D	137	VAL	O-C-N	-9.64	107.27	122.70
2	B	60	VAL	CA-C-O	9.64	140.34	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	ASN	N-CA-CB	9.62	127.92	110.60
1	C	56	LYS	CB-CG-CD	-9.62	86.59	111.60
2	B	47	ASP	CA-C-N	-9.61	96.06	117.20
1	C	49	SER	CA-C-O	9.61	140.28	120.10
2	D	54	VAL	O-C-N	-9.61	107.33	122.70
1	C	64	ASP	OD1-CG-OD2	9.61	141.55	123.30
2	B	53	ALA	O-C-N	-9.59	107.36	122.70
1	C	70	VAL	CA-C-O	-9.59	99.96	120.10
2	D	65	LYS	CA-CB-CG	-9.58	92.33	113.40
1	A	76	MET	CA-CB-CG	-9.56	97.05	113.30
2	D	85	PHE	CZ-CE2-CD2	9.54	131.55	120.10
2	B	139	ASN	CB-CA-C	-9.54	91.33	110.40
1	A	89	HIS	O-C-N	-9.53	107.46	122.70
2	B	122	PHE	CB-CG-CD2	-9.52	114.14	120.80
1	C	138	SER	N-CA-CB	-9.52	96.22	110.50
1	C	38	THR	CA-CB-CG2	-9.52	99.08	112.40
2	D	18	VAL	CA-C-O	-9.51	100.12	120.10
1	C	138	SER	O-C-N	9.49	137.89	122.70
1	C	109	LEU	CB-CA-C	9.49	128.23	110.20
2	D	143	HIS	CG-ND1-CE1	-9.49	93.37	105.70
2	D	19	ASN	CB-CG-OD1	-9.47	102.65	121.60
2	D	79	ASP	CB-CG-OD1	-9.47	109.77	118.30
2	B	126	VAL	CG1-CB-CG2	-9.47	95.75	110.90
2	B	73	ASP	CB-CG-OD1	9.47	126.82	118.30
1	A	42	TYR	CG-CD1-CE1	-9.46	113.73	121.30
2	B	134	VAL	CA-CB-CG1	-9.45	96.72	110.90
1	A	96	VAL	CA-CB-CG2	-9.45	96.72	110.90
2	B	144	LYS	CA-C-N	9.43	137.95	117.20
1	C	96	VAL	CA-CB-CG2	9.42	125.03	110.90
1	A	127	LYS	CB-CA-C	9.41	129.22	110.40
1	C	105	LEU	CD1-CG-CD2	-9.39	82.32	110.50
2	D	48	LEU	CB-CG-CD2	9.38	126.95	111.00
1	A	19	ALA	CB-CA-C	-9.36	96.05	110.10
2	D	89	SER	CA-C-O	9.36	139.75	120.10
2	B	49	SER	CA-C-N	9.35	137.76	117.20
2	D	99	ASP	OD1-CG-OD2	9.35	141.06	123.30
1	C	103	HIS	CG-ND1-CE1	-9.34	93.55	105.70
2	D	35	TYR	CB-CG-CD2	9.34	126.60	121.00
2	B	130	TYR	CB-CG-CD1	9.34	126.60	121.00
2	D	40	ARG	CA-CB-CG	9.33	133.93	113.40
1	C	94	ASP	CB-CG-OD2	-9.33	109.91	118.30
2	B	127	GLN	O-C-N	-9.32	107.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	5	ALA	N-CA-CB	9.32	123.14	110.10
2	D	1	VAL	CA-C-O	-9.31	100.55	120.10
1	A	56	LYS	CB-CG-CD	-9.31	87.40	111.60
2	B	3	LEU	N-CA-CB	-9.31	91.78	110.40
1	A	52	SER	O-C-N	-9.29	107.83	122.70
1	A	24	TYR	CG-CD2-CE2	9.29	128.73	121.30
1	C	48	LEU	C-N-CA	9.29	144.92	121.70
2	D	67	VAL	N-CA-CB	-9.29	91.07	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	145	TYR	CG-CD2-CE2	-9.28	113.88	121.30
1	A	6	ASP	O-C-N	9.25	137.51	122.70
2	B	81	LEU	CA-CB-CG	9.24	136.56	115.30
2	D	23	VAL	CA-CB-CG2	-9.24	97.04	110.90
2	D	116	HIS	ND1-CG-CD2	9.24	121.74	108.80
1	C	112	HIS	O-C-N	-9.22	107.95	122.70
2	B	10	ALA	CB-CA-C	-9.21	96.29	110.10
2	D	122	PHE	CG-CD2-CE2	9.19	130.91	120.80
1	A	11	LYS	C-N-CA	-9.16	98.80	121.70
1	A	19	ALA	O-C-N	-9.16	108.05	122.70
2	D	53	ALA	CA-C-O	9.16	139.33	120.10
2	D	90	GLU	CB-CG-CD	-9.15	89.48	114.20
1	C	72	HIS	O-C-N	-9.15	108.06	122.70
2	D	51	PRO	N-CD-CG	-9.15	89.48	103.20
2	D	41	PHE	CA-C-O	-9.14	100.90	120.10
1	A	43	PHE	CD1-CE1-CZ	9.14	131.07	120.10
1	A	7	LYS	CA-C-N	-9.13	97.12	117.20
1	C	45	HIS	O-C-N	9.12	137.29	122.70
2	B	118	PHE	CE1-CZ-CE2	-9.12	103.59	120.00
1	C	131	SER	CA-C-O	-9.11	100.97	120.10
2	B	146	HIS	CB-CG-ND1	-9.10	100.45	123.20
2	D	10	ALA	N-CA-CB	-9.10	97.36	110.10
1	A	29	LEU	CB-CG-CD1	-9.10	95.54	111.00
2	D	95	LYS	CA-C-O	9.09	139.19	120.10
1	A	86	LEU	CB-CG-CD2	9.07	126.41	111.00
1	A	14	TRP	C-N-CA	-9.06	103.27	122.30
2	B	66	LYS	CD-CE-NZ	-9.06	90.86	111.70
1	C	38	THR	CA-CB-OG1	-9.06	89.98	109.00
1	C	86	LEU	CA-C-O	9.06	139.12	120.10
1	C	12	ALA	N-CA-C	9.03	135.37	111.00
1	C	112	HIS	C-N-CA	9.03	144.26	121.70
1	A	118	THR	CA-CB-OG1	9.02	127.94	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	38	THR	CA-CB-CG2	-9.01	99.79	112.40
2	B	15	TRP	O-C-N	9.01	138.51	123.20
1	C	44	PRO	CA-N-CD	9.00	124.30	111.70
2	B	41	PHE	CG-CD2-CE2	-9.00	110.90	120.80
2	B	90	GLU	CA-C-N	-8.99	97.42	117.20
1	A	134	THR	O-C-N	-8.98	108.33	122.70
2	D	77	HIS	CA-C-N	-8.98	97.44	117.20
2	D	17	LYS	CD-CE-NZ	-8.97	91.08	111.70
2	B	144	LYS	C-N-CA	8.96	144.11	121.70
1	C	117	PHE	CB-CG-CD2	8.96	127.07	120.80
1	A	62	VAL	CG1-CB-CG2	-8.96	96.57	110.90
1	A	2	LEU	N-CA-CB	-8.95	92.49	110.40
2	B	2	HIS	CA-C-N	-8.95	97.52	117.20
2	D	52	ASP	CA-C-O	-8.95	101.31	120.10
2	D	53	ALA	CB-CA-C	-8.94	96.69	110.10
1	A	78	ASN	CB-CG-ND2	8.94	138.16	116.70
2	B	37	TRP	CZ3-CH2-CZ2	8.92	132.31	121.60
1	C	87	HIS	O-C-N	8.92	136.97	122.70
2	B	5	PRO	O-C-N	8.92	136.97	122.70
1	A	112	HIS	CA-C-O	-8.91	101.39	120.10
2	D	21	ASP	O-C-N	-8.91	108.45	122.70
2	D	120	LYS	CB-CG-CD	8.89	134.73	111.60
2	B	12	THR	CA-CB-CG2	-8.88	99.97	112.40
1	A	56	LYS	CA-C-O	8.87	138.73	120.10
1	C	77	PRO	O-C-N	-8.87	108.51	122.70
2	B	42	PHE	CE1-CZ-CE2	-8.86	104.05	120.00
2	D	2	HIS	C-N-CA	-8.86	99.56	121.70
2	D	44	SER	CA-C-N	8.85	136.68	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	3	LEU	C-N-CA	8.84	143.80	121.70
2	B	47	ASP	N-CA-CB	-8.83	94.70	110.60
1	A	98	PHE	CB-CG-CD2	8.83	126.98	120.80
1	C	77	PRO	N-CA-C	8.82	135.04	112.10
1	A	62	VAL	CA-C-N	-8.81	97.82	117.20
1	C	128	PHE	CD1-CE1-CZ	8.80	130.66	120.10
1	C	82	ALA	CA-C-O	8.78	138.54	120.10
1	C	50	HIS	O-C-N	8.78	138.12	123.20
1	C	53	ALA	CA-C-N	-8.76	97.92	117.20
2	D	57	ASN	O-C-N	-8.75	104.47	121.10
1	C	112	HIS	CA-C-N	8.74	136.42	117.20
2	B	111	VAL	O-C-N	-8.73	108.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	130	TYR	CZ-CE2-CD2	-8.73	111.94	119.80
1	A	50	HIS	CG-CD2-NE2	-8.72	92.62	109.20
2	B	47	ASP	CB-CA-C	-8.72	92.95	110.40
1	C	1	VAL	N-CA-C	-8.71	87.48	111.00
2	D	122	PHE	CE1-CZ-CE2	8.71	135.68	120.00
2	D	35	TYR	CB-CG-CD1	-8.71	115.78	121.00
2	D	108	ASN	OD1-CG-ND2	8.71	141.93	121.90
2	B	6	GLU	CG-CD-OE1	-8.70	100.90	118.30
1	C	84	SER	CB-CA-C	-8.70	93.58	110.10
1	A	106	LEU	CB-CG-CD1	8.69	125.77	111.00
2	D	93	CYS	CA-CB-SG	-8.69	98.36	114.00
1	C	11	LYS	CA-CB-CG	8.68	132.50	113.40
1	C	74	ASP	O-C-N	8.68	136.59	122.70
2	D	16	GLY	CA-C-N	8.67	136.28	117.20
1	A	56	LYS	O-C-N	-8.65	108.49	123.20
1	A	50	HIS	CA-C-N	8.64	133.49	116.20
2	B	5	PRO	CA-C-N	-8.63	98.21	117.20
2	B	60	VAL	CG1-CB-CG2	8.63	124.71	110.90
1	C	137	THR	OG1-CB-CG2	8.62	129.84	110.00
2	B	3	LEU	CA-C-N	-8.62	98.23	117.20
2	B	48	LEU	C-N-CA	-8.61	100.19	121.70
1	C	18	GLY	CA-C-N	-8.60	98.27	117.20
2	D	43	GLU	CA-C-N	-8.59	98.30	117.20
1	A	128	PHE	CE1-CZ-CE2	8.59	135.45	120.00
2	B	40	ARG	CA-C-N	8.58	136.08	117.20
2	D	55	MET	CA-C-O	-8.57	102.10	120.10
2	D	40	ARG	O-C-N	-8.56	109.00	122.70
2	B	51	PRO	O-C-N	-8.56	109.01	122.70
1	C	36	PHE	CG-CD2-CE2	-8.53	111.42	120.80
2	D	143	HIS	CG-CD2-NE2	-8.53	92.99	109.20
2	D	122	PHE	CB-CG-CD1	8.51	126.75	120.80
1	C	46	PHE	CD1-CE1-CZ	8.50	130.30	120.10
1	A	13	ALA	O-C-N	8.49	136.29	122.70
1	C	114	PRO	N-CD-CG	-8.49	90.46	103.20
2	B	71	PHE	CZ-CE2-CD2	8.49	130.29	120.10
2	D	95	LYS	CB-CG-CD	-8.48	89.54	111.60
1	C	62	VAL	CA-C-N	-8.48	98.55	117.20
2	B	80	ASN	CB-CG-ND2	-8.47	96.38	116.70
2	D	146	HIS	N-CA-CB	-8.46	95.37	110.60
2	D	71	PHE	CZ-CE2-CD2	8.45	130.24	120.10
2	D	119	GLY	CA-C-O	8.45	135.81	120.60
1	C	50	HIS	CB-CG-CD2	8.45	156.98	130.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	36	PRO	N-CD-CG	8.44	115.86	103.20
1	C	124	SER	O-C-N	8.43	136.19	122.70
2	B	88	LEU	CB-CG-CD2	-8.43	96.67	111.00
1	A	60	LYS	CA-C-O	8.42	137.78	120.10
1	A	62	VAL	C-N-CA	-8.42	100.66	121.70
1	A	63	ALA	O-C-N	-8.41	109.24	122.70
1	C	69	ALA	O-C-N	8.40	136.13	122.70
1	A	71	ALA	O-C-N	-8.38	109.30	122.70
1	A	77	PRO	CA-CB-CG	-8.36	88.11	104.00
2	B	9	SER	N-CA-CB	8.36	123.04	110.50
2	B	50	THR	N-CA-CB	-8.36	94.41	110.30
2	D	2	HIS	ND1-CG-CD2	-8.36	94.29	106.00
2	B	115	ALA	N-CA-CB	-8.36	98.39	110.10
2	B	35	TYR	CD1-CG-CD2	-8.35	108.71	117.90
2	D	59	LYS	CA-C-N	-8.34	98.86	117.20
1	A	54	GLN	O-C-N	8.33	136.03	122.70
2	D	7	GLU	OE1-CD-OE2	-8.32	113.31	123.30
1	A	126	ASP	CB-CG-OD1	-8.32	110.81	118.30
2	B	85	PHE	CB-CG-CD1	8.31	126.62	120.80
2	B	114	LEU	CB-CA-C	8.31	125.99	110.20
1	A	90	LYS	N-CA-C	8.31	133.43	111.00
2	D	60	VAL	CA-CB-CG1	-8.31	98.44	110.90
2	B	73	ASP	CA-C-N	8.30	132.81	116.20
1	C	81	SER	CA-CB-OG	-8.30	88.78	111.20
1	A	75	ASP	N-CA-CB	-8.30	95.66	110.60
2	B	103	PHE	CB-CG-CD1	-8.30	114.99	120.80
2	B	146	HIS	CA-CB-CG	-8.29	99.50	113.60
1	C	95	PRO	CA-C-N	8.29	135.44	117.20
2	D	90	GLU	CA-CB-CG	-8.28	95.18	113.40
1	C	50	HIS	ND1-CG-CD2	-8.28	94.41	106.00
2	D	55	MET	CB-CG-SD	8.28	137.22	112.40
1	A	4	PRO	N-CD-CG	-8.27	90.80	103.20
2	D	52	ASP	O-C-N	8.26	135.92	122.70
2	B	99	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	A	58	HIS	C-N-CA	-8.26	104.96	122.30
1	A	1	VAL	C-N-CA	-8.25	101.08	121.70
2	B	48	LEU	CB-CA-C	8.24	125.86	110.20
1	A	117	PHE	CD1-CG-CD2	8.24	129.01	118.30
2	D	118	PHE	CG-CD2-CE2	-8.24	111.74	120.80
2	B	89	SER	N-CA-CB	-8.23	98.15	110.50
1	A	117	PHE	CB-CG-CD2	-8.23	115.04	120.80
2	D	6	GLU	CA-C-N	-8.23	99.10	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	HIS	N-CA-CB	-8.22	95.80	110.60
1	C	25	GLY	CA-C-N	8.22	135.28	117.20
1	C	83	LEU	CB-CA-C	-8.22	94.59	110.20
1	C	22	GLY	C-N-CA	8.21	142.24	121.70
1	C	7	LYS	CB-CA-C	8.20	126.79	110.40
2	D	93	CYS	CB-CA-C	8.19	126.78	110.40
1	A	16	LYS	N-CA-CB	8.19	125.33	110.60
2	D	37	TRP	CE3-CZ3-CH2	-8.18	112.20	121.20
1	A	72	HIS	O-C-N	-8.18	109.61	122.70
1	C	117	PHE	CG-CD2-CE2	8.18	129.80	120.80
1	A	7	LYS	N-CA-C	8.18	133.07	111.00
2	B	41	PHE	CB-CG-CD1	-8.17	115.08	120.80
2	B	94	ASP	CA-C-N	8.16	135.16	117.20
2	D	92	HIS	ND1-CE1-NE2	8.16	127.86	109.90
2	B	23	VAL	CG1-CB-CG2	8.15	123.94	110.90
2	B	127	GLN	CA-C-O	8.15	137.22	120.10
2	D	9	SER	CA-CB-OG	8.15	133.20	111.20
2	B	67	VAL	CG1-CB-CG2	8.15	123.93	110.90
2	D	2	HIS	CB-CA-C	8.15	126.69	110.40
2	D	20	VAL	CB-CA-C	8.14	126.87	111.40
1	A	70	VAL	CG1-CB-CG2	-8.14	97.88	110.90
2	B	40	ARG	CA-C-O	-8.13	103.02	120.10
1	C	54	GLN	O-C-N	8.13	135.71	122.70
2	D	143	HIS	O-C-N	8.12	135.70	122.70
1	C	141	ARG	CA-C-O	-8.12	103.04	120.10
1	A	114	PRO	N-CA-CB	-8.12	93.56	103.30
1	A	6	ASP	C-N-CA	-8.12	101.41	121.70
1	A	117	PHE	CG-CD1-CE1	-8.11	111.88	120.80
1	C	50	HIS	CE1-NE2-CD2	-8.11	86.31	106.60
2	D	86	ALA	CB-CA-C	-8.12	97.93	110.10
1	A	114	PRO	CA-CB-CG	8.11	120.21	104.80
2	D	93	CYS	N-CA-CB	-8.11	96.00	110.60
1	C	90	LYS	CG-CD-CE	-8.10	87.59	111.90
1	C	138	SER	CA-C-O	-8.10	103.08	120.10
2	D	68	LEU	CB-CG-CD1	8.10	124.77	111.00
2	D	92	HIS	CB-CA-C	-8.10	94.20	110.40
2	D	85	PHE	O-C-N	-8.10	109.75	122.70
1	A	33	PHE	CG-CD1-CE1	8.09	129.69	120.80
2	D	146	HIS	CB-CG-CD2	8.09	155.87	130.80
2	D	47	ASP	CA-CB-CG	-8.08	95.63	113.40
2	D	16	GLY	O-C-N	-8.06	109.80	122.70
2	D	110	LEU	CA-C-O	8.06	137.02	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	19	ASN	CB-CG-ND2	-8.06	97.37	116.70
2	B	118	PHE	CD1-CG-CD2	-8.05	107.83	118.30
1	C	74	ASP	CA-CB-CG	8.05	131.12	113.40
1	C	117	PHE	CZ-CE2-CD2	-8.04	110.45	120.10
1	A	42	TYR	CB-CG-CD2	-8.04	116.18	121.00
1	A	70	VAL	CA-CB-CG1	8.04	122.96	110.90
1	C	17	VAL	C-N-CA	-8.04	105.42	122.30
1	A	52	SER	CA-C-O	8.02	136.93	120.10
2	B	54	VAL	CG1-CB-CG2	8.01	123.72	110.90
1	A	52	SER	CB-CA-C	8.00	125.30	110.10
2	D	121	GLU	O-C-N	7.99	135.49	122.70
2	D	92	HIS	CG-CD2-NE2	7.99	124.38	109.20
2	B	134	VAL	O-C-N	-7.99	109.92	122.70
2	D	144	LYS	CG-CD-CE	7.96	135.79	111.90
2	D	6	GLU	N-CA-CB	7.96	124.93	110.60
2	D	108	ASN	CB-CG-ND2	-7.96	97.59	116.70
1	C	26	ALA	CA-C-O	7.96	136.82	120.10
2	D	63	HIS	O-C-N	7.96	136.73	123.20
1	A	24	TYR	CG-CD1-CE1	-7.95	114.94	121.30
1	A	59	GLY	O-C-N	-7.95	109.99	122.70
1	C	49	SER	N-CA-CB	7.94	122.41	110.50
1	C	43	PHE	CD1-CE1-CZ	7.93	129.62	120.10
1	A	81	SER	O-C-N	-7.92	110.03	122.70
2	B	38	THR	N-CA-CB	7.92	125.34	110.30
1	A	1	VAL	O-C-N	7.90	135.34	122.70
1	A	110	ALA	CA-C-O	7.90	136.69	120.10
1	C	98	PHE	CE1-CZ-CE2	-7.90	105.78	120.00
2	B	64	GLY	O-C-N	-7.90	110.06	122.70
2	D	17	LYS	CG-CD-CE	7.88	135.55	111.90
1	A	63	ALA	N-CA-CB	-7.88	99.07	110.10
2	B	12	THR	O-C-N	-7.88	110.09	122.70
1	C	114	PRO	N-CA-C	-7.88	91.63	112.10
2	B	79	ASP	N-CA-CB	-7.87	96.43	110.60
1	A	4	PRO	CA-CB-CG	-7.87	89.06	104.00
1	C	12	ALA	CB-CA-C	-7.86	98.31	110.10
2	D	72	SER	CA-CB-OG	-7.86	89.98	111.20
2	B	78	LEU	CA-CB-CG	-7.85	97.25	115.30
2	D	15	TRP	NE1-CE2-CZ2	7.85	139.03	130.40
2	B	26	GLU	O-C-N	7.84	135.25	122.70
1	A	110	ALA	C-N-CA	7.84	141.29	121.70
1	C	110	ALA	O-C-N	-7.84	110.16	122.70
1	A	106	LEU	O-C-N	-7.83	110.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	87	THR	CB-CA-C	-7.83	90.47	111.60
2	D	40	ARG	CA-C-N	7.82	134.40	117.20
2	D	92	HIS	N-CA-CB	-7.82	96.53	110.60
1	A	19	ALA	N-CA-C	-7.81	89.91	111.00
2	B	57	ASN	O-C-N	-7.81	106.26	121.10
1	C	14	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	117	PHE	CB-CG-CD1	-7.81	115.33	120.80
2	B	99	ASP	CB-CG-OD1	-7.81	111.27	118.30
1	A	27	GLU	OE1-CD-OE2	7.80	132.66	123.30
2	D	9	SER	C-N-CA	-7.80	102.20	121.70
1	A	21	ALA	N-CA-CB	7.79	121.00	110.10
1	A	16	LYS	CD-CE-NZ	7.77	129.57	111.70
1	C	43	PHE	CG-CD1-CE1	-7.77	112.26	120.80
2	B	66	LYS	CG-CD-CE	-7.76	88.62	111.90
1	C	115	ALA	N-CA-CB	7.76	120.96	110.10
2	D	66	LYS	CG-CD-CE	-7.76	88.63	111.90
1	A	93	VAL	O-C-N	-7.73	110.33	122.70
1	A	132	VAL	CG1-CB-CG2	-7.73	98.53	110.90
2	D	78	LEU	C-N-CA	-7.73	102.38	121.70
1	A	98	PHE	CZ-CE2-CD2	-7.73	110.83	120.10
2	D	99	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	20	HIS	CG-CD2-NE2	-7.71	94.55	109.20
2	D	146	HIS	CA-C-O	7.71	136.28	120.10
1	A	3	SER	O-C-N	-7.70	106.46	121.10
2	D	50	THR	CA-CB-OG1	7.69	125.15	109.00
1	C	17	VAL	CB-CA-C	7.69	126.01	111.40
1	A	69	ALA	N-CA-CB	-7.68	99.34	110.10
2	D	122	PHE	CD1-CG-CD2	-7.68	108.31	118.30
1	A	92	ARG	O-C-N	-7.68	110.41	122.70
1	A	56	LYS	CD-CE-NZ	-7.68	94.04	111.70
1	C	23	GLU	CB-CG-CD	-7.67	93.48	114.20
2	D	141	LEU	CB-CG-CD2	-7.67	97.96	111.00
1	A	75	ASP	CA-C-N	-7.67	100.32	117.20
1	C	42	TYR	CD1-CE1-CZ	7.67	126.70	119.80
1	A	51	GLY	O-C-N	7.67	134.97	122.70
2	D	3	LEU	CD1-CG-CD2	-7.66	87.52	110.50
2	B	79	ASP	OD1-CG-OD2	-7.66	108.75	123.30
2	B	80	ASN	CA-C-O	-7.66	104.02	120.10
1	A	2	LEU	CB-CG-CD1	7.65	124.01	111.00
2	B	45	PHE	O-C-N	-7.64	110.21	123.20
1	A	48	LEU	CB-CG-CD1	-7.64	98.01	111.00
2	B	122	PHE	CD1-CE1-CZ	-7.64	110.93	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	THR	CA-CB-CG2	-7.64	101.71	112.40
1	A	108	THR	CA-CB-CG2	-7.63	101.71	112.40
1	A	17	VAL	C-N-CA	-7.63	106.28	122.30
2	B	99	ASP	OD1-CG-OD2	7.63	137.79	123.30
1	C	3	SER	CB-CA-C	7.63	124.60	110.10
2	B	55	MET	O-C-N	7.62	136.15	123.20
1	C	63	ALA	CA-C-O	7.60	136.06	120.10
1	A	3	SER	CA-C-O	7.59	136.04	120.10
1	A	101	LEU	O-C-N	-7.59	110.56	122.70
2	B	130	TYR	CD1-CE1-CZ	7.58	126.62	119.80
2	D	89	SER	O-C-N	-7.57	110.58	122.70
1	C	3	SER	O-C-N	-7.57	106.73	121.10
2	D	131	GLN	CG-CD-OE1	-7.55	106.49	121.60
2	D	94	ASP	N-CA-CB	-7.55	97.01	110.60
2	B	13	ALA	O-C-N	-7.55	110.62	122.70
2	D	97	HIS	ND1-CG-CD2	7.55	119.37	108.80
1	C	99	LYS	CG-CD-CE	-7.55	89.26	111.90
1	C	72	HIS	CA-C-O	7.54	135.94	120.10
1	C	49	SER	O-C-N	-7.54	110.63	122.70
2	D	72	SER	CA-C-N	-7.54	100.61	117.20
1	A	7	LYS	N-CA-CB	-7.53	97.04	110.60
2	D	50	THR	CA-CB-CG2	-7.53	101.86	112.40
1	C	42	TYR	CA-CB-CG	-7.53	99.10	113.40
2	D	92	HIS	CG-ND1-CE1	-7.52	95.92	105.70
1	C	106	LEU	C-N-CA	7.52	140.50	121.70
2	D	48	LEU	CA-CB-CG	-7.51	98.02	115.30
1	C	75	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	C	67	THR	CA-CB-CG2	-7.51	101.89	112.40
1	A	84	SER	O-C-N	7.49	134.69	122.70
1	C	110	ALA	CB-CA-C	7.49	121.33	110.10
2	D	117	HIS	O-C-N	-7.49	110.72	122.70
1	A	85	ASP	OD1-CG-OD2	-7.47	109.10	123.30
1	C	137	THR	CA-CB-CG2	-7.47	101.94	112.40
1	C	17	VAL	CA-C-N	-7.47	101.25	116.20
1	A	61	LYS	CB-CA-C	-7.47	95.46	110.40
1	C	74	ASP	CB-CG-OD1	7.47	125.02	118.30
1	C	95	PRO	O-C-N	-7.45	110.78	122.70
2	B	140	ALA	O-C-N	-7.45	110.78	122.70
2	D	98	VAL	CA-CB-CG2	-7.44	99.74	110.90
1	C	40	LYS	CD-CE-NZ	-7.44	94.60	111.70
2	B	3	LEU	O-C-N	7.43	134.59	122.70
1	C	51	GLY	CA-C-O	7.43	133.98	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	17	LYS	CB-CG-CD	-7.43	92.29	111.60
1	A	77	PRO	O-C-N	-7.42	110.84	122.70
2	D	2	HIS	N-CA-C	7.40	130.99	111.00
2	B	46	GLY	O-C-N	7.40	134.54	122.70
1	C	141	ARG	NH1-CZ-NH2	7.39	127.53	119.40
2	B	71	PHE	CG-CD2-CE2	-7.38	112.68	120.80
2	B	17	LYS	CA-C-N	7.37	133.42	117.20
1	A	28	ALA	CA-C-N	-7.37	100.99	117.20
1	C	56	LYS	CA-C-O	7.37	135.57	120.10
2	D	110	LEU	O-C-N	-7.37	110.91	122.70
1	A	105	LEU	O-C-N	7.37	134.49	122.70
1	A	87	HIS	CA-CB-CG	-7.36	101.08	113.60
1	C	107	VAL	O-C-N	-7.36	110.92	122.70
