Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:52 AM UTC

PDB ID	:	1HDS / pdb_00001hds
Title	:	MACROMOLECULAR STRUCTURE REFINEMENT BY RESTRAINED LEAST-SQUARES AND INTERACTIVE GRAPHICS AS APPLIED TO SICKLING DEER TYPE III HEMOGLOBIN
Authors	:	Amma, E.L.; Girling, R.L.
Deposited on	:	1979-10-01
Resolution	:	1.98 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

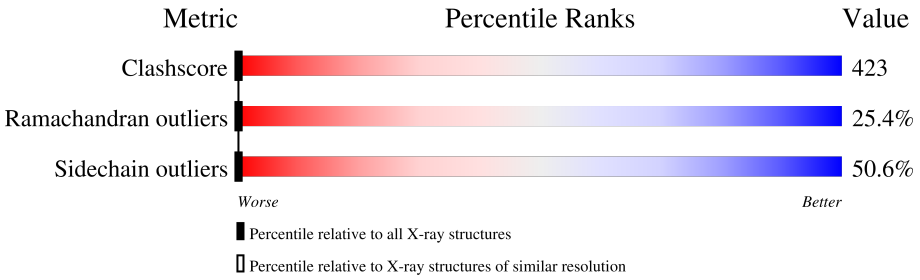
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	. 33% 65%
1	C	141	. 37% 62%
2	B	145	. 42% 56%
2	D	145	. 27% 72%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4556 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called HEMOGLOBIN S (DEOXY) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1076	684	199	192	1			
1	C	141	Total	C	N	O	S	0	0	0
			1076	684	199	192	1			

There are 32 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

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

There are 36 discrepancies between the modelled and reference sequences:

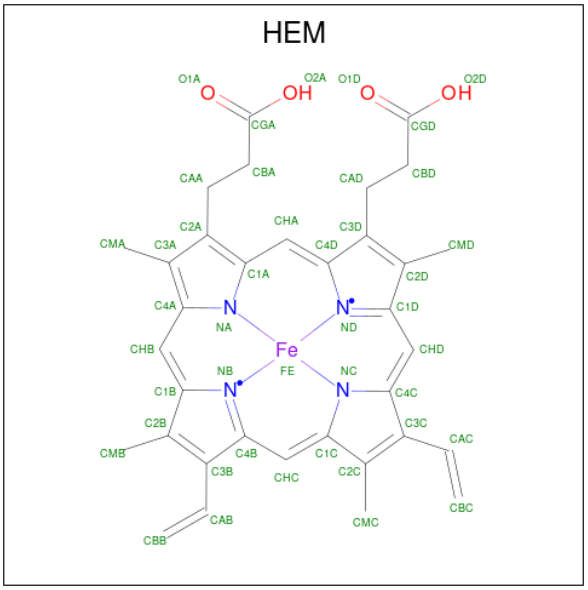
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	ASP	ASN	conflict	UNP P02074
B	25	GLN	GLU	conflict	UNP P02074
B	42	GLN	GLU	conflict	UNP P02074
B	46	ASN	ASP	conflict	UNP P02074
B	55	ASN	GLY	conflict	UNP P02074
B	71	THR	SER	conflict	UNP P02074
B	72	GLN	GLU	conflict	UNP P02074
B	86	GLN	GLU	conflict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

Continued on next page...

Continued from previous page...

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

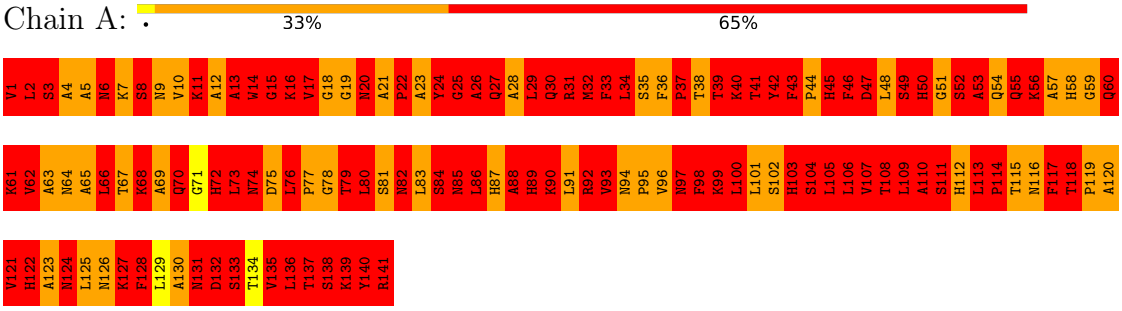
3 Residue-property plots (i)

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

Note EDS was not executed.

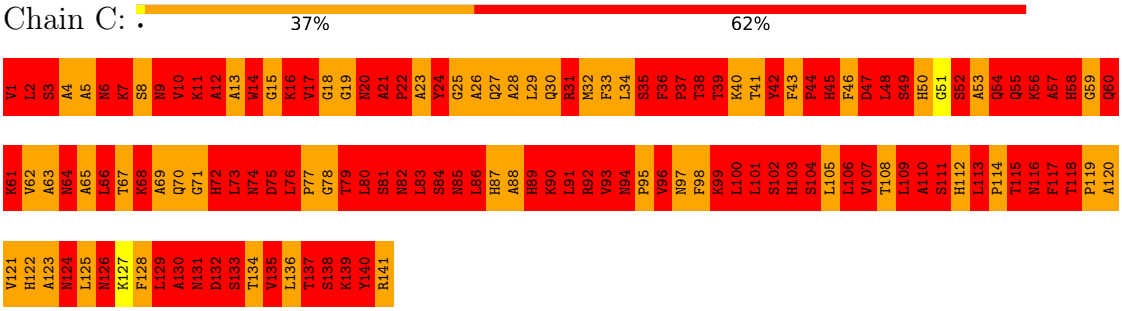
• Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)

Chain A:



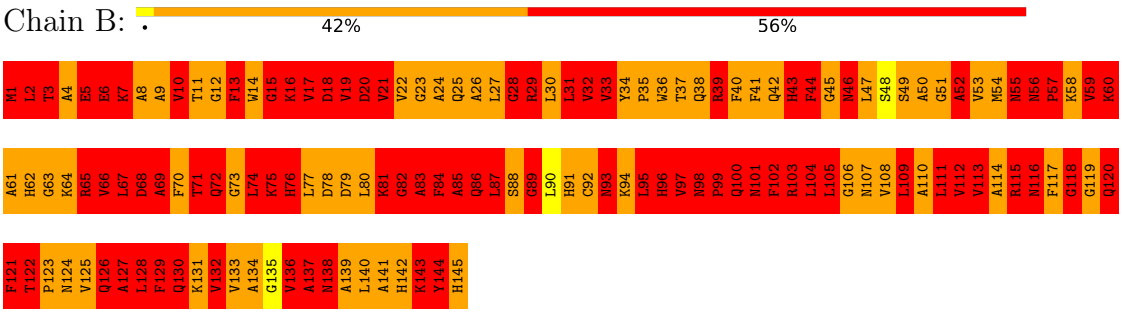
• Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)

Chain C:



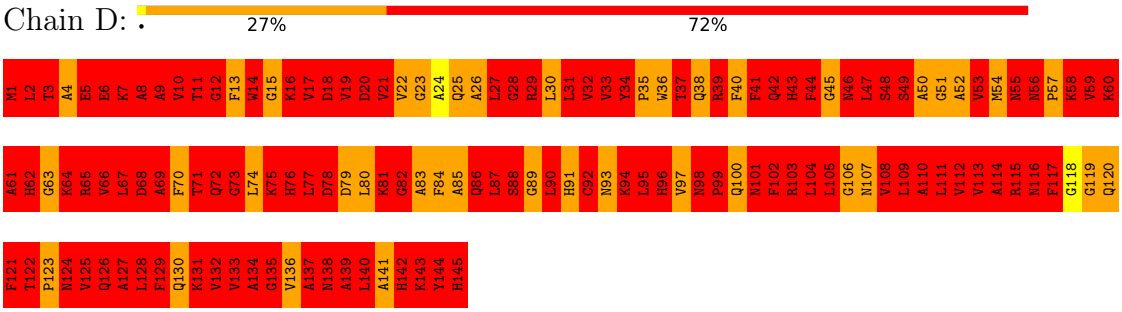
• Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain B:



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

Chain D:


27%
72%
M1 L2 T3 A4 E5 E6 K7 A8 A9 V10 T11 G12 F13 W14 G15 K16 V17 D18 V19 D20 V21 V22 G23 A24 Q25 A26 L27 G28 R29 L30 L31 V32 V33 Y34 P35 W36 T37 Q38 R39 F40 F41 Q42 H43 F44 G45 N46 L47 S48 S49 A50 G51 A52 V53 M54 N55 N56 P57 K58 V59 K60
A61 H62 G63 K64 R65 V66 L67 D68 A69 F70 T71 Q72 G73 L74 K75 H76 L77 D78 D79 L80 K81 G82 A83 F84 A85 Q86 L87 S88 G89 L90 H91 C92 N93 K94 L95 H96 V97 N98 P99 Q100 N101 F102 R103 L104 L105 G106 N107 V108 L109 A110 L111 V112 V113 A114 R115 N116 F117 G118 G119 Q120
F121 T122 P123 N124 V125 Q126 A127 L128 F129 Q130 K131 V132 V133 A134 G135 V136 A137 N138 A139 L140 A141 H142 K143 Y144 H145

4 Data and refinement statistics (i)

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

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	14.76	785/1103 (71.2%)	11.56	941/1498 (62.8%)
1	C	13.93	776/1103 (70.4%)	11.39	970/1498 (64.8%)
2	B	14.29	782/1142 (68.5%)	11.25	964/1545 (62.4%)
2	D	14.94	798/1142 (69.9%)	12.74	1002/1545 (64.9%)
All	All	14.49	3141/4490 (70.0%)	11.75	3877/6086 (63.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	9	52
1	C	2	41
2	B	2	40
2	D	6	51
All	All	19	184