1	C	99	LYS	CA-C-N	-7.36	101.01	117.20
2	D	47	ASP	C-N-CA	-7.36	103.31	121.70
1	C	24	TYR	OH-CZ-CE2	-7.36	100.24	120.10
2	B	77	HIS	ND1-CE1-NE2	7.35	126.06	109.90
1	A	65	ALA	C-N-CA	-7.33	103.39	121.70
1	A	61	LYS	CD-CE-NZ	7.32	128.54	111.70
2	D	126	VAL	O-C-N	7.32	134.41	122.70
2	D	131	GLN	OE1-CD-NE2	7.32	138.73	121.90
1	A	127	LYS	CG-CD-CE	-7.31	89.97	111.90
1	C	44	PRO	N-CD-CG	-7.31	92.24	103.20
2	D	6	GLU	C-N-CA	-7.31	103.43	121.70
1	A	89	HIS	CG-CD2-NE2	-7.30	95.32	109.20
2	D	130	TYR	CZ-CE2-CD2	7.30	126.37	119.80
1	C	15	GLY	O-C-N	-7.29	111.03	122.70
1	C	24	TYR	CG-CD2-CE2	-7.29	115.46	121.30
2	B	38	THR	CA-CB-CG2	-7.29	102.20	112.40
2	D	5	PRO	O-C-N	-7.28	111.05	122.70
2	D	57	ASN	C-N-CD	7.28	143.69	128.40
1	A	136	LEU	CD1-CG-CD2	7.27	132.31	110.50
2	D	35	TYR	CG-CD1-CE1	7.25	127.10	121.30
2	D	65	LYS	N-CA-CB	-7.24	97.56	110.60
2	B	95	LYS	N-CA-CB	-7.24	97.56	110.60
2	D	112	CYS	CA-C-N	-7.24	101.28	117.20
1	C	74	ASP	CA-C-N	-7.23	101.29	117.20
2	D	7	GLU	CA-C-O	-7.23	104.92	120.10
2	D	144	LYS	O-C-N	-7.23	111.13	122.70
2	B	35	TYR	CZ-CE2-CD2	7.21	126.29	119.80
1	A	5	ALA	CB-CA-C	-7.21	99.28	110.10
2	D	36	PRO	N-CD-CG	7.21	114.01	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	141	LEU	CB-CG-CD1	-7.19	98.77	111.00
1	A	6	ASP	CB-CG-OD1	7.19	124.77	118.30
1	C	60	LYS	CA-CB-CG	-7.19	97.59	113.40
2	B	84	THR	CA-C-O	7.18	135.17	120.10
2	D	45	PHE	CG-CD1-CE1	-7.17	112.91	120.80
2	B	20	VAL	CA-C-N	7.17	132.97	117.20
1	C	117	PHE	CE1-CZ-CE2	7.17	132.90	120.00
2	D	122	PHE	CG-CD1-CE1	7.16	128.68	120.80
2	D	143	HIS	ND1-CG-CD2	7.16	118.83	108.80
2	B	126	VAL	O-C-N	-7.16	111.24	122.70
1	A	103	HIS	CA-C-O	7.16	135.13	120.10
2	B	61	LYS	O-C-N	-7.16	111.25	122.70
2	D	43	GLU	CB-CG-CD	-7.16	94.87	114.20
2	B	36	PRO	CA-N-CD	-7.15	101.49	111.50
2	D	38	THR	CA-CB-CG2	-7.15	102.40	112.40
1	A	10	VAL	O-C-N	7.14	134.13	122.70
2	D	144	LYS	CB-CA-C	7.14	124.69	110.40
1	A	134	THR	N-CA-CB	-7.14	96.73	110.30
1	A	23	GLU	N-CA-CB	-7.14	97.75	110.60
1	C	37	PRO	N-CD-CG	7.13	113.90	103.20
1	A	83	LEU	CD1-CG-CD2	-7.13	89.11	110.50
2	B	77	HIS	CB-CG-CD2	-7.12	108.71	130.80
2	D	93	CYS	CA-C-N	-7.12	101.53	117.20
2	B	9	SER	CA-C-N	-7.11	101.56	117.20
1	A	42	TYR	CA-CB-CG	-7.09	99.92	113.40
2	B	6	GLU	CG-CD-OE2	7.09	132.48	118.30
1	A	17	VAL	CA-CB-CG2	7.09	121.53	110.90
1	C	94	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	49	SER	CA-C-O	7.08	134.97	120.10
1	C	49	SER	N-CA-C	-7.07	91.91	111.00
1	C	47	ASP	N-CA-CB	-7.07	97.88	110.60
2	D	3	LEU	CB-CG-CD1	-7.07	98.99	111.00
1	C	118	THR	N-CA-CB	-7.07	96.88	110.30
2	B	12	THR	CA-CB-OG1	-7.06	94.17	109.00
2	D	92	HIS	CA-C-O	-7.06	105.28	120.10
1	C	17	VAL	CA-C-O	7.05	134.90	120.10
2	B	31	LEU	CB-CG-CD1	-7.04	99.02	111.00
2	D	1	VAL	CB-CA-C	-7.04	98.02	111.40
1	C	78	ASN	N-CA-C	7.04	130.00	111.00
2	D	80	ASN	CB-CA-C	-7.03	96.34	110.40
1	A	50	HIS	O-C-N	-7.02	111.26	123.20
2	B	130	TYR	CB-CG-CD2	-7.01	116.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	86	LEU	CA-C-N	-7.01	101.78	117.20
2	D	13	ALA	CA-C-O	7.00	134.81	120.10
2	B	50	THR	CA-CB-OG1	7.00	123.70	109.00
1	C	14	TRP	CD2-CE3-CZ3	7.00	127.90	118.80
1	C	129	LEU	O-C-N	-7.00	111.51	122.70
2	D	137	VAL	CB-CA-C	-6.99	98.11	111.40
1	C	99	LYS	CB-CG-CD	6.99	129.76	111.60
1	A	58	HIS	CA-CB-CG	-6.98	101.73	113.60
1	A	39	THR	O-C-N	6.98	133.86	122.70
1	C	112	HIS	CG-CD2-NE2	6.96	122.43	109.20
2	B	28	LEU	CA-C-O	6.96	134.71	120.10
2	B	65	LYS	CB-CG-CD	-6.95	93.52	111.60
1	A	17	VAL	N-CA-CB	6.95	126.79	111.50
2	B	15	TRP	CG-CD1-NE1	6.94	117.04	110.10
2	D	45	PHE	C-N-CA	-6.94	107.73	122.30
1	A	81	SER	CA-C-N	6.94	132.46	117.20
1	A	61	LYS	CA-C-N	-6.92	101.97	117.20
1	C	99	LYS	CA-CB-CG	6.92	128.62	113.40
2	D	71	PHE	CD1-CE1-CZ	6.91	128.39	120.10
2	D	19	ASN	CB-CG-ND2	-6.91	100.13	116.70
2	B	112	CYS	N-CA-CB	6.90	123.02	110.60
1	C	107	VAL	CA-C-O	6.90	134.58	120.10
1	A	105	LEU	N-CA-CB	-6.90	96.61	110.40
1	A	138	SER	CB-CA-C	-6.89	97.00	110.10
2	B	82	LYS	O-C-N	-6.89	111.49	123.20
1	A	60	LYS	CA-C-N	-6.89	102.05	117.20
2	D	39	GLN	O-C-N	-6.88	111.69	122.70
2	B	126	VAL	CA-C-N	6.88	132.33	117.20
1	C	33	PHE	CZ-CE2-CD2	6.88	128.35	120.10
2	D	85	PHE	CB-CG-CD2	6.87	125.61	120.80
1	C	52	SER	CA-C-N	6.87	132.31	117.20
2	B	76	ALA	CA-C-O	6.86	134.51	120.10
1	C	76	MET	N-CA-CB	-6.86	98.25	110.60
1	A	18	GLY	CA-C-O	-6.85	108.27	120.60
2	B	15	TRP	NE1-CE2-CD2	-6.85	100.45	107.30
2	B	69	GLY	CA-C-N	-6.85	102.13	117.20
2	B	20	VAL	CA-CB-CG1	-6.84	100.63	110.90
1	C	43	PHE	CE1-CZ-CE2	-6.84	107.68	120.00
1	A	73	VAL	CA-CB-CG1	6.84	121.16	110.90
2	D	52	ASP	CA-CB-CG	6.84	128.46	113.40
2	D	56	GLY	CA-C-O	6.84	132.91	120.60
2	B	77	HIS	CB-CG-ND1	6.84	140.29	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	14	LEU	O-C-N	6.83	133.63	122.70
1	A	43	PHE	CG-CD1-CE1	-6.83	113.29	120.80
2	B	84	THR	N-CA-CB	6.82	123.27	110.30
1	C	128	PHE	O-C-N	6.82	133.62	122.70
2	D	76	ALA	N-CA-C	-6.82	92.58	111.00
2	B	80	ASN	N-CA-C	-6.81	92.62	111.00
1	A	31	ARG	O-C-N	6.80	133.59	122.70
2	B	66	LYS	O-C-N	6.80	133.58	122.70
2	B	52	ASP	OD1-CG-OD2	-6.80	110.38	123.30
2	D	42	PHE	C-N-CA	-6.79	104.72	121.70
1	A	113	LEU	CB-CG-CD1	6.79	122.54	111.00
1	A	129	LEU	CB-CG-CD2	-6.78	99.47	111.00
2	B	84	THR	O-C-N	-6.78	111.85	122.70
1	C	141	ARG	CG-CD-NE	-6.78	97.56	111.80
2	D	4	THR	OG1-CB-CG2	6.76	125.56	110.00
2	B	41	PHE	CA-C-O	-6.76	105.90	120.10
1	C	131	SER	CB-CA-C	-6.76	97.25	110.10
2	D	60	VAL	O-C-N	-6.76	111.88	122.70
2	B	2	HIS	ND1-CG-CD2	6.76	118.26	108.80
2	D	85	PHE	CE1-CZ-CE2	-6.76	107.83	120.00
1	A	68	ASN	O-C-N	-6.75	111.89	122.70
2	B	113	VAL	CA-C-N	6.75	132.06	117.20
1	C	45	HIS	CB-CG-ND1	-6.75	106.33	123.20
2	D	81	LEU	CB-CG-CD2	6.75	122.47	111.00
2	D	48	LEU	C-N-CA	-6.75	104.84	121.70
2	B	142	ALA	CA-C-O	-6.74	105.94	120.10
2	D	126	VAL	CA-CB-CG1	-6.74	100.79	110.90
2	B	49	SER	N-CA-C	-6.74	92.80	111.00
2	D	84	THR	CA-C-N	-6.74	102.37	117.20
2	B	58	PRO	O-C-N	6.74	133.48	122.70
2	D	76	ALA	CA-C-O	-6.74	105.95	120.10
1	C	29	LEU	CA-C-O	6.74	134.25	120.10
2	D	100	PRO	O-C-N	6.74	133.48	122.70
1	C	21	ALA	N-CA-CB	-6.72	100.69	110.10
1	A	61	LYS	C-N-CA	-6.71	104.91	121.70
1	C	58	HIS	O-C-N	6.71	134.61	123.20
1	C	4	PRO	CA-C-N	-6.71	102.44	117.20
1	C	83	LEU	N-CA-CB	-6.70	97.00	110.40
2	D	92	HIS	CE1-NE2-CD2	-6.70	89.86	106.60
1	C	55	VAL	CA-CB-CG1	-6.69	100.86	110.90
2	D	19	ASN	CB-CA-C	6.69	123.78	110.40
2	B	139	ASN	CA-CB-CG	-6.69	98.69	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	40	ARG	NH1-CZ-NH2	6.69	126.76	119.40
1	C	31	ARG	NH1-CZ-NH2	6.69	126.76	119.40
2	D	41	PHE	C-N-CA	-6.68	105.00	121.70
2	D	26	GLU	O-C-N	6.67	133.38	122.70
2	B	66	LYS	CB-CA-C	-6.67	97.05	110.40
2	B	90	GLU	CG-CD-OE2	-6.67	104.95	118.30
2	D	75	LEU	CB-CA-C	6.67	122.88	110.20
2	D	80	ASN	C-N-CA	-6.65	105.08	121.70
1	A	96	VAL	CA-CB-CG1	6.64	120.87	110.90
2	D	91	LEU	CA-C-O	6.64	134.05	120.10
2	B	90	GLU	CA-CB-CG	-6.64	98.79	113.40
1	C	130	ALA	N-CA-CB	6.63	119.39	110.10
1	C	38	THR	CB-CA-C	6.63	129.50	111.60
2	B	44	SER	CA-C-O	-6.63	106.18	120.10
2	B	88	LEU	CB-CG-CD1	-6.63	99.73	111.00
1	C	10	VAL	CG1-CB-CG2	-6.63	100.29	110.90
1	C	7	LYS	CA-C-N	-6.63	102.62	117.20
1	A	33	PHE	CD1-CE1-CZ	-6.62	112.16	120.10
2	B	141	LEU	CB-CA-C	6.62	122.77	110.20
1	A	24	TYR	CA-CB-CG	-6.61	100.84	113.40
2	D	103	PHE	N-CA-CB	6.60	122.48	110.60
2	D	1	VAL	CG1-CB-CG2	-6.60	100.34	110.90
1	A	78	ASN	O-C-N	-6.59	112.16	122.70
1	C	140	TYR	CD1-CG-CD2	-6.58	110.66	117.90
1	C	64	ASP	CA-CB-CG	6.58	127.89	113.40
2	D	13	ALA	CA-C-N	-6.58	102.72	117.20
2	D	23	VAL	CG1-CB-CG2	6.58	121.43	110.90
2	B	28	LEU	O-C-N	-6.58	112.02	123.20
2	B	74	GLY	N-CA-C	6.58	129.54	113.10
1	A	84	SER	CB-CA-C	-6.57	97.62	110.10
1	C	6	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	140	TYR	CD1-CG-CD2	-6.57	110.68	117.90
2	D	137	VAL	CG1-CB-CG2	6.56	121.40	110.90
2	D	51	PRO	CA-C-O	6.56	135.94	120.20
1	A	81	SER	C-N-CA	6.55	138.09	121.70
1	A	126	ASP	CA-C-O	6.55	133.86	120.10
2	D	8	LYS	CA-C-O	6.55	133.86	120.10
1	A	83	LEU	CB-CA-C	-6.55	97.76	110.20
2	B	103	PHE	N-CA-CB	6.55	122.38	110.60
1	A	71	ALA	CB-CA-C	6.54	119.92	110.10
1	A	77	PRO	N-CA-CB	6.54	111.15	103.30
1	A	50	HIS	ND1-CG-CD2	-6.54	96.84	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	101	GLU	O-C-N	-6.54	112.24	122.70
1	C	139	LYS	CA-CB-CG	-6.54	99.02	113.40
2	B	101	GLU	CG-CD-OE1	-6.54	105.23	118.30
2	B	141	LEU	O-C-N	-6.53	112.25	122.70
1	C	42	TYR	CB-CG-CD2	6.53	124.92	121.00
2	D	51	PRO	O-C-N	-6.53	112.25	122.70
2	D	144	LYS	N-CA-CB	6.53	122.35	110.60
2	B	17	LYS	C-N-CA	6.52	138.00	121.70
2	B	95	LYS	O-C-N	-6.52	112.27	122.70
1	A	46	PHE	CD1-CE1-CZ	6.51	127.92	120.10
2	B	27	ALA	N-CA-CB	-6.51	100.99	110.10
1	C	140	TYR	O-C-N	6.51	133.11	122.70
1	A	23	GLU	CG-CD-OE2	-6.50	105.30	118.30
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
2	D	92	HIS	CB-CG-CD2	6.50	150.95	130.80
1	A	3	SER	N-CA-CB	-6.49	100.76	110.50
2	B	90	GLU	CA-C-O	6.49	133.73	120.10
1	A	84	SER	N-CA-CB	6.48	120.23	110.50
2	D	66	LYS	CB-CA-C	6.48	123.37	110.40
2	B	138	ALA	CA-C-O	6.48	133.71	120.10
2	B	24	GLY	CA-C-O	6.47	132.25	120.60
2	B	91	LEU	C-N-CA	-6.46	105.54	121.70
1	A	51	GLY	C-N-CA	-6.46	105.55	121.70
2	D	15	TRP	CZ3-CH2-CZ2	6.45	129.34	121.60
2	D	100	PRO	CA-N-CD	-6.45	102.47	111.50
2	D	135	ALA	N-CA-CB	6.45	119.14	110.10
1	A	36	PHE	O-C-N	6.45	133.36	121.10
2	D	49	SER	CA-C-N	-6.45	103.01	117.20
2	B	99	ASP	N-CA-C	-6.45	93.60	111.00
2	B	2	HIS	CA-C-O	6.44	133.63	120.10
2	B	3	LEU	CB-CG-CD2	-6.44	100.06	111.00
2	B	37	TRP	CD2-CE3-CZ3	-6.44	110.43	118.80
2	B	59	LYS	CG-CD-CE	-6.43	92.60	111.90
1	C	1	VAL	CA-C-O	6.43	133.61	120.10
1	A	76	MET	N-CA-CB	-6.42	99.04	110.60
2	D	100	PRO	CB-CA-C	6.42	128.06	112.00
2	B	65	LYS	CA-CB-CG	-6.42	99.27	113.40
2	B	118	PHE	CZ-CE2-CD2	6.42	127.81	120.10
1	A	72	HIS	ND1-CE1-NE2	-6.42	95.78	109.90
1	C	96	VAL	CA-CB-CG1	-6.42	101.27	110.90
1	C	36	PHE	C-N-CD	6.41	141.87	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	107	VAL	N-CA-CB	6.41	125.61	111.50
2	D	145	TYR	CD1-CE1-CZ	-6.41	114.03	119.80
2	B	81	LEU	CB-CG-CD1	6.41	121.89	111.00
2	D	105	LEU	CA-CB-CG	6.40	130.03	115.30
1	C	58	HIS	CE1-NE2-CD2	-6.40	90.60	106.60
2	D	59	LYS	CD-CE-NZ	-6.40	96.99	111.70
1	C	61	LYS	O-C-N	6.39	132.93	122.70
2	D	90	GLU	C-N-CA	-6.39	105.73	121.70
1	C	18	GLY	C-N-CA	-6.39	105.74	121.70
2	D	122	PHE	N-CA-CB	-6.38	99.11	110.60
1	C	16	LYS	N-CA-C	-6.38	93.78	111.00
2	D	24	GLY	CA-C-N	6.38	128.95	116.20
2	B	142	ALA	N-CA-CB	6.37	119.02	110.10
2	D	18	VAL	CG1-CB-CG2	-6.37	100.71	110.90
1	C	11	LYS	CB-CA-C	6.37	123.13	110.40
2	D	60	VAL	CA-CB-CG2	6.37	120.45	110.90
1	C	13	ALA	CB-CA-C	6.36	119.65	110.10
1	A	86	LEU	C-N-CA	-6.36	105.80	121.70
2	B	80	ASN	C-N-CA	-6.36	105.80	121.70
1	C	91	LEU	N-CA-CB	-6.36	97.68	110.40
1	C	133	SER	N-CA-CB	6.36	120.04	110.50
1	C	80	LEU	CB-CG-CD2	-6.36	100.20	111.00
1	C	47	ASP	CA-CB-CG	-6.35	99.42	113.40
1	C	112	HIS	CA-CB-CG	-6.35	102.81	113.60
1	A	125	LEU	O-C-N	-6.34	112.55	122.70
1	C	98	PHE	CB-CG-CD1	-6.34	116.36	120.80
1	A	33	PHE	CA-C-O	6.34	133.41	120.10
1	A	74	ASP	OD1-CG-OD2	-6.34	111.26	123.30
1	C	2	LEU	CB-CG-CD2	6.33	121.77	111.00
2	B	13	ALA	N-CA-C	6.33	128.10	111.00
2	B	14	LEU	CD1-CG-CD2	6.33	129.48	110.50
2	B	5	PRO	N-CD-CG	-6.33	93.71	103.20
2	D	64	GLY	CA-C-O	6.32	131.98	120.60
2	B	79	ASP	CB-CG-OD2	6.32	123.99	118.30
2	D	45	PHE	CE1-CZ-CE2	-6.32	108.62	120.00
1	A	99	LYS	CB-CG-CD	6.31	128.01	111.60
1	A	64	ASP	CB-CA-C	-6.31	97.78	110.40
1	C	103	HIS	O-C-N	-6.31	112.60	122.70
2	B	37	TRP	CD1-CG-CD2	-6.30	101.26	106.30
2	B	66	LYS	CA-CB-CG	6.30	127.27	113.40
2	B	36	PRO	N-CA-CB	6.30	110.86	103.30
1	C	109	LEU	CD1-CG-CD2	6.30	129.40	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	74	GLY	CA-C-O	6.30	131.94	120.60
2	B	6	GLU	CB-CA-C	-6.30	97.81	110.40
2	B	103	PHE	CG-CD2-CE2	-6.29	113.88	120.80
1	A	30	GLU	CG-CD-OE2	-6.29	105.72	118.30
1	A	22	GLY	N-CA-C	6.29	128.82	113.10
2	B	78	LEU	CA-C-O	-6.29	106.89	120.10
1	C	50	HIS	CA-C-O	-6.29	106.90	120.10
1	C	118	THR	O-C-N	6.28	133.03	121.10
1	C	65	ALA	CB-CA-C	-6.27	100.70	110.10
2	D	4	THR	CA-C-N	6.27	134.66	117.10
1	A	7	LYS	C-N-CA	-6.27	106.03	121.70
1	A	56	LYS	CA-C-N	-6.27	103.67	116.20
1	A	112	HIS	CB-CG-ND1	-6.27	107.53	123.20
2	D	139	ASN	CA-C-O	6.26	133.25	120.10
1	A	86	LEU	CD1-CG-CD2	-6.26	91.73	110.50
2	B	71	PHE	CG-CD1-CE1	6.25	127.68	120.80
1	C	47	ASP	CA-C-N	-6.25	103.45	117.20
1	C	69	ALA	CB-CA-C	6.24	119.47	110.10
1	A	132	VAL	CA-CB-CG1	6.24	120.26	110.90
1	A	64	ASP	N-CA-C	6.24	127.85	111.00
1	A	99	LYS	CD-CE-NZ	-6.24	97.35	111.70
2	D	85	PHE	CA-CB-CG	-6.24	98.93	113.90
2	D	6	GLU	N-CA-C	-6.24	94.16	111.00
2	B	145	TYR	O-C-N	6.24	132.68	122.70
2	D	41	PHE	CB-CG-CD1	-6.24	116.44	120.80
1	C	58	HIS	CG-CD2-NE2	6.23	121.04	109.20
2	D	96	LEU	O-C-N	6.23	132.67	122.70
1	A	83	LEU	O-C-N	-6.23	112.73	122.70
2	B	95	LYS	N-CA-C	6.23	127.81	111.00
1	A	138	SER	O-C-N	6.22	132.66	122.70
2	B	61	LYS	CG-CD-CE	-6.22	93.24	111.90
1	A	24	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	C	5	ALA	CA-C-N	-6.22	103.53	117.20
2	B	93	CYS	O-C-N	6.21	132.64	122.70
1	A	128	PHE	CG-CD1-CE1	-6.21	113.97	120.80
1	A	15	GLY	O-C-N	-6.21	112.77	122.70
2	D	77	HIS	CG-ND1-CE1	-6.20	97.64	105.70
1	C	1	VAL	CB-CA-C	-6.20	99.62	111.40
1	C	54	GLN	CA-C-N	-6.20	103.56	117.20
2	D	39	GLN	N-CA-CB	-6.20	99.44	110.60
2	D	141	LEU	CD1-CG-CD2	-6.20	91.91	110.50
2	D	131	GLN	CA-C-O	6.19	133.10	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	21	ASP	OD1-CG-OD2	6.19	135.06	123.30
2	D	80	ASN	CB-CG-OD1	-6.19	109.22	121.60
1	C	50	HIS	CA-CB-CG	-6.18	103.09	113.60
1	C	74	ASP	N-CA-CB	-6.18	99.47	110.60
1	A	75	ASP	C-N-CA	-6.18	106.26	121.70
1	A	4	PRO	O-C-N	-6.18	112.82	122.70
1	A	28	ALA	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	61	LYS	CB-CA-C	-6.17	98.06	110.40
2	B	63	HIS	CA-CB-CG	6.17	124.09	113.60
2	B	81	LEU	C-N-CA	-6.17	106.28	121.70
2	B	8	LYS	CG-CD-CE	6.17	130.40	111.90
2	D	24	GLY	C-N-CA	6.17	135.25	122.30
1	A	117	PHE	CZ-CE2-CD2	-6.15	112.72	120.10
2	B	14	LEU	N-CA-CB	-6.15	98.09	110.40
2	B	37	TRP	N-CA-CB	-6.15	99.53	110.60
1	C	100	LEU	CB-CA-C	6.15	121.89	110.20
2	B	44	SER	C-N-CA	6.15	137.08	121.70
2	B	103	PHE	CD1-CG-CD2	6.14	126.29	118.30
2	D	7	GLU	CB-CG-CD	-6.14	97.61	114.20
1	C	122	HIS	CB-CA-C	6.14	122.69	110.40
2	D	19	ASN	CA-C-O	-6.14	107.20	120.10
2	B	19	ASN	CB-CG-OD1	6.14	133.88	121.60
2	B	120	LYS	CB-CA-C	-6.13	98.13	110.40
2	B	35	TYR	O-C-N	6.13	132.74	121.10
2	B	120	LYS	CG-CD-CE	-6.12	93.53	111.90
2	D	15	TRP	NE1-CE2-CD2	-6.12	101.18	107.30
1	C	21	ALA	CA-C-N	6.12	128.44	116.20
2	D	1	VAL	C-N-CA	-6.12	106.40	121.70
1	A	58	HIS	CG-ND1-CE1	-6.11	97.75	105.70
1	C	11	LYS	O-C-N	-6.11	112.92	122.70
1	A	96	VAL	CA-C-O	6.11	132.93	120.10
1	A	79	ALA	O-C-N	6.11	132.47	122.70
2	D	48	LEU	CB-CG-CD1	-6.11	100.62	111.00
2	B	76	ALA	N-CA-C	6.10	127.47	111.00
1	C	77	PRO	CA-C-O	6.10	134.83	120.20
2	D	93	CYS	C-N-CA	-6.10	106.46	121.70
2	B	90	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	C	38	THR	N-CA-CB	-6.09	98.73	110.30
2	B	73	ASP	C-N-CA	6.09	135.09	122.30
2	D	12	THR	N-CA-CB	-6.08	98.76	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	36	PRO	O-C-N	-6.07	112.99	122.70
1	C	25	GLY	C-N-CA	6.06	136.85	121.70
2	B	12	THR	CA-C-O	6.06	132.83	120.10
2	B	50	THR	N-CA-C	6.06	127.36	111.00
1	C	72	HIS	CE1-NE2-CD2	-6.06	91.46	106.60
1	A	83	LEU	CB-CG-CD2	6.06	121.30	111.00
1	A	18	GLY	CA-C-N	-6.05	103.88	117.20
2	D	7	GLU	CA-CB-CG	-6.05	100.08	113.40
1	A	58	HIS	CA-C-N	-6.05	104.10	116.20
2	B	41	PHE	CG-CD1-CE1	-6.05	114.14	120.80
1	C	43	PHE	CD1-CG-CD2	6.05	126.16	118.30
1	C	103	HIS	ND1-CE1-NE2	6.05	123.20	109.90
1	C	138	SER	CB-CA-C	-6.05	98.61	110.10
1	A	89	HIS	C-N-CA	6.04	136.81	121.70
1	A	1	VAL	CA-C-N	-6.04	103.91	117.20
2	B	104	ARG	CG-CD-NE	-6.04	99.13	111.80
2	B	97	HIS	CG-CD2-NE2	-6.03	97.74	109.20
2	D	102	ASN	CA-C-N	6.03	130.46	117.20
2	D	17	LYS	N-CA-CB	6.02	121.44	110.60
1	A	45	HIS	CB-CG-ND1	-6.02	108.15	123.20
1	A	109	LEU	CD1-CG-CD2	6.02	128.56	110.50
1	A	99	LYS	CA-CB-CG	6.02	126.64	113.40
1	A	56	LYS	CB-CA-C	6.01	122.43	110.40
1	A	85	ASP	CA-CB-CG	-6.01	100.18	113.40
1	A	26	ALA	O-C-N	-6.00	113.09	122.70
1	A	15	GLY	C-N-CA	6.00	136.70	121.70
2	D	92	HIS	CA-CB-CG	-6.00	103.40	113.60
1	A	40	LYS	CB-CA-C	-6.00	98.40	110.40
1	C	47	ASP	O-C-N	6.00	132.30	122.70
2	D	125	PRO	CA-C-N	-6.00	104.00	117.20
2	B	30	ARG	CD-NE-CZ	5.99	131.99	123.60
1	C	39	THR	CA-CB-CG2	-5.98	104.02	112.40
1	C	75	ASP	N-CA-CB	-5.98	99.84	110.60
1	A	126	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	49	SER	N-CA-C	-5.96	94.91	111.00
1	A	84	SER	CA-CB-OG	-5.96	95.12	111.20
1	A	27	GLU	N-CA-CB	-5.95	99.89	110.60
1	A	46	PHE	CG-CD1-CE1	5.95	127.35	120.80
1	A	117	PHE	O-C-N	5.95	132.22	122.70
2	B	108	ASN	CB-CG-OD1	-5.95	109.70	121.60
2	B	46	GLY	CA-C-O	-5.95	109.89	120.60
2	D	19	ASN	O-C-N	-5.95	113.18	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	126	VAL	CA-C-N	-5.95	104.11	117.20
2	D	103	PHE	CG-CD2-CE2	-5.95	114.26	120.80
2	B	140	ALA	CA-C-N	5.94	130.27	117.20
1	C	45	HIS	CA-C-O	-5.94	107.63	120.10
2	D	88	LEU	CB-CG-CD1	-5.94	100.91	111.00
2	B	91	LEU	N-CA-CB	-5.93	98.53	110.40
2	D	21	ASP	C-N-CA	5.93	136.53	121.70
2	B	28	LEU	CB-CA-C	5.93	121.46	110.20
2	D	103	PHE	CZ-CE2-CD2	5.92	127.21	120.10
1	C	77	PRO	CA-CB-CG	5.92	116.05	104.80
1	C	124	SER	CA-C-O	-5.92	107.67	120.10
1	A	14	TRP	CB-CG-CD1	-5.92	119.31	127.00
2	B	69	GLY	CA-C-O	5.92	131.25	120.60
2	D	78	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	134	THR	CA-CB-OG1	5.91	121.41	109.00
2	B	33	VAL	O-C-N	5.91	132.15	122.70
1	A	54	GLN	OE1-CD-NE2	-5.91	108.31	121.90
2	D	57	ASN	CB-CG-OD1	5.91	133.41	121.60
2	D	95	LYS	CG-CD-CE	5.91	129.62	111.90
1	A	7	LYS	O-C-N	5.90	132.14	122.70
1	A	67	THR	CA-CB-OG1	5.90	121.39	109.00
1	A	89	HIS	CA-C-O	5.90	132.49	120.10
2	D	130	TYR	CD1-CG-CD2	-5.90	111.41	117.90
2	B	50	THR	CA-C-O	-5.89	107.72	120.10
1	A	134	THR	CA-C-N	5.89	130.16	117.20
1	A	135	VAL	CA-C-N	5.89	130.16	117.20
2	B	11	VAL	O-C-N	5.89	132.12	122.70
1	C	14	TRP	CA-CB-CG	-5.89	102.51	113.70
1	C	50	HIS	CB-CG-ND1	-5.89	108.47	123.20
1	A	28	ALA	CA-C-O	5.89	132.46	120.10
1	C	37	PRO	CA-N-CD	-5.89	103.26	111.50
2	D	91	LEU	CB-CG-CD2	5.89	121.01	111.00
1	A	131	SER	CA-C-O	-5.88	107.75	120.10
2	B	123	THR	O-C-N	5.87	132.26	121.10
1	C	90	LYS	CA-CB-CG	-5.87	100.49	113.40
1	A	64	ASP	N-CA-CB	-5.86	100.05	110.60
2	B	24	GLY	O-C-N	-5.86	113.23	123.20
1	C	92	ARG	CG-CD-NE	-5.86	99.49	111.80
2	D	141	LEU	O-C-N	-5.86	113.33	122.70
1	C	89	HIS	CB-CA-C	5.85	122.11	110.40
1	A	8	THR	N-CA-CB	-5.85	99.18	110.30
2	D	137	VAL	CA-CB-CG2	-5.84	102.14	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	79	ASP	CA-CB-CG	-5.84	100.55	113.40
1	A	98	PHE	N-CA-CB	5.84	121.11	110.60
1	A	81	SER	CB-CA-C	-5.83	99.01	110.10
1	A	73	VAL	CB-CA-C	5.83	122.47	111.40
1	C	77	PRO	N-CA-CB	-5.83	96.19	102.60
2	B	132	LYS	O-C-N	-5.82	113.38	122.70
2	B	37	TRP	CE3-CZ3-CH2	5.82	127.60	121.20
1	C	136	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	A	103	HIS	CG-ND1-CE1	-5.82	98.14	105.70
2	D	60	VAL	CA-C-O	5.81	132.31	120.10
2	D	53	ALA	CA-C-N	-5.81	104.42	117.20
1	A	44	PRO	CA-N-CD	5.81	119.83	111.70
2	B	17	LYS	CA-CB-CG	-5.81	100.62	113.40
1	A	54	GLN	CA-C-O	-5.80	107.92	120.10
2	D	97	HIS	N-CA-CB	5.80	121.04	110.60
1	C	11	LYS	CA-C-O	5.80	132.27	120.10
2	D	12	THR	C-N-CA	5.79	136.18	121.70
1	A	11	LYS	CD-CE-NZ	-5.79	98.38	111.70
1	A	16	LYS	CA-C-N	-5.78	104.48	117.20
2	D	22	GLU	CB-CA-C	5.78	121.96	110.40
1	C	15	GLY	CA-C-N	5.78	129.91	117.20
1	C	89	HIS	ND1-CG-CD2	5.77	116.88	108.80
1	A	21	ALA	N-CA-C	-5.77	95.43	111.00
1	A	132	VAL	CA-C-N	5.77	129.89	117.20
2	D	82	LYS	CA-C-N	5.76	127.73	116.20
2	D	112	CYS	CA-C-O	5.76	132.20	120.10
1	C	83	LEU	CB-CG-CD1	-5.76	101.21	111.00
2	B	8	LYS	CA-C-N	5.75	129.86	117.20
1	C	46	PHE	CA-C-O	5.75	132.18	120.10
2	D	68	LEU	CB-CA-C	-5.75	99.28	110.20
2	D	56	GLY	C-N-CA	5.75	136.06	121.70
2	B	36	PRO	CA-C-N	5.74	129.83	117.20
2	B	75	LEU	CD1-CG-CD2	-5.74	93.28	110.50
1	C	47	ASP	CB-CA-C	-5.74	98.92	110.40
1	A	103	HIS	N-CA-CB	5.74	120.92	110.60
2	B	96	LEU	N-CA-C	5.74	126.48	111.00
1	C	118	THR	CB-CA-C	-5.73	96.12	111.60
1	C	12	ALA	N-CA-CB	5.73	118.12	110.10
1	A	4	PRO	CA-C-N	-5.73	104.60	117.20
2	B	9	SER	C-N-CA	-5.73	107.38	121.70
1	A	32	MET	CA-CB-CG	5.73	123.04	113.30
2	B	13	ALA	CB-CA-C	-5.73	101.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	THR	CA-C-N	5.73	129.80	117.20
2	B	17	LYS	CB-CA-C	-5.72	98.95	110.40
1	A	104	CYS	CA-C-O	-5.72	108.08	120.10
1	C	116	GLU	CA-C-O	-5.72	108.09	120.10
1	A	14	TRP	NE1-CE2-CD2	-5.72	101.58	107.30
2	B	97	HIS	ND1-CG-CD2	5.72	116.80	108.80
1	C	41	THR	C-N-CA	5.71	135.99	121.70
2	D	13	ALA	CB-CA-C	-5.71	101.54	110.10
2	D	20	VAL	CA-C-N	-5.71	104.64	117.20
2	B	39	GLN	OE1-CD-NE2	5.71	135.02	121.90
1	C	78	ASN	CB-CA-C	5.70	121.80	110.40
2	D	108	ASN	CB-CG-OD1	-5.70	110.20	121.60
1	C	36	PHE	CZ-CE2-CD2	5.70	126.94	120.10
2	D	28	LEU	O-C-N	-5.69	113.53	123.20
2	B	62	ALA	C-N-CA	-5.68	107.49	121.70
2	D	54	VAL	CA-C-N	5.68	129.70	117.20
2	B	110	LEU	CB-CA-C	5.68	120.99	110.20
1	C	27	GLU	OE1-CD-OE2	-5.68	116.48	123.30
1	A	35	SER	CB-CA-C	-5.68	99.31	110.10
1	A	88	ALA	N-CA-CB	5.68	118.05	110.10
1	A	52	SER	N-CA-CB	-5.67	101.99	110.50
2	D	15	TRP	CE3-CZ3-CH2	-5.67	114.96	121.20
2	D	33	VAL	CA-CB-CG1	-5.67	102.39	110.90
2	D	92	HIS	ND1-CG-CD2	-5.67	98.06	106.00
2	B	91	LEU	CB-CA-C	5.67	120.97	110.20
1	A	33	PHE	O-C-N	-5.66	113.64	122.70
2	B	50	THR	O-C-N	5.66	131.86	121.10
2	D	143	HIS	CB-CG-CD2	-5.66	113.25	130.80
2	B	39	GLN	CG-CD-OE1	-5.66	110.28	121.60
1	A	2	LEU	C-N-CA	-5.66	107.55	121.70
2	B	131	GLN	CG-CD-NE2	5.65	130.27	116.70
2	D	39	GLN	C-N-CA	5.65	135.82	121.70
2	D	54	VAL	CA-CB-CG2	5.65	119.37	110.90
1	A	77	PRO	N-CA-C	5.65	126.78	112.10
2	B	131	GLN	CG-CD-OE1	-5.65	110.31	121.60
1	C	88	ALA	CA-C-N	-5.63	104.81	117.20
2	D	121	GLU	CA-C-N	-5.63	104.80	117.20
1	A	8	THR	O-C-N	-5.63	113.69	122.70
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	83	LEU	CA-CB-CG	-5.63	102.35	115.30
1	C	125	LEU	O-C-N	-5.63	113.69	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	ASP	C-N-CA	-5.63	107.63	121.70
1	A	71	ALA	CA-C-O	-5.63	108.28	120.10
1	A	13	ALA	C-N-CA	-5.62	107.64	121.70
1	A	55	VAL	CA-C-O	5.62	131.90	120.10
1	C	47	ASP	C-N-CA	-5.62	107.66	121.70
2	D	143	HIS	CA-C-O	-5.62	108.30	120.10
1	A	13	ALA	CA-C-N	-5.62	104.85	117.20
1	C	3	SER	N-CA-CB	-5.62	102.08	110.50
2	D	6	GLU	CB-CG-CD	5.61	129.35	114.20
2	D	58	PRO	CA-C-O	-5.61	106.73	120.20
2	D	63	HIS	CB-CG-ND1	-5.61	109.17	123.20
1	A	8	THR	CA-C-N	-5.61	104.87	117.20
1	C	69	ALA	CA-C-O	-5.61	108.33	120.10
1	A	113	LEU	CB-CA-C	-5.60	99.55	110.20
2	B	143	HIS	CB-CG-CD2	-5.60	113.44	130.80
1	A	48	LEU	CA-C-N	-5.60	104.88	117.20
2	B	4	THR	O-C-N	-5.59	110.47	121.10
2	B	91	LEU	CB-CG-CD2	5.59	120.51	111.00
1	C	72	HIS	CG-CD2-NE2	5.59	119.82	109.20
2	B	33	VAL	CA-CB-CG2	-5.59	102.52	110.90
2	B	92	HIS	CB-CA-C	-5.58	99.23	110.40
1	C	131	SER	CA-CB-OG	-5.58	96.12	111.20
2	B	124	PRO	CA-C-N	5.58	132.72	117.10
1	C	35	SER	N-CA-C	5.58	126.06	111.00
1	C	106	LEU	CA-CB-CG	5.58	128.12	115.30
2	B	3	LEU	CB-CA-C	-5.57	99.61	110.20
2	B	79	ASP	N-CA-C	-5.56	95.98	111.00
2	D	139	ASN	O-C-N	-5.56	113.81	122.70
2	B	117	HIS	C-N-CA	5.55	135.59	121.70
1	C	44	PRO	CA-C-O	-5.55	106.87	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	5.54	118.42	110.10
2	B	80	ASN	O-C-N	5.53	131.55	122.70
2	B	13	ALA	CA-C-O	5.53	131.72	120.10
1	C	98	PHE	N-CA-CB	5.53	120.55	110.60
2	D	72	SER	O-C-N	-5.52	113.86	122.70
1	A	26	ALA	CA-C-N	-5.52	105.06	117.20
2	D	11	VAL	CA-CB-CG1	-5.51	102.63	110.90
2	D	44	SER	CA-CB-OG	5.51	126.07	111.20
1	C	99	LYS	CA-C-O	5.50	131.66	120.10
1	A	94	ASP	CB-CG-OD1	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	GLU	CB-CG-CD	-5.50	99.35	114.20
2	D	118	PHE	CA-C-N	5.50	127.20	116.20
1	A	57	GLY	CA-C-O	-5.50	110.71	120.60
2	D	62	ALA	CA-C-N	-5.49	105.11	117.20
2	D	44	SER	N-CA-CB	5.49	118.74	110.50
2	B	68	LEU	CB-CG-CD2	5.49	120.33	111.00
1	A	16	LYS	CB-CG-CD	-5.48	97.35	111.60
1	C	19	ALA	CA-C-O	5.48	131.61	120.10
1	A	109	LEU	O-C-N	5.47	131.45	122.70
1	C	89	HIS	CB-CG-CD2	-5.47	113.85	130.80
1	A	139	LYS	CA-C-N	5.47	129.23	117.20
1	C	113	LEU	CD1-CG-CD2	5.47	126.90	110.50
2	D	64	GLY	CA-C-N	-5.46	105.18	117.20
1	C	24	TYR	CA-C-O	5.46	131.56	120.10
2	B	92	HIS	CG-ND1-CE1	-5.45	98.61	105.70
2	D	45	PHE	CD1-CG-CD2	-5.45	111.21	118.30
2	D	59	LYS	C-N-CA	-5.45	108.07	121.70
1	A	20	HIS	ND1-CG-CD2	-5.44	98.38	106.00
2	B	124	PRO	N-CD-CG	-5.44	95.03	103.20
1	C	58	HIS	ND1-CE1-NE2	5.44	121.88	109.90
1	A	5	ALA	N-CA-CB	-5.44	102.48	110.10
1	C	29	LEU	C-N-CA	5.44	135.30	121.70
1	C	121	VAL	CB-CA-C	5.44	121.74	111.40
1	C	65	ALA	O-C-N	-5.44	114.00	122.70
2	D	73	ASP	CB-CA-C	-5.43	99.53	110.40
2	B	143	HIS	ND1-CE1-NE2	5.43	121.85	109.90
1	C	133	SER	CA-CB-OG	-5.43	96.53	111.20
2	D	85	PHE	CG-CD2-CE2	-5.43	114.82	120.80
1	A	84	SER	C-N-CA	-5.42	108.15	121.70
1	C	14	TRP	CB-CA-C	-5.42	99.56	110.40
1	C	14	TRP	CE2-CD2-CE3	5.41	125.19	118.70
2	D	66	LYS	N-CA-C	-5.41	96.40	111.00
2	B	91	LEU	CA-CB-CG	-5.41	102.86	115.30
1	C	98	PHE	CG-CD1-CE1	5.41	126.75	120.80
1	A	12	ALA	CA-C-N	5.40	129.09	117.20
1	C	53	ALA	C-N-CA	-5.39	108.21	121.70
1	C	111	ALA	CA-C-O	-5.39	108.78	120.10
1	C	12	ALA	CA-C-N	-5.39	105.35	117.20
1	A	4	PRO	C-N-CA	-5.38	108.24	121.70
2	D	3	LEU	CB-CA-C	5.38	120.42	110.20
1	C	92	ARG	CA-C-O	5.37	131.37	120.10
1	A	61	LYS	CA-C-O	-5.36	108.84	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	84	THR	CA-CB-OG1	-5.36	97.74	109.00
2	D	91	LEU	N-CA-C	5.36	125.48	111.00
1	A	67	THR	CA-CB-CG2	-5.36	104.90	112.40
1	A	85	ASP	O-C-N	-5.36	114.13	122.70
1	A	60	LYS	N-CA-C	5.35	125.45	111.00
1	A	88	ALA	CA-C-O	-5.35	108.86	120.10
2	B	71	PHE	N-CA-CB	-5.35	100.97	110.60
1	A	112	HIS	O-C-N	5.35	131.26	122.70
2	D	74	GLY	CA-C-N	-5.35	105.43	117.20
2	D	119	GLY	CA-C-N	-5.35	105.44	117.20
1	C	79	ALA	O-C-N	5.34	131.25	122.70
1	C	119	PRO	N-CA-CB	5.34	109.71	103.30
2	D	75	LEU	N-CA-CB	-5.34	99.71	110.40
2	D	5	PRO	CB-CG-CD	5.34	127.34	106.50
2	B	77	HIS	N-CA-C	-5.33	96.60	111.00
1	C	78	ASN	CA-C-N	-5.33	105.48	117.20
1	C	35	SER	CA-C-O	5.33	131.28	120.10
2	B	41	PHE	CD1-CE1-CZ	5.32	126.48	120.10
1	C	48	LEU	N-CA-CB	-5.32	99.77	110.40
2	D	68	LEU	CA-C-O	5.32	131.26	120.10
1	A	10	VAL	CA-CB-CG2	5.31	118.87	110.90
1	A	64	ASP	CA-C-N	-5.31	105.51	117.20
2	B	118	PHE	CB-CA-C	5.31	121.03	110.40
2	D	54	VAL	N-CA-CB	-5.31	99.82	111.50
2	D	78	LEU	O-C-N	-5.31	114.20	122.70
1	A	89	HIS	N-CA-C	5.30	125.32	111.00
1	A	89	HIS	ND1-CG-CD2	-5.29	98.59	106.00
1	C	139	LYS	CB-CG-CD	-5.29	97.85	111.60
1	A	71	ALA	N-CA-CB	-5.28	102.71	110.10
1	C	50	HIS	ND1-CE1-NE2	5.28	121.52	109.90
1	A	24	TYR	CB-CA-C	-5.28	99.84	110.40
2	B	124	PRO	N-CA-CB	5.28	109.63	103.30
2	D	83	GLY	CA-C-N	5.28	128.81	117.20
2	D	92	HIS	N-CA-C	-5.28	96.76	111.00
1	A	140	TYR	N-CA-CB	5.27	120.08	110.60
1	A	83	LEU	CA-C-N	5.27	128.79	117.20
2	B	89	SER	CB-CA-C	5.27	120.11	110.10
2	B	77	HIS	CE1-NE2-CD2	5.26	119.75	106.60
2	D	66	LYS	CB-CG-CD	5.26	125.27	111.60
1	A	62	VAL	CA-CB-CG2	-5.26	103.02	110.90
2	B	101	GLU	CA-C-O	5.25	131.13	120.10
2	D	117	HIS	ND1-CE1-NE2	5.25	121.46	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	75	LEU	CA-CB-CG	5.25	127.38	115.30
2	D	117	HIS	CB-CG-CD2	5.25	147.08	130.80
1	C	20	HIS	ND1-CG-CD2	5.25	116.15	108.80
1	A	2	LEU	CA-C-N	-5.25	105.66	117.20
1	A	95	PRO	CA-C-N	5.24	128.74	117.20
1	C	20	HIS	ND1-CE1-NE2	-5.24	98.37	109.90
1	A	90	LYS	CG-CD-CE	-5.24	96.18	111.90
2	D	77	HIS	CB-CG-ND1	-5.24	110.11	123.20
2	D	139	ASN	CB-CG-ND2	-5.24	104.13	116.70
1	A	50	HIS	CA-CB-CG	-5.24	104.70	113.60
2	D	74	GLY	C-N-CA	-5.24	108.61	121.70
1	A	11	LYS	O-C-N	-5.23	114.33	122.70
2	B	20	VAL	C-N-CA	5.23	134.78	121.70
1	C	28	ALA	O-C-N	5.23	131.07	122.70
2	D	41	PHE	CD1-CG-CD2	5.23	125.10	118.30
1	A	141	ARG	CB-CG-CD	-5.23	98.00	111.60
2	D	63	HIS	C-N-CA	-5.23	111.33	122.30
2	D	127	GLN	CB-CA-C	5.23	120.85	110.40
1	A	73	VAL	CG1-CB-CG2	5.22	119.26	110.90
1	C	7	LYS	N-CA-CB	-5.22	101.20	110.60
1	A	72	HIS	CB-CA-C	-5.22	99.96	110.40
2	B	54	VAL	CA-CB-CG1	-5.22	103.07	110.90
1	A	112	HIS	CE1-NE2-CD2	-5.22	93.56	106.60
2	B	122	PHE	CZ-CE2-CD2	-5.22	113.84	120.10
2	D	102	ASN	C-N-CA	5.21	134.73	121.70
1	A	23	GLU	CB-CG-CD	-5.21	100.13	114.20
1	A	24	TYR	CA-C-N	5.21	126.61	116.20
1	A	41	THR	CA-C-N	5.20	128.65	117.20
1	A	71	ALA	C-N-CA	5.20	134.71	121.70
1	C	140	TYR	CD1-CE1-CZ	5.20	124.48	119.80
2	B	45	PHE	CD1-CG-CD2	-5.20	111.54	118.30
2	B	119	GLY	O-C-N	-5.20	114.39	122.70
1	A	82	ALA	O-C-N	-5.19	114.39	122.70
1	C	137	THR	O-C-N	5.19	131.01	122.70
2	B	7	GLU	CA-CB-CG	5.19	124.82	113.40
2	D	91	LEU	CA-C-N	-5.19	105.78	117.20
2	B	85	PHE	CB-CA-C	5.19	120.77	110.40
1	C	75	ASP	CA-C-N	-5.18	105.79	117.20
2	B	22	GLU	N-CA-CB	-5.18	101.27	110.60
1	C	76	MET	CB-CG-SD	-5.18	96.86	112.40
2	B	54	VAL	O-C-N	-5.18	114.42	122.70
2	B	145	TYR	CB-CG-CD1	-5.18	117.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	LYS	CD-CE-NZ	-5.17	99.80	111.70
2	B	17	LYS	N-CA-CB	5.17	119.91	110.60
2	D	143	HIS	CB-CA-C	5.17	120.74	110.40
2	D	90	GLU	N-CA-CB	-5.16	101.31	110.60
2	B	89	SER	CA-CB-OG	-5.16	97.26	111.20
2	D	58	PRO	N-CA-CB	5.16	109.49	103.30
2	B	95	LYS	CA-C-O	5.15	130.91	120.10
1	C	40	LYS	CB-CG-CD	-5.15	98.21	111.60
2	D	100	PRO	N-CA-CB	5.15	109.48	103.30
2	B	75	LEU	CB-CA-C	-5.15	100.42	110.20
2	D	106	LEU	CB-CG-CD2	-5.15	102.25	111.00
1	A	19	ALA	CA-C-N	5.14	128.52	117.20
1	A	101	LEU	CB-CG-CD1	5.14	119.75	111.00
1	C	58	HIS	C-N-CA	-5.14	111.50	122.30
1	C	75	ASP	N-CA-C	-5.14	97.11	111.00
1	A	74	ASP	C-N-CA	5.14	134.54	121.70
1	C	17	VAL	N-CA-CB	5.14	122.80	111.50
1	C	36	PHE	O-C-N	5.14	130.86	121.10
2	B	82	LYS	CG-CD-CE	-5.13	96.50	111.90
1	A	30	GLU	CA-CB-CG	-5.13	102.12	113.40
1	A	39	THR	C-N-CA	-5.13	108.88	121.70
2	B	15	TRP	CZ3-CH2-CZ2	5.13	127.75	121.60
2	B	66	LYS	C-N-CA	-5.13	108.88	121.70
2	B	55	MET	C-N-CA	-5.12	111.54	122.30
1	A	106	LEU	CB-CG-CD2	5.12	119.71	111.00
2	B	26	GLU	C-N-CA	-5.12	108.89	121.70
2	D	44	SER	C-N-CA	5.12	134.51	121.70
2	B	106	LEU	O-C-N	-5.12	114.49	123.20
1	C	65	ALA	CA-C-O	5.12	130.85	120.10
1	A	16	LYS	CA-C-O	5.11	130.83	120.10
1	A	14	TRP	O-C-N	5.11	131.88	123.20
1	C	62	VAL	CA-C-O	5.10	130.82	120.10
2	D	83	GLY	N-CA-C	-5.10	100.34	113.10
1	C	75	ASP	CA-CB-CG	5.10	124.62	113.40
2	D	9	SER	CA-C-O	-5.09	109.40	120.10
2	B	111	VAL	CA-CB-CG1	-5.09	103.26	110.90
2	B	116	HIS	CG-CD2-NE2	5.09	118.88	109.20
2	D	77	HIS	O-C-N	-5.09	114.56	122.70
1	C	117	PHE	CD1-CE1-CZ	-5.09	113.99	120.10
2	D	132	LYS	CG-CD-CE	-5.09	96.64	111.90
2	B	62	ALA	O-C-N	5.09	130.84	122.70
1	A	103	HIS	ND1-CE1-NE2	5.08	121.08	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	VAL	O-C-N	5.08	130.83	122.70
1	C	3	SER	CA-C-O	5.08	130.77	120.10
1	A	47	ASP	CA-C-N	-5.08	106.03	117.20
2	B	93	CYS	N-CA-CB	-5.08	101.46	110.60
2	D	73	ASP	N-CA-CB	5.08	119.74	110.60
2	B	145	TYR	C-N-CA	5.08	134.39	121.70
1	A	58	HIS	CA-C-O	-5.07	109.45	120.10
2	B	35	TYR	CB-CG-CD1	5.07	124.04	121.00
2	B	145	TYR	CA-CB-CG	5.07	123.03	113.40
1	A	25	GLY	CA-C-O	5.07	129.72	120.60
2	B	27	ALA	O-C-N	-5.07	114.59	122.70
1	A	44	PRO	CB-CA-C	-5.07	99.33	112.00
1	A	83	LEU	N-CA-CB	-5.07	100.27	110.40
1	A	92	ARG	C-N-CA	5.06	134.36	121.70
2	D	9	SER	N-CA-CB	-5.06	102.91	110.50
1	A	88	ALA	CA-C-N	-5.06	106.07	117.20
2	B	76	ALA	CA-C-N	-5.06	106.07	117.20
1	A	59	GLY	CA-C-O	5.06	129.70	120.60
1	C	35	SER	O-C-N	-5.05	114.62	122.70
1	A	119	PRO	O-C-N	-5.05	114.63	122.70
2	D	40	ARG	N-CA-C	-5.04	97.38	111.00
2	D	42	PHE	CD1-CG-CD2	5.04	124.86	118.30
1	A	82	ALA	CA-C-O	5.04	130.68	120.10
1	A	136	LEU	CB-CG-CD2	5.04	119.56	111.00
1	A	90	LYS	CB-CG-CD	5.04	124.69	111.60
2	D	30	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	109	LEU	C-N-CA	-5.03	109.12	121.70
2	B	8	LYS	C-N-CA	5.03	134.28	121.70
1	A	14	TRP	CD1-CG-CD2	-5.03	102.28	106.30
2	D	48	LEU	CA-C-N	-5.03	106.14	117.20
1	A	34	LEU	CA-CB-CG	5.03	126.86	115.30
1	C	36	PHE	CA-C-N	-5.03	103.03	117.10
2	D	137	VAL	N-CA-C	5.03	124.57	111.00
1	A	100	LEU	CD1-CG-CD2	-5.02	95.43	110.50
2	B	3	LEU	CD1-CG-CD2	-5.02	95.44	110.50
2	B	103	PHE	CG-CD1-CE1	-5.01	115.28	120.80
2	D	88	LEU	CD1-CG-CD2	5.01	125.54	110.50
2	B	15	TRP	CB-CG-CD2	-5.01	120.08	126.60
2	B	37	TRP	O-C-N	-5.01	114.69	122.70
2	D	123	THR	OG1-CB-CG2	-5.01	98.48	110.00
1	C	26	ALA	O-C-N	-5.01	114.69	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
2	B	12	THR	CB
2	B	50	THR	CB
1	C	78	ASN	CA
1	C	118	THR	CB
2	D	2	HIS	CA
2	D	72	SER	CA
2	D	73	ASP	CA
2	D	78	LEU	CA
2	D	144	LYS	CA