All (3141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	145	HIS	CD2-NE2	81.18	2.27	1.37
1	A	72	HIS	CE1-NE2	62.40	1.95	1.32
2	D	145	HIS	CG-ND1	61.95	2.06	1.38
2	D	70	PHE	C-O	60.24	1.98	1.23
2	B	43	HIS	ND1-CE1	59.63	1.92	1.32
1	A	50	HIS	CE1-NE2	56.45	1.89	1.32
2	B	62	HIS	CB-CG	55.78	2.28	1.50
1	A	29	LEU	CA-C	-54.70	0.79	1.52
2	D	123	PRO	N-CD	53.22	2.22	1.47
2	D	75	LYS	C-O	52.44	1.90	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	43	HIS	CE1-NE2	52.40	1.84	1.32
1	C	38	THR	C-O	51.91	1.92	1.24
2	D	85	ALA	N-CA	51.18	2.08	1.46
1	A	74	ASN	C-O	50.23	1.87	1.24
1	A	109	LEU	CA-C	49.87	2.19	1.52
2	B	118	GLY	N-CA	-49.67	0.73	1.45
1	A	131	ASN	N-CA	49.41	2.05	1.46
2	B	15	GLY	C-O	48.31	1.89	1.23
2	B	71	THR	N-CA	-47.73	0.85	1.46
1	A	87	HIS	CB-CG	47.63	2.16	1.50
1	C	98	PHE	C-N	47.55	1.99	1.33
2	B	75	LYS	N-CA	47.46	2.07	1.46
2	B	145	HIS	CE1-NE2	46.64	1.79	1.32
2	D	76	HIS	CG-ND1	-46.21	0.87	1.38
1	A	124	ASN	C-O	45.57	1.76	1.24
2	D	5	GLU	N-CA	-45.38	0.60	1.46
1	C	72	HIS	CG-CD2	45.02	1.85	1.35
2	D	55	ASN	N-CA	-44.55	0.94	1.46
2	D	68	ASP	N-CA	-44.39	0.92	1.46
2	B	42	GLN	C-N	43.22	1.93	1.33
2	D	108	VAL	C-O	-43.11	0.73	1.24
2	D	7	LYS	C-O	-42.84	0.69	1.24
1	A	45	HIS	CD2-NE2	42.77	1.84	1.37
2	D	42	GLN	CD-OE1	42.75	2.04	1.23
2	D	111	LEU	C-N	-42.64	0.84	1.33
2	B	55	ASN	CA-C	42.60	2.07	1.52
2	D	8	ALA	C-O	42.44	2.08	1.23
2	B	49	SER	C-O	42.25	1.75	1.23
1	A	77	PRO	CA-C	42.18	2.12	1.52
1	A	104	SER	CB-OG	42.16	2.26	1.42
2	D	54	MET	C-O	41.89	1.73	1.24
1	A	11	LYS	C-O	-41.70	0.73	1.24
2	D	4	ALA	CA-C	41.68	2.04	1.52
2	B	79	ASP	C-O	41.25	1.75	1.24
2	B	71	THR	CA-CB	41.03	2.06	1.52
2	D	65	ARG	CZ-NH1	40.89	1.90	1.32
2	D	55	ASN	CA-CB	40.72	2.17	1.53
1	C	75	ASP	N-CA	-40.60	0.93	1.46
1	A	124	ASN	CA-CB	-40.36	0.90	1.53
1	C	112	HIS	ND1-CE1	-40.29	0.92	1.32
2	B	41	PHE	C-O	-40.21	0.74	1.23
2	B	33	VAL	CA-CB	-39.66	1.00	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	7	LYS	CA-CB	39.57	2.20	1.53
2	B	65	ARG	CZ-NH2	39.48	1.84	1.33
2	B	76	HIS	CG-ND1	39.47	1.81	1.38
1	A	4	ALA	N-CA	39.40	1.97	1.46
2	B	59	VAL	C-O	39.15	1.70	1.24
1	A	31	ARG	CA-C	-39.14	1.00	1.52
1	A	2	LEU	CA-C	39.00	2.05	1.52
1	C	89	HIS	ND1-CE1	-38.95	0.93	1.32
2	D	53	VAL	N-CA	-38.87	0.95	1.46
1	A	94	ASN	C-O	-38.86	0.74	1.24
1	C	75	ASP	CA-C	38.76	2.04	1.52
1	C	8	SER	C-O	38.69	1.72	1.24
2	B	142	HIS	N-CA	-38.41	0.95	1.46
1	C	51	GLY	C-O	-38.22	0.89	1.24
2	D	109	LEU	N-CA	-38.09	0.97	1.46
2	B	103	ARG	CZ-NH2	38.08	1.82	1.33
1	C	100	LEU	CA-CB	-38.06	0.98	1.53
2	B	43	HIS	CD2-NE2	37.85	1.79	1.37
2	D	4	ALA	N-CA	37.79	1.94	1.46
2	B	69	ALA	CA-CB	-37.76	0.89	1.53
1	C	33	PHE	C-O	37.66	1.69	1.24
1	C	137	THR	C-O	37.63	1.71	1.24
1	C	98	PHE	C-O	-37.63	0.78	1.24
2	D	76	HIS	CG-CD2	37.51	1.77	1.35
2	D	18	ASP	C-O	-37.47	0.76	1.24
2	B	11	THR	C-O	-37.47	0.80	1.24
2	D	102	PHE	N-CA	37.29	1.90	1.46
1	A	127	LYS	C-N	-36.94	0.81	1.33
2	D	110	ALA	CA-C	36.86	2.02	1.52
1	A	42	TYR	C-O	-36.82	0.77	1.24
2	B	133	VAL	C-O	-36.82	0.80	1.24
1	C	45	HIS	CD2-NE2	36.77	1.78	1.37
2	B	41	PHE	C-N	36.59	1.85	1.33
1	C	74	ASN	C-N	36.56	1.84	1.33
2	D	36	TRP	NE1-CE2	-36.50	0.97	1.37
2	D	142	HIS	ND1-CE1	36.33	1.68	1.32
2	B	7	LYS	CA-C	36.22	2.01	1.52
1	A	85	ASN	C-O	36.17	1.69	1.24
1	A	3	SER	C-O	36.09	1.68	1.23
2	D	62	HIS	CE1-NE2	36.02	1.68	1.32
1	A	89	HIS	CE1-NE2	35.89	1.68	1.32
2	D	51	GLY	C-N	35.82	1.88	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	32	VAL	N-CA	35.72	1.90	1.46
2	B	56	ASN	C-O	-35.68	0.78	1.24
1	A	30	GLN	CD-NE2	35.58	2.08	1.33
2	B	96	HIS	CE1-NE2	35.49	1.68	1.32
1	A	113	LEU	CA-C	-35.43	1.12	1.53
2	D	74	LEU	N-CA	-35.39	1.03	1.46
1	C	90	LYS	N-CA	35.33	1.90	1.46
1	A	54	GLN	C-O	35.28	1.65	1.24
1	A	53	ALA	C-O	35.22	1.68	1.24
2	B	5	GLU	N-CA	35.22	1.93	1.46
1	C	31	ARG	CA-C	35.16	1.99	1.52
1	C	130	ALA	N-CA	34.72	1.91	1.46
1	A	12	ALA	C-O	-34.63	0.80	1.24
1	A	41	THR	N-CA	-34.63	1.01	1.45
2	D	44	PHE	N-CA	-34.51	1.01	1.46
1	A	77	PRO	CA-CB	-34.32	1.05	1.53
2	D	108	VAL	N-CA	34.32	1.86	1.46
1	C	41	THR	CA-C	-34.25	1.07	1.52
2	D	84	PHE	CA-CB	34.13	1.99	1.53
1	A	56	LYS	C-O	34.06	1.63	1.24
2	B	139	ALA	C-O	34.01	1.66	1.24
2	B	1	MET	N-CA	34.00	2.10	1.46
1	C	102	SER	C-N	33.96	1.78	1.34
1	A	131	ASN	CA-CB	-33.92	0.99	1.53
1	C	93	VAL	CA-CB	33.90	2.00	1.54
2	B	45	GLY	C-O	33.88	1.69	1.23
1	A	108	THR	C-O	-33.84	0.81	1.24
2	D	138	ASN	CA-C	-33.81	1.21	1.52
2	D	43	HIS	CD2-NE2	33.78	1.75	1.37
2	B	145	HIS	CG-CD2	33.75	1.73	1.35
1	C	135	VAL	C-O	33.67	1.65	1.24
2	D	126	GLN	CD-OE1	33.59	1.87	1.23
2	D	70	PHE	N-CA	-33.58	1.03	1.46
1	A	132	ASP	CG-OD2	33.46	1.89	1.25
2	D	41	PHE	C-N	33.45	1.83	1.33
2	B	43	HIS	CG-ND1	33.45	1.75	1.38
2	B	22	VAL	CA-CB	-33.43	1.08	1.54
1	C	80	LEU	C-O	33.30	1.73	1.24
2	D	44	PHE	CA-C	33.29	1.97	1.52
2	B	110	ALA	N-CA	33.21	1.87	1.46
2	D	43	HIS	CG-CD2	33.18	1.72	1.35
1	C	59	GLY	CA-C	33.13	1.92	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	30	LEU	CA-C	33.11	1.94	1.52
1	C	20	ASN	CA-C	-33.06	1.17	1.53
2	B	103	ARG	CZ-NH1	-32.98	0.86	1.32
2	D	79	ASP	CA-CB	32.98	1.97	1.53
1	C	12	ALA	C-O	32.92	1.66	1.24
2	B	17	VAL	C-O	32.88	1.63	1.24
1	A	141	ARG	CZ-NH2	32.87	1.76	1.33
2	D	125	VAL	C-O	32.79	1.63	1.24
1	A	42	TYR	C-N	32.78	1.73	1.33
1	A	106	LEU	CA-CB	-32.71	0.98	1.53
2	D	56	ASN	C-O	32.70	1.66	1.24
2	D	57	PRO	N-CD	32.70	1.93	1.47
2	B	76	HIS	CG-CD2	-32.51	1.00	1.35
1	A	46	PHE	CA-C	-32.49	1.22	1.53
2	B	32	VAL	CB-CG2	32.41	2.59	1.52
1	A	57	ALA	C-O	-32.32	0.90	1.23
1	C	84	SER	CB-OG	32.24	2.06	1.42
1	C	130	ALA	C-O	32.24	1.64	1.24
2	D	21	VAL	N-CA	-32.24	1.08	1.46
2	B	50	ALA	CA-CB	-32.16	1.01	1.53
1	A	122	HIS	CG-ND1	-32.14	1.02	1.38
1	A	31	ARG	C-O	32.08	1.64	1.24
1	C	115	THR	C-O	31.93	1.66	1.24
2	D	64	LYS	C-O	-31.82	0.83	1.24
1	A	78	GLY	N-CA	31.76	1.91	1.45
1	A	16	LYS	C-N	31.75	1.76	1.33
2	B	4	ALA	C-O	-31.72	0.82	1.24
1	C	93	VAL	C-O	31.66	1.61	1.24
2	D	6	GLU	C-O	31.43	1.63	1.24
1	C	119	PRO	CA-CB	-31.42	1.07	1.53
1	A	82	ASN	N-CA	31.41	1.86	1.46
1	A	127	LYS	C-O	31.39	1.63	1.24
1	A	31	ARG	C-N	31.30	1.81	1.33
1	A	76	LEU	C-O	31.27	1.55	1.24
2	D	138	ASN	N-CA	31.18	1.82	1.46
1	C	87	HIS	CB-CG	-31.15	1.06	1.50
1	A	84	SER	N-CA	31.14	1.86	1.46
1	C	103	HIS	CG-CD2	-31.13	1.01	1.35
1	C	140	TYR	N-CA	-31.07	1.07	1.46
1	C	117	PHE	CA-C	31.07	1.88	1.53
1	C	74	ASN	N-CA	31.05	1.86	1.46