All (206) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Mainchain
1	A	101	LEU	Mainchain
1	A	11	LYS	Mainchain
1	A	111	ALA	Mainchain
1	A	114	PRO	Mainchain
1	A	118	THR	Mainchain
1	A	12	ALA	Mainchain
1	A	122	HIS	Mainchain
1	A	126	ASP	Sidechain
1	A	141	ARG	Sidechain
1	A	15	GLY	Mainchain
1	A	18	GLY	Peptide
1	A	19	ALA	Mainchain
1	A	20	HIS	Sidechain
1	A	21	ALA	Mainchain
1	A	22	GLY	Mainchain
1	A	23	GLU	Sidechain
1	A	24	TYR	Sidechain
1	A	3	SER	Mainchain
1	A	36	PHE	Sidechain
1	A	4	PRO	Mainchain
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	Sidechain,Mainchain
1	A	81	SER	Mainchain
1	A	82	ALA	Mainchain
1	A	83	LEU	Mainchain
1	A	85	ASP	Sidechain,Mainchain
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	Sidechain,Mainchain
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	Sidechain,Mainchain
2	B	49	SER	Peptide,Mainchain
2	B	52	ASP	Sidechain
2	B	56	GLY	Mainchain
2	B	59	LYS	Mainchain
2	B	6	GLU	Sidechain
2	B	60	VAL	Mainchain
2	B	61	LYS	Mainchain
2	B	62	ALA	Mainchain
2	B	63	HIS	Sidechain,Mainchain
2	B	7	GLU	Mainchain
2	B	78	LEU	Mainchain
2	B	79	ASP	Sidechain,Mainchain
2	B	80	ASN	Sidechain,Mainchain
2	B	84	THR	Mainchain
2	B	90	GLU	Sidechain,Mainchain
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	Sidechain,Mainchain
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	Sidechain,Mainchain
1	C	46	PHE	Sidechain,Mainchain
1	C	47	ASP	Sidechain,Mainchain
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	Sidechain,Mainchain
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	Sidechain,Mainchain
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	Sidechain,Mainchain
2	D	21	ASP	Sidechain,Mainchain
2	D	22	GLU	Sidechain,Mainchain
2	D	26	GLU	Sidechain
2	D	3	LEU	Peptide,Mainchain
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	Peptide,Mainchain
2	D	49	SER	Peptide,Mainchain
2	D	5	PRO	Mainchain
2	D	52	ASP	Sidechain,Mainchain
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	Sidechain,Mainchain
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	Sidechain,Mainchain
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	241	0
1	C	1069	0	1063	254	1
2	B	1123	0	1104	324	0
2	D	1123	0	1108	419	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	15	0
3	D	43	0	30	12	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	56	0	0	1	0
5	B	57	0	0	1	2
5	C	59	0	0	0	1
5	D	49	0	0	1	0
All	All	4779	0	4456	1272	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 (1272) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:CA	1:C:118:THR:CB	1.75	1.63
1:C:113:LEU:CD1	1:C:113:LEU:CG	1.75	1.63
2:D:2:HIS:CD2	2:D:2:HIS:CG	1.85	1.63
2:B:50:THR:CG2	2:B:50:THR:CB	1.75	1.63
1:A:40:LYS:CA	1:A:40:LYS:CB	1.75	1.61
2:D:48:LEU:CG	2:D:48:LEU:CD1	1.75	1.61
2:D:67:VAL:CA	2:D:67:VAL:CB	1.76	1.61
1:A:29:LEU:CB	1:A:29:LEU:CA	1.79	1.60
2:D:113:VAL:CG2	2:D:113:VAL:CB	1.74	1.60
2:B:8:LYS:CD	2:B:8:LYS:CG	1.78	1.59
2:B:8:LYS:CB	2:B:8:LYS:CA	1.74	1.59
2:B:9:SER:CB	2:B:9:SER:CA	1.79	1.59
1:C:105:LEU:CD1	1:C:105:LEU:CG	1.79	1.59
1:C:16:LYS:CD	1:C:16:LYS:CG	1.81	1.58
2:D:77:HIS:CB	2:D:77:HIS:CA	1.75	1.58
1:C:48:LEU:CD2	1:C:48:LEU:CG	1.74	1.58
2:D:126:VAL:CB	2:D:126:VAL:CA	1.81	1.58
2:B:7:GLU:CG	2:B:7:GLU:CB	1.77	1.57
2:B:143:HIS:ND1	2:B:143:HIS:CG	1.70	1.57
2:B:104:ARG:CD	2:B:104:ARG:CG	1.76	1.57
1:C:38:THR:CB	1:C:38:THR:CA	1.81	1.57
1:A:5:ALA:CB	1:A:5:ALA:CA	1.77	1.57
1:C:73:VAL:CB	1:C:73:VAL:CA	1.80	1.56
2:B:65:LYS:CB	2:B:65:LYS:CA	1.80	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:C	1:C:70:VAL:CA	1.74	1.56
2:D:78:LEU:CA	2:D:78:LEU:CB	1.79	1.56
2:D:121:GLU:CB	2:D:121:GLU:CA	1.79	1.56
1:A:14:TRP:CA	1:A:14:TRP:CB	1.83	1.56
1:C:54:GLN:CA	1:C:54:GLN:C	1.75	1.55
2:D:18:VAL:CB	2:D:18:VAL:CG2	1.80	1.55
1:A:141:ARG:CB	1:A:141:ARG:CG	1.79	1.55
1:C:84:SER:CB	1:C:84:SER:CA	1.79	1.55
2:D:123:THR:CG2	2:D:123:THR:CB	1.80	1.55
2:D:8:LYS:CA	2:D:8:LYS:CB	1.85	1.55
1:C:70:VAL:CA	1:C:70:VAL:N	1.68	1.55
2:D:52:ASP:CG	2:D:52:ASP:CB	1.75	1.55
2:D:141:LEU:CG	2:D:141:LEU:CD2	1.78	1.55
1:A:72:HIS:CA	1:A:72:HIS:CB	1.78	1.54
2:B:145:TYR:C	2:B:145:TYR:CA	1.75	1.54
1:C:61:LYS:CE	1:C:61:LYS:CD	1.81	1.54
2:B:49:SER:CA	2:B:49:SER:CB	1.83	1.54
2:B:90:GLU:CB	2:B:90:GLU:CA	1.84	1.54
2:D:59:LYS:C	2:D:59:LYS:CA	1.76	1.54
1:A:62:VAL:C	1:A:62:VAL:CA	1.75	1.54
1:C:40:LYS:CE	1:C:40:LYS:NZ	1.69	1.54
2:D:4:THR:CB	2:D:4:THR:CA	1.82	1.54
2:D:8:LYS:CB	2:D:8:LYS:CG	1.79	1.54
2:D:92:HIS:C	2:D:92:HIS:CA	1.76	1.54
2:B:1:VAL:N	2:B:1:VAL:CA	1.68	1.53
1:C:8:THR:CB	1:C:8:THR:CA	1.84	1.53
1:C:99:LYS:CD	1:C:99:LYS:CG	1.82	1.53
1:A:84:SER:CB	1:A:84:SER:CA	1.82	1.53
2:B:3:LEU:CA	2:B:3:LEU:CB	1.77	1.53
2:D:47:ASP:CG	2:D:47:ASP:CB	1.76	1.53
2:B:117:HIS:CE1	2:B:117:HIS:ND1	1.75	1.53
1:A:87:HIS:C	1:A:87:HIS:CA	1.75	1.53
2:B:47:ASP:CA	2:B:47:ASP:C	1.75	1.53
2:B:52:ASP:CG	2:B:52:ASP:CB	1.77	1.53
2:D:22:GLU:CG	2:D:22:GLU:CA	1.85	1.53
2:D:50:THR:N	2:D:50:THR:CA	1.71	1.53
2:D:73:ASP:CA	2:D:73:ASP:CB	1.86	1.53
2:B:47:ASP:CA	2:B:47:ASP:N	1.67	1.52
1:A:90:LYS:CE	1:A:90:LYS:CD	1.84	1.52
2:B:41:PHE:C	2:B:41:PHE:CA	1.77	1.52
2:D:53:ALA:C	2:D:53:ALA:CA	1.76	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:ASP:N	2:D:94:ASP:CA	1.68	1.52
1:A:2:LEU:C	1:A:2:LEU:CA	1.77	1.52
2:B:81:LEU:N	2:B:81:LEU:CA	1.68	1.52
1:C:72:HIS:CB	1:C:72:HIS:CA	1.86	1.52
1:A:56:LYS:CE	1:A:56:LYS:CD	1.84	1.51
2:B:10:ALA:C	2:B:10:ALA:CA	1.78	1.51
2:B:49:SER:CA	2:B:49:SER:N	1.67	1.51
1:A:31:ARG:NE	1:A:31:ARG:CD	1.68	1.51
1:C:137:THR:C	1:C:137:THR:CA	1.74	1.51
2:B:5:PRO:C	2:B:5:PRO:CA	1.78	1.51
2:B:1:VAL:CA	2:B:1:VAL:CB	1.86	1.51
1:A:1:VAL:CB	1:A:1:VAL:CA	1.84	1.51
1:C:61:LYS:C	1:C:61:LYS:CA	1.76	1.51
2:D:8:LYS:CA	2:D:8:LYS:N	1.68	1.51
2:D:10:ALA:C	2:D:10:ALA:CA	1.75	1.51
2:D:48:LEU:CA	2:D:48:LEU:N	1.72	1.51
2:D:12:THR:N	2:D:12:THR:CA	1.68	1.50
1:A:58:HIS:C	1:A:58:HIS:CA	1.76	1.50
1:C:78:ASN:CB	1:C:78:ASN:CG	1.77	1.50
2:D:7:GLU:C	2:D:7:GLU:CA	1.75	1.50
2:D:18:VAL:N	2:D:18:VAL:CA	1.70	1.50
2:B:80:ASN:CA	2:B:80:ASN:N	1.73	1.50
2:B:12:THR:CG2	2:B:12:THR:CA	1.89	1.50
1:C:56:LYS:NZ	1:C:56:LYS:CE	1.72	1.50
2:D:131:GLN:CD	2:D:131:GLN:CG	1.77	1.50
2:B:80:ASN:CG	2:B:80:ASN:CB	1.75	1.50
2:D:7:GLU:CG	2:D:7:GLU:CB	1.88	1.50
2:D:21:ASP:CG	2:D:21:ASP:CB	1.78	1.49
3:B:148:HEM:CBD	3:B:148:HEM:CGD	1.85	1.49
2:D:80:ASN:N	2:D:80:ASN:CA	1.75	1.49
1:A:52:SER:N	1:A:52:SER:CA	1.75	1.49
2:B:6:GLU:C	2:B:6:GLU:CA	1.77	1.49
1:C:16:LYS:CE	1:C:16:LYS:NZ	1.71	1.49
1:C:10:VAL:C	1:C:10:VAL:CA	1.81	1.49
2:D:82:LYS:CD	2:D:82:LYS:CG	1.89	1.49
2:D:45:PHE:C	2:D:46:GLY:CA	1.78	1.48
2:B:77:HIS:CG	2:B:77:HIS:CD2	1.83	1.48
1:C:2:LEU:C	1:C:2:LEU:CA	1.79	1.48
1:C:90:LYS:CE	1:C:90:LYS:CD	1.91	1.48
1:C:131:SER:C	1:C:131:SER:CA	1.76	1.48
1:A:76:MET:CG	1:A:76:MET:SD	2.02	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:HIS:C	2:B:143:HIS:CA	1.76	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:46:GLY:CA	2:D:46:GLY:C	1.82	1.48
2:D:59:LYS:CE	2:D:59:LYS:CD	1.88	1.48
1:A:16:LYS:CD	1:A:16:LYS:CE	1.92	1.48
1:A:61:LYS:CE	1:A:61:LYS:NZ	1.74	1.48
2:B:80:ASN:CA	2:B:80:ASN:C	1.80	1.48
1:C:7:LYS:N	1:C:7:LYS:CA	1.75	1.47
2:B:61:LYS:NZ	2:B:61:LYS:CE	1.75	1.47
1:C:20:HIS:CE1	1:C:20:HIS:ND1	1.79	1.47
2:D:117:HIS:CG	2:D:117:HIS:ND1	1.74	1.47
1:C:75:ASP:N	1:C:75:ASP:CA	1.71	1.47
2:D:12:THR:CA	2:D:12:THR:CB	1.93	1.47
2:D:52:ASP:N	2:D:52:ASP:CA	1.76	1.46
2:B:142:ALA:C	2:B:142:ALA:CA	1.82	1.46
3:B:148:HEM:CBA	3:B:148:HEM:CGA	1.91	1.46
1:C:90:LYS:CD	1:C:90:LYS:CG	1.90	1.46
1:A:74:ASP:CG	1:A:74:ASP:CB	1.80	1.46
2:D:22:GLU:CA	2:D:22:GLU:C	1.83	1.46
1:C:82:ALA:C	1:C:83:LEU:N	1.69	1.46
3:C:142:HEM:CGD	3:C:142:HEM:CBD	1.93	1.46
2:D:79:ASP:C	2:D:79:ASP:CA	1.83	1.46
1:A:137:THR:CB	1:A:137:THR:CA	1.91	1.45
2:D:1:VAL:N	2:D:1:VAL:CA	1.77	1.45
2:B:61:LYS:CD	2:B:61:LYS:CG	1.93	1.45
2:D:108:ASN:CG	2:D:108:ASN:CB	1.83	1.45
1:C:7:LYS:CD	1:C:7:LYS:CG	1.95	1.45
1:C:139:LYS:CE	1:C:139:LYS:CD	1.95	1.45
2:B:74:GLY:C	2:B:75:LEU:N	1.70	1.44
1:C:76:MET:CG	1:C:76:MET:SD	2.05	1.44
2:B:108:ASN:CB	2:B:108:ASN:CG	1.84	1.44
1:A:60:LYS:CE	1:A:60:LYS:CD	1.93	1.44
2:B:82:LYS:CE	2:B:82:LYS:CG	1.93	1.44
2:D:49:SER:C	2:D:49:SER:CA	1.86	1.44
1:A:18:GLY:C	1:A:18:GLY:CA	1.86	1.44
2:B:22:GLU:CD	2:B:22:GLU:CG	1.85	1.44
2:D:43:GLU:CG	2:D:43:GLU:CA	1.95	1.44
1:A:44:PRO:C	1:A:44:PRO:CA	1.83	1.43
2:B:2:HIS:C	2:B:2:HIS:CA	1.84	1.43
2:B:21:ASP:CG	2:B:21:ASP:CB	1.84	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:VAL:C	1:C:1:VAL:CA	1.83	1.43
2:D:19:ASN:ND2	2:D:19:ASN:CG	1.71	1.43
2:D:47:ASP:CB	2:D:47:ASP:CA	1.94	1.43
1:A:11:LYS:CE	1:A:11:LYS:CD	1.96	1.43
1:A:99:LYS:CE	1:A:99:LYS:CD	1.95	1.43
2:B:87:THR:CB	2:B:87:THR:CA	1.95	1.43
1:C:16:LYS:CG	1:C:16:LYS:CB	1.93	1.43
2:D:146:HIS:CG	2:D:146:HIS:ND1	1.85	1.43
1:A:137:THR:CB	1:A:137:THR:OG1	1.66	1.42
2:B:2:HIS:CG	2:B:2:HIS:CD2	2.05	1.42
2:D:58:PRO:CD	2:D:58:PRO:N	1.71	1.42
1:A:127:LYS:CD	1:A:127:LYS:CG	1.97	1.42
1:C:72:HIS:CG	1:C:72:HIS:ND1	1.80	1.42
2:B:65:LYS:CA	2:B:65:LYS:CG	1.98	1.42
1:A:75:ASP:CG	1:A:75:ASP:CA	1.88	1.41
2:B:9:SER:CA	2:B:9:SER:C	1.87	1.41
2:D:77:HIS:CD2	2:D:77:HIS:NE2	1.88	1.41
2:B:66:LYS:CE	2:B:66:LYS:NZ	1.81	1.41
2:D:104:ARG:CD	2:D:104:ARG:NE	1.84	1.41
1:A:138:SER:CA	1:A:138:SER:OG	1.69	1.41
2:B:2:HIS:CG	2:B:2:HIS:ND1	1.88	1.40
1:C:139:LYS:CE	1:C:139:LYS:NZ	1.84	1.40
2:B:139:ASN:CG	2:B:139:ASN:CA	1.87	1.40
1:A:20:HIS:ND1	1:A:20:HIS:CG	1.70	1.40
2:D:5:PRO:N	2:D:5:PRO:CA	1.84	1.39
1:C:114:PRO:C	1:C:114:PRO:CA	1.90	1.39
2:D:2:HIS:ND1	2:D:2:HIS:CE1	1.90	1.39
1:A:75:ASP:CA	1:A:75:ASP:CB	1.97	1.39
1:A:81:SER:CB	1:A:81:SER:CA	2.00	1.39
2:B:49:SER:CB	2:B:49:SER:OG	1.71	1.38
2:B:125:PRO:N	2:B:125:PRO:CD	1.67	1.38
1:A:16:LYS:CD	1:A:16:LYS:CG	2.01	1.38
2:B:146:HIS:CB	2:B:146:HIS:CG	2.05	1.38
3:D:148:HEM:CGD	3:D:148:HEM:CBD	2.01	1.38
2:B:2:HIS:CA	2:B:2:HIS:CB	2.01	1.38
2:B:124:PRO:CD	2:B:124:PRO:N	1.70	1.38
2:D:43:GLU:CG	2:D:43:GLU:CD	1.92	1.38
2:B:144:LYS:CE	2:B:144:LYS:CD	2.01	1.38
1:A:92:ARG:CD	1:A:92:ARG:CZ	2.01	1.38
2:D:26:GLU:CD	2:D:26:GLU:CG	1.90	1.38
2:D:55:MET:C	2:D:55:MET:CA	1.90	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:HIS:CE1	2:D:2:HIS:NE2	1.90	1.37
2:D:143:HIS:CD2	2:D:143:HIS:CG	1.85	1.37
2:B:87:THR:CB	2:B:87:THR:CG2	2.02	1.37
2:D:77:HIS:CE1	2:D:77:HIS:ND1	1.91	1.37
1:C:92:ARG:NH1	1:C:92:ARG:CZ	1.87	1.37
2:D:146:HIS:ND1	2:D:146:HIS:CD2	1.91	1.36
1:C:138:SER:CA	1:C:138:SER:OG	1.73	1.36
2:D:43:GLU:CA	2:D:43:GLU:C	1.94	1.36
1:A:50:HIS:CB	1:A:50:HIS:CA	2.02	1.36
2:B:1:VAL:CB	2:B:1:VAL:CG1	2.03	1.36
2:B:117:HIS:ND1	2:B:117:HIS:CG	1.94	1.35
1:A:127:LYS:CG	1:A:127:LYS:CA	2.02	1.35
1:A:64:ASP:CG	1:A:64:ASP:CB	1.95	1.35
2:D:8:LYS:CD	2:D:8:LYS:CE	2.03	1.35
2:B:104:ARG:CZ	2:B:104:ARG:NH1	1.87	1.34
2:D:90:GLU:OE1	2:D:90:GLU:CD	1.64	1.34
2:B:132:LYS:NZ	2:B:132:LYS:CE	1.88	1.34
2:D:20:VAL:CA	2:D:20:VAL:CG2	2.05	1.34
1:A:17:VAL:C	1:A:17:VAL:CA	1.96	1.34
2:D:80:ASN:CG	2:D:80:ASN:OD1	1.66	1.33
1:A:16:LYS:CE	1:A:16:LYS:CG	2.06	1.33
2:B:59:LYS:CE	2:B:59:LYS:NZ	1.92	1.33
2:B:146:HIS:CE1	2:B:146:HIS:ND1	1.84	1.33
1:C:30:GLU:CD	1:C:30:GLU:CG	1.96	1.33
1:A:56:LYS:CD	1:A:56:LYS:CG	2.06	1.32
1:A:15:GLY:O	1:A:15:GLY:C	1.67	1.32
1:A:61:LYS:CE	1:A:61:LYS:CG	2.06	1.32
1:A:72:HIS:CA	1:A:72:HIS:CG	2.12	1.32
2:D:66:LYS:CD	2:D:66:LYS:CG	2.06	1.32
2:B:6:GLU:OE1	2:B:6:GLU:CD	1.67	1.32
1:C:11:LYS:CE	1:C:11:LYS:NZ	1.91	1.32
1:A:78:ASN:CB	1:A:78:ASN:ND2	1.87	1.31
2:B:79:ASP:CG	2:B:79:ASP:OD2	1.67	1.31
2:B:143:HIS:ND1	2:B:143:HIS:CE1	1.99	1.31
2:D:82:LYS:NZ	2:D:82:LYS:CE	1.94	1.31
2:D:6:GLU:CD	2:D:6:GLU:CG	1.97	1.30
2:D:20:VAL:CA	2:D:20:VAL:CB	2.10	1.30
1:C:40:LYS:CE	1:C:40:LYS:CG	2.07	1.30
2:D:66:LYS:NZ	2:D:66:LYS:CE	1.95	1.29
2:D:139:ASN:CG	2:D:139:ASN:OD1	1.68	1.29
2:D:121:GLU:CD	2:D:121:GLU:CG	2.01	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:142:HEM:CGD	3:A:142:HEM:CBD	2.09	1.29
3:D:148:HEM:CGA	3:D:148:HEM:O2A	1.77	1.29
2:D:50:THR:CA	2:D:50:THR:CB	2.11	1.29
2:D:8:LYS:CE	2:D:8:LYS:NZ	1.94	1.29
2:D:26:GLU:CD	2:D:26:GLU:OE2	1.71	1.29
2:D:76:ALA:N	2:D:76:ALA:CA	1.94	1.29
1:A:30:GLU:CD	1:A:30:GLU:CG	2.00	1.28
1:C:40:LYS:NZ	1:C:40:LYS:CD	1.95	1.28
2:B:1:VAL:O	2:B:1:VAL:C	1.70	1.28
1:A:139:LYS:CE	1:A:139:LYS:NZ	1.96	1.28
1:A:138:SER:CA	1:A:138:SER:CB	2.12	1.28
2:D:43:GLU:C	2:D:43:GLU:HB2	1.53	1.28
2:B:101:GLU:CG	2:B:101:GLU:CD	2.02	1.27
1:C:105:LEU:CG	1:C:105:LEU:CD2	2.12	1.27
1:A:1:VAL:CA	1:A:1:VAL:CG2	2.13	1.27
1:A:23:GLU:OE1	1:A:23:GLU:CD	1.72	1.26
1:C:61:LYS:CE	1:C:61:LYS:NZ	1.98	1.26
2:D:1:VAL:CA	2:D:1:VAL:C	2.02	1.26
1:C:114:PRO:CA	1:C:114:PRO:N	1.72	1.26
1:A:85:ASP:CG	1:A:85:ASP:OD2	1.73	1.26
1:C:1:VAL:CG1	1:C:1:VAL:CG2	2.13	1.26
2:D:17:LYS:CE	2:D:17:LYS:NZ	1.98	1.26
2:B:104:ARG:CZ	2:B:104:ARG:NH2	1.97	1.25
2:D:125:PRO:CD	2:D:125:PRO:N	1.67	1.25
2:B:8:LYS:CG	2:B:8:LYS:CA	2.13	1.25
1:C:138:SER:CA	1:C:138:SER:CB	2.14	1.24
2:D:4:THR:HB	2:D:6:GLU:OE2	1.29	1.24
2:B:144:LYS:CE	2:B:144:LYS:NZ	1.99	1.24
1:C:1:VAL:CG2	1:C:1:VAL:HG13	1.64	1.24
2:D:95:LYS:NZ	2:D:95:LYS:CE	1.99	1.24
2:B:5:PRO:N	2:B:5:PRO:CD	1.81	1.23
2:B:12:THR:CG2	2:B:12:THR:OG1	1.78	1.23
2:D:101:GLU:CD	2:D:101:GLU:CG	2.07	1.23
2:B:22:GLU:CD	2:B:22:GLU:OE1	1.77	1.22
1:A:14:TRP:CA	1:A:14:TRP:CG	2.22	1.22
2:D:95:LYS:CD	2:D:95:LYS:CG	2.16	1.22
2:B:90:GLU:CD	2:B:90:GLU:CG	2.07	1.22
1:C:46:PHE:CE2	1:C:46:PHE:CG	2.02	1.22
2:D:3:LEU:O	2:D:3:LEU:C	1.77	1.22
1:A:21:ALA:C	1:A:21:ALA:CA	2.09	1.21
1:C:60:LYS:NZ	1:C:60:LYS:CE	2.02	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:VAL:CA	2:B:1:VAL:C	2.09	1.21
2:B:6:GLU:CD	2:B:6:GLU:CG	2.07	1.21
2:B:121:GLU:CD	2:B:121:GLU:CG	2.07	1.21
1:C:112:HIS:CG	1:C:112:HIS:ND1	1.78	1.21
2:B:2:HIS:CD2	2:B:2:HIS:NE2	2.09	1.21
1:C:1:VAL:CA	1:C:1:VAL:CG1	2.18	1.21
2:D:26:GLU:CG	2:D:26:GLU:CB	2.18	1.21
1:C:99:LYS:CG	1:C:99:LYS:CA	2.17	1.20
1:A:23:GLU:CD	1:A:23:GLU:CG	2.10	1.20
2:B:47:ASP:CG	2:B:47:ASP:OD2	1.78	1.19
2:D:58:PRO:CD	2:D:58:PRO:CB	2.20	1.19
1:A:92:ARG:CD	1:A:92:ARG:NH1	2.03	1.19
2:B:49:SER:C	2:B:49:SER:O	1.79	1.19
2:D:26:GLU:CD	2:D:26:GLU:OE1	1.79	1.19
1:C:90:LYS:CE	1:C:90:LYS:NZ	2.06	1.18
1:C:113:LEU:CD1	1:C:113:LEU:CB	2.22	1.18
2:D:65:LYS:CE	2:D:65:LYS:CD	2.20	1.18
1:A:78:ASN:CG	1:A:78:ASN:CA	2.11	1.17
1:C:92:ARG:HH21	1:C:92:ARG:NE	1.42	1.17
2:D:43:GLU:CD	2:D:43:GLU:CB	2.13	1.17
1:C:16:LYS:CD	1:C:16:LYS:CE	2.23	1.17
2:D:2:HIS:CB	2:D:2:HIS:CA	2.21	1.17
1:A:127:LYS:CD	1:A:127:LYS:CB	2.23	1.16
1:C:1:VAL:CG1	1:C:1:VAL:CB	2.22	1.16
1:A:75:ASP:CG	1:A:75:ASP:OD1	1.82	1.16
2:B:104:ARG:CD	2:B:104:ARG:CZ	2.24	1.15
2:B:108:ASN:CB	2:B:108:ASN:ND2	2.10	1.15
2:D:73:ASP:CA	2:D:73:ASP:CG	2.14	1.15
1:A:1:VAL:HG23	1:A:1:VAL:N	1.61	1.15
2:B:26:GLU:HG2	2:B:26:GLU:OE2	1.46	1.15
1:C:23:GLU:CG	1:C:23:GLU:CD	2.15	1.15
2:D:77:HIS:NE2	2:D:77:HIS:CG	2.15	1.15
2:B:58:PRO:CD	2:B:58:PRO:N	1.78	1.14
1:A:1:VAL:CG2	1:A:1:VAL:N	2.09	1.14
2:B:26:GLU:OE2	2:B:26:GLU:CG	1.95	1.14
2:B:49:SER:CB	2:B:49:SER:C	2.15	1.14
1:C:73:VAL:CA	1:C:73:VAL:CG1	2.26	1.14
1:A:72:HIS:CG	1:A:72:HIS:ND1	1.85	1.14
2:D:47:ASP:CA	2:D:47:ASP:N	2.09	1.13
1:C:56:LYS:CD	1:C:56:LYS:CG	2.27	1.13
1:C:99:LYS:CD	1:C:99:LYS:CE	2.26	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:LYS:CD	2:D:82:LYS:NZ	2.12	1.13
2:D:66:LYS:CD	2:D:66:LYS:CE	2.27	1.12
1:A:92:ARG:NH1	1:A:92:ARG:HD3	1.60	1.12
2:D:49:SER:C	2:D:50:THR:CA	2.17	1.12
2:B:104:ARG:CZ	2:B:104:ARG:NE	2.13	1.12
2:B:139:ASN:CG	2:B:139:ASN:ND2	2.01	1.12
2:B:121:GLU:CD	2:B:121:GLU:OE1	1.87	1.12
2:D:65:LYS:CD	2:D:65:LYS:CG	2.27	1.11
3:C:142:HEM:CGA	3:C:142:HEM:O2A	0.82	1.11
2:B:2:HIS:ND1	2:B:2:HIS:CE1	2.18	1.11
2:D:8:LYS:CA	2:D:8:LYS:CG	2.29	1.11
2:D:6:GLU:CG	2:D:6:GLU:CA	2.28	1.10
3:C:142:HEM:CGA	3:C:142:HEM:CBA	2.29	1.10
2:D:22:GLU:CA	2:D:22:GLU:HG3	1.61	1.10
2:D:4:THR:CB	2:D:6:GLU:OE2	2.00	1.10
2:D:78:LEU:CD2	2:D:78:LEU:CD1	2.30	1.09
2:D:46:GLY:C	2:D:47:ASP:CA	2.20	1.09
2:D:43:GLU:CD	2:D:43:GLU:HB3	1.71	1.09
1:A:90:LYS:CE	1:A:90:LYS:CG	2.29	1.08
2:D:144:LYS:CE	2:D:144:LYS:NZ	2.16	1.08
1:A:78:ASN:CG	1:A:78:ASN:HB2	1.50	1.08
2:B:117:HIS:NE2	2:B:117:HIS:CD2	2.21	1.08
1:A:75:ASP:HB3	1:A:75:ASP:OD2	1.54	1.08
1:A:92:ARG:CD	1:A:92:ARG:HH11	1.65	1.07
1:C:1:VAL:CG1	1:C:1:VAL:HG22	1.77	1.07
2:D:5:PRO:CA	2:D:5:PRO:CB	2.31	1.07
1:A:16:LYS:CG	1:A:16:LYS:HE2	1.82	1.07
3:A:142:HEM:CGA	3:A:142:HEM:CBA	2.32	1.07
1:C:16:LYS:CD	1:C:16:LYS:CB	2.33	1.07
2:D:76:ALA:N	2:D:76:ALA:CB	2.17	1.07
2:D:6:GLU:CG	2:D:6:GLU:HB3	1.55	1.07
2:D:8:LYS:CB	2:D:8:LYS:CD	2.33	1.06
1:A:75:ASP:CB	1:A:75:ASP:OD2	2.02	1.06
1:C:116:GLU:CG	1:C:116:GLU:CB	2.33	1.06
2:D:6:GLU:CG	2:D:6:GLU:HB2	1.55	1.06
2:D:10:ALA:C	2:D:10:ALA:CB	2.23	1.05
2:D:43:GLU:C	2:D:43:GLU:CB	2.23	1.05
1:A:78:ASN:CG	1:A:78:ASN:HB3	1.50	1.05
2:D:26:GLU:CG	2:D:26:GLU:OE1	2.05	1.05
1:C:84:SER:CA	1:C:84:SER:OG	2.04	1.05
2:D:78:LEU:CB	2:D:78:LEU:CD2	2.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:CE	1:A:99:LYS:NZ	2.20	1.05
2:B:65:LYS:CD	2:B:65:LYS:CE	2.35	1.04
1:C:40:LYS:CD	1:C:40:LYS:HE3	1.53	1.04
1:A:16:LYS:HE2	1:A:16:LYS:HG3	1.38	1.04
2:D:141:LEU:CD2	2:D:141:LEU:CD1	2.34	1.04
2:D:6:GLU:CB	2:D:6:GLU:HG2	1.51	1.03
2:B:48:LEU:C	2:B:49:SER:CA	2.27	1.03
2:B:59:LYS:CE	2:B:59:LYS:CD	2.36	1.03
2:B:66:LYS:CE	2:B:66:LYS:CD	2.37	1.02
2:B:81:LEU:N	2:B:81:LEU:CB	2.22	1.02
1:C:1:VAL:CB	1:C:1:VAL:N	2.22	1.02
2:B:139:ASN:ND2	2:B:139:ASN:OD1	1.91	1.02
1:C:99:LYS:CD	1:C:99:LYS:CB	2.36	1.02
2:B:8:LYS:CG	2:B:8:LYS:HB2	1.52	1.02
1:C:40:LYS:CD	1:C:40:LYS:HE2	1.53	1.02
1:C:38:THR:H	1:C:38:THR:HG22	1.23	1.01
1:C:92:ARG:HH21	1:C:92:ARG:CD	1.72	1.01
1:C:40:LYS:CE	1:C:40:LYS:HD2	1.50	1.01
2:D:58:PRO:CD	2:D:58:PRO:CA	2.37	1.01
2:D:79:ASP:CG	2:D:79:ASP:OD2	1.98	1.01
1:A:75:ASP:CG	1:A:75:ASP:HB2	1.42	1.01
2:B:1:VAL:CA	2:B:2:HIS:N	2.23	1.01
2:D:4:THR:C	2:D:5:PRO:CA	2.27	1.01
2:D:6:GLU:CB	2:D:6:GLU:HG3	1.51	1.01
3:D:148:HEM:CGA	3:D:148:HEM:CBA	2.39	1.01
2:B:101:GLU:CG	2:B:101:GLU:OE2	2.09	1.00
2:B:46:GLY:C	2:B:47:ASP:CA	2.29	1.00
1:C:90:LYS:CD	1:C:90:LYS:CB	2.39	1.00
2:D:79:ASP:CG	2:D:79:ASP:OD1	1.99	1.00
1:A:92:ARG:CZ	1:A:92:ARG:NH2	0.85	1.00
2:D:78:LEU:CG	2:D:78:LEU:HD21	1.51	1.00