2	D	16	LYS	CA-CB	31.03	2.06	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	143	LYS	C-O	31.03	1.63	1.24
2	B	106	GLY	N-CA	-31.03	1.00	1.45
2	D	103	ARG	NE-CZ	31.02	1.67	1.33
1	A	58	HIS	C-N	30.96	1.71	1.33
1	A	41	THR	CB-OG1	-30.78	0.94	1.43
2	D	118	GLY	CA-C	-30.76	1.19	1.52
1	C	4	ALA	CA-CB	30.73	1.94	1.53
1	C	96	VAL	CA-C	-30.67	1.13	1.52
2	D	145	HIS	ND1-CE1	30.67	1.63	1.32
1	A	32	MET	N-CA	30.60	1.86	1.46
2	B	43	HIS	CG-CD2	30.59	1.69	1.35
1	C	121	VAL	C-N	30.58	1.74	1.34
1	A	112	HIS	CG-ND1	30.57	1.71	1.38
1	A	107	VAL	CA-CB	-30.52	1.12	1.54
2	D	57	PRO	CA-CB	30.52	1.97	1.53
2	D	87	LEU	N-CA	-30.47	1.05	1.45
2	B	74	LEU	C-N	-30.44	0.91	1.33
1	A	114	PRO	N-CD	30.41	1.90	1.47
1	C	141	ARG	C-O	30.41	1.84	1.23
1	C	44	PRO	N-CA	30.39	1.86	1.47
1	A	49	SER	CA-C	-30.36	1.12	1.52
2	B	144	TYR	CE2-CZ	30.30	2.10	1.38
1	A	103	HIS	CG-ND1	30.28	1.71	1.38
1	A	94	ASN	CA-CB	30.25	2.00	1.53
1	A	70	GLN	CD-OE1	30.12	1.80	1.23
2	D	26	ALA	CA-C	30.09	1.90	1.52
2	B	58	LYS	C-N	30.04	1.71	1.33
2	D	90	LEU	C-O	-30.00	0.87	1.24
1	C	108	THR	CA-C	29.97	1.85	1.53
1	A	59	GLY	N-CA	-29.81	1.08	1.45
1	C	6	ASN	C-N	29.79	1.75	1.33
1	C	16	LYS	N-CA	29.77	1.83	1.46
1	C	100	LEU	N-CA	29.75	1.82	1.46
1	A	9	ASN	N-CA	29.72	1.82	1.46
2	B	138	ASN	C-O	29.68	1.58	1.24
2	B	19	VAL	C-N	-29.66	0.92	1.33
2	B	103	ARG	N-CA	-29.65	1.08	1.46
2	D	116	ASN	C-N	29.64	1.72	1.33
1	C	116	ASN	CA-C	29.61	1.77	1.52
1	A	60	GLN	C-O	-29.55	0.86	1.24
1	A	38	THR	C-O	-29.49	0.87	1.24
2	D	65	ARG	C-N	-29.48	0.93	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	143	LYS	CA-C	-29.48	1.13	1.52
1	C	59	GLY	C-N	-29.45	0.98	1.33
1	A	87	HIS	CD2-NE2	29.43	1.70	1.37
1	A	14	TRP	NE1-CE2	-29.43	1.05	1.37
1	A	7	LYS	CA-C	29.39	1.90	1.52
1	C	88	ALA	C-O	29.30	1.60	1.24
2	B	71	THR	C-O	29.27	1.55	1.23
1	A	114	PRO	CA-C	-29.27	1.10	1.52
2	B	55	ASN	C-O	-29.25	0.89	1.24
2	B	45	GLY	C-N	-29.23	0.92	1.33
2	D	109	LEU	CA-C	29.21	1.92	1.52
1	C	15	GLY	C-O	-29.18	0.90	1.24
2	D	62	HIS	CG-ND1	29.13	1.70	1.38
1	C	122	HIS	CG-ND1	29.12	1.70	1.38
1	A	65	ALA	CA-C	-29.12	1.14	1.52
2	B	110	ALA	C-N	29.05	1.74	1.34
1	C	134	THR	CA-CB	29.04	1.99	1.53
2	D	14	TRP	N-CA	-29.02	1.08	1.46
1	C	107	VAL	CA-CB	-29.02	1.15	1.54
1	A	26	ALA	CA-CB	29.00	2.07	1.53
2	B	128	LEU	C-N	-28.98	0.94	1.33
2	D	20	ASP	C-N	28.91	1.70	1.33
1	A	100	LEU	N-CA	-28.78	1.09	1.46
1	C	55	GLN	C-O	28.72	1.57	1.24
2	D	11	THR	N-CA	28.68	1.83	1.46
1	C	50	HIS	ND1-CE1	28.68	1.61	1.32
1	C	59	GLY	C-O	28.67	1.60	1.23
2	B	124	ASN	C-N	28.62	1.68	1.33
2	B	115	ARG	CZ-NH1	-28.56	0.92	1.32
2	D	50	ALA	CA-C	28.53	1.91	1.52
1	C	119	PRO	CA-C	28.47	1.93	1.52
2	B	123	PRO	CA-CB	-28.45	1.14	1.53
1	C	86	LEU	CA-CB	28.41	2.10	1.53
1	C	87	HIS	CG-ND1	28.41	1.69	1.38
2	B	109	LEU	C-N	-28.37	0.95	1.34
1	C	110	ALA	C-N	-28.32	0.97	1.33
2	D	135	GLY	CA-C	-28.28	1.18	1.52
1	A	22	PRO	N-CD	28.27	1.87	1.47
2	B	82	GLY	C-N	-28.26	0.94	1.33
2	D	42	GLN	C-N	-28.21	0.94	1.33
2	B	133	VAL	CA-CB	-28.14	1.18	1.54
1	A	139	LYS	C-O	28.07	1.59	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83	LEU	C-N	-28.05	0.94	1.33
2	B	10	VAL	N-CA	28.05	1.83	1.46
2	B	142	HIS	CG-CD2	28.00	1.66	1.35
1	C	115	THR	CA-C	27.97	1.90	1.52
2	D	87	LEU	CA-CB	27.96	1.92	1.54
1	A	67	THR	C-N	-27.88	0.95	1.33
1	A	141	ARG	NE-CZ	27.77	1.63	1.33
1	A	26	ALA	C-O	27.70	1.59	1.24
1	A	12	ALA	CA-C	27.69	1.89	1.52
2	B	81	LYS	CG-CD	27.63	2.35	1.52
2	D	142	HIS	C-O	-27.63	0.91	1.23
2	B	126	GLN	CA-C	27.62	1.89	1.52
1	C	120	ALA	N-CA	-27.60	1.09	1.46
1	C	61	LYS	CA-CB	27.59	2.00	1.53
1	C	43	PHE	CG-CD1	27.56	1.96	1.38
1	C	3	SER	N-CA	-27.55	1.10	1.46
1	C	116	ASN	C-N	-27.49	0.99	1.33
1	A	34	LEU	CA-CB	27.47	1.94	1.54
2	B	63	GLY	C-O	-27.45	0.90	1.24
2	D	3	THR	N-CA	27.44	1.81	1.46
1	C	45	HIS	N-CA	27.43	1.81	1.46
2	B	62	HIS	CG-ND1	27.41	1.68	1.38
2	D	83	ALA	CA-C	27.38	1.90	1.52
2	B	23	GLY	N-CA	27.29	1.84	1.45
2	D	108	VAL	CA-C	-27.29	1.17	1.52
1	A	45	HIS	CE1-NE2	27.28	1.59	1.32
2	D	143	LYS	CA-CB	27.26	1.99	1.53
2	B	80	LEU	C-N	27.25	1.71	1.33
1	A	32	MET	C-N	27.25	1.69	1.33
1	C	57	ALA	C-O	27.21	1.58	1.24
2	D	36	TRP	N-CA	27.08	1.80	1.46
2	B	95	LEU	N-CA	27.08	1.81	1.46
2	D	136	VAL	C-O	27.07	1.57	1.24
1	C	138	SER	CB-OG	27.05	1.96	1.42
1	A	91	LEU	N-CA	27.03	1.77	1.46
1	C	22	PRO	N-CA	27.02	1.81	1.47
1	A	67	THR	N-CA	-26.99	1.10	1.46
2	D	95	LEU	CB-CG	26.98	2.07	1.53
2	B	41	PHE	CA-C	26.97	1.85	1.53
1	A	119	PRO	C-N	26.97	1.69	1.33
1	C	87	HIS	CA-C	-26.95	1.18	1.53
2	D	142	HIS	CA-CB	26.92	1.87	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	ALA	C-O	-26.92	0.90	1.23
1	C	55	GLN	N-CA	-26.89	1.14	1.46
2	D	88	SER	CA-CB	26.86	1.85	1.52
1	A	40	LYS	CA-CB	-26.86	1.08	1.53
2	D	94	LYS	C-N	-26.83	0.92	1.33
1	C	135	VAL	CA-CB	-26.75	1.17	1.54
1	C	17	VAL	CA-C	26.74	1.86	1.52
2	D	92	CYS	CA-C	26.71	1.88	1.52
2	B	96	HIS	CG-CD2	-26.71	1.06	1.35
2	D	142	HIS	CB-CG	-26.70	1.12	1.50
2	D	28	GLY	C-N	-26.68	0.95	1.33
1	C	133	SER	N-CA	-26.66	1.11	1.46
1	A	24	TYR	CA-C	-26.66	1.28	1.53
2	D	96	HIS	N-CA	26.64	1.80	1.46
1	C	44	PRO	N-CD	26.61	1.84	1.47
1	A	50	HIS	CB-CG	26.51	1.87	1.50
2	D	89	GLY	C-N	-26.49	0.96	1.33
1	A	7	LYS	C-N	-26.43	0.98	1.33
1	C	110	ALA	CA-C	26.39	2.08	1.52
1	C	89	HIS	CD2-NE2	26.35	1.66	1.37
2	D	128	LEU	CB-CG	-26.33	1.00	1.53
1	A	28	ALA	N-CA	-26.32	1.12	1.46
1	C	43	PHE	CA-CB	26.28	1.83	1.53
1	A	137	THR	N-CA	-26.25	1.12	1.45
1	C	79	THR	CA-CB	26.24	1.94	1.53
1	A	106	LEU	N-CA	26.21	1.83	1.46
2	D	55	ASN	CG-OD1	26.19	1.73	1.23
1	A	50	HIS	CG-CD2	-26.17	1.07	1.35
2	B	32	VAL	CA-C	-26.16	1.24	1.52
2	D	76	HIS	CB-CG	26.12	1.86	1.50
2	B	75	LYS	C-O	26.08	1.56	1.24
1	A	78	GLY	C-N	-26.04	0.99	1.33
2	B	25	GLN	C-N	-26.04	0.99	1.33
1	A	86	LEU	C-N	26.00	1.68	1.33
2	D	25	GLN	C-O	-26.00	0.91	1.24
1	C	104	SER	CB-OG	-25.97	0.90	1.42
2	D	63	GLY	C-N	-25.90	0.97	1.33
1	C	84	SER	CA-C	25.88	1.87	1.52
2	B	130	GLN	CD-NE2	-25.86	0.79	1.33
1	C	58	HIS	CB-CG	-25.85	1.14	1.50
1	A	108	THR	CB-OG1	-25.85	1.02	1.43
2	D	145	HIS	C-O	25.79	1.75	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	46	ASN	CA-CB	25.75	1.97	1.53
1	A	49	SER	CB-OG	25.73	1.93	1.42
1	A	103	HIS	CD2-NE2	25.72	1.66	1.37
2	B	58	LYS	N-CA	-25.72	1.15	1.46
1	A	122	HIS	ND1-CE1	25.70	1.58	1.32
1	A	75	ASP	C-O	25.70	1.52	1.24
2	D	67	LEU	CA-C	25.68	1.86	1.52