2:B:8:LYS:CG	2:B:8:LYS:HB3	1.52	1.00
1:C:56:LYS:CE	1:C:56:LYS:CD	2.39	1.00
2:D:6:GLU:CA	2:D:6:GLU:C	2.31	1.00
2:D:53:ALA:C	2:D:53:ALA:CB	2.30	1.00
1:C:30:GLU:CD	1:C:30:GLU:OE2	0.80	1.00
2:D:18:VAL:CG2	2:D:18:VAL:CG1	2.40	1.00
2:D:77:HIS:CB	2:D:77:HIS:C	2.29	1.00
1:A:75:ASP:CG	1:A:75:ASP:HB3	1.43	0.99
1:C:40:LYS:CE	1:C:40:LYS:HD3	1.50	0.99
2:D:1:VAL:CA	2:D:2:HIS:N	2.23	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ASP:CB	2:D:47:ASP:N	2.25	0.99
2:D:47:ASP:C	2:D:48:LEU:CA	2.30	0.99
2:D:12:THR:CA	2:D:12:THR:CG2	2.39	0.99
1:A:74:ASP:CG	1:A:74:ASP:OD1	0.80	0.99
2:D:104:ARG:CD	2:D:104:ARG:HH11	1.76	0.99
2:B:90:GLU:CA	2:B:90:GLU:CG	2.41	0.98
2:D:20:VAL:CA	2:D:20:VAL:HG22	1.92	0.98
2:D:82:LYS:CD	2:D:82:LYS:CE	2.41	0.98
2:D:146:HIS:ND1	2:D:146:HIS:NE2	2.10	0.98
1:A:2:LEU:CA	1:A:3:SER:N	2.27	0.98
2:B:139:ASN:CG	2:B:139:ASN:HB3	1.37	0.98
2:D:79:ASP:C	2:D:79:ASP:CB	2.31	0.98
2:D:43:GLU:CB	2:D:43:GLU:HG3	1.47	0.97
1:A:78:ASN:CB	1:A:78:ASN:CG	0.88	0.97
2:B:8:LYS:NZ	2:B:8:LYS:CE	2.27	0.97
2:B:132:LYS:NZ	2:B:132:LYS:CD	2.26	0.97
2:D:45:PHE:CA	2:D:46:GLY:N	2.27	0.97
2:D:52:ASP:CB	2:D:52:ASP:N	2.28	0.97
1:C:139:LYS:CD	1:C:139:LYS:NZ	2.27	0.97
2:D:43:GLU:CB	2:D:43:GLU:HG2	1.47	0.97
1:A:92:ARG:NH1	1:A:92:ARG:HD2	1.75	0.97
2:B:49:SER:N	2:B:49:SER:C	2.18	0.97
1:A:92:ARG:CZ	1:A:92:ARG:HD2	1.94	0.96
3:C:142:HEM:O2A	3:C:142:HEM:CBA	2.14	0.96
3:B:148:HEM:CGA	3:B:148:HEM:O2A	0.66	0.96
1:A:75:ASP:CG	1:A:75:ASP:OD2	2.04	0.95
2:B:2:HIS:CA	2:B:3:LEU:N	2.28	0.95
1:A:127:LYS:CG	1:A:127:LYS:CE	2.44	0.95
2:D:45:PHE:C	2:D:46:GLY:HA3	1.85	0.95
2:D:78:LEU:HG	2:D:78:LEU:HD22	0.96	0.95
1:A:61:LYS:CE	1:A:61:LYS:HD2	1.44	0.95
1:C:38:THR:CA	1:C:38:THR:CG2	2.44	0.95
2:D:20:VAL:CA	2:D:20:VAL:HG23	1.91	0.95
2:D:20:VAL:CA	2:D:20:VAL:CG1	2.45	0.95
1:A:85:ASP:CG	1:A:85:ASP:OD1	0.75	0.95
1:C:61:LYS:CD	1:C:61:LYS:NZ	2.29	0.95
1:A:1:VAL:HG23	1:A:1:VAL:H3	1.12	0.95
1:C:7:LYS:CG	1:C:7:LYS:CE	2.45	0.95
2:B:9:SER:CA	2:B:9:SER:OG	2.13	0.95
2:D:79:ASP:C	2:D:80:ASN:CA	2.35	0.94
1:A:17:VAL:C	1:A:17:VAL:O	0.75	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:VAL:N	1:C:1:VAL:HB	1.81	0.94
1:A:61:LYS:CE	1:A:61:LYS:HD3	1.44	0.94
2:D:120:LYS:NZ	2:D:120:LYS:CE	2.29	0.94
2:B:139:ASN:CG	2:B:139:ASN:HB2	1.37	0.94
3:B:148:HEM:CBA	3:B:148:HEM:O2A	2.15	0.94
1:A:138:SER:CA	1:A:138:SER:HG	1.76	0.94
2:B:8:LYS:CB	2:B:8:LYS:HG2	1.44	0.94
2:D:22:GLU:CG	2:D:22:GLU:HB2	1.43	0.94
2:B:8:LYS:CB	2:B:8:LYS:HG3	1.44	0.93
2:D:121:GLU:CA	2:D:121:GLU:CG	2.45	0.93
1:A:85:ASP:OD1	1:A:85:ASP:CB	2.15	0.93
1:C:1:VAL:HG13	1:C:1:VAL:HG22	0.95	0.93
2:D:6:GLU:CG	2:D:6:GLU:CB	0.94	0.93
1:A:78:ASN:CG	1:A:78:ASN:OD1	2.07	0.93
2:D:141:LEU:CD2	2:D:141:LEU:CB	2.45	0.93
2:D:22:GLU:CG	2:D:22:GLU:HB3	1.43	0.93
2:D:78:LEU:CG	2:D:78:LEU:HD22	1.51	0.93
1:A:90:LYS:CE	1:A:90:LYS:HG3	1.98	0.93
2:D:92:HIS:C	2:D:92:HIS:CB	2.37	0.92
2:D:126:VAL:CA	2:D:126:VAL:CG2	2.46	0.92
3:D:148:HEM:CBA	3:D:148:HEM:O1A	2.18	0.92
2:D:73:ASP:CB	2:D:73:ASP:C	2.38	0.92
1:A:61:LYS:CD	1:A:61:LYS:HE2	1.42	0.92
2:B:82:LYS:CE	2:B:82:LYS:HD3	1.40	0.92
2:B:104:ARG:CZ	2:B:104:ARG:HD3	1.98	0.92
2:D:45:PHE:C	2:D:46:GLY:N	0.87	0.92
2:D:79:ASP:CA	2:D:80:ASN:N	2.33	0.92
1:A:137:THR:CA	1:A:137:THR:CG2	2.45	0.92
1:A:62:VAL:CA	1:A:63:ALA:N	2.33	0.92
1:C:1:VAL:CG2	1:C:1:VAL:CB	2.48	0.92
2:D:52:ASP:CB	2:D:52:ASP:OD1	2.17	0.92
2:D:126:VAL:CA	2:D:126:VAL:CG1	2.48	0.91
1:C:46:PHE:CE2	1:C:46:PHE:CD2	0.92	0.91
1:A:61:LYS:CD	1:A:61:LYS:HE3	1.42	0.91
2:B:80:ASN:CB	2:B:80:ASN:ND2	2.33	0.91
2:D:108:ASN:CB	2:D:108:ASN:ND2	2.33	0.91
2:B:65:LYS:CA	2:B:65:LYS:HG2	2.01	0.91
2:B:87:THR:CG2	2:B:87:THR:OG1	2.16	0.91
1:C:1:VAL:C	1:C:1:VAL:CB	2.38	0.91
2:D:67:VAL:CA	2:D:67:VAL:CG1	2.47	0.91
2:B:2:HIS:C	2:B:2:HIS:CB	2.39	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:GLU:C	2:D:8:LYS:CA	2.37	0.91
2:D:22:GLU:CG	2:D:22:GLU:CD	2.39	0.91
2:D:22:GLU:HG3	2:D:22:GLU:CB	1.39	0.91
2:D:65:LYS:CD	2:D:65:LYS:CB	2.48	0.91
2:B:2:HIS:CD2	2:B:2:HIS:CB	2.53	0.91
2:B:65:LYS:CA	2:B:65:LYS:HG3	2.01	0.91
2:B:82:LYS:CD	2:B:82:LYS:HE3	1.39	0.91
2:D:77:HIS:CE1	2:D:77:HIS:CG	2.52	0.91
1:A:127:LYS:CB	1:A:127:LYS:HG3	1.40	0.90
2:B:82:LYS:CD	2:B:82:LYS:HE2	1.39	0.90
2:B:82:LYS:CG	2:B:82:LYS:HE2	1.74	0.90
2:B:82:LYS:CE	2:B:82:LYS:NZ	2.35	0.90
1:C:1:VAL:CA	1:C:1:VAL:N	2.33	0.90
2:B:82:LYS:CE	2:B:82:LYS:HD2	1.40	0.90
1:A:137:THR:OG1	1:A:137:THR:CG2	2.14	0.90
2:B:139:ASN:OD1	2:B:139:ASN:CB	2.20	0.90
2:D:139:ASN:OD1	2:D:139:ASN:CB	2.19	0.90
2:B:8:LYS:CD	2:B:8:LYS:CB	2.49	0.90
2:B:65:LYS:CG	2:B:65:LYS:CD	2.49	0.90
2:D:3:LEU:O	2:D:4:THR:N	2.03	0.90
1:A:61:LYS:NZ	1:A:61:LYS:CD	2.34	0.89
1:C:30:GLU:CG	1:C:30:GLU:OE2	2.20	0.89
2:D:26:GLU:CG	2:D:26:GLU:OE2	2.20	0.89
1:A:127:LYS:CB	1:A:127:LYS:HG2	1.40	0.89
2:B:80:ASN:C	2:B:81:LEU:CA	2.40	0.89
1:A:56:LYS:CD	1:A:56:LYS:CB	2.50	0.89
1:C:84:SER:CB	1:C:84:SER:C	2.39	0.89
2:D:104:ARG:HH11	2:D:104:ARG:HD2	1.37	0.89
2:D:76:ALA:N	2:D:76:ALA:C	2.26	0.89
1:A:127:LYS:CG	1:A:127:LYS:HB2	1.37	0.89
2:D:22:GLU:CB	2:D:22:GLU:HG2	1.39	0.89
2:D:66:LYS:NZ	3:D:148:HEM:O1A	2.06	0.89
1:A:1:VAL:CA	1:A:1:VAL:CG1	2.51	0.89
1:C:72:HIS:CA	1:C:72:HIS:CG	2.54	0.88
2:B:12:THR:C	2:B:12:THR:HG23	1.93	0.88
2:D:78:LEU:CD2	2:D:78:LEU:CG	0.88	0.88
2:D:80:ASN:N	2:D:80:ASN:HB3	1.89	0.88
2:B:2:HIS:CG	2:B:2:HIS:CB	0.83	0.88
1:C:1:VAL:CA	1:C:1:VAL:CG2	2.51	0.88
2:B:8:LYS:CA	2:B:8:LYS:HG3	2.02	0.88
1:C:16:LYS:CD	1:C:16:LYS:HB3	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:GLU:CD	2:B:22:GLU:OE2	2.12	0.88
1:A:127:LYS:CG	1:A:127:LYS:HB3	1.37	0.88
2:B:2:HIS:CG	2:B:2:HIS:HB3	1.42	0.88
2:B:2:HIS:CG	2:B:2:HIS:HB2	1.42	0.88
1:C:70:VAL:CA	1:C:71:ALA:N	2.36	0.88
1:C:99:LYS:CB	1:C:99:LYS:HG3	1.36	0.87
2:D:67:VAL:CB	2:D:67:VAL:N	2.36	0.87
2:B:47:ASP:C	2:B:47:ASP:CB	2.41	0.87
1:C:72:HIS:CB	1:C:72:HIS:C	2.41	0.87
2:B:43:GLU:CD	2:B:43:GLU:CG	2.43	0.87
1:C:38:THR:H	1:C:38:THR:CG2	1.88	0.87
1:C:99:LYS:CG	1:C:99:LYS:HB3	1.36	0.87
2:D:90:GLU:CD	2:D:90:GLU:CG	2.43	0.87
2:B:8:LYS:CG	2:B:8:LYS:CB	0.87	0.87
2:B:10:ALA:C	2:B:10:ALA:CB	2.41	0.87
2:D:47:ASP:CA	2:D:47:ASP:C	2.43	0.87
2:D:94:ASP:N	2:D:94:ASP:CB	2.38	0.87
1:A:51:GLY:C	1:A:52:SER:CA	2.43	0.86
1:A:72:HIS:CB	1:A:72:HIS:C	2.42	0.86
2:D:146:HIS:ND1	2:D:146:HIS:CE1	0.67	0.86
1:A:141:ARG:CG	1:A:141:ARG:CA	2.53	0.86
2:B:117:HIS:ND1	2:B:117:HIS:CB	2.37	0.86
3:C:142:HEM:O2A	3:C:142:HEM:O1A	1.92	0.86
1:C:99:LYS:CB	1:C:99:LYS:HG2	1.36	0.86
1:C:99:LYS:CG	1:C:99:LYS:HB2	1.36	0.86
1:A:17:VAL:CA	1:A:18:GLY:N	2.38	0.85
1:A:50:HIS:CB	1:A:50:HIS:N	2.37	0.85
2:B:12:THR:CG2	2:B:12:THR:C	2.45	0.85
1:C:38:THR:HG22	1:C:38:THR:N	1.91	0.85
2:D:49:SER:C	2:D:49:SER:CB	2.44	0.85
1:C:40:LYS:CE	1:C:40:LYS:CD	0.85	0.85
1:A:58:HIS:CA	1:A:59:GLY:N	2.39	0.85
2:B:108:ASN:CB	2:B:108:ASN:HD22	1.88	0.85
1:C:38:THR:CG2	1:C:38:THR:N	2.39	0.85
1:C:46:PHE:CE2	1:C:46:PHE:HD2	1.59	0.85
2:B:5:PRO:CA	2:B:6:GLU:N	2.40	0.85
2:B:47:ASP:N	2:B:47:ASP:CB	2.39	0.84
1:C:56:LYS:CE	1:C:56:LYS:CG	2.55	0.84
1:A:31:ARG:CD	1:A:31:ARG:CZ	2.54	0.84
2:D:59:LYS:CA	2:D:60:VAL:N	2.40	0.84
1:A:44:PRO:C	1:A:44:PRO:CB	2.46	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:CB	1:C:118:THR:N	2.40	0.84
1:C:8:THR:CA	1:C:8:THR:CG2	2.55	0.84
1:C:40:LYS:NZ	1:C:40:LYS:HD3	1.92	0.84
2:D:7:GLU:CB	2:D:7:GLU:CD	2.45	0.84
2:D:20:VAL:CG2	2:D:20:VAL:C	2.45	0.84
1:A:127:LYS:CD	1:A:127:LYS:HB2	2.06	0.84
1:A:141:ARG:CB	1:A:141:ARG:CD	2.55	0.84
2:B:49:SER:CA	2:B:49:SER:O	2.26	0.84
3:B:148:HEM:CBA	3:B:148:HEM:O1A	2.24	0.84
1:C:60:LYS:NZ	1:C:60:LYS:CD	2.41	0.84
2:D:93:CYS:C	2:D:94:ASP:CA	2.45	0.84
1:A:75:ASP:CB	1:A:75:ASP:C	2.45	0.83
1:A:99:LYS:CE	1:A:99:LYS:CG	2.52	0.83
1:C:139:LYS:CE	1:C:139:LYS:CG	2.56	0.83
2:D:19:ASN:ND2	2:D:19:ASN:OD1	2.10	0.83
2:D:77:HIS:CA	2:D:77:HIS:CG	2.61	0.83
1:A:137:THR:CA	1:A:137:THR:OG1	2.25	0.83
2:B:61:LYS:NZ	2:B:61:LYS:CD	2.42	0.83
2:D:78:LEU:HG	2:D:78:LEU:HD23	0.83	0.83
1:A:92:ARG:CZ	1:A:92:ARG:HD3	1.96	0.82
2:B:5:PRO:C	2:B:5:PRO:N	2.31	0.82
2:B:8:LYS:CA	2:B:8:LYS:HG2	2.08	0.82
2:D:78:LEU:CD2	2:D:78:LEU:HG	0.56	0.82
1:A:92:ARG:HD3	1:A:92:ARG:HH11	1.20	0.82
2:B:143:HIS:ND1	2:B:143:HIS:CB	2.43	0.82
2:D:48:LEU:N	2:D:48:LEU:CB	2.42	0.82
2:B:65:LYS:CB	2:B:65:LYS:HG2	1.32	0.82
2:B:65:LYS:CB	2:B:65:LYS:HG3	1.32	0.82
1:C:105:LEU:CD2	1:C:105:LEU:CB	2.56	0.82
2:B:47:ASP:CA	2:B:48:LEU:N	2.41	0.82
2:D:146:HIS:ND1	2:D:146:HIS:HE1	1.35	0.82
2:D:80:ASN:N	2:D:80:ASN:CB	2.40	0.82
1:C:48:LEU:CD2	1:C:48:LEU:CD1	2.57	0.81
2:D:2:HIS:CG	2:D:2:HIS:ND1	2.48	0.81
1:A:61:LYS:CE	1:A:61:LYS:CD	0.81	0.81
1:A:92:ARG:CZ	1:A:92:ARG:HH22	1.48	0.81
2:B:65:LYS:CG	2:B:65:LYS:HB2	1.31	0.81
2:D:113:VAL:CG2	2:D:113:VAL:CG1	2.58	0.81
1:A:21:ALA:CA	1:A:22:GLY:N	2.43	0.81
2:B:3:LEU:CB	2:B:3:LEU:N	2.42	0.81
2:B:65:LYS:CG	2:B:65:LYS:CE	2.58	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:CD1	1:C:105:LEU:CB	2.58	0.81
2:D:45:PHE:O	2:D:46:GLY:N	2.14	0.81
1:A:5:ALA:CB	1:A:5:ALA:N	2.43	0.81
1:A:92:ARG:CZ	1:A:92:ARG:HH21	1.48	0.81
1:C:76:MET:SD	1:C:76:MET:CB	2.68	0.81
2:D:4:THR:CA	2:D:4:THR:CG2	2.54	0.81
2:B:121:GLU:CG	2:B:121:GLU:OE2	2.27	0.81
1:A:60:LYS:CE	1:A:60:LYS:CG	2.57	0.81
2:D:18:VAL:CG2	2:D:18:VAL:CA	2.58	0.81
1:A:72:HIS:CG	1:A:72:HIS:N	2.48	0.81
2:B:2:HIS:ND1	2:B:2:HIS:CB	2.44	0.81
1:C:23:GLU:OE2	1:C:23:GLU:CB	2.29	0.81
2:D:48:LEU:CD1	2:D:48:LEU:CB	2.58	0.81
1:C:23:GLU:CG	1:C:23:GLU:OE2	2.28	0.80
2:D:8:LYS:CG	2:D:8:LYS:CE	2.59	0.80
2:D:49:SER:O	2:D:50:THR:HA	1.81	0.80
2:D:55:MET:CA	2:D:56:GLY:N	2.43	0.80
1:A:84:SER:CA	1:A:84:SER:OG	2.28	0.80
2:B:65:LYS:CG	2:B:65:LYS:HB3	1.31	0.80
1:C:105:LEU:CD1	1:C:105:LEU:CD2	2.58	0.80
2:D:43:GLU:CG	2:D:43:GLU:HB2	1.29	0.80
2:D:20:VAL:HG23	2:D:20:VAL:C	2.01	0.80
2:B:7:GLU:CG	2:B:7:GLU:CA	2.47	0.80
1:C:92:ARG:NE	1:C:92:ARG:NH2	2.27	0.80
2:B:65:LYS:CB	2:B:65:LYS:CD	2.59	0.80
1:A:76:MET:SD	1:A:76:MET:CB	2.66	0.80
2:B:12:THR:HG23	2:B:12:THR:CB	1.28	0.80
2:B:65:LYS:HG3	2:B:65:LYS:C	2.03	0.79
1:A:1:VAL:CA	1:A:1:VAL:HG22	2.12	0.79
2:B:12:THR:CB	2:B:12:THR:HG22	1.28	0.79
1:A:50:HIS:CB	1:A:50:HIS:C	2.50	0.79
2:B:59:LYS:CE	2:B:59:LYS:CG	2.61	0.79
1:C:73:VAL:CA	1:C:73:VAL:CG2	2.59	0.79
3:A:142:HEM:CBA	3:A:142:HEM:O1A	2.31	0.79
1:C:74:ASP:C	1:C:75:ASP:CA	2.51	0.79
1:A:81:SER:CB	1:A:81:SER:N	2.45	0.79
2:D:17:LYS:NZ	2:D:17:LYS:CD	2.46	0.79
1:A:74:ASP:OD1	1:A:74:ASP:OD2	2.00	0.79
2:D:43:GLU:CG	2:D:43:GLU:HB3	1.29	0.79
1:C:61:LYS:CE	1:C:61:LYS:CG	2.59	0.79
2:D:50:THR:CB	2:D:50:THR:C	2.51	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ALA:C	1:C:70:VAL:CA	2.50	0.79
2:D:82:LYS:CD	2:D:82:LYS:HZ2	1.97	0.78
2:B:146:HIS:CB	2:B:146:HIS:CD2	2.66	0.78
2:D:11:VAL:C	2:D:12:THR:CA	2.52	0.78
2:D:49:SER:O	2:D:50:THR:CA	2.31	0.78
1:C:1:VAL:CG2	1:C:1:VAL:HA	2.12	0.78
2:B:2:HIS:CA	2:B:2:HIS:CG	2.65	0.78
2:B:82:LYS:HE2	2:B:82:LYS:CB	2.14	0.78
2:B:80:ASN:CA	2:B:80:ASN:O	2.31	0.78
1:A:75:ASP:CG	1:A:75:ASP:CB	0.68	0.77
2:B:2:HIS:CD2	2:B:2:HIS:CE1	2.72	0.77
2:D:43:GLU:CG	2:D:43:GLU:CB	0.78	0.77
2:B:121:GLU:CD	2:B:121:GLU:CB	2.52	0.77
2:B:139:ASN:ND2	2:B:139:ASN:CB	2.47	0.77
1:C:46:PHE:CD2	1:C:46:PHE:HE2	1.48	0.77
2:D:82:LYS:NZ	2:D:82:LYS:HD2	1.98	0.77
2:B:117:HIS:CG	2:B:117:HIS:NE2	2.52	0.77
1:C:90:LYS:CE	1:C:90:LYS:CG	2.63	0.77
1:A:40:LYS:CB	1:A:40:LYS:C	2.53	0.77
2:D:7:GLU:CA	2:D:7:GLU:CG	2.63	0.76
2:B:41:PHE:CA	2:B:42:PHE:N	2.46	0.76
2:B:87:THR:CB	2:B:87:THR:C	2.52	0.76
2:B:41:PHE:CA	2:B:41:PHE:O	2.31	0.76
2:B:87:THR:CA	2:B:87:THR:OG1	2.32	0.76
1:C:70:VAL:CA	1:C:70:VAL:O	2.32	0.76
1:C:118:THR:CB	1:C:118:THR:C	2.52	0.76
2:D:6:GLU:OE2	2:D:6:GLU:OE1	2.02	0.76
1:C:131:SER:CA	1:C:131:SER:O	2.34	0.76
1:A:40:LYS:CA	1:A:40:LYS:CG	2.61	0.76
3:A:142:HEM:CBA	3:A:142:HEM:O2A	2.33	0.76
2:D:46:GLY:CA	2:D:46:GLY:O	2.33	0.76
2:D:47:ASP:CB	2:D:47:ASP:OD1	2.34	0.76
2:B:146:HIS:CB	2:B:146:HIS:ND1	2.42	0.76
1:A:50:HIS:CA	1:A:50:HIS:CG	2.68	0.76
2:B:61:LYS:CE	2:B:61:LYS:CG	2.64	0.76
2:D:22:GLU:CG	2:D:22:GLU:CB	0.76	0.75
1:A:138:SER:OG	1:A:138:SER:HA	1.81	0.75
2:B:139:ASN:CG	2:B:139:ASN:CB	0.66	0.75
2:D:78:LEU:CB	2:D:78:LEU:N	2.49	0.75
2:D:132:LYS:NZ	2:D:132:LYS:CE	2.49	0.75
2:D:101:GLU:CG	2:D:101:GLU:OE2	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:148:HEM:CBD	3:D:148:HEM:O1D	2.34	0.75
1:A:2:LEU:CA	1:A:2:LEU:O	2.33	0.75
2:B:61:LYS:CD	2:B:61:LYS:CB	2.62	0.75
1:A:17:VAL:CA	1:A:17:VAL:O	2.34	0.75
2:B:5:PRO:C	2:B:5:PRO:CB	2.54	0.75
2:B:49:SER:O	2:B:50:THR:N	2.19	0.75
1:A:11:LYS:CE	1:A:11:LYS:CG	2.64	0.75
2:B:43:GLU:O	2:B:44:SER:C	2.23	0.75
1:A:18:GLY:CA	1:A:19:ALA:N	2.49	0.74
1:A:133:SER:O	1:A:137:THR:HG22	1.85	0.74
2:D:73:ASP:CG	2:D:73:ASP:OD2	2.26	0.74
2:D:104:ARG:NE	2:D:104:ARG:CG	2.49	0.74
1:C:30:GLU:CG	1:C:30:GLU:OE1	2.35	0.74
2:D:12:THR:C	2:D:12:THR:HG22	2.07	0.74
1:C:2:LEU:CA	1:C:2:LEU:O	2.36	0.74
1:C:99:LYS:CG	1:C:99:LYS:CB	0.74	0.74
2:D:59:LYS:CE	2:D:59:LYS:CG	2.52	0.74
1:A:81:SER:CA	1:A:81:SER:OG	2.35	0.74
1:C:7:LYS:N	1:C:7:LYS:CB	2.49	0.74
2:D:22:GLU:C	2:D:22:GLU:HG3	2.09	0.74
2:B:43:GLU:CG	2:B:43:GLU:OE2	2.36	0.73
3:A:142:HEM:CBD	3:A:142:HEM:O1D	2.35	0.73
2:D:82:LYS:CD	2:D:82:LYS:HZ3	2.02	0.73
1:C:54:GLN:CA	1:C:55:VAL:N	2.51	0.73
2:D:104:ARG:CD	2:D:104:ARG:NH1	2.52	0.73
2:B:74:GLY:CA	2:B:75:LEU:N	2.51	0.73
1:A:74:ASP:CB	1:A:74:ASP:OD1	2.37	0.73
1:A:84:SER:CB	1:A:84:SER:C	2.57	0.73
1:A:1:VAL:CG2	1:A:1:VAL:H1	1.99	0.73
2:D:95:LYS:CD	2:D:95:LYS:CB	2.67	0.73
3:B:148:HEM:CBD	3:B:148:HEM:O1D	2.35	0.73
2:D:7:GLU:C	2:D:7:GLU:CB	2.57	0.73
2:D:79:ASP:OD2	2:D:79:ASP:CB	2.37	0.73
2:D:10:ALA:C	2:D:10:ALA:HB3	2.08	0.73
1:C:70:VAL:N	1:C:70:VAL:CB	2.49	0.72
2:D:49:SER:CA	2:D:50:THR:N	2.52	0.72
2:B:12:THR:HG21	2:B:12:THR:HB	0.75	0.72
1:C:75:ASP:N	1:C:75:ASP:C	2.43	0.72
2:D:143:HIS:CD2	2:D:143:HIS:CB	2.68	0.72
1:A:56:LYS:CD	1:A:56:LYS:NZ	2.52	0.72
1:C:16:LYS:HB3	1:C:16:LYS:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:HIS:CG	2:D:2:HIS:CA	2.70	0.72
2:D:113:VAL:CG2	2:D:113:VAL:CA	2.65	0.72
2:B:6:GLU:C	2:B:6:GLU:CB	2.58	0.72
1:C:116:GLU:CB	1:C:116:GLU:CD	2.57	0.72
2:D:7:GLU:CA	2:D:7:GLU:O	2.38	0.72
2:D:132:LYS:NZ	2:D:132:LYS:CD	2.53	0.72
2:B:59:LYS:NZ	2:B:59:LYS:CD	2.53	0.72
1:C:40:LYS:NZ	1:C:40:LYS:HD2	2.01	0.72
2:B:8:LYS:CB	2:B:8:LYS:N	2.49	0.72
2:D:47:ASP:N	2:D:47:ASP:HB3	2.04	0.72
2:D:50:THR:N	2:D:50:THR:CB	2.53	0.72
1:C:92:ARG:CD	1:C:92:ARG:NH2	2.52	0.71
2:D:12:THR:CG2	2:D:12:THR:C	2.58	0.71
2:D:78:LEU:CG	2:D:78:LEU:HD23	1.51	0.71
2:B:2:HIS:CG	2:B:2:HIS:CE1	2.77	0.71
2:D:43:GLU:CA	2:D:44:SER:N	2.53	0.71
1:A:87:HIS:CA	1:A:88:ALA:N	2.50	0.71
2:B:146:HIS:CG	2:B:146:HIS:CA	2.73	0.71
1:A:52:SER:N	1:A:52:SER:CB	2.54	0.71
1:A:50:HIS:C	1:A:50:HIS:CG	2.64	0.71
1:A:127:LYS:CG	1:A:127:LYS:CB	0.71	0.71
2:B:7:GLU:CG	2:B:7:GLU:HA	2.19	0.71
1:C:16:LYS:C	1:C:16:LYS:N	2.43	0.71
2:B:6:GLU:C	2:B:6:GLU:N	2.43	0.71
2:B:7:GLU:CB	2:B:7:GLU:CD	2.56	0.71
2:B:145:TYR:CA	2:B:145:TYR:O	2.38	0.71
2:D:139:ASN:OD1	2:D:139:ASN:HB3	1.91	0.71
2:D:59:LYS:C	2:D:59:LYS:CB	2.57	0.71
2:B:12:THR:CB	2:B:12:THR:HG21	1.28	0.71
1:C:75:ASP:N	1:C:75:ASP:CB	2.54	0.71
1:C:82:ALA:C	1:C:83:LEU:CA	2.58	0.71
2:B:1:VAL:CA	2:B:1:VAL:CG2	2.64	0.70
1:C:30:GLU:CD	1:C:50:HIS:HD2	1.94	0.70
2:D:22:GLU:CA	2:D:23:VAL:N	2.53	0.70
2:D:141:LEU:CD2	2:D:141:LEU:HD13	2.21	0.70
1:C:2:LEU:C	1:C:2:LEU:CB	2.57	0.70
2:B:49:SER:OG	2:B:49:SER:C	2.29	0.70
1:C:113:LEU:CD1	1:C:113:LEU:HB3	2.21	0.70
3:C:142:HEM:CBD	3:C:142:HEM:O1D	2.32	0.70
1:C:1:VAL:C	1:C:1:VAL:CG1	2.59	0.70
2:B:65:LYS:CG	2:B:65:LYS:C	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:THR:O	2:D:5:PRO:CA	2.40	0.70
2:D:1:VAL:HB	2:D:2:HIS:N	2.06	0.70
2:D:45:PHE:O	2:D:46:GLY:HA3	1.90	0.70
2:B:8:LYS:HG2	2:B:8:LYS:C	2.12	0.70
2:B:82:LYS:CE	2:B:82:LYS:CD	0.70	0.70
1:C:1:VAL:CA	1:C:2:LEU:N	2.55	0.70
2:B:3:LEU:CB	2:B:3:LEU:C	2.61	0.69
1:C:10:VAL:CA	1:C:11:LYS:N	2.52	0.69
2:B:12:THR:CA	2:B:12:THR:HG23	1.88	0.69
1:C:1:VAL:C	1:C:1:VAL:HG12	2.12	0.69
2:B:5:PRO:N	2:B:6:GLU:N	2.40	0.69
2:D:73:ASP:OD2	5:D:174:HOH:O	2.10	0.69
2:B:90:GLU:CG	2:B:90:GLU:OE1	2.38	0.69
1:C:56:LYS:NZ	1:C:56:LYS:CD	2.56	0.69
2:D:131:GLN:CG	2:D:131:GLN:NE2	2.49	0.69
1:A:74:ASP:CG	1:A:74:ASP:CA	2.60	0.69
1:C:61:LYS:C	1:C:61:LYS:CB	2.60	0.69
1:A:127:LYS:CG	1:A:127:LYS:HA	2.15	0.69
1:C:46:PHE:CD2	1:C:46:PHE:CZ	2.39	0.69
2:D:17:LYS:NZ	2:D:17:LYS:HD3	2.07	0.69
2:D:47:ASP:CA	2:D:48:LEU:N	2.55	0.69
1:C:56:LYS:CD	1:C:56:LYS:CB	2.70	0.69
1:A:11:LYS:CD	1:A:11:LYS:NZ	2.56	0.68
1:A:92:ARG:CD	1:A:92:ARG:NH2	2.56	0.68
3:B:148:HEM:CBD	3:B:148:HEM:O2D	2.38	0.68
1:A:87:HIS:C	1:A:87:HIS:CB	2.60	0.68
2:B:12:THR:CA	2:B:12:THR:HG22	1.88	0.68
3:C:142:HEM:CBD	3:C:142:HEM:O2D	2.35	0.68
1:C:38:THR:CB	1:C:38:THR:N	2.56	0.68
2:D:8:LYS:CB	2:D:8:LYS:N	2.55	0.68
2:D:82:LYS:CD	2:D:82:LYS:CB	2.68	0.68
1:A:78:ASN:ND2	1:A:78:ASN:OD1	2.26	0.68
2:B:52:ASP:CB	2:B:52:ASP:OD2	2.41	0.68
2:D:12:THR:CA	2:D:12:THR:OG1	2.40	0.68
1:A:85:ASP:OD2	1:A:85:ASP:OD1	2.10	0.68
2:B:9:SER:CA	2:B:10:ALA:N	2.56	0.68
2:D:7:GLU:CA	2:D:8:LYS:N	2.49	0.68
1:C:16:LYS:CG	1:C:16:LYS:HA	2.22	0.68
1:A:92:ARG:CZ	1:A:92:ARG:NE	2.57	0.68
2:B:2:HIS:C	2:B:2:HIS:CG	2.66	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)
2:D:131:GLN:CG	2:D:131:GLN:OE1	2.39	0.68
2:D:8:LYS:CB	2:D:8:LYS:HD3	2.21	0.68
2:B:145:TYR:C	2:B:145:TYR:CB	2.55	0.68
1:A:137:THR:OG1	1:A:137:THR:HG22	1.93	0.68
2:D:24:GLY:HA2	2:D:68:LEU:HD22	1.76	0.67
1:C:1:VAL:CG1	1:C:1:VAL:HA	2.23	0.67
2:B:117:HIS:CE1	2:B:117:HIS:CG	2.82	0.67
1:C:38:THR:CA	1:C:38:THR:OG1	2.42	0.67
2:D:123:THR:CG2	2:D:123:THR:OG1	2.42	0.67
1:A:5:ALA:CB	1:A:5:ALA:C	2.62	0.67
2:D:8:LYS:CB	2:D:8:LYS:C	2.60	0.67
2:D:121:GLU:CG	2:D:121:GLU:OE2	2.42	0.67
2:D:104:ARG:NE	2:D:104:ARG:CZ	2.58	0.67
2:D:123:THR:CG2	2:D:123:THR:CA	2.70	0.67
2:B:49:SER:CB	2:B:49:SER:N	2.57	0.67
2:D:78:LEU:CB	2:D:78:LEU:C	2.58	0.67
2:D:92:HIS:CA	2:D:92:HIS:O	2.40	0.67
1:C:113:LEU:HD22	1:C:116:GLU:HG3	1.77	0.67
2:D:1:VAL:CB	2:D:2:HIS:N	2.57	0.67
3:C:142:HEM:HBB2	3:C:142:HEM:CMB	2.25	0.66
2:D:92:HIS:C	2:D:92:HIS:N	2.49	0.66
2:D:82:LYS:CG	2:D:82:LYS:CE	2.73	0.66
1:A:30:GLU:CD	1:A:30:GLU:CB	2.63	0.66
2:D:43:GLU:HB3	2:D:43:GLU:OE1	1.95	0.66
2:D:79:ASP:N	2:D:80:ASN:N	2.43	0.66
2:B:65:LYS:CE	2:B:65:LYS:NZ	2.59	0.66
2:D:24:GLY:CA	2:D:68:LEU:HD22	2.24	0.66
1:A:75:ASP:CB	1:A:75:ASP:OD1	2.44	0.66
2:B:65:LYS:CE	2:B:65:LYS:HG3	2.24	0.66
2:D:26:GLU:OE2	2:D:26:GLU:CB	2.43	0.66
1:C:135:VAL:O	1:C:138:SER:HB2	1.95	0.65
2:B:82:LYS:CD	2:B:82:LYS:NZ	2.59	0.65
1:A:21:ALA:CA	1:A:21:ALA:O	2.44	0.65
1:A:44:PRO:CA	1:A:45:HIS:N	2.55	0.65
1:A:139:LYS:NZ	1:A:139:LYS:CD	2.57	0.65
1:C:10:VAL:C	1:C:10:VAL:CB	2.65	0.65
1:C:137:THR:CA	1:C:137:THR:O	2.42	0.65
2:D:55:MET:CA	2:D:55:MET:O	2.42	0.65
2:B:6:GLU:CA	2:B:7:GLU:N	2.54	0.65
1:C:6:ASP:C	1:C:7:LYS:CA	2.62	0.65
2:D:104:ARG:HD2	2:D:104:ARG:NH1	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:LEU:CD1	2:D:48:LEU:CD2	2.72	0.65
1:C:27:GLU:OE2	1:C:112:HIS:HE1	1.80	0.64
2:D:101:GLU:CG	2:D:101:GLU:OE1	2.43	0.64
2:D:65:LYS:CD	2:D:65:LYS:NZ	2.59	0.64
2:D:82:LYS:HZ2	2:D:82:LYS:HD2	1.59	0.64
2:B:50:THR:CG2	2:B:50:THR:OG1	2.43	0.64
2:B:57:ASN:C	2:B:58:PRO:CD	2.64	0.64
2:B:74:GLY:O	2:B:75:LEU:N	2.28	0.64
1:C:92:ARG:NH1	1:C:92:ARG:HD2	2.12	0.64
2:D:1:VAL:CA	2:D:2:HIS:H	2.07	0.64
2:D:8:LYS:CG	2:D:8:LYS:C	2.65	0.64
1:C:16:LYS:CB	1:C:16:LYS:HD3	2.22	0.64
2:D:8:LYS:CA	2:D:8:LYS:HG3	2.26	0.64
1:A:137:THR:CB	1:A:137:THR:C	2.64	0.64
3:C:142:HEM:CGD	3:C:142:HEM:CAD	2.73	0.64
1:C:54:GLN:C	1:C:54:GLN:CB	2.59	0.64
2:D:67:VAL:CG1	2:D:67:VAL:C	2.66	0.64
2:B:104:ARG:CG	2:B:104:ARG:NE	2.60	0.64
1:C:105:LEU:CD2	1:C:105:LEU:HD13	2.28	0.64
2:D:6:GLU:CD	2:D:6:GLU:CB	2.67	0.64
2:B:21:ASP:CB	2:B:21:ASP:OD1	2.42	0.63
1:C:48:LEU:CD2	1:C:48:LEU:CB	2.66	0.63
2:D:21:ASP:CB	2:D:21:ASP:OD2	2.42	0.63
1:A:127:LYS:HG3	1:A:127:LYS:HA	1.77	0.63
2:B:6:GLU:OE1	2:B:6:GLU:OE2	2.09	0.63
1:C:23:GLU:OE2	1:C:23:GLU:HB2	1.96	0.63
3:C:142:HEM:HBB2	3:C:142:HEM:HMB1	1.80	0.63
1:C:8:THR:CA	1:C:8:THR:OG1	2.46	0.63
1:A:81:SER:CB	1:A:81:SER:C	2.66	0.63
2:D:52:ASP:N	2:D:52:ASP:HB2	2.12	0.63
1:C:60:LYS:NZ	1:C:60:LYS:HD3	2.13	0.63
2:D:80:ASN:OD1	2:D:80:ASN:CB	2.39	0.63
2:B:52:ASP:CG	2:B:52:ASP:CA	2.64	0.63
1:C:7:LYS:CG	1:C:7:LYS:HE3	2.27	0.63
1:C:73:VAL:H	1:C:73:VAL:HG12	1.64	0.63
1:C:138:SER:CA	1:C:138:SER:HG	2.05	0.63
2:D:65:LYS:CE	2:D:65:LYS:CG	2.77	0.63
1:A:29:LEU:CA	1:A:29:LEU:CG	2.70	0.62
2:D:121:GLU:CB	2:D:121:GLU:C	2.68	0.62
1:A:62:VAL:C	1:A:62:VAL:CB	2.63	0.62
2:B:82:LYS:CE	2:B:82:LYS:HG2	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLU:CD	1:C:23:GLU:OE1	2.37	0.62
1:C:87:HIS:CA	1:C:88:ALA:N	2.61	0.62
2:D:77:HIS:CD2	2:D:77:HIS:CE1	2.70	0.62
2:B:41:PHE:C	2:B:41:PHE:CB	2.67	0.62
2:B:48:LEU:O	2:B:49:SER:CA	2.47	0.62
2:B:143:HIS:C	2:B:143:HIS:CB	2.60	0.62
1:C:61:LYS:CA	1:C:62:VAL:N	2.62	0.62
1:C:87:HIS:C	1:C:87:HIS:CB	2.66	0.62
2:B:80:ASN:OD1	2:B:80:ASN:HA	2.00	0.62
2:D:59:LYS:CD	2:D:59:LYS:NZ	2.63	0.62
1:C:139:LYS:CD	1:C:139:LYS:HZ3	2.13	0.62
2:D:58:PRO:CG	2:D:58:PRO:HD3	1.11	0.62
1:A:99:LYS:CE	1:A:99:LYS:HG3	2.29	0.62
1:C:82:ALA:CA	1:C:83:LEU:N	2.58	0.62
3:C:142:HEM:CBA	3:C:142:HEM:O1A	2.48	0.62
2:D:5:PRO:CB	2:D:5:PRO:C	2.68	0.62
2:D:4:THR:CA	2:D:4:THR:OG1	2.46	0.61
1:A:15:GLY:O	1:A:16:LYS:N	2.19	0.61
1:A:90:LYS:CD	1:A:90:LYS:NZ	2.62	0.61
1:C:105:LEU:CD2	1:C:105:LEU:HB2	2.30	0.61
2:D:76:ALA:N	2:D:76:ALA:HB3	2.13	0.61
2:D:46:GLY:CA	2:D:47:ASP:N	2.60	0.61
2:D:58:PRO:CG	2:D:58:PRO:HD2	1.11	0.61
1:A:87:HIS:CA	1:A:87:HIS:O	2.44	0.61
2:B:65:LYS:HG3	2:B:65:LYS:HE2	1.82	0.61
2:B:142:ALA:CA	2:B:143:HIS:N	2.54	0.61
1:C:92:ARG:HD2	1:C:92:ARG:HH11	1.65	0.61
1:A:17:VAL:N	1:A:18:GLY:N	2.48	0.61
2:B:80:ASN:CA	2:B:80:ASN:CG	2.62	0.61
2:D:45:PHE:O	2:D:46:GLY:CA	2.44	0.61
2:B:108:ASN:CG	2:B:108:ASN:CA	2.64	0.61
1:A:127:LYS:CG	1:A:127:LYS:HE2	2.27	0.61
2:D:4:THR:OG1	2:D:6:GLU:OE2	2.19	0.61
1:A:16:LYS:CD	1:A:16:LYS:CB	2.78	0.60
2:D:19:ASN:ND2	2:D:19:ASN:CB	2.63	0.60
2:B:65:LYS:CB	2:B:65:LYS:C	2.66	0.60
1:C:73:VAL:CA	1:C:73:VAL:HG12	2.30	0.60
2:D:18:VAL:CB	2:D:18:VAL:N	2.53	0.60
1:A:75:ASP:CB	1:A:75:ASP:N	2.64	0.60
2:D:53:ALA:CA	2:D:54:VAL:N	2.63	0.60
1:A:16:LYS:CE	1:A:16:LYS:HG2	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:LEU:HD13	2:D:141:LEU:HD22	1.82	0.60
1:C:118:THR:CA	1:C:118:THR:CG2	2.59	0.60
2:D:7:GLU:C	2:D:7:GLU:N	2.55	0.60
2:B:80:ASN:N	2:B:80:ASN:C	2.55	0.59
1:A:92:ARG:HH11	1:A:92:ARG:HD2	1.47	0.59
2:B:63:HIS:HE1	3:B:148:HEM:C4D	2.20	0.59
2:B:90:GLU:CB	2:B:90:GLU:CD	2.69	0.59
2:D:78:LEU:CD1	2:D:78:LEU:HD21	2.19	0.59
2:D:94:ASP:N	2:D:94:ASP:C	2.50	0.59
2:D:51:PRO:C	2:D:52:ASP:CA	2.71	0.59
2:B:66:LYS:CE	2:B:66:LYS:HG3	2.32	0.59
2:D:76:ALA:N	2:D:76:ALA:HB2	2.13	0.59
2:B:66:LYS:CE	2:B:66:LYS:CG	2.80	0.59
2:D:2:HIS:CG	2:D:2:HIS:NE2	2.67	0.59
2:D:12:THR:CB	2:D:12:THR:C	2.66	0.59
2:B:82:LYS:HE2	2:B:82:LYS:HB3	1.82	0.59
2:B:124:PRO:C	2:B:125:PRO:CD	2.60	0.59
1:C:131:SER:CA	1:C:132:VAL:N	2.60	0.59
2:D:12:THR:N	2:D:12:THR:C	2.49	0.59
1:C:56:LYS:CD	1:C:56:LYS:HB3	2.32	0.58
2:D:52:ASP:N	2:D:52:ASP:C	2.56	0.58
2:D:1:VAL:HB	2:D:2:HIS:H	1.67	0.58
2:B:2:HIS:CB	2:B:2:HIS:N	2.66	0.58
1:C:73:VAL:CA	1:C:73:VAL:HG13	2.30	0.58
2:D:132:LYS:NZ	2:D:132:LYS:HD3	2.18	0.58
2:B:80:ASN:CB	2:B:80:ASN:OD1	2.50	0.58
1:A:40:LYS:CB	1:A:40:LYS:N	2.59	0.58
1:A:90:LYS:CE	1:A:90:LYS:NZ	2.67	0.58
1:C:92:ARG:HH21	1:C:92:ARG:HD2	1.68	0.58
2:D:79:ASP:O	2:D:80:ASN:CA	2.51	0.58
2:D:50:THR:CA	2:D:50:THR:CG2	2.81	0.58
2:B:12:THR:CG2	2:B:12:THR:CB	0.58	0.58
1:A:14:TRP:CB	1:A:14:TRP:N	2.63	0.57
1:A:62:VAL:CA	1:A:62:VAL:O	2.44	0.57
2:B:65:LYS:CB	2:B:65:LYS:CG	0.58	0.57
2:B:90:GLU:CB	2:B:90:GLU:C	2.67	0.57
1:A:14:TRP:CG	1:A:14:TRP:HA	2.34	0.57
1:C:113:LEU:CD1	1:C:113:LEU:HB2	2.28	0.57
1:C:73:VAL:HG12	1:C:73:VAL:N	2.19	0.57
1:C:76:MET:CG	1:C:76:MET:CE	2.81	0.57
2:B:26:GLU:OE2	2:B:26:GLU:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:HIS:CD2	2:B:77:HIS:CB	2.84	0.57
1:C:137:THR:CA	1:C:138:SER:N	2.58	0.57
2:D:10:ALA:C	2:D:10:ALA:N	2.57	0.57
1:A:127:LYS:CD	1:A:127:LYS:HB3	2.28	0.57
2:D:22:GLU:C	2:D:22:GLU:N	2.52	0.57
1:C:73:VAL:CG1	1:C:73:VAL:N	2.68	0.57
1:A:58:HIS:CA	1:A:58:HIS:O	2.45	0.57
2:B:9:SER:C	2:B:9:SER:OG	2.43	0.57
2:B:80:ASN:N	2:B:80:ASN:CB	2.57	0.57
2:B:26:GLU:OE2	2:B:26:GLU:CD	2.43	0.56
1:C:16:LYS:CD	1:C:16:LYS:NZ	2.68	0.56
2:B:146:HIS:CG	2:B:146:HIS:C	2.79	0.56
1:A:60:LYS:CE	1:A:60:LYS:NZ	2.69	0.56
2:D:126:VAL:CB	2:D:126:VAL:N	2.66	0.56
2:B:142:ALA:C	2:B:142:ALA:N	2.54	0.56
2:D:43:GLU:HB2	2:D:44:SER:N	2.16	0.56
2:B:90:GLU:CG	2:B:90:GLU:N	2.68	0.56
1:C:118:THR:CA	1:C:118:THR:HB	2.16	0.56
2:D:20:VAL:HG22	2:D:20:VAL:C	2.18	0.56
1:A:1:VAL:HG22	1:A:1:VAL:H1	1.70	0.56
1:A:64:ASP:CB	1:A:64:ASP:OD2	2.51	0.56
1:C:7:LYS:CG	1:C:7:LYS:HE2	2.34	0.56
1:C:118:THR:HG23	1:C:121:VAL:H	1.71	0.56
2:D:21:ASP:OD1	2:D:65:LYS:HG3	2.06	0.56
1:A:52:SER:N	1:A:52:SER:C	2.46	0.56
2:B:143:HIS:CA	2:B:144:LYS:N	2.62	0.56
2:D:52:ASP:CG	2:D:52:ASP:OD2	2.44	0.56
2:D:90:GLU:OE1	2:D:90:GLU:CG	2.53	0.56
2:D:47:ASP:CG	2:D:47:ASP:CA	2.74	0.56
2:B:12:THR:CG2	2:B:12:THR:HB	1.04	0.55
2:D:47:ASP:N	2:D:47:ASP:C	2.60	0.55
1:A:75:ASP:HB3	1:A:75:ASP:O	2.07	0.55
1:C:47:ASP:C	1:C:47:ASP:OD1	2.43	0.55
1:A:75:ASP:CB	1:A:75:ASP:O	2.53	0.55
2:B:4:THR:C	2:B:5:PRO:CD	2.73	0.55
2:B:142:ALA:C	2:B:142:ALA:CB	2.72	0.55
2:B:143:HIS:ND1	2:B:143:HIS:HB3	2.21	0.55
1:A:78:ASN:CG	1:A:78:ASN:HA	2.20	0.55
2:B:145:TYR:CA	2:B:146:HIS:N	2.46	0.55
2:B:8:LYS:CG	2:B:8:LYS:C	2.70	0.55
2:D:65:LYS:CD	2:D:65:LYS:HB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:VAL:CG2	1:A:1:VAL:H3	1.89	0.55
2:B:41:PHE:C	2:B:41:PHE:N	2.57	0.55
2:B:90:GLU:HG3	2:B:90:GLU:H	1.72	0.55
1:C:61:LYS:NZ	1:C:61:LYS:HD2	2.19	0.55
2:D:124:PRO:C	2:D:125:PRO:CD	2.67	0.54
2:D:58:PRO:CD	2:D:58:PRO:HG2	1.03	0.54
1:A:15:GLY:O	1:A:15:GLY:CA	2.56	0.54
3:A:142:HEM:CGA	3:A:142:HEM:CAA	2.82	0.54
1:C:114:PRO:C	1:C:114:PRO:N	2.60	0.54
2:D:102:ASN:HB3	3:D:148:HEM:HMC1	1.90	0.54
1:C:138:SER:OG	1:C:138:SER:HA	1.96	0.54
2:B:101:GLU:CD	2:B:101:GLU:CB	2.75	0.54
2:D:59:LYS:CE	2:D:59:LYS:HG2	2.38	0.54
2:D:79:ASP:N	2:D:80:ASN:H	2.04	0.54
2:B:61:LYS:CD	2:B:61:LYS:HZ2	2.19	0.54
2:B:108:ASN:HD22	2:B:108:ASN:HB2	1.70	0.54
1:C:84:SER:HB2	1:C:139:LYS:HD2	1.90	0.54
1:C:90:LYS:CD	1:C:90:LYS:NZ	2.71	0.53
2:D:67:VAL:C	2:D:67:VAL:HG12	2.29	0.53
2:D:18:VAL:CG2	2:D:18:VAL:HG11	2.37	0.53
2:D:67:VAL:CB	2:D:67:VAL:C	2.64	0.53
1:C:8:THR:CB	1:C:8:THR:N	2.67	0.53
1:C:10:VAL:CA	1:C:10:VAL:O	2.47	0.53
2:D:58:PRO:CD	2:D:58:PRO:HG3	1.03	0.53
1:C:82:ALA:O	1:C:83:LEU:N	2.36	0.53
1:A:20:HIS:O	1:A:21:ALA:C	2.46	0.53
2:B:47:ASP:C	2:B:47:ASP:HB3	2.29	0.53
1:C:7:LYS:CD	1:C:7:LYS:CB	2.80	0.53
2:D:76:ALA:CB	2:D:76:ALA:H	2.12	0.53
1:A:133:SER:O	1:A:137:THR:CG2	2.57	0.53
1:C:138:SER:CB	1:C:138:SER:N	2.72	0.53
2:D:3:LEU:O	2:D:4:THR:CA	2.55	0.53
2:D:73:ASP:O	2:D:76:ALA:HB3	2.08	0.53
3:D:148:HEM:O1A	3:D:148:HEM:CAA	2.56	0.53
2:D:10:ALA:HB3	2:D:11:VAL:N	2.24	0.53
2:B:80:ASN:CA	2:B:80:ASN:OD1	2.57	0.52
2:D:95:LYS:HA	2:D:95:LYS:HD3	1.92	0.52
2:B:143:HIS:C	2:B:143:HIS:N	2.60	0.52
1:A:23:GLU:OE1	1:A:23:GLU:CG	2.57	0.52
2:B:79:ASP:OD2	2:B:79:ASP:CA	2.56	0.52
2:D:18:VAL:N	2:D:18:VAL:C	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:VAL:CA	2:D:67:VAL:CG2	2.77	0.52
2:D:79:ASP:C	2:D:79:ASP:HB2	2.25	0.52
2:D:104:ARG:NE	2:D:104:ARG:HH21	2.06	0.52
2:B:81:LEU:N	2:B:81:LEU:HB2	2.18	0.52
1:A:75:ASP:CG	1:A:75:ASP:C	2.65	0.52
2:B:22:GLU:OE1	2:B:22:GLU:OE2	2.28	0.52
1:A:137:THR:CB	1:A:137:THR:HG1	2.10	0.52
2:B:41:PHE:N	2:B:42:PHE:N	2.57	0.52
2:D:2:HIS:ND1	2:D:2:HIS:NE2	2.57	0.52
2:D:79:ASP:O	2:D:80:ASN:HA	2.10	0.52
2:B:1:VAL:CA	2:B:1:VAL:CG1	2.88	0.52
1:C:92:ARG:CZ	1:C:92:ARG:HD2	2.40	0.52
2:D:90:GLU:CB	2:D:90:GLU:OE2	2.58	0.52
1:C:78:ASN:CB	1:C:78:ASN:OD1	2.48	0.52
1:C:99:LYS:CG	1:C:99:LYS:CE	2.89	0.52
2:D:3:LEU:O	2:D:3:LEU:CA	2.58	0.51
1:C:2:LEU:C	1:C:2:LEU:N	2.55	0.51
2:B:1:VAL:O	2:B:2:HIS:HA	2.11	0.51
2:B:8:LYS:CB	2:B:8:LYS:C	2.69	0.51
2:B:50:THR:O	2:B:54:VAL:HG23	2.11	0.51
1:C:92:ARG:CZ	1:C:92:ARG:CD	2.89	0.51
2:B:2:HIS:ND1	2:B:2:HIS:HB3	2.20	0.51
1:C:139:LYS:NZ	1:C:139:LYS:HD2	2.20	0.51
2:D:20:VAL:HG13	2:D:20:VAL:N	2.26	0.51
2:B:22:GLU:CG	2:B:22:GLU:OE1	2.59	0.51
2:D:73:ASP:CB	2:D:73:ASP:OD2	2.59	0.51
1:A:2:LEU:HA	1:A:3:SER:N	2.21	0.50
2:B:65:LYS:CG	2:B:65:LYS:HE2	2.39	0.50
1:C:90:LYS:CD	1:C:90:LYS:HB3	2.38	0.50
2:D:104:ARG:NE	2:D:104:ARG:NH2	2.59	0.50
2:D:121:GLU:CA	2:D:121:GLU:HG3	2.37	0.50
1:C:8:THR:CB	1:C:8:THR:C	2.67	0.50
1:A:29:LEU:CB	1:A:29:LEU:C	2.74	0.50
1:A:81:SER:CB	1:A:81:SER:H	2.22	0.50
2:B:21:ASP:CB	2:B:21:ASP:OD2	2.56	0.50
2:D:58:PRO:HD3	2:D:58:PRO:HG2	1.04	0.50
1:C:16:LYS:C	1:C:16:LYS:CB	2.71	0.50
2:D:5:PRO:CA	2:D:5:PRO:CG	2.81	0.50
2:D:55:MET:N	2:D:56:GLY:N	2.59	0.50
2:D:121:GLU:CB	2:D:121:GLU:N	2.60	0.50
1:C:40:LYS:HG2	1:C:48:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:HIS:HE1	2:D:131:GLN:OE1	1.94	0.50
2:D:1:VAL:CB	2:D:2:HIS:H	2.23	0.50
2:D:73:ASP:OD2	2:D:73:ASP:OD1	2.30	0.50
2:B:3:LEU:CA	2:B:3:LEU:CG	2.81	0.50
1:C:40:LYS:HD3	1:C:40:LYS:HZ3	1.75	0.50
2:B:12:THR:CG2	2:B:12:THR:HG1	2.16	0.49
2:D:121:GLU:CG	2:D:121:GLU:OE1	2.60	0.49
2:D:12:THR:N	2:D:12:THR:CB	2.75	0.49
2:D:26:GLU:OE2	2:D:26:GLU:OE1	2.29	0.49
1:C:105:LEU:HD13	1:C:105:LEU:HD22	1.93	0.49
1:C:61:LYS:CD	1:C:61:LYS:HZ3	2.24	0.49
1:C:82:ALA:O	1:C:83:LEU:CA	2.59	0.49
2:D:43:GLU:HB2	2:D:43:GLU:HG3	1.34	0.49
2:D:123:THR:HB	2:D:124:PRO:CD	2.42	0.49
1:C:16:LYS:N	1:C:17:VAL:N	2.61	0.49
2:D:4:THR:CB	2:D:4:THR:C	2.76	0.49
2:D:8:LYS:C	2:D:8:LYS:HG2	2.33	0.49
2:D:82:LYS:CE	2:D:82:LYS:HG3	2.41	0.49
1:A:17:VAL:C	1:A:17:VAL:CG1	2.81	0.48
2:B:65:LYS:CB	2:B:65:LYS:CE	2.91	0.48
2:B:132:LYS:CD	2:B:132:LYS:HZ2	2.25	0.48
2:B:142:ALA:CA	2:B:142:ALA:O	2.55	0.48
2:B:96:LEU:HD13	3:B:148:HEM:C3D	2.49	0.48
1:C:137:THR:C	1:C:137:THR:CB	2.76	0.48
2:D:1:VAL:C	2:D:1:VAL:CB	2.81	0.48
1:A:16:LYS:CG	1:A:16:LYS:NZ	2.71	0.48
1:A:138:SER:CB	1:A:138:SER:C	2.81	0.48
1:C:7:LYS:N	1:C:7:LYS:CG	2.76	0.48
1:C:56:LYS:CG	1:C:56:LYS:HE3	2.42	0.48
1:C:118:THR:CA	1:C:118:THR:OG1	2.54	0.48
1:C:78:ASN:CB	1:C:78:ASN:ND2	2.66	0.48
3:D:148:HEM:CGD	3:D:148:HEM:CAD	2.85	0.48
1:A:50:HIS:HA	5:A:173:HOH:O	2.13	0.48
2:B:65:LYS:CB	2:B:65:LYS:N	2.65	0.48
2:D:6:GLU:CB	2:D:6:GLU:C	2.81	0.48
3:C:142:HEM:HMB1	3:C:142:HEM:CBB	2.44	0.48
2:D:12:THR:CA	2:D:12:THR:HG23	2.41	0.48
2:D:47:ASP:CA	2:D:47:ASP:OD2	2.62	0.48
2:B:22:GLU:CG	2:B:22:GLU:OE2	2.61	0.48
1:A:29:LEU:CB	1:A:29:LEU:N	2.74	0.48
1:C:137:THR:C	1:C:137:THR:N	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:OD1	1:A:75:ASP:OD2	2.33	0.47
2:D:20:VAL:CA	2:D:20:VAL:HG12	2.41	0.47
1:A:18:GLY:C	1:A:18:GLY:N	2.61	0.47
2:B:87:THR:CA	2:B:87:THR:CG2	2.92	0.47
1:A:50:HIS:CB	1:A:50:HIS:H	2.23	0.47
2:B:4:THR:HA	2:B:5:PRO:CD	2.44	0.47
1:A:137:THR:CG2	1:A:137:THR:N	2.78	0.47
2:B:5:PRO:N	2:B:6:GLU:H	2.10	0.47
2:B:80:ASN:O	2:B:81:LEU:CA	2.63	0.47
2:D:49:SER:N	2:D:50:THR:N	2.63	0.47
2:D:73:ASP:CG	2:D:73:ASP:N	2.65	0.47
2:B:123:THR:C	2:B:124:PRO:CD	2.63	0.47
2:D:5:PRO:HA	2:D:8:LYS:HB3	1.96	0.47
2:B:2:HIS:ND1	2:B:2:HIS:O	2.48	0.47
1:C:70:VAL:C	1:C:70:VAL:CB	2.70	0.47
1:A:23:GLU:CD	1:A:23:GLU:CB	2.80	0.46
2:D:82:LYS:HD3	2:D:143:HIS:NE2	2.31	0.46
2:D:108:ASN:CG	2:D:108:ASN:CA	2.74	0.46
2:B:10:ALA:C	2:B:10:ALA:N	2.54	0.46
2:D:47:ASP:CB	2:D:47:ASP:C	2.84	0.46
2:D:92:HIS:C	2:D:92:HIS:HB3	2.29	0.46
1:A:72:HIS:CB	1:A:72:HIS:O	2.62	0.46
2:B:90:GLU:CB	2:B:90:GLU:N	2.64	0.46
2:B:10:ALA:CA	2:B:11:VAL:N	2.66	0.46
1:C:116:GLU:CB	1:C:116:GLU:OE1	2.63	0.46
2:D:10:ALA:CA	2:D:10:ALA:O	2.52	0.46
2:D:8:LYS:HG3	2:D:8:LYS:HA	1.95	0.46
1:A:51:GLY:C	1:A:52:SER:C	2.71	0.46
1:A:64:ASP:CB	1:A:64:ASP:OD1	2.62	0.46
2:B:2:HIS:CG	2:B:2:HIS:O	2.69	0.46
1:C:3:SER:O	1:C:7:LYS:HG3	2.16	0.46
2:D:48:LEU:N	2:D:49:SER:N	2.63	0.46
1:A:84:SER:CA	1:A:84:SER:HG	2.28	0.46
2:D:20:VAL:HG22	2:D:21:ASP:N	2.30	0.46
1:A:76:MET:O	1:A:77:PRO:C	2.49	0.46
1:C:1:VAL:HB	1:C:1:VAL:H3	1.74	0.46
1:A:87:HIS:C	1:A:87:HIS:N	2.62	0.45
1:C:56:LYS:HE3	1:C:56:LYS:HG3	1.98	0.45
1:A:84:SER:HB2	1:A:139:LYS:HD2	1.97	0.45
2:D:15:TRP:HE1	2:D:72:SER:HB3	1.80	0.45
2:D:141:LEU:CD2	2:D:141:LEU:HB3	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLU:CA	2:D:7:GLU:N	2.77	0.45
1:A:17:VAL:C	1:A:18:GLY:C	2.75	0.45
1:A:44:PRO:C	1:A:44:PRO:HB2	2.33	0.45
2:D:2:HIS:ND1	2:D:2:HIS:CB	2.76	0.45
1:C:113:LEU:HB3	1:C:113:LEU:HD13	1.96	0.45
1:C:16:LYS:CA	1:C:17:VAL:N	2.72	0.45
1:C:56:LYS:CE	1:C:56:LYS:HG3	2.46	0.45
3:D:148:HEM:CBD	3:D:148:HEM:O2D	2.42	0.45
1:A:30:GLU:CD	1:A:50:HIS:HD1	2.20	0.45
2:B:1:VAL:N	5:B:197:HOH:O	2.50	0.45
2:B:57:ASN:CA	2:B:58:PRO:CD	2.95	0.45
2:D:90:GLU:CD	2:D:90:GLU:CB	2.85	0.45
2:B:1:VAL:O	2:B:2:HIS:CA	2.63	0.45
2:B:79:ASP:O	2:B:80:ASN:CA	2.65	0.45
2:B:90:GLU:CB	2:B:90:GLU:OE1	2.63	0.45
2:B:80:ASN:ND2	2:B:80:ASN:HB3	2.27	0.44
2:B:89:SER:OG	2:B:144:LYS:HB2	2.17	0.44
1:A:16:LYS:HG2	1:A:16:LYS:NZ	2.31	0.44
1:A:43:PHE:N	1:A:44:PRO:CD	2.80	0.44
2:D:17:LYS:HE3	2:D:121:GLU:OE1	2.17	0.44
2:D:121:GLU:CB	2:D:121:GLU:OE2	2.65	0.44
1:A:103:HIS:HE1	2:B:131:GLN:OE1	2.00	0.44
3:C:142:HEM:CGA	3:C:142:HEM:CAA	2.95	0.44
1:A:61:LYS:CG	1:A:61:LYS:HE2	2.11	0.44
2:B:6:GLU:C	2:B:6:GLU:HB2	2.36	0.44
2:B:90:GLU:N	2:B:90:GLU:HG3	2.32	0.44
1:A:56:LYS:CD	1:A:56:LYS:HB3	2.44	0.44
3:D:148:HEM:O1D	3:D:148:HEM:HBD1	2.17	0.44
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.82	0.44
2:B:41:PHE:N	2:B:42:PHE:H	2.16	0.44
2:B:79:ASP:OD2	2:B:79:ASP:HA	2.17	0.44
2:B:2:HIS:CB	2:B:2:HIS:O	2.66	0.44
1:C:30:GLU:OE2	1:C:50:HIS:HD2	1.99	0.44
1:C:72:HIS:CG	1:C:72:HIS:N	2.86	0.44
1:C:105:LEU:HD23	1:C:129:LEU:HD22	2.00	0.44
2:B:144:LYS:CE	2:B:144:LYS:HD2	2.29	0.43
1:A:78:ASN:ND2	1:A:78:ASN:HA	2.31	0.43
2:D:6:GLU:HB2	2:D:6:GLU:C	2.38	0.43
1:C:30:GLU:OE1	1:C:30:GLU:CB	2.66	0.43
2:D:8:LYS:CE	2:D:8:LYS:HG2	2.46	0.43
2:D:20:VAL:CA	2:D:20:VAL:HG13	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:HIS:CE1	3:D:148:HEM:C4D	3.06	0.43
2:D:67:VAL:CB	2:D:67:VAL:H	2.24	0.43
1:A:55:VAL:O	1:A:56:LYS:C	2.53	0.43
2:B:144:LYS:CE	2:B:144:LYS:HD3	2.29	0.43
1:A:7:LYS:O	1:A:11:LYS:HG3	2.19	0.43
1:A:28:ALA:CB	1:A:105:LEU:HD23	2.48	0.43
1:C:113:LEU:HD13	1:C:116:GLU:HB2	1.99	0.43
2:B:82:LYS:CE	2:B:82:LYS:CB	2.78	0.43
1:C:40:LYS:CG	1:C:40:LYS:HE2	2.20	0.43
1:C:94:ASP:OD2	1:C:96:VAL:HG13	2.18	0.43
2:D:47:ASP:CA	2:D:48:LEU:H	2.29	0.43
1:C:72:HIS:CB	1:C:72:HIS:N	2.63	0.43
1:A:44:PRO:C	1:A:44:PRO:N	2.63	0.42
2:B:52:ASP:CB	2:B:52:ASP:OD1	2.44	0.42
2:D:22:GLU:CG	2:D:22:GLU:C	2.80	0.42
2:B:123:THR:CA	2:B:124:PRO:CD	2.97	0.42
2:D:6:GLU:N	2:D:7:GLU:N	2.67	0.42
2:D:22:GLU:CD	2:D:22:GLU:CB	2.87	0.42
2:D:43:GLU:CG	2:D:43:GLU:N	2.78	0.42
2:D:47:ASP:HB3	2:D:47:ASP:O	2.19	0.42
2:B:139:ASN:CA	2:B:139:ASN:OD1	2.61	0.42
2:D:47:ASP:HB3	2:D:47:ASP:H	1.80	0.42
1:C:76:MET:SD	1:C:76:MET:HB3	2.55	0.42
2:D:78:LEU:HD21	2:D:78:LEU:HD11	2.00	0.42
2:B:74:GLY:O	2:B:75:LEU:CA	2.67	0.42
2:D:10:ALA:CA	2:D:11:VAL:N	2.65	0.42
2:D:52:ASP:CB	2:D:52:ASP:H	2.28	0.42
1:A:85:ASP:OD1	1:A:85:ASP:CA	2.67	0.42
2:D:59:LYS:N	2:D:60:VAL:N	2.67	0.42
2:B:65:LYS:CD	2:B:65:LYS:HB3	2.45	0.42
2:D:1:VAL:CA	2:D:1:VAL:O	2.61	0.42
1:A:56:LYS:CE	1:A:56:LYS:CG	2.98	0.42
2:B:49:SER:CB	2:B:49:SER:HG	2.14	0.42
2:B:63:HIS:CE1	3:B:148:HEM:C4D	3.05	0.42
2:D:123:THR:HB	2:D:124:PRO:HD2	2.02	0.42
1:C:86:LEU:CD2	3:C:142:HEM:HBA2	2.49	0.41
2:B:101:GLU:CG	2:B:101:GLU:OE1	2.59	0.41
3:C:142:HEM:CMB	3:C:142:HEM:CBB	2.98	0.41
1:A:16:LYS:HG3	1:A:16:LYS:O	2.20	0.41
2:B:8:LYS:CD	2:B:8:LYS:HG3	2.21	0.41
2:D:20:VAL:HG23	2:D:20:VAL:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:N	1:A:88:ALA:N	2.67	0.41
1:C:43:PHE:N	1:C:44:PRO:CD	2.84	0.41
2:D:80:ASN:OD1	2:D:80:ASN:HB2	2.19	0.41
1:A:85:ASP:OD2	1:A:85:ASP:CB	2.62	0.41
1:C:138:SER:CB	1:C:138:SER:C	2.89	0.41
2:D:28:LEU:HD12	2:D:28:LEU:HA	1.88	0.41
1:A:60:LYS:CD	1:A:60:LYS:NZ	2.84	0.41
2:D:79:ASP:CA	2:D:79:ASP:OD2	2.68	0.41
2:D:92:HIS:HA	2:D:96:LEU:HB2	2.02	0.41
2:D:94:ASP:N	2:D:94:ASP:HB2	2.29	0.41
1:A:2:LEU:C	1:A:2:LEU:CB	2.75	0.41
2:B:77:HIS:CD2	2:B:77:HIS:HA	2.56	0.41
2:D:3:LEU:HD23	2:D:3:LEU:HA	1.72	0.41
2:D:17:LYS:O	2:D:18:VAL:CA	2.68	0.41
2:D:141:LEU:HD23	2:D:141:LEU:HA	2.03	0.40
2:B:6:GLU:N	2:B:7:GLU:N	2.65	0.40
2:B:145:TYR:C	2:B:145:TYR:N	2.62	0.40
2:B:57:ASN:HA	2:B:58:PRO:CD	2.52	0.40