1	A	11	LYS	C-N	25.67	1.69	1.33
1	C	45	HIS	CA-C	-25.65	1.18	1.52
2	B	105	LEU	CA-C	25.62	1.87	1.52
2	D	123	PRO	CA-C	25.60	1.89	1.52
2	D	34	TYR	N-CA	25.50	1.73	1.46
1	A	102	SER	CA-C	-25.50	1.19	1.52
1	A	125	LEU	C-O	-25.48	0.94	1.24
2	B	22	VAL	CA-C	25.47	1.93	1.52
1	A	8	SER	C-O	25.46	1.64	1.23
2	D	137	ALA	C-N	-25.45	0.99	1.33
2	B	6	GLU	N-CA	25.44	1.79	1.46
2	D	68	ASP	C-N	-25.44	1.02	1.33
1	A	25	GLY	CA-C	25.43	1.87	1.51
1	C	3	SER	C-O	25.41	1.55	1.24
1	A	9	ASN	CG-OD1	25.40	1.71	1.23
1	A	74	ASN	CG-ND2	25.40	1.86	1.33
2	D	125	VAL	CA-CB	-25.39	1.20	1.54
2	D	6	GLU	C-N	-25.34	0.98	1.33
2	B	125	VAL	CA-C	25.30	1.89	1.52
1	A	50	HIS	CD2-NE2	25.30	1.65	1.37
1	A	81	SER	C-N	-25.27	0.98	1.33
2	D	37	THR	C-O	25.27	1.53	1.24
2	B	62	HIS	ND1-CE1	25.20	1.57	1.32
1	C	114	PRO	C-O	-25.14	0.91	1.24
2	B	114	ALA	N-CA	-25.12	1.15	1.46
2	B	1	MET	C-N	-25.02	0.98	1.33
2	B	96	HIS	CA-C	-24.99	1.19	1.52
1	A	109	LEU	CA-CB	-24.99	1.11	1.53
2	D	115	ARG	CA-CB	24.98	1.93	1.53
1	A	48	LEU	CA-CB	24.97	1.86	1.52
2	B	59	VAL	N-CA	-24.94	1.16	1.46
1	C	58	HIS	C-O	-24.93	0.94	1.24
2	B	137	ALA	C-O	24.89	1.55	1.24
1	C	9	ASN	CG-OD1	-24.89	0.76	1.23
1	C	111	SER	CA-C	24.88	1.86	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	39	ARG	C-N	-24.87	0.98	1.33
1	A	29	LEU	CB-CG	24.86	2.03	1.53
1	A	92	ARG	CZ-NH2	24.86	1.65	1.33
1	C	122	HIS	ND1-CE1	24.85	1.57	1.32
2	B	65	ARG	C-O	24.84	1.53	1.24
2	B	96	HIS	CD2-NE2	24.79	1.65	1.37
1	C	69	ALA	N-CA	-24.77	1.14	1.46
1	C	53	ALA	CA-CB	24.76	1.99	1.53
1	C	56	LYS	CB-CG	24.74	2.26	1.52
2	D	59	VAL	CA-C	24.72	1.84	1.52
1	A	32	MET	CA-CB	-24.64	1.09	1.53
2	D	124	ASN	CG-OD1	24.64	1.70	1.23
2	B	20	ASP	CG-OD1	24.60	1.72	1.25
2	D	3	THR	CB-OG1	24.57	1.83	1.43
1	C	74	ASN	C-O	-24.56	0.93	1.24
2	B	142	HIS	C-N	-24.55	0.99	1.33
1	C	74	ASN	CB-CG	24.54	2.13	1.52
2	B	141	ALA	C-O	24.53	1.57	1.24
2	D	103	ARG	CA-CB	24.40	1.96	1.53
1	C	3	SER	CA-CB	24.39	1.94	1.53
1	A	69	ALA	N-CA	24.35	1.76	1.46
2	B	76	HIS	CE1-NE2	-24.34	1.08	1.32
2	D	63	GLY	C-O	24.32	1.56	1.23
2	D	141	ALA	CA-C	24.30	1.86	1.52
1	A	100	LEU	C-O	24.29	1.54	1.24
1	A	85	ASN	CA-CB	-24.28	1.12	1.53
2	B	29	ARG	C-O	-24.23	0.94	1.24
1	C	111	SER	C-N	24.22	1.65	1.33
1	C	31	ARG	NE-CZ	-24.22	1.06	1.33
1	C	81	SER	C-N	24.20	1.64	1.33
1	A	71	GLY	N-CA	-24.12	1.10	1.45
2	D	57	PRO	N-CA	-24.10	1.16	1.47
1	A	99	LYS	CG-CD	24.09	2.24	1.52
1	A	77	PRO	C-N	24.09	1.68	1.33
1	C	85	ASN	CA-C	24.09	1.83	1.52
2	D	114	ALA	C-N	-24.05	1.03	1.33
1	C	95	PRO	C-O	24.04	1.54	1.24
1	C	10	VAL	C-N	24.03	1.64	1.33
2	D	96	HIS	CA-C	24.02	1.84	1.52
2	B	136	VAL	CA-C	24.01	1.81	1.52
1	C	33	PHE	C-N	24.00	1.67	1.33
1	C	40	LYS	C-N	-23.98	0.99	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASN	C-N	-23.98	1.00	1.33
1	C	28	ALA	CA-C	-23.94	1.19	1.52
2	D	73	GLY	N-CA	-23.93	1.10	1.45
1	C	94	ASN	CG-OD1	23.91	1.69	1.23
1	C	101	LEU	C-O	23.91	1.52	1.24
1	A	72	HIS	C-O	23.90	1.54	1.24
2	B	136	VAL	CA-CB	-23.90	1.25	1.54
1	C	87	HIS	CE1-NE2	23.89	1.56	1.32
1	C	6	ASN	CA-C	-23.88	1.20	1.52
2	B	70	PHE	CA-C	-23.87	1.31	1.53
2	B	102	PHE	CG-CD1	23.86	1.89	1.38
2	D	75	LYS	CD-CE	23.86	2.24	1.52
2	D	73	GLY	C-N	23.85	1.65	1.33
1	A	107	VAL	C-O	-23.83	0.95	1.24
2	B	133	VAL	C-N	-23.82	1.03	1.33
2	B	14	TRP	C-O	-23.79	0.94	1.24
1	C	30	GLN	CD-NE2	23.77	1.83	1.33
1	C	112	HIS	C-O	23.76	1.55	1.23
2	D	62	HIS	CD2-NE2	23.75	1.64	1.37
2	D	7	LYS	CA-C	-23.73	1.21	1.52
2	D	11	THR	CA-C	23.73	1.79	1.53
2	D	95	LEU	C-O	23.71	1.55	1.24
2	B	140	LEU	N-CA	-23.70	1.14	1.46
2	D	123	PRO	C-O	-23.70	0.94	1.24
2	B	115	ARG	C-N	-23.70	1.04	1.33
2	B	36	TRP	CE2-CZ2	-23.69	0.90	1.39
1	A	62	VAL	CA-CB	-23.67	1.22	1.54
2	D	131	LYS	C-N	23.66	1.62	1.33
2	D	14	TRP	C-N	-23.65	0.98	1.33
2	D	129	PHE	N-CA	23.63	1.76	1.46
2	D	76	HIS	CE1-NE2	23.63	1.56	1.32
2	B	139	ALA	C-N	23.61	1.66	1.33
1	C	28	ALA	C-N	23.57	1.66	1.33
2	D	144	TYR	C-O	23.56	1.53	1.24
2	B	83	ALA	CA-C	-23.54	1.21	1.52
2	D	70	PHE	C-N	-23.52	1.00	1.33
2	D	88	SER	CA-C	-23.52	1.27	1.53
2	D	125	VAL	CA-C	-23.52	1.22	1.52
2	B	82	GLY	C-O	23.50	1.55	1.23
2	D	144	TYR	CE1-CZ	23.49	1.94	1.38
1	A	84	SER	C-O	-23.47	0.94	1.24
1	A	89	HIS	CG-ND1	23.46	1.64	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	55	ASN	N-CA	-23.40	1.17	1.46
1	C	46	PHE	CB-CG	23.36	2.04	1.50
2	D	75	LYS	CB-CG	-23.35	0.82	1.52
1	C	92	ARG	C-O	23.35	1.54	1.23
1	A	85	ASN	CB-CG	23.34	2.10	1.52
2	B	142	HIS	ND1-CE1	23.33	1.55	1.32
2	B	1	MET	SD-CE	23.33	2.37	1.79
2	B	145	HIS	CA-CB	23.32	2.00	1.53
1	C	25	GLY	N-CA	23.31	1.75	1.45
2	D	86	GLN	CA-C	23.28	1.83	1.52
2	B	98	ASN	CG-OD1	23.27	1.67	1.23
2	B	36	TRP	CG-CD2	23.27	1.85	1.43
1	A	7	LYS	C-O	-23.26	0.97	1.24
2	B	125	VAL	N-CA	-23.26	1.16	1.46
1	A	95	PRO	N-CA	-23.24	1.16	1.47
2	B	29	ARG	CZ-NH2	-23.23	1.03	1.33
1	A	29	LEU	CA-CB	23.22	1.92	1.53
1	C	116	ASN	CG-ND2	23.21	1.81	1.33
1	C	11	LYS	N-CA	23.20	1.73	1.46
2	B	106	GLY	CA-C	23.20	1.79	1.51
2	B	101	ASN	CA-C	23.19	1.85	1.52
1	A	2	LEU	C-N	23.18	1.65	1.33
2	B	141	ALA	C-N	23.12	1.68	1.33
2	D	13	PHE	C-N	23.07	1.66	1.33
1	C	10	VAL	CA-CB	-23.05	1.23	1.54
1	C	122	HIS	CA-C	-23.04	1.20	1.52
2	B	144	TYR	C-O	23.04	1.51	1.23
2	D	35	PRO	N-CD	23.03	1.79	1.47
1	C	17	VAL	N-CA	-23.01	1.17	1.46
2	D	67	LEU	C-N	-23.01	1.03	1.33
2	D	31	LEU	CA-C	23.00	1.81	1.52
2	D	131	LYS	CA-CB	23.00	1.94	1.53
1	C	108	THR	CB-OG1	-22.99	1.06	1.43
1	C	116	ASN	CA-CB	-22.97	1.15	1.53
2	B	52	ALA	N-CA	22.96	1.75	1.46
1	C	43	PHE	N-CA	-22.89	1.21	1.46
2	D	68	ASP	CA-C	22.86	1.82	1.52
2	B	72	GLN	C-N	-22.83	1.00	1.33
1	A	112	HIS	CD2-NE2	22.82	1.62	1.37
1	A	43	PHE	CA-CB	22.80	1.77	1.53
1	C	20	ASN	N-CA	22.80	1.71	1.46
2	D	4	ALA	C-N	-22.79	1.01	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	54	MET	C-N	22.79	1.61	1.33
2	B	39	ARG	CA-C	-22.78	1.24	1.52
2	B	126	GLN	C-O	-22.74	0.95	1.24
1	C	122	HIS	CB-CG	-22.73	1.18	1.50
2	D	48	SER	C-O	22.71	1.52	1.24
2	D	130	GLN	CB-CG	-22.70	0.84	1.52
1	A	79	THR	C-O	22.70	1.50	1.24
1	A	109	LEU	C-O	-22.69	0.95	1.24
1	C	131	ASN	N-CA	-22.67	1.17	1.46
2	B	110	ALA	CA-CB	22.67	1.90	1.53
2	D	124	ASN	CA-C	22.66	1.83	1.52
1	A	43	PHE	CG-CD2	22.65	1.86	1.38
1	C	2	LEU	C-O	-22.65	0.98	1.24
1	A	119	PRO	CG-CD	22.64	2.27	1.50
2	B	16	LYS	CA-C	-22.64	1.22	1.52
2	B	102	PHE	CB-CG	-22.63	0.98	1.50
2	B	102	PHE	C-N	22.62	1.66	1.33