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

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	139/141 (99%)	122 (88%)	14 (10%)	3 (2%)	6 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	139/141 (99%)	126 (91%)	13 (9%)	0	100 100
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	113/113 (100%)	105 (93%)	8 (7%)	14 2
1	C	113/113 (100%)	110 (97%)	3 (3%)	44 21
2	B	118/118 (100%)	107 (91%)	11 (9%)	9 1
2	D	118/118 (100%)	101 (86%)	17 (14%)	3 0
All	All	462/462 (100%)	423 (92%)	39 (8%)	11 1

All (39) 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

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Mol	Chain	Res	Type
1	A	75	ASP
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	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	41,50,50	8.85	30 (73%)	45,82,82	5.37	31 (68%)
3	HEM	C	142	1	41,50,50	7.23	27 (65%)	45,82,82	5.21	34 (75%)
3	HEM	A	142	1	41,50,50	7.96	23 (56%)	45,82,82	6.55	28 (62%)
3	HEM	B	148	2	41,50,50	5.74	21 (51%)	45,82,82	6.71	31 (68%)

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	-	5/12/54/54	-
3	HEM	C	142	1	-	3/12/54/54	-
3	HEM	A	142	1	-	4/12/54/54	-
3	HEM	B	148	2	-	3/12/54/54	-

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	148	HEM	CBA-CGA	38.20	2.39	1.50
3	A	142	HEM	CBA-CGA	35.42	2.32	1.50
3	C	142	HEM	CBA-CGA	33.89	2.29	1.50
3	A	142	HEM	CBD-CGD	25.19	2.09	1.50
3	D	148	HEM	CBD-CGD	22.04	2.01	1.50
3	B	148	HEM	O2A-CGA	-19.08	0.66	1.30
3	C	142	HEM	CBD-CGD	18.35	1.93	1.50
3	B	148	HEM	CBA-CGA	17.76	1.91	1.50
3	B	148	HEM	CBD-CGD	15.10	1.85	1.50
3	C	142	HEM	O2A-CGA	-14.41	0.82	1.30
3	D	148	HEM	O2A-CGA	13.97	1.77	1.30
3	A	142	HEM	O2D-CGD	-12.82	0.87	1.30
3	D	148	HEM	O2D-CGD	-11.87	0.90	1.30
3	D	148	HEM	O1D-CGD	11.85	1.61	1.22
3	D	148	HEM	CAA-C2A	11.33	1.68	1.52
3	D	148	HEM	C2C-C1C	9.70	1.64	1.42
3	B	148	HEM	C3C-C2C	9.33	1.53	1.40
3	A	142	HEM	C4D-C3D	-8.74	1.30	1.45
3	D	148	HEM	C3D-C2D	8.11	1.54	1.36
3	A	142	HEM	CBD-CAD	-8.08	1.26	1.52
3	C	142	HEM	O1D-CGD	-7.55	0.97	1.22
3	B	148	HEM	O1A-CGA	7.41	1.46	1.22
3	C	142	HEM	C1D-C2D	7.37	1.58	1.44
3	A	142	HEM	O2A-CGA	7.26	1.55	1.30
3	D	148	HEM	C4A-NA	-7.05	1.21	1.36
3	B	148	HEM	CMB-C2B	-6.82	1.36	1.50
3	D	148	HEM	CHD-C1D	6.78	1.60	1.41
3	A	142	HEM	O1A-CGA	6.66	1.44	1.22
3	B	148	HEM	C3B-C4B	6.60	1.58	1.44
3	D	148	HEM	CBB-CAB	-6.41	0.98	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	148	HEM	C1B-C2B	5.92	1.56	1.44
3	A	142	HEM	C1D-C2D	5.86	1.55	1.44
3	D	148	HEM	CAA-CBA	-5.80	1.23	1.52
3	C	142	HEM	CMB-C2B	-5.75	1.38	1.50
3	C	142	HEM	CAB-C3B	5.71	1.63	1.47
3	D	148	HEM	C3C-CAC	-5.71	1.36	1.47
3	D	148	HEM	C1B-C2B	-5.70	1.33	1.44
3	C	142	HEM	C1B-C2B	5.55	1.55	1.44
3	A	142	HEM	C4D-ND	5.53	1.49	1.40
3	D	148	HEM	CHA-C4D	-5.32	1.21	1.35
3	A	142	HEM	C1A-CHA	-5.18	1.26	1.41
3	A	142	HEM	FE-NB	5.18	2.22	1.96
3	B	148	HEM	CAB-C3B	5.11	1.61	1.47
3	C	142	HEM	O1A-CGA	5.06	1.38	1.22
3	C	142	HEM	C2C-C1C	5.00	1.53	1.42
3	D	148	HEM	O1A-CGA	4.97	1.38	1.22
3	C	142	HEM	O2D-CGD	-4.96	1.14	1.30
3	D	148	HEM	C4D-ND	4.96	1.48	1.40
3	D	148	HEM	CAB-C3B	4.87	1.60	1.47
3	A	142	HEM	C1D-ND	-4.86	1.28	1.38
3	A	142	HEM	CAA-CBA	-4.69	1.29	1.52
3	D	148	HEM	CMB-C2B	-4.56	1.41	1.50
3	A	142	HEM	C3B-C2B	4.53	1.46	1.37
3	B	148	HEM	CMA-C3A	-4.51	1.42	1.51
3	C	142	HEM	C3C-CAC	-4.45	1.38	1.47
3	C	142	HEM	C4D-C3D	-4.41	1.37	1.45
3	D	148	HEM	C3B-C2B	-4.36	1.28	1.37
3	B	148	HEM	CAD-C3D	4.34	1.62	1.51
3	A	142	HEM	CMD-C2D	4.23	1.59	1.50
3	B	148	HEM	C3B-C2B	-4.13	1.28	1.37
3	D	148	HEM	CMA-C3A	-4.10	1.43	1.51
3	D	148	HEM	C1B-NB	4.04	1.47	1.40
3	C	142	HEM	C4B-NB	-4.00	1.30	1.38
3	A	142	HEM	C4B-NB	3.96	1.47	1.38
3	D	148	HEM	CMC-C2C	3.95	1.61	1.51
3	A	142	HEM	C1B-C2B	-3.90	1.37	1.44
3	A	142	HEM	FE-ND	3.84	2.15	1.96
3	D	148	HEM	C4D-C3D	-3.84	1.38	1.45
3	D	148	HEM	CBD-CAD	-3.61	1.40	1.52
3	C	142	HEM	CBD-CAD	-3.53	1.40	1.52
3	C	142	HEM	CAD-C3D	3.49	1.60	1.51
3	B	148	HEM	CAA-C2A	3.32	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	CHB-C1B	-3.30	1.26	1.35
3	D	148	HEM	C1D-C2D	-3.26	1.38	1.44
3	C	142	HEM	FE-NB	3.19	2.12	1.96
3	D	148	HEM	C2A-C3A	-3.13	1.28	1.37
3	C	142	HEM	C3B-C4B	3.00	1.50	1.44
3	B	148	HEM	C4D-ND	3.00	1.45	1.40
3	C	142	HEM	FE-ND	2.96	2.11	1.96
3	B	148	HEM	CHB-C1B	2.93	1.42	1.35
3	B	148	HEM	C3C-CAC	-2.92	1.41	1.47
3	C	142	HEM	CBC-CAC	2.76	1.47	1.29
3	B	148	HEM	C4B-NB	-2.70	1.33	1.38
3	B	148	HEM	C1A-NA	2.68	1.41	1.36
3	B	148	HEM	C1D-ND	-2.67	1.33	1.38
3	C	142	HEM	CMA-C3A	-2.66	1.46	1.51
3	C	142	HEM	C4D-ND	-2.64	1.35	1.40
3	C	142	HEM	C3B-C2B	-2.58	1.32	1.37
3	C	142	HEM	C1B-NB	2.54	1.44	1.40
3	A	142	HEM	C3C-CAC	-2.40	1.42	1.47
3	A	142	HEM	CMC-C2C	-2.28	1.46	1.51
3	D	148	HEM	FE-ND	2.27	2.08	1.96
3	C	142	HEM	CHD-C1D	2.27	1.47	1.41
3	C	142	HEM	C3C-C2C	2.25	1.43	1.40
3	A	142	HEM	CMA-C3A	-2.22	1.47	1.51
3	A	142	HEM	C3D-C2D	-2.20	1.32	1.36
3	B	148	HEM	C1A-CHA	-2.19	1.34	1.41
3	B	148	HEM	C4A-NA	2.18	1.40	1.36
3	D	148	HEM	CHC-C4B	-2.09	1.35	1.41
3	C	142	HEM	C2A-C3A	-2.05	1.31	1.37
3	D	148	HEM	C4B-NB	-2.05	1.34	1.38