1	C	100	LEU	CB-CG	22.60	1.98	1.53
1	C	10	VAL	N-CA	-22.59	1.18	1.46
2	D	141	ALA	C-N	22.57	1.71	1.33
2	D	122	THR	CA-C	-22.52	1.24	1.52
1	A	126	ASN	C-O	22.52	1.50	1.24
1	A	112	HIS	C-N	22.52	1.61	1.33
1	A	130	ALA	C-O	-22.52	0.96	1.24
1	A	103	HIS	CA-CB	22.48	1.88	1.53
1	A	67	THR	C-O	22.48	1.53	1.24
2	D	138	ASN	CG-OD1	22.46	1.66	1.23
1	A	80	LEU	CB-CG	22.44	1.98	1.53
1	A	14	TRP	CZ2-CH2	22.42	1.79	1.37
2	D	66	VAL	C-O	22.38	1.50	1.24
2	B	34	TYR	N-CA	22.36	1.77	1.46
2	B	102	PHE	CA-C	-22.34	1.22	1.52
1	C	94	ASN	CA-C	-22.32	1.30	1.53
1	A	61	LYS	CA-CB	22.30	1.88	1.53
1	A	12	ALA	C-N	22.29	1.64	1.33
1	C	57	ALA	CA-C	-22.29	1.23	1.52
1	A	112	HIS	CE1-NE2	22.29	1.54	1.32
1	C	18	GLY	N-CA	22.28	1.77	1.45
1	A	71	GLY	C-O	-22.23	0.94	1.23
2	B	109	LEU	CB-CG	22.23	1.98	1.53
1	C	67	THR	CB-OG1	-22.22	1.08	1.43
2	D	120	GLN	C-O	-22.21	0.95	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	GLU	CD-OE2	22.18	1.67	1.25
1	A	34	LEU	C-O	22.18	1.51	1.24
1	A	64	ASN	CA-C	22.17	1.81	1.52
2	D	93	ASN	CA-C	22.14	1.80	1.52
1	C	17	VAL	C-N	-22.11	1.01	1.33
1	A	13	ALA	C-O	-22.10	0.96	1.24
1	C	124	ASN	CG-ND2	22.09	1.79	1.33
1	A	77	PRO	N-CA	22.08	1.75	1.47
1	C	131	ASN	CG-OD1	22.08	1.65	1.23
1	C	39	THR	N-CA	-22.01	1.16	1.46
1	C	81	SER	CA-CB	21.97	1.89	1.53
2	B	132	VAL	C-O	21.96	1.50	1.24
2	D	52	ALA	CA-CB	21.95	1.82	1.53
2	D	84	PHE	CG-CD1	21.93	1.84	1.38
2	D	71	THR	CB-OG1	21.92	1.78	1.43
1	C	44	PRO	C-O	21.92	1.52	1.24
2	B	84	PHE	CG-CD2	-21.87	0.93	1.38
2	B	40	PHE	C-O	21.86	1.52	1.24
1	C	69	ALA	CA-C	21.86	1.83	1.52
1	C	11	LYS	CA-C	-21.86	1.25	1.52
2	B	121	PHE	CA-CB	-21.85	1.22	1.52
2	D	127	ALA	CA-CB	21.82	1.81	1.53
2	B	104	LEU	N-CA	21.81	1.74	1.46
2	B	39	ARG	N-CA	-21.80	1.18	1.46
2	D	11	THR	CB-OG1	21.79	1.78	1.43
2	B	62	HIS	N-CA	21.78	1.74	1.46
2	B	27	LEU	C-O	21.77	1.49	1.24
2	D	7	LYS	CE-NZ	21.77	2.14	1.49
1	A	59	GLY	C-O	-21.76	0.97	1.23
2	B	142	HIS	CB-CG	-21.76	1.19	1.50
2	D	7	LYS	C-N	-21.74	1.02	1.33
1	A	87	HIS	ND1-CE1	21.73	1.54	1.32
2	B	92	CYS	C-N	21.71	1.64	1.33
2	B	69	ALA	N-CA	-21.70	1.18	1.46
2	B	99	PRO	C-N	21.68	1.61	1.33
1	A	47	ASP	C-O	21.63	1.51	1.24
2	B	95	LEU	CA-CB	21.60	1.90	1.53
1	A	118	THR	CA-CB	-21.60	1.19	1.53
1	A	122	HIS	C-O	21.55	1.49	1.24
2	B	51	GLY	C-N	21.55	1.63	1.33
2	B	76	HIS	N-CA	21.55	1.74	1.46
1	A	70	GLN	C-O	-21.54	0.99	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	VAL	C-N	21.53	1.61	1.33
2	B	55	ASN	C-N	21.52	1.78	1.33
2	D	119	GLY	N-CA	21.51	1.72	1.45
2	D	61	ALA	N-CA	-21.50	1.18	1.46
2	D	37	THR	CB-OG1	-21.48	1.09	1.43
1	A	74	ASN	CA-C	-21.47	1.24	1.52
1	C	47	ASP	C-O	21.46	1.50	1.24
1	A	90	LYS	C-O	21.46	1.48	1.24
2	B	66	VAL	C-N	-21.40	1.03	1.33
2	B	115	ARG	CA-CB	21.36	2.08	1.54
2	B	143	LYS	C-O	21.33	1.50	1.24
1	A	68	LYS	C-N	-21.32	1.04	1.33
1	A	105	LEU	N-CA	21.32	1.73	1.46
1	A	67	THR	CA-C	21.32	1.82	1.52
1	A	19	GLY	CA-C	21.27	1.78	1.51
1	C	134	THR	N-CA	21.24	1.71	1.46
1	C	85	ASN	N-CA	-21.23	1.17	1.46
1	C	50	HIS	CE1-NE2	21.23	1.53	1.32
2	D	76	HIS	N-CA	21.20	1.72	1.46
1	C	45	HIS	CG-ND1	21.19	1.61	1.38
2	B	36	TRP	C-O	-21.16	0.98	1.24
2	D	142	HIS	CE1-NE2	21.16	1.53	1.32
2	D	78	ASP	CA-CB	-21.14	1.11	1.53
2	D	142	HIS	CG-ND1	21.14	1.61	1.38
2	D	46	ASN	C-N	-21.12	1.00	1.33
2	B	78	ASP	CG-OD2	21.12	1.65	1.25
2	D	5	GLU	CG-CD	21.12	2.04	1.52
1	A	78	GLY	C-O	21.11	1.52	1.23
2	D	38	GLN	C-O	-21.09	0.99	1.24
1	A	21	ALA	C-N	-21.09	1.03	1.33
2	D	19	VAL	CA-CB	-21.06	1.25	1.54
1	A	51	GLY	C-O	21.06	1.52	1.23
2	B	64	LYS	CA-C	-21.01	1.24	1.52
1	A	37	PRO	N-CD	21.01	1.77	1.47
1	A	17	VAL	C-O	21.00	1.49	1.24
1	C	117	PHE	C-N	-20.99	0.90	1.33
2	D	115	ARG	CA-C	-20.99	1.31	1.53
2	D	144	TYR	CZ-OH	20.96	1.82	1.38
2	D	16	LYS	CA-C	-20.96	1.24	1.52
1	A	94	ASN	N-CA	20.95	1.75	1.46
2	B	65	ARG	N-CA	20.93	1.72	1.46
1	A	136	LEU	CA-C	20.93	1.80	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	PHE	CE2-CZ	20.90	2.01	1.38
1	A	78	GLY	CA-C	20.88	1.81	1.51
1	A	3	SER	CB-OG	20.86	1.83	1.42
1	A	126	ASN	CG-ND2	20.84	1.77	1.33
2	B	54	MET	N-CA	20.82	1.72	1.46
1	A	96	VAL	N-CA	-20.80	1.20	1.46
2	D	17	VAL	N-CA	-20.79	1.20	1.46
1	C	14	TRP	N-CA	-20.78	1.20	1.46
2	B	29	ARG	NE-CZ	20.72	1.55	1.33
2	B	23	GLY	C-O	-20.71	0.95	1.23
1	C	9	ASN	CB-CG	20.71	2.03	1.52
2	D	128	LEU	N-CA	20.71	1.73	1.46
2	D	57	PRO	C-O	-20.70	0.97	1.24
2	D	41	PHE	CA-C	-20.70	1.29	1.53
2	D	120	GLN	CD-OE1	20.69	1.62	1.23
1	A	121	VAL	C-N	20.68	1.61	1.33
1	A	128	PHE	C-O	-20.66	0.97	1.24
1	C	107	VAL	N-CA	-20.66	1.20	1.46
2	B	29	ARG	CD-NE	-20.66	1.17	1.46
2	B	136	VAL	C-O	20.64	1.44	1.24
1	C	111	SER	C-O	20.62	1.48	1.24
2	B	139	ALA	CA-CB	-20.60	1.18	1.53
1	C	103	HIS	CB-CG	20.55	1.78	1.50
1	A	55	GLN	C-N	-20.54	1.07	1.33
2	D	101	ASN	CG-OD1	20.52	1.62	1.23
1	A	27	GLN	CD-OE1	-20.51	0.84	1.23
2	B	25	GLN	N-CA	20.51	1.69	1.46
2	B	53	VAL	C-N	-20.50	1.06	1.33
1	A	120	ALA	N-CA	-20.43	1.21	1.46
2	B	2	LEU	CA-CB	20.41	1.88	1.53
2	B	24	ALA	CA-CB	20.37	1.85	1.53
2	B	58	LYS	C-O	20.36	1.47	1.24
1	C	85	ASN	CG-ND2	20.33	1.75	1.33
1	C	72	HIS	CD2-NE2	20.32	1.60	1.37
1	A	52	SER	CB-OG	20.31	1.82	1.42
2	D	45	GLY	C-O	-20.31	0.96	1.23
1	A	20	ASN	CG-ND2	20.30	1.75	1.33
1	C	44	PRO	CA-CB	-20.30	1.25	1.53
2	B	145	HIS	CD2-NE2	-20.27	1.15	1.37
1	A	80	LEU	CA-C	-20.27	1.16	1.52
1	C	77	PRO	CA-C	-20.27	1.17	1.52
2	D	132	VAL	N-CA	20.26	1.72	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	77	LEU	CB-CG	20.21	1.93	1.53
2	B	6	GLU	CA-CB	20.21	1.87	1.53
1	C	76	LEU	C-O	20.21	1.50	1.24
2	B	117	PHE	CG-CD1	20.18	1.81	1.38
1	A	116	ASN	CG-OD1	20.16	1.61	1.23
1	A	87	HIS	C-N	20.16	1.61	1.33
2	D	110	ALA	C-O	20.16	1.49	1.24
1	C	128	PHE	C-N	-20.16	1.07	1.33
2	D	67	LEU	CA-CB	20.15	1.84	1.53
2	B	134	ALA	CA-CB	-20.14	1.21	1.53
2	D	18	ASP	N-CA	-20.12	1.21	1.46
2	B	115	ARG	CZ-NH2	-20.08	1.07	1.33
2	D	4	ALA	C-O	20.05	1.48	1.24
1	C	30	GLN	N-CA	-20.05	1.20	1.46
1	A	58	HIS	CA-CB	20.04	1.85	1.53
1	A	141	ARG	CA-C	20.02	1.95	1.52
1	C	58	HIS	CE1-NE2	-20.02	1.12	1.32
2	B	91	HIS	CD2-NE2	20.02	1.59	1.37
1	A	70	GLN	CD-NE2	20.00	1.75	1.33
1	A	5	ALA	C-O	-19.95	0.97	1.24
2	B	61	ALA	CA-C	-19.95	1.26	1.52
2	B	137	ALA	N-CA	19.92	1.71	1.46
1	A	126	ASN	CA-C	19.92	1.79	1.52
1	C	55	GLN	CA-CB	19.92	1.84	1.53
2	D	130	GLN	CG-CD	19.91	2.01	1.52
1	C	132	ASP	CG-OD1	19.91	1.63	1.25
1	A	45	HIS	C-O	19.89	1.49	1.24
2	D	115	ARG	C-N	19.87	1.61	1.33
2	B	100	GLN	CA-CB	-19.85	1.22	1.53
1	A	131	ASN	CG-OD1	19.84	1.61	1.23
1	A	135	VAL	CA-C	19.80	1.77	1.52
2	B	25	GLN	C-O	19.80	1.44	1.23
1	C	19	GLY	C-O	-19.79	0.99	1.23
1	C	1	VAL	CA-C	19.79	1.94	1.52
2	B	1	MET	CG-SD	19.78	2.30	1.80
1	A	40	LYS	C-N	19.77	1.62	1.33
1	A	69	ALA	CA-C	-19.77	1.27	1.52
2	B	88	SER	CA-C	-19.76	1.26	1.52
2	D	94	LYS	C-O	19.76	1.40	1.23
2	B	19	VAL	CA-CB	19.75	1.81	1.54
2	D	86	GLN	C-O	-19.75	0.99	1.24
2	D	48	SER	CB-OG	19.70	1.81	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	117	PHE	C-O	19.70	1.51	1.24
2	D	91	HIS	CD2-NE2	-19.70	1.16	1.37
2	D	35	PRO	C-O	-19.69	0.98	1.24
1	A	18	GLY	C-O	-19.68	0.82	1.23
2	D	59	VAL	CA-CB	-19.67	1.27	1.54
1	A	60	GLN	C-N	-19.66	1.07	1.33
2	B	130	GLN	CD-OE1	19.65	1.60	1.23
1	C	67	THR	C-O	-19.63	1.01	1.24
2	D	44	PHE	CA-CB	19.61	1.86	1.53
2	D	107	ASN	N-CA	19.60	1.69	1.46
2	B	40	PHE	CA-C	19.59	1.79	1.52
2	B	20	ASP	CA-C	-19.58	1.26	1.52
1	A	140	TYR	CE2-CZ	-19.58	0.91	1.38
1	A	116	ASN	C-N	-19.56	1.07	1.33
2	D	36	TRP	CA-C	19.55	1.79	1.52
2	B	12	GLY	C-O	19.54	1.50	1.23
1	C	36	PHE	CA-CB	19.54	1.84	1.53
1	C	104	SER	CA-C	19.52	1.77	1.52
2	D	93	ASN	N-CA	-19.51	1.23	1.46
2	B	83	ALA	CA-CB	19.50	1.86	1.53
1	C	141	ARG	CG-CD	19.50	2.10	1.52
2	D	111	LEU	N-CA	-19.49	1.21	1.46
2	B	130	GLN	CA-CB	19.48	1.84	1.53
2	B	2	LEU	C-O	-19.44	0.99	1.24
2	B	128	LEU	N-CA	-19.42	1.21	1.46
2	D	88	SER	C-N	-19.40	1.05	1.33
2	D	140	LEU	C-O	-19.40	1.00	1.24
2	B	70	PHE	C-N	19.40	1.58	1.33
1	C	75	ASP	CG-OD2	19.38	1.62	1.25
1	C	29	LEU	CG-CD2	19.37	2.16	1.52
1	C	85	ASN	CG-OD1	19.36	1.60	1.23
1	C	16	LYS	C-O	-19.36	1.00	1.24
2	B	65	ARG	CA-C	-19.34	1.27	1.52
2	B	13	PHE	CA-C	19.31	1.79	1.52
1	A	40	LYS	CB-CG	19.31	2.10	1.52
2	B	64	LYS	CA-CB	-19.30	1.20	1.53
1	C	79	THR	N-CA	19.29	1.69	1.46
2	B	112	VAL	C-O	-19.28	1.01	1.24
1	C	36	PHE	CA-C	-19.28	1.28	1.52
1	A	55	GLN	CD-NE2	19.28	1.73	1.33
1	C	137	THR	N-CA	19.28	1.71	1.46
1	A	84	SER	CA-CB	-19.26	1.21	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	THR	C-N	-19.26	1.08	1.33
1	A	117	PHE	C-O	-19.26	0.92	1.23
2	B	141	ALA	N-CA	19.26	1.69	1.46
2	D	29	ARG	C-O	-19.26	1.00	1.24
1	A	87	HIS	CG-ND1	19.25	1.59	1.38
1	C	108	THR	C-N	-19.24	1.06	1.33
2	B	57	PRO	N-CD	19.24	1.74	1.47
2	B	126	GLN	CD-OE1	19.24	1.60	1.23
1	A	73	LEU	CA-CB	-19.24	1.28	1.53
2	B	66	VAL	C-O	19.23	1.47	1.24
1	C	98	PHE	CG-CD1	19.23	1.79	1.38
1	A	19	GLY	C-O	-19.22	1.06	1.24
2	D	104	LEU	CB-CG	19.22	1.91	1.53
1	A	3	SER	CA-C	-19.22	1.30	1.52
1	A	25	GLY	N-CA	-19.22	1.17	1.45
2	B	55	ASN	CG-OD1	19.18	1.59	1.23
2	D	25	GLN	C-N	19.16	1.58	1.33
1	C	128	PHE	C-O	19.15	1.48	1.24
2	D	105	LEU	C-O	19.14	1.49	1.24
1	A	60	GLN	CD-OE1	19.11	1.59	1.23
1	A	63	ALA	CA-C	-19.11	1.26	1.52
2	B	144	TYR	C-N	19.11	1.60	1.33
1	A	59	GLY	CA-C	19.10	1.73	1.52
2	D	10	VAL	CA-C	19.09	1.76	1.52
2	D	15	GLY	C-N	-19.04	1.07	1.33
2	B	64	LYS	CD-CE	19.04	2.09	1.52
1	C	130	ALA	CA-C	-19.03	1.27	1.52
2	B	98	ASN	CG-ND2	19.01	1.73	1.33
1	A	43	PHE	C-N	19.01	1.78	1.33
1	C	91	LEU	N-CA	18.99	1.69	1.46
1	A	20	ASN	CA-CB	-18.99	1.24	1.53
2	D	75	LYS	CA-CB	18.99	1.85	1.53
2	D	92	CYS	C-O	-18.96	1.00	1.24
2	D	73	GLY	C-O	-18.93	0.98	1.23
2	D	106	GLY	C-N	18.93	1.59	1.33
2	D	25	GLN	CG-CD	18.92	1.99	1.52
1	A	115	THR	C-O	-18.90	0.97	1.23
2	D	43	HIS	CE1-NE2	-18.89	1.13	1.32
1	C	14	TRP	CD1-NE1	-18.88	0.98	1.37
2	D	95	LEU	CG-CD1	18.88	2.14	1.52
2	B	131	LYS	C-N	18.84	1.59	1.33
2	B	126	GLN	CG-CD	18.83	1.99	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	ALA	C-O	-18.82	1.00	1.24
1	A	70	GLN	C-N	18.77	1.60	1.33
1	C	75	ASP	CG-OD1	18.77	1.61	1.25
1	C	70	GLN	N-CA	-18.75	1.29	1.46
1	A	119	PRO	CA-CB	18.73	1.81	1.53
2	B	72	GLN	N-CA	18.68	1.70	1.46
2	B	49	SER	CA-C	18.66	1.75	1.52
2	B	33	VAL	C-O	-18.64	1.01	1.24
1	A	10	VAL	CA-C	18.62	1.76	1.52
2	B	105	LEU	C-O	18.62	1.47	1.24
2	D	34	TYR	CE2-CZ	-18.61	0.93	1.38
1	C	82	ASN	C-O	-18.59	1.02	1.24
2	D	145	HIS	CB-CG	-18.59	1.24	1.50
1	C	111	SER	N-CA	-18.59	1.23	1.46
1	A	10	VAL	CA-CB	-18.59	1.29	1.54
2	D	14	TRP	CA-C	18.58	1.77	1.52
2	B	79	ASP	CG-OD2	18.58	1.60	1.25
1	A	99	LYS	C-O	18.57	1.47	1.24
1	A	141	ARG	CZ-NH1	18.55	1.58	1.32
1	A	41	THR	CA-CB	18.53	1.80	1.54
2	B	14	TRP	N-CA	-18.52	1.22	1.46
2	D	120	GLN	CD-NE2	18.52	1.72	1.33
2	B	104	LEU	CA-C	-18.52	1.27	1.52
1	C	106	LEU	N-CA	-18.52	1.21	1.46
1	C	87	HIS	CG-CD2	-18.51	1.15	1.35
1	C	133	SER	CA-C	18.50	1.77	1.52
2	D	38	GLN	C-N	18.48	1.58	1.34
2	D	48	SER	CA-CB	-18.46	1.22	1.53
1	A	36	PHE	CG-CD2	-18.45	1.00	1.38
2	B	63	GLY	CA-C	-18.44	1.25	1.51
2	B	107	ASN	CG-ND2	18.44	1.72	1.33
2	B	17	VAL	CA-C	18.44	1.76	1.52
1	A	39	THR	CA-C	-18.43	1.28	1.52
1	C	36	PHE	C-N	18.42	1.76	1.33
1	A	60	GLN	CA-C	18.42	1.77	1.52
1	C	93	VAL	C-N	-18.42	1.04	1.33
1	C	22	PRO	C-O	18.41	1.47	1.24
2	D	100	GLN	CA-CB	18.40	1.82	1.53
2	D	110	ALA	CA-CB	-18.40	1.22	1.53
1	C	134	THR	C-O	18.37	1.45	1.24
1	C	20	ASN	C-N	18.36	1.71	1.33
2	B	62	HIS	CG-CD2	18.34	1.56	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	61	ALA	CA-CB	18.32	1.84	1.53
2	D	8	ALA	N-CA	-18.30	1.11	1.46
2	B	87	LEU	CB-CG	-18.30	1.16	1.53
1	C	11	LYS	CD-CE	18.29	2.07	1.52
2	D	104	LEU	C-N	-18.27	1.05	1.33
2	B	138	ASN	CA-C	-18.26	1.30	1.52
2	D	43	HIS	CA-CB	18.23	1.84	1.53
2	B	7	LYS	CE-NZ	18.22	2.04	1.49
2	B	24	ALA	N-CA	18.22	1.68	1.46
2	B	97	VAL	C-O	18.18	1.49	1.23
2	D	55	ASN	C-N	-18.16	0.95	1.33
2	B	52	ALA	C-N	18.14	1.56	1.34
2	D	50	ALA	C-N	-18.13	1.07	1.33
2	B	116	ASN	CG-OD1	-18.13	0.89	1.23
2	B	6	GLU	C-O	18.12	1.46	1.24
2	B	62	HIS	CD2-NE2	18.11	1.57	1.37
1	C	108	THR	C-O	18.10	1.42	1.23
2	D	90	LEU	C-N	18.10	1.58	1.33
2	D	110	ALA	N-CA	18.10	1.69	1.46
2	B	30	LEU	C-N	18.06	1.58	1.33
1	C	53	ALA	N-CA	18.05	1.70	1.46
1	C	82	ASN	CG-OD1	18.05	1.57	1.23
1	C	11	LYS	CE-NZ	-18.04	0.95	1.49
1	A	14	TRP	CA-C	-18.03	1.28	1.52
2	D	22	VAL	CA-CB	-18.03	1.35	1.54
2	B	36	TRP	C-N	18.03	1.58	1.33
1	A	92	ARG	C-O	18.02	1.44	1.23
2	B	21	VAL	CA-C	-18.02	1.29	1.52
1	C	126	ASN	CA-C	18.02	1.75	1.52
1	C	54	GLN	CA-C	18.00	1.76	1.52
1	C	61	LYS	CE-NZ	18.00	2.03	1.49
1	A	93	VAL	C-O	-18.00	1.01	1.23
2	B	39	ARG	C-O	-17.99	0.96	1.23
1	C	28	ALA	N-CA	17.98	1.69	1.46
2	D	97	VAL	CA-CB	-17.98	1.32	1.54
1	C	112	HIS	CA-CB	-17.97	1.25	1.53
1	A	140	TYR	CE1-CZ	-17.97	0.95	1.38