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	142	HEM	O2A-CGA-O1A	-24.59	62.01	123.30
3	B	148	HEM	C2C-C3C-C4C	-21.01	92.23	106.90
3	D	148	HEM	O1A-CGA-CBA	-18.35	64.13	123.08
3	A	142	HEM	O1A-CGA-CBA	-16.11	71.34	123.08
3	B	148	HEM	C4A-C3A-C2A	-15.58	96.16	107.00
3	C	142	HEM	O2A-CGA-CBA	-13.90	69.38	114.03
3	D	148	HEM	O1D-CGD-CBD	-13.58	79.45	123.08
3	A	142	HEM	O2A-CGA-CBA	-13.43	70.86	114.03
3	C	142	HEM	O1A-CGA-CBA	-13.20	80.66	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	148	HEM	O1A-CGA-CBA	-12.77	82.05	123.08
3	B	148	HEM	O2A-CGA-O1A	11.26	151.37	123.30
3	A	142	HEM	O1D-CGD-CBD	-11.10	87.41	123.08
3	A	142	HEM	CHD-C1D-ND	11.04	136.43	124.43
3	C	142	HEM	CHD-C1D-ND	10.49	135.83	124.43
3	D	148	HEM	O2A-CGA-O1A	-10.40	97.39	123.30
3	B	148	HEM	C3C-C4C-NC	10.34	130.47	110.94
3	B	148	HEM	CHA-C4D-ND	10.22	137.00	124.38
3	B	148	HEM	CAD-C3D-C2D	-9.36	110.45	127.88
3	B	148	HEM	C1D-C2D-C3D	-9.10	97.39	106.96
3	D	148	HEM	CHB-C1B-NB	-8.80	113.51	124.38
3	B	148	HEM	O1D-CGD-CBD	-8.16	96.88	123.08
3	A	142	HEM	CHA-C4D-ND	-8.02	114.47	124.38
3	D	148	HEM	CHA-C4D-ND	-7.95	114.56	124.38
3	D	148	HEM	C2C-C3C-C4C	-7.92	101.36	106.90
3	A	142	HEM	C3D-C4D-ND	-7.89	101.38	110.17
3	A	142	HEM	O2D-CGD-O1D	7.88	142.95	123.30
3	B	148	HEM	C3B-C2B-C1B	-7.75	100.74	106.49
3	C	142	HEM	CMA-C3A-C2A	7.50	139.09	124.94
3	B	148	HEM	C3D-C4D-ND	-7.37	101.96	110.17
3	B	148	HEM	CHC-C4B-NB	7.24	132.30	124.43
3	A	142	HEM	CHB-C1B-NB	-7.23	115.44	124.38
3	C	142	HEM	C4A-C3A-C2A	-7.11	102.05	107.00
3	C	142	HEM	CMB-C2B-C1B	-7.10	114.22	125.04
3	A	142	HEM	CHC-C4B-NB	6.92	131.95	124.43
3	A	142	HEM	C4D-ND-C1D	6.92	112.22	105.07
3	A	142	HEM	C2D-C1D-ND	-6.90	101.61	109.88
3	C	142	HEM	O1D-CGD-CBD	-6.68	101.63	123.08
3	C	142	HEM	C1B-NB-C4B	6.60	111.89	105.07
3	C	142	HEM	O2D-CGD-O1D	6.58	139.69	123.30
3	B	148	HEM	CMB-C2B-C1B	-6.56	115.05	125.04
3	B	148	HEM	C4B-C3B-C2B	6.52	112.29	107.11
3	C	142	HEM	CMA-C3A-C4A	-6.48	118.51	128.46
3	D	148	HEM	C1D-C2D-C3D	-6.47	100.16	106.96
3	D	148	HEM	O2D-CGD-O1D	-6.45	107.23	123.30
3	B	148	HEM	CMB-C2B-C3B	6.39	143.95	128.30
3	A	142	HEM	CHA-C4D-C3D	6.12	136.82	125.33
3	D	148	HEM	C3D-C4D-ND	-5.99	103.50	110.17
3	B	148	HEM	C2D-C1D-ND	5.97	117.03	109.88
3	C	142	HEM	C1D-C2D-C3D	-5.89	100.77	106.96
3	D	148	HEM	CHD-C1D-C2D	-5.80	115.92	124.98
3	D	148	HEM	CAD-C3D-C2D	-5.66	117.34	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	148	HEM	C4D-C3D-C2D	5.43	114.81	106.90
3	A	142	HEM	CAA-CBA-CGA	-5.42	98.57	113.76
3	C	142	HEM	C2B-C1B-NB	-5.40	103.44	109.84
3	B	148	HEM	CMA-C3A-C2A	5.38	135.08	124.94
3	D	148	HEM	C3B-C2B-C1B	5.32	110.44	106.49
3	C	142	HEM	O2D-CGD-CBD	-5.30	97.01	114.03
3	C	142	HEM	CAA-CBA-CGA	-5.27	99.00	113.76
3	A	142	HEM	C4D-C3D-C2D	5.26	114.57	106.90
3	D	148	HEM	C4A-C3A-C2A	-4.95	103.55	107.00
3	C	142	HEM	CHC-C4B-NB	4.95	129.81	124.43
3	D	148	HEM	O2A-CGA-CBA	-4.94	98.14	114.03
3	B	148	HEM	C4B-CHC-C1C	-4.87	116.13	122.56
3	B	148	HEM	O2D-CGD-CBD	-4.78	98.65	114.03
3	B	148	HEM	CHD-C1D-ND	-4.74	119.28	124.43
3	D	148	HEM	CBA-CAA-C2A	-4.74	104.54	112.62
3	B	148	HEM	O2D-CGD-O1D	4.73	135.09	123.30
3	D	148	HEM	C1B-NB-C4B	-4.71	100.20	105.07
3	C	142	HEM	CAD-C3D-C2D	-4.71	119.11	127.88
3	B	148	HEM	CAA-CBA-CGA	4.71	126.95	113.76
3	C	142	HEM	CHD-C1D-C2D	-4.65	117.71	124.98
3	B	148	HEM	CMD-C2D-C3D	4.60	138.60	126.12
3	C	142	HEM	C4D-C3D-C2D	4.55	113.52	106.90
3	C	142	HEM	CAA-C2A-C3A	-4.51	114.29	127.25
3	D	148	HEM	C4C-CHD-C1D	-4.29	116.90	122.56
3	C	142	HEM	C4D-ND-C1D	4.04	109.25	105.07
3	A	142	HEM	CMB-C2B-C1B	-4.03	118.90	125.04
3	D	148	HEM	CHA-C4D-C3D	4.01	132.84	125.33
3	C	142	HEM	C4B-C3B-C2B	3.99	110.28	107.11
3	A	142	HEM	C3B-C2B-C1B	3.99	109.44	106.49
3	A	142	HEM	C1B-NB-C4B	3.91	109.11	105.07
3	C	142	HEM	CHA-C4D-ND	-3.90	119.57	124.38
3	C	142	HEM	C4C-CHD-C1D	-3.88	117.44	122.56
3	A	142	HEM	C2C-C3C-C4C	-3.83	104.22	106.90
3	A	142	HEM	C4C-CHD-C1D	-3.80	117.54	122.56
3	B	148	HEM	CHA-C4D-C3D	-3.79	118.21	125.33
3	C	142	HEM	C2D-C1D-ND	-3.75	105.38	109.88
3	A	142	HEM	C3C-C4C-NC	-3.70	103.96	110.94
3	C	142	HEM	C2C-C3C-C4C	3.70	109.48	106.90
3	D	148	HEM	CMB-C2B-C1B	-3.63	119.51	125.04
3	B	148	HEM	O2A-CGA-CBA	-3.62	102.40	114.03
3	D	148	HEM	CMA-C3A-C2A	3.59	131.71	124.94
3	A	142	HEM	CAD-C3D-C2D	-3.54	121.28	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	142	HEM	CMB-C2B-C3B	3.49	136.85	128.30
3	D	148	HEM	C4B-CHC-C1C	3.46	127.12	122.56
3	C	142	HEM	CMD-C2D-C3D	3.31	135.11	126.12
3	D	148	HEM	C4D-C3D-C2D	3.31	111.72	106.90
3	C	142	HEM	CBB-CAB-C3B	-3.26	111.40	127.62
3	A	142	HEM	O2D-CGD-CBD	-3.05	104.23	114.03
3	B	148	HEM	CAA-C2A-C3A	-3.01	118.61	127.25
3	B	148	HEM	CHC-C4B-C3B	-2.99	119.99	124.57
3	B	148	HEM	C2B-C1B-NB	2.97	113.36	109.84
3	C	142	HEM	C3C-C4C-NC	-2.91	105.44	110.94
3	D	148	HEM	CMD-C2D-C1D	2.80	129.31	125.04
3	D	148	HEM	CHB-C1B-C2B	2.78	134.41	126.72
3	C	142	HEM	CHA-C4D-C3D	2.74	130.47	125.33
3	D	148	HEM	O2D-CGD-CBD	-2.68	105.41	114.03
3	B	148	HEM	CBD-CAD-C3D	2.61	119.88	112.63
3	D	148	HEM	CAA-CBA-CGA	2.61	121.07	113.76
3	A	142	HEM	CMC-C2C-C3C	-2.59	119.83	124.68
3	D	148	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
3	D	148	HEM	C4D-ND-C1D	2.59	107.75	105.07
3	A	142	HEM	CBA-CAA-C2A	-2.59	108.21	112.62
3	A	142	HEM	CAD-CBD-CGD	2.53	119.06	113.60
3	C	142	HEM	CHB-C1B-NB	-2.51	121.28	124.38
3	D	148	HEM	CBB-CAB-C3B	-2.47	115.34	127.62
3	C	142	HEM	C4B-CHC-C1C	2.45	125.79	122.56
3	D	148	HEM	CHC-C4B-NB	-2.34	121.89	124.43
3	D	148	HEM	C2D-C1D-ND	2.32	112.66	109.88
3	A	142	HEM	C2B-C1B-NB	-2.27	107.14	109.84
3	A	142	HEM	CHB-C1B-C2B	2.24	132.93	126.72
3	C	142	HEM	CHB-C1B-C2B	2.10	132.53	126.72
3	C	142	HEM	CAD-CBD-CGD	-2.04	109.20	113.60
3	B	148	HEM	CAD-CBD-CGD	2.01	117.94	113.60

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	148	HEM	C4D-C3D-CAD-CBD
3	A	142	HEM	C2B-C3B-CAB-CBB
3	D	148	HEM	C2B-C3B-CAB-CBB
3	C	142	HEM	CAD-CBD-CGD-O2D
3	D	148	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAD-CBD-CGD-O1D

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

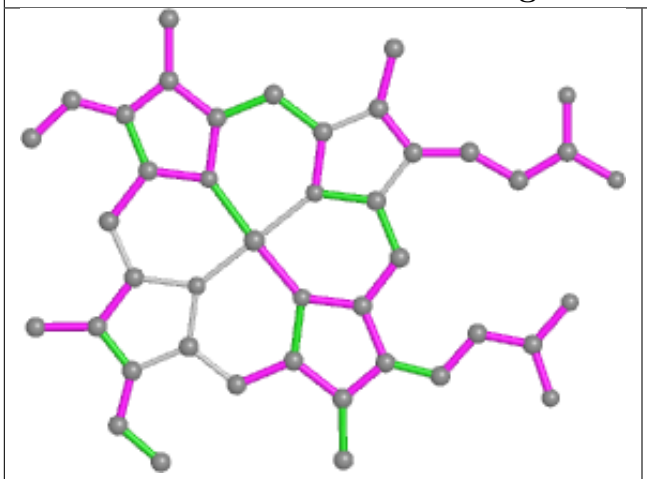
There are no ring outliers.

4 monomers are involved in 43 short contacts:

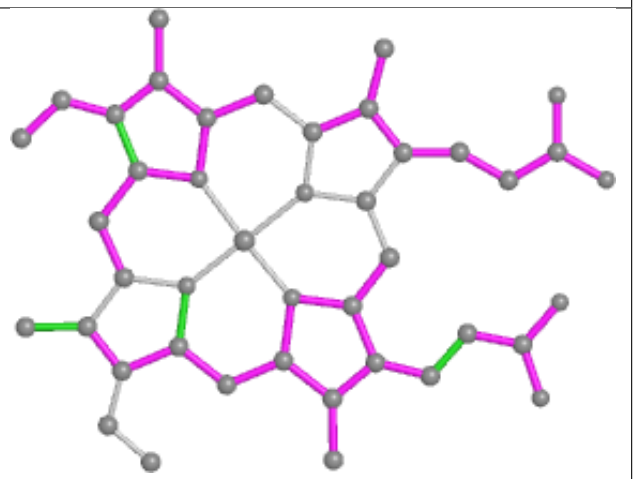
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	148	HEM	12	0
3	C	142	HEM	15	0
3	A	142	HEM	6	0
3	B	148	HEM	10	0

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

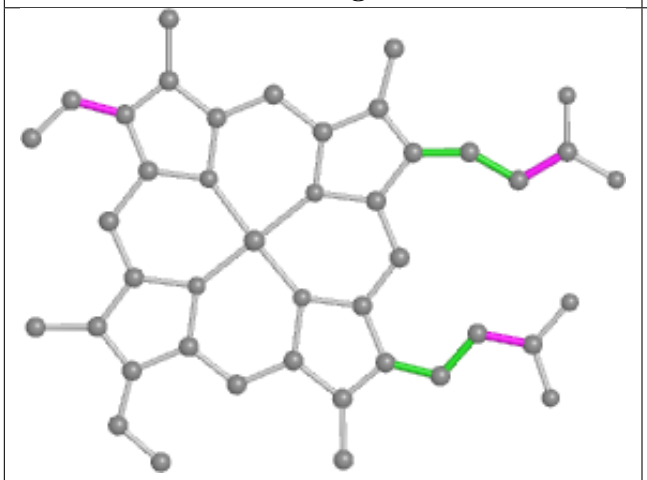
Ligand HEM D 148



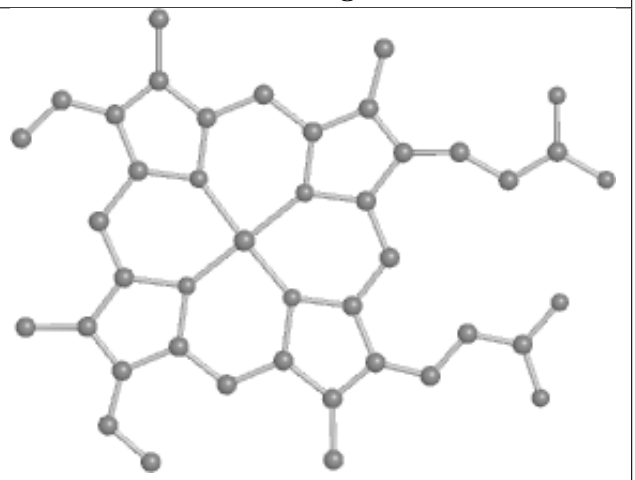
Bond lengths



Bond angles

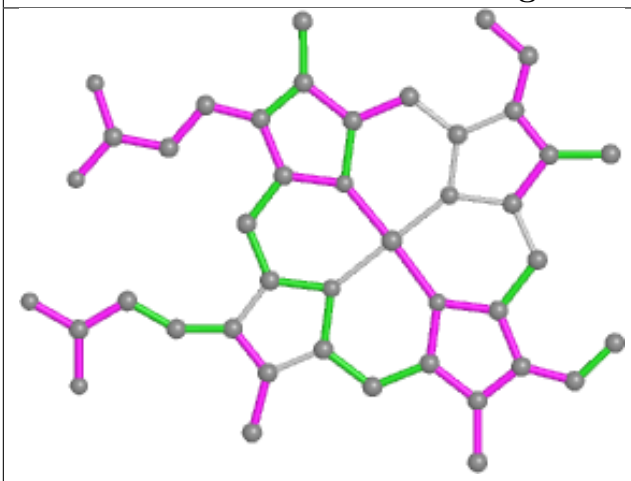


Torsions

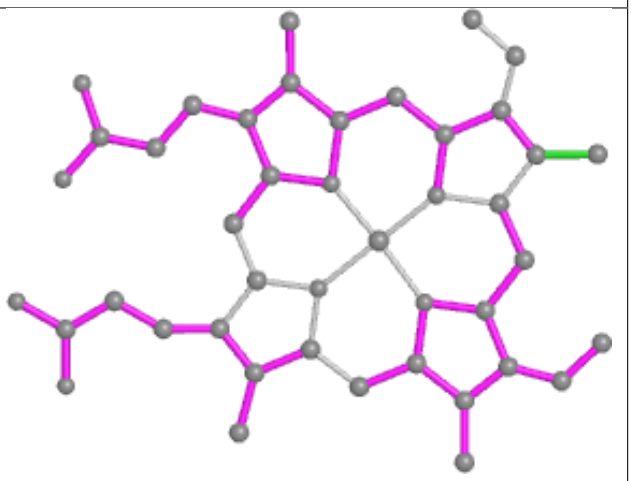


Rings

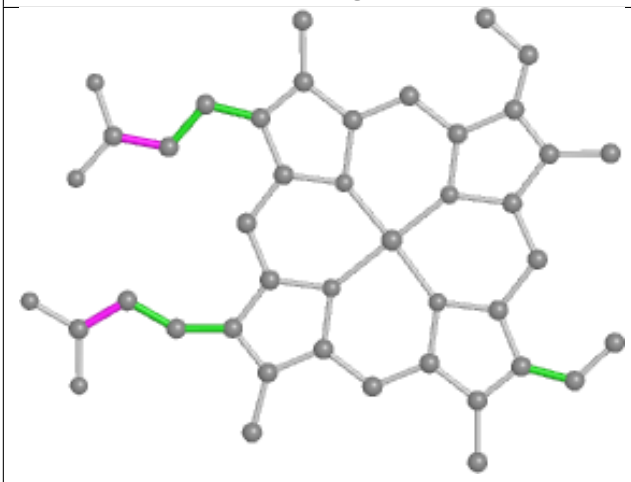
Ligand HEM C 142



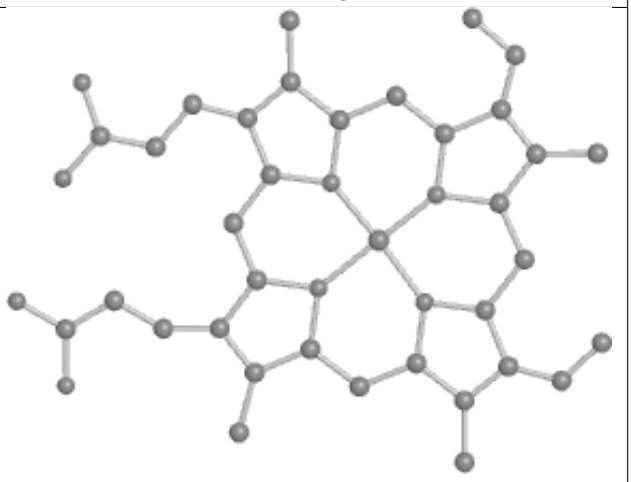
Bond lengths



Bond angles

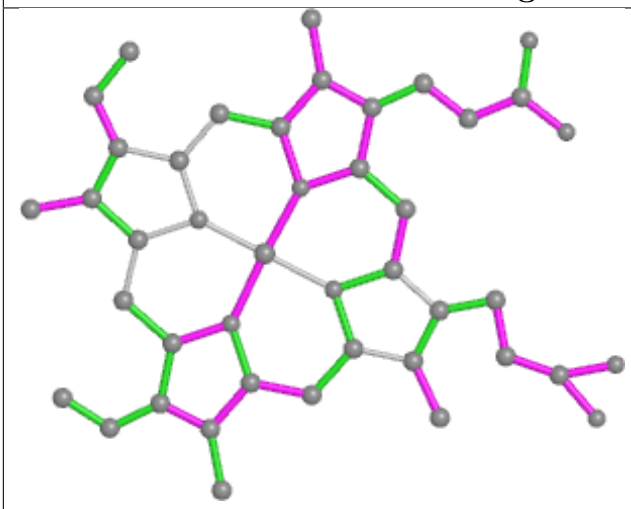


Torsions

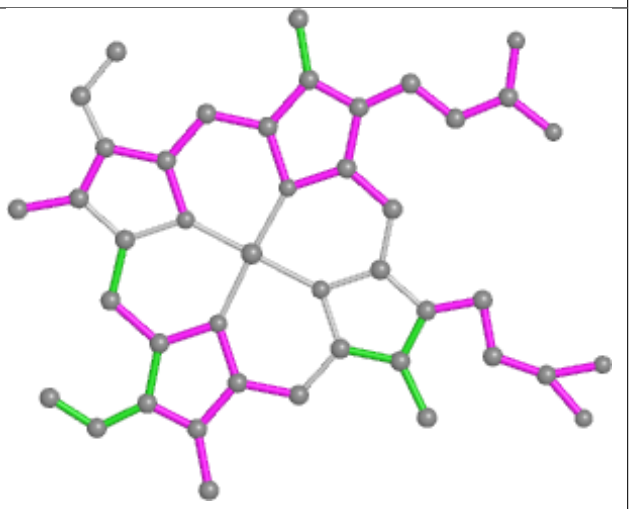


Rings

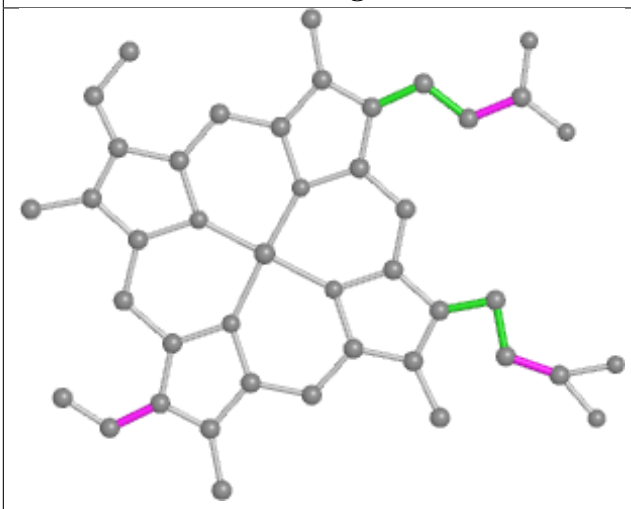
Ligand HEM A 142



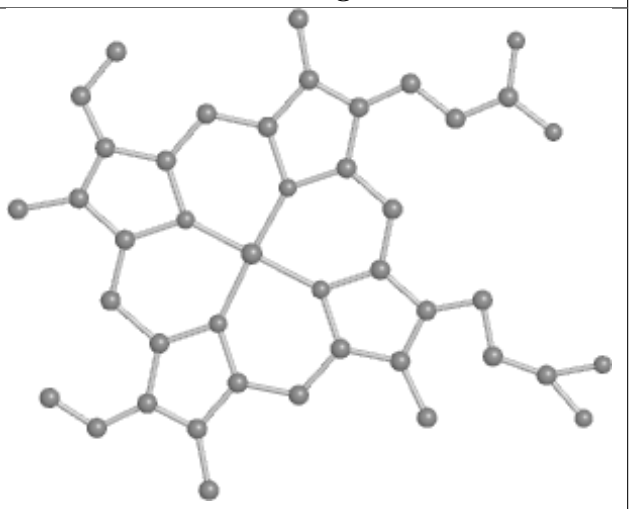
Bond lengths



Bond angles

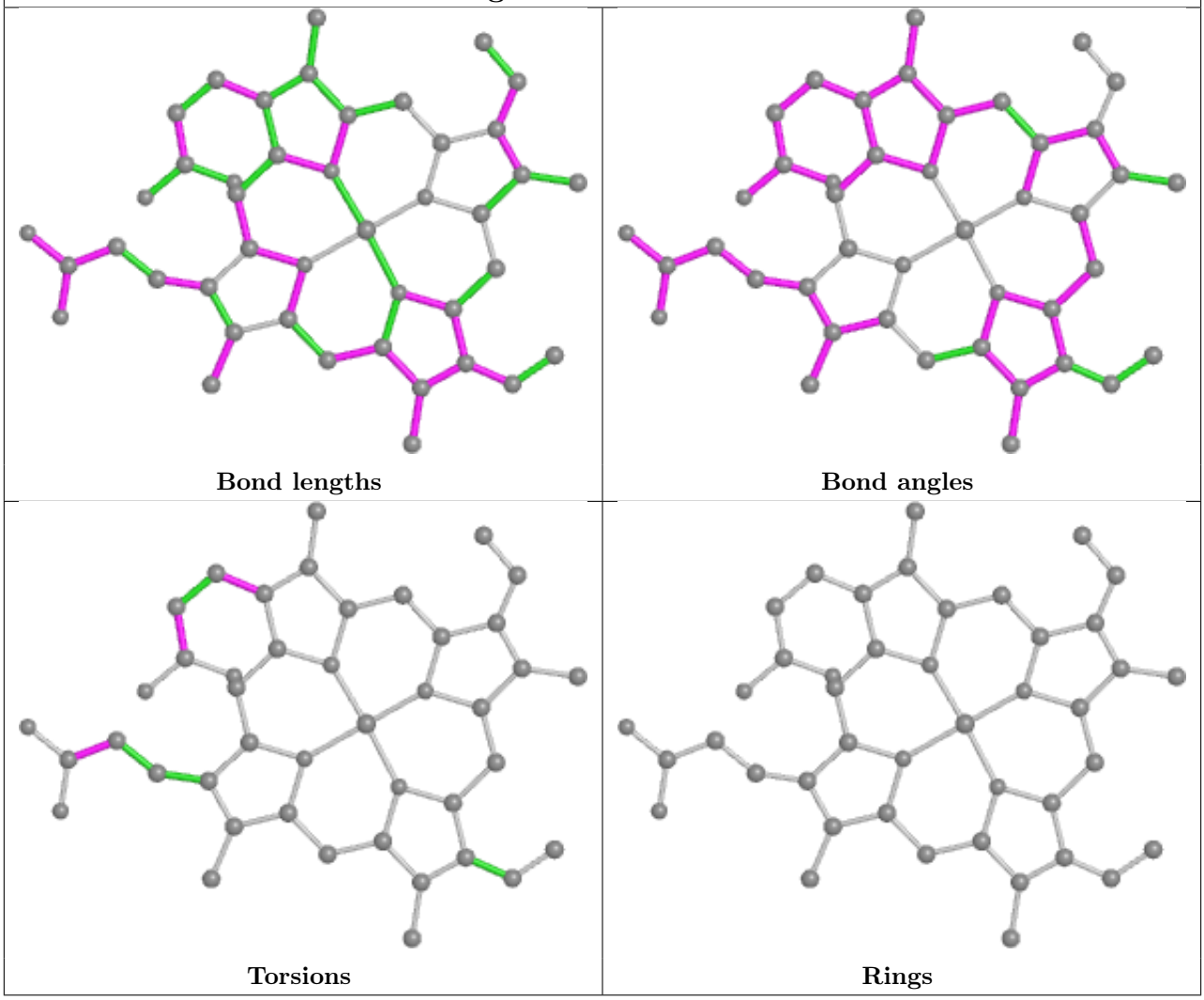


Torsions



Rings

Ligand HEM B 148



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

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

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.