1	C	87	HIS	CD2-NE2	-17.93	1.18	1.37
1	C	103	HIS	CD2-NE2	-17.93	1.18	1.37
2	D	1	MET	N-CA	17.92	1.80	1.46
1	A	137	THR	CA-CB	17.91	1.79	1.54
2	D	121	PHE	CA-CB	17.91	1.83	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	144	TYR	N-CA	-17.89	1.23	1.46
1	A	45	HIS	CA-CB	17.88	1.85	1.53
2	B	113	VAL	C-O	-17.88	1.01	1.24
1	A	80	LEU	C-O	17.87	1.50	1.24
2	B	4	ALA	N-CA	17.87	1.69	1.46
2	B	20	ASP	CG-OD2	17.86	1.59	1.25
1	C	141	ARG	CD-NE	17.86	1.71	1.46
2	D	60	LYS	C-O	17.85	1.46	1.24
2	B	46	ASN	CB-CG	17.84	1.96	1.52
1	A	98	PHE	CA-C	-17.83	1.31	1.53
1	C	97	ASN	CA-C	17.82	1.76	1.52
1	A	35	SER	CA-CB	17.81	1.79	1.54
1	C	42	TYR	C-N	-17.79	1.09	1.33
2	D	14	TRP	CG-CD1	17.78	1.81	1.36
1	C	126	ASN	CG-ND2	17.78	1.70	1.33
1	C	140	TYR	C-O	17.78	1.44	1.23
1	C	98	PHE	CE1-CZ	-17.77	0.85	1.38
1	A	8	SER	CA-C	-17.75	1.23	1.52
1	C	54	GLN	C-O	17.75	1.45	1.24
1	C	131	ASN	CA-CB	17.75	1.81	1.53
1	C	66	LEU	CB-CG	-17.75	1.18	1.53
1	A	61	LYS	CG-CD	-17.73	0.99	1.52
2	D	52	ALA	C-N	17.71	1.50	1.33
2	B	86	GLN	CD-NE2	17.70	1.70	1.33
2	B	138	ASN	N-CA	-17.70	1.25	1.46
1	A	79	THR	CB-OG1	-17.68	1.15	1.43
1	A	48	LEU	CB-CG	-17.67	1.18	1.53
2	B	128	LEU	CA-CB	17.67	1.82	1.53
1	A	116	ASN	N-CA	17.66	1.69	1.46
2	B	23	GLY	C-N	-17.65	1.11	1.33
2	D	46	ASN	N-CA	17.64	1.69	1.46
1	C	6	ASN	C-O	-17.63	1.01	1.24
1	A	14	TRP	CZ3-CH2	-17.62	0.96	1.40
2	B	37	THR	N-CA	17.62	1.69	1.46
1	C	65	ALA	C-O	17.61	1.44	1.24
1	C	2	LEU	N-CA	-17.60	1.24	1.46
2	D	31	LEU	CA-CB	17.59	1.81	1.53
1	A	36	PHE	C-O	17.58	1.46	1.24
1	A	45	HIS	CG-ND1	17.57	1.57	1.38
2	D	56	ASN	CB-CG	-17.57	1.08	1.52
2	B	111	LEU	C-O	-17.56	1.01	1.24
2	B	144	TYR	CG-CD2	17.56	1.76	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	19	VAL	CB-CG2	17.56	2.10	1.52
1	A	88	ALA	CA-C	17.55	1.76	1.52
2	B	138	ASN	CG-ND2	17.54	1.70	1.33
1	C	46	PHE	C-O	-17.53	1.03	1.23
2	D	17	VAL	CA-C	17.53	1.75	1.52
1	C	58	HIS	CG-CD2	17.51	1.55	1.35
2	D	69	ALA	CA-C	17.50	1.74	1.52
1	A	120	ALA	C-O	17.50	1.44	1.24
2	D	14	TRP	CD2-CE3	-17.50	1.12	1.40
2	D	23	GLY	CA-C	-17.48	1.31	1.52
1	A	85	ASN	CA-C	17.48	1.76	1.52
2	B	31	LEU	C-N	17.47	1.55	1.33
2	D	39	ARG	CA-CB	-17.46	1.24	1.53
1	A	97	ASN	N-CA	17.44	1.69	1.46
1	A	74	ASN	CB-CG	17.43	1.95	1.52
2	B	39	ARG	CB-CG	17.43	2.04	1.52
1	C	26	ALA	N-CA	-17.43	1.25	1.46
1	A	23	ALA	N-CA	-17.42	1.24	1.46
1	C	99	LYS	CA-CB	-17.42	1.23	1.53
1	A	108	THR	CA-CB	17.39	1.82	1.53
2	D	122	THR	CB-OG1	-17.38	1.16	1.43
2	B	87	LEU	CA-C	17.38	1.76	1.52
1	C	128	PHE	CG-CD1	-17.36	1.02	1.38
2	B	14	TRP	C-N	17.35	1.58	1.33
2	B	111	LEU	CA-CB	-17.34	1.24	1.53
2	D	32	VAL	C-N	-17.34	1.11	1.33
2	D	39	ARG	CZ-NH2	17.32	1.55	1.33
2	D	16	LYS	C-O	17.32	1.45	1.24
2	D	101	ASN	N-CA	17.32	1.68	1.46
1	C	12	ALA	CA-CB	-17.31	1.22	1.53
2	D	68	ASP	CG-OD2	17.29	1.58	1.25
2	B	34	TYR	CE2-CZ	17.29	1.79	1.38
2	D	93	ASN	CA-CB	-17.28	1.26	1.53
2	B	136	VAL	C-N	-17.28	1.09	1.33
2	D	42	GLN	CB-CG	17.27	2.04	1.52
1	C	64	ASN	CA-CB	17.25	1.82	1.53
1	C	16	LYS	C-N	17.23	1.57	1.33
2	B	42	GLN	CD-NE2	17.23	1.69	1.33
2	D	67	LEU	CB-CG	-17.23	1.19	1.53
1	C	129	LEU	CB-CG	17.21	1.87	1.53
2	D	1	MET	SD-CE	17.21	2.22	1.79
1	C	9	ASN	C-N	17.20	1.57	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	LYS	C-O	17.19	1.45	1.24
2	D	28	GLY	C-O	17.17	1.47	1.23
2	B	77	LEU	CA-CB	17.15	1.79	1.53
1	C	38	THR	CB-CG2	17.15	2.09	1.52
1	A	131	ASN	CB-CG	-17.15	1.09	1.52
1	C	82	ASN	C-N	17.15	1.57	1.33
1	C	58	HIS	C-N	-17.14	1.09	1.33
2	D	40	PHE	CE2-CZ	17.13	1.90	1.38
1	A	41	THR	CA-C	-17.12	1.30	1.52
2	D	39	ARG	CD-NE	17.12	1.70	1.46
2	B	21	VAL	CA-CB	17.10	1.77	1.54
1	A	110	ALA	C-O	17.10	1.45	1.24
2	D	1	MET	C-N	17.10	1.57	1.33
1	A	92	ARG	CZ-NH1	-17.09	1.08	1.32
2	B	8	ALA	CA-CB	17.08	1.82	1.53
1	C	132	ASP	C-O	17.07	1.44	1.24
2	B	16	LYS	N-CA	17.07	1.68	1.46
2	D	47	LEU	CA-CB	17.07	1.77	1.53
2	B	11	THR	CA-CB	17.07	1.79	1.53
2	B	7	LYS	N-CA	-17.05	1.24	1.46
1	C	15	GLY	N-CA	17.04	1.69	1.45
1	C	45	HIS	C-O	17.04	1.45	1.24
2	D	24	ALA	CA-C	-17.04	1.29	1.52
1	C	77	PRO	C-O	17.03	1.46	1.24
2	B	116	ASN	CA-C	17.01	1.74	1.52
1	C	138	SER	CA-CB	17.00	1.82	1.53
1	A	122	HIS	CA-C	16.99	1.74	1.52
2	D	100	GLN	C-N	-16.98	1.11	1.34
1	A	137	THR	C-N	16.96	1.57	1.33
2	D	18	ASP	CG-OD1	16.95	1.57	1.25
1	C	132	ASP	C-N	-16.94	1.09	1.33
2	B	26	ALA	CA-C	16.93	1.74	1.52
2	D	95	LEU	C-N	-16.92	1.10	1.33
1	C	45	HIS	C-N	16.91	1.57	1.33
2	B	128	LEU	CA-C	16.90	1.75	1.52
2	B	16	LYS	C-O	16.85	1.45	1.24
2	B	64	LYS	N-CA	16.83	1.68	1.46
2	B	42	GLN	CD-OE1	16.82	1.55	1.23
1	C	61	LYS	C-N	-16.81	1.10	1.33
1	A	136	LEU	CB-CG	-16.80	1.19	1.53
1	C	24	TYR	CD2-CE2	16.80	1.89	1.38
2	B	94	LYS	CA-C	16.79	1.74	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	140	LEU	CB-CG	-16.79	1.19	1.53
1	C	25	GLY	CA-C	-16.78	1.33	1.52
2	B	91	HIS	C-O	16.77	1.43	1.24
2	D	130	GLN	CD-OE1	16.77	1.55	1.23
1	A	128	PHE	C-N	16.76	1.56	1.34
2	D	40	PHE	C-O	16.76	1.44	1.24
1	C	70	GLN	CA-CB	16.76	2.00	1.54
2	B	108	VAL	CB-CG2	16.75	2.07	1.52
1	A	134	THR	CA-C	16.73	1.73	1.52
1	C	91	LEU	C-O	16.73	1.43	1.24
2	D	32	VAL	C-O	-16.71	1.04	1.24
1	A	122	HIS	CE1-NE2	-16.70	1.15	1.32
1	C	114	PRO	N-CD	16.70	1.71	1.47
2	D	73	GLY	CA-C	16.68	1.75	1.51
1	C	35	SER	CB-OG	16.65	1.75	1.42
2	D	88	SER	CB-OG	-16.65	1.08	1.42
2	B	38	GLN	C-O	-16.64	0.82	1.24
1	A	58	HIS	CE1-NE2	16.63	1.49	1.32
2	B	117	PHE	CD1-CE1	-16.61	0.88	1.38
2	D	119	GLY	C-N	16.60	1.56	1.33
1	C	62	VAL	CA-C	-16.59	1.31	1.52
1	C	126	ASN	C-N	-16.59	1.12	1.33
2	B	5	GLU	C-N	-16.57	1.10	1.33
2	B	140	LEU	C-N	16.56	1.55	1.33
1	C	32	MET	C-O	-16.55	1.02	1.24
1	A	12	ALA	CA-CB	16.54	1.81	1.53
2	D	94	LYS	N-CA	-16.54	1.26	1.47
1	C	45	HIS	CA-CB	16.51	1.81	1.53
2	B	103	ARG	CG-CD	16.50	2.02	1.52
1	C	119	PRO	C-O	-16.50	1.03	1.24
1	C	79	THR	C-N	16.49	1.56	1.33
2	D	2	LEU	CA-CB	16.49	1.81	1.53
2	D	74	LEU	CA-C	16.47	1.74	1.52
2	D	13	PHE	CG-CD2	-16.47	1.04	1.38
2	D	32	VAL	CA-C	16.44	1.74	1.52
1	A	1	VAL	CA-C	16.43	1.87	1.52
1	A	129	LEU	C-O	-16.43	1.03	1.24
1	C	19	GLY	CA-C	16.43	1.79	1.51
2	D	96	HIS	ND1-CE1	-16.41	1.16	1.32
1	A	100	LEU	CB-CG	16.40	1.86	1.53
1	C	10	VAL	C-O	-16.38	1.04	1.24
2	D	105	LEU	CG-CD2	-16.34	0.98	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	130	GLN	C-N	-16.34	1.13	1.33
2	D	97	VAL	C-O	-16.32	1.06	1.24
2	D	25	GLN	CA-C	-16.32	1.30	1.52
1	C	3	SER	CA-C	16.31	1.74	1.52
1	A	73	LEU	C-N	-16.27	1.10	1.33
2	B	70	PHE	N-CA	16.27	1.67	1.47
2	B	4	ALA	CA-C	16.26	1.75	1.52
2	D	47	LEU	CA-C	16.25	1.74	1.52
1	A	57	ALA	CA-CB	16.24	1.74	1.53
1	A	29	LEU	N-CA	16.24	1.67	1.46
2	D	80	LEU	C-O	-16.23	1.05	1.24
1	A	70	GLN	CG-CD	16.22	1.92	1.52
2	D	102	PHE	C-N	-16.21	1.09	1.33
2	D	50	ALA	C-O	16.19	1.43	1.24
1	C	13	ALA	N-CA	-16.19	1.25	1.46
1	A	28	ALA	CA-CB	-16.19	1.26	1.53
1	A	137	THR	C-O	-16.17	1.03	1.23
2	B	144	TYR	CA-C	-16.16	1.35	1.53
1	C	117	PHE	CB-CG	-16.16	1.13	1.50
2	B	113	VAL	CA-CB	-16.15	1.31	1.54
1	A	46	PHE	N-CA	-16.14	1.25	1.47
2	B	96	HIS	CB-CG	16.13	1.72	1.50
2	B	36	TRP	CD2-CE2	16.13	1.68	1.41
1	A	88	ALA	C-O	16.13	1.44	1.24
1	C	115	THR	N-CA	-16.11	1.24	1.46
2	B	143	LYS	CB-CG	16.11	2.00	1.52
2	B	79	ASP	CA-C	-16.09	1.31	1.52
1	C	140	TYR	C-N	16.09	1.55	1.33
1	C	1	VAL	C-O	-16.08	0.91	1.23
2	D	81	LYS	CG-CD	16.07	2.00	1.52
1	C	8	SER	CB-OG	-16.05	1.10	1.42
1	A	11	LYS	CA-C	16.05	1.74	1.52
1	A	138	SER	N-CA	16.05	1.66	1.46
2	D	95	LEU	N-CA	-16.05	1.24	1.46
1	C	84	SER	CA-CB	-16.01	1.26	1.53
2	D	34	TYR	CB-CG	-16.01	1.16	1.51
2	D	10	VAL	C-O	-15.99	1.05	1.24
1	A	104	SER	CA-CB	15.98	1.78	1.53
1	C	114	PRO	N-CA	15.98	1.67	1.47
2	D	61	ALA	CA-C	-15.96	1.31	1.52
1	A	83	LEU	C-N	-15.95	1.11	1.34
2	D	65	ARG	CB-CG	15.94	2.00	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	PHE	CA-CB	-15.93	1.28	1.53
1	C	9	ASN	CG-ND2	15.93	1.66	1.33
1	A	136	LEU	C-O	15.92	1.44	1.24
1	A	117	PHE	CA-C	15.92	1.69	1.53
2	B	25	GLN	CA-CB	-15.91	1.33	1.53
2	D	65	ARG	CA-C	15.91	1.75	1.52
1	A	10	VAL	C-N	-15.90	1.11	1.33
1	C	88	ALA	C-N	-15.88	1.10	1.33
1	C	72	HIS	CA-C	15.88	1.74	1.52
2	D	113	VAL	CA-C	-15.87	1.33	1.52
1	A	3	SER	N-CA	15.87	1.64	1.45
2	B	80	LEU	C-O	15.87	1.55	1.23
1	A	44	PRO	CA-CB	15.86	1.76	1.53
2	B	46	ASN	CG-OD1	15.85	1.53	1.23
2	B	116	ASN	C-O	15.85	1.42	1.24
2	D	140	LEU	CA-CB	-15.84	1.28	1.53
2	D	31	LEU	C-N	-15.82	1.14	1.33
2	D	49	SER	N-CA	15.82	1.66	1.46
1	C	107	VAL	C-N	-15.81	1.14	1.33
1	A	39	THR	CA-CB	-15.79	1.28	1.53
2	D	107	ASN	C-O	-15.79	1.05	1.24
2	D	131	LYS	C-O	-15.79	1.03	1.24
2	B	118	GLY	C-O	15.78	1.45	1.23
1	A	70	GLN	CB-CG	-15.76	1.05	1.52
1	A	10	VAL	C-O	15.76	1.42	1.24
1	A	20	ASN	CG-OD1	15.75	1.53	1.23
1	C	82	ASN	CG-ND2	15.75	1.66	1.33
1	A	44	PRO	C-N	-15.73	1.12	1.33
2	B	85	ALA	CA-CB	-15.73	1.26	1.53
2	D	76	HIS	CA-CB	15.72	1.73	1.53
2	B	116	ASN	C-N	-15.72	1.12	1.33
1	C	91	LEU	CA-CB	-15.71	1.28	1.53
2	D	138	ASN	C-O	15.70	1.43	1.24
1	C	117	PHE	CG-CD2	15.69	1.71	1.38
1	A	99	LYS	C-N	-15.68	1.11	1.33
2	D	130	GLN	CA-C	15.67	1.73	1.52
1	A	93	VAL	N-CA	-15.67	1.24	1.46
2	B	76	HIS	CA-C	15.67	1.73	1.52
2	B	110	ALA	CA-C	15.66	1.74	1.52
2	B	34	TYR	CD2-CE2	-15.66	0.91	1.38
1	A	82	ASN	C-O	15.65	1.43	1.24
2	B	38	GLN	C-N	-15.64	1.11	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	VAL	C-O	15.63	1.43	1.24
1	C	76	LEU	N-CA	-15.63	1.24	1.46
2	B	61	ALA	N-CA	15.60	1.66	1.46
1	A	134	THR	C-N	-15.59	1.12	1.33
1	C	124	ASN	CG-OD1	-15.57	0.94	1.23
2	D	132	VAL	C-N	-15.57	1.14	1.34
2	D	93	ASN	CG-ND2	15.56	1.66	1.33
2	B	11	THR	CB-OG1	15.56	1.68	1.43
1	A	121	VAL	N-CA	-15.54	1.26	1.46
1	C	56	LYS	CE-NZ	15.54	1.96	1.49
1	A	105	LEU	CA-C	-15.54	1.31	1.52
2	D	90	LEU	CB-CG	15.52	1.84	1.53
1	A	103	HIS	C-N	-15.52	1.13	1.33
1	A	55	GLN	CA-CB	15.52	1.81	1.53
2	D	78	ASP	CA-C	15.50	1.85	1.52
1	C	83	LEU	CA-CB	15.49	1.79	1.53
1	C	29	LEU	CB-CG	-15.48	1.22	1.53
2	D	26	ALA	CA-CB	-15.48	1.29	1.53
1	A	139	LYS	N-CA	-15.47	1.26	1.46
2	B	116	ASN	CA-CB	15.45	1.77	1.53
1	C	94	ASN	N-CA	15.45	1.63	1.45
2	D	11	THR	C-N	15.44	1.54	1.33
1	A	36	PHE	CA-C	-15.44	1.33	1.52
1	C	38	THR	CA-CB	-15.44	1.27	1.53
1	C	29	LEU	CA-CB	15.43	1.77	1.53
2	D	81	LYS	C-O	-15.43	1.04	1.24
1	C	101	LEU	N-CA	15.42	1.65	1.46
2	B	144	TYR	CZ-OH	15.41	1.70	1.38
2	B	70	PHE	CE2-CZ	15.41	1.84	1.38
1	A	61	LYS	C-N	15.41	1.54	1.33
1	C	66	LEU	C-N	15.40	1.52	1.33
1	C	24	TYR	CG-CD2	-15.39	1.07	1.39
1	C	61	LYS	CB-CG	-15.39	1.06	1.52
2	D	30	LEU	N-CA	-15.38	1.27	1.46
2	D	87	LEU	CB-CG	-15.38	1.22	1.53
2	B	18	ASP	CA-C	15.38	1.73	1.52
2	D	33	VAL	CA-CB	15.38	1.72	1.54
1	A	71	GLY	C-N	15.37	1.55	1.33
1	C	41	THR	CB-CG2	15.36	2.03	1.52
2	D	14	TRP	NE1-CE2	15.36	1.54	1.37
2	B	143	LYS	CA-C	-15.36	1.32	1.52
1	C	62	VAL	C-O	-15.35	1.05	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	GLU	CA-CB	15.34	1.79	1.53
1	C	1	VAL	CA-CB	-15.34	1.13	1.54
1	A	13	ALA	N-CA	15.33	1.66	1.46
2	D	137	ALA	C-O	-15.33	1.01	1.23
1	C	128	PHE	CE1-CZ	15.33	1.84	1.38
1	C	1	VAL	C-N	15.28	1.54	1.33
2	B	45	GLY	N-CA	15.27	1.67	1.45
2	D	41	PHE	C-O	-15.25	1.07	1.23
1	A	47	ASP	CG-OD2	-15.24	0.96	1.25
1	C	136	LEU	C-N	-15.23	1.12	1.33
1	A	94	ASN	C-N	15.22	1.56	1.33
2	B	108	VAL	CA-C	15.21	1.71	1.52
2	D	121	PHE	C-O	-15.21	1.04	1.24
1	C	101	LEU	CA-CB	15.21	1.77	1.53
1	A	101	LEU	CA-C	15.19	1.73	1.52
1	C	14	TRP	CD2-CE3	15.19	1.64	1.40
2	D	128	LEU	CA-C	15.18	1.73	1.52
1	C	84	SER	C-O	15.18	1.43	1.24
2	B	74	LEU	CB-CG	15.18	1.83	1.53
2	B	7	LYS	C-O	-15.17	1.04	1.24
2	D	91	HIS	N-CA	15.16	1.65	1.46
1	A	112	HIS	ND1-CE1	15.16	1.47	1.32
2	D	91	HIS	CG-ND1	-15.11	1.21	1.38
2	D	112	VAL	CA-C	15.10	1.74	1.52
2	B	15	GLY	CA-C	15.10	1.73	1.51
1	A	128	PHE	CD1-CE1	15.10	1.83	1.38
1	C	141	ARG	CZ-NH2	15.10	1.53	1.33
2	D	130	GLN	CD-NE2	-15.07	1.01	1.33
2	B	13	PHE	C-O	-15.07	1.04	1.24
2	B	18	ASP	C-O	-15.06	1.05	1.24
1	A	138	SER	C-O	15.05	1.43	1.24
2	B	97	VAL	CA-CB	15.04	1.75	1.54
1	C	101	LEU	C-N	-15.04	1.12	1.33
1	C	41	THR	N-CA	15.02	1.65	1.46
2	B	34	TYR	CG-CD2	15.01	1.70	1.39
1	A	84	SER	CA-C	-14.99	1.32	1.52
1	A	85	ASN	N-CA	14.99	1.65	1.46
2	B	131	LYS	CD-CE	14.98	1.97	1.52
1	C	48	LEU	C-N	14.96	1.54	1.33
1	A	37	PRO	C-N	-14.96	1.14	1.34
2	D	33	VAL	CA-C	14.96	1.71	1.52
2	B	10	VAL	C-O	-14.95	1.04	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	113	VAL	CB-CG2	14.95	2.01	1.52
2	B	101	ASN	C-N	-14.94	1.14	1.33
1	C	114	PRO	C-N	14.94	1.55	1.33
2	B	115	ARG	C-O	-14.94	1.01	1.23
2	D	90	LEU	CA-C	-14.92	1.33	1.52
1	C	134	THR	C-N	-14.90	1.14	1.33
2	D	116	ASN	N-CA	-14.90	1.26	1.46
2	D	100	GLN	CG-CD	-14.89	1.14	1.52
2	B	117	PHE	C-O	-14.89	1.06	1.24
1	C	70	GLN	C-O	14.88	1.40	1.24
1	A	75	ASP	CG-OD1	14.86	1.53	1.25
2	D	108	VAL	C-N	14.85	1.54	1.33
2	D	127	ALA	C-O	14.82	1.39	1.23
1	A	103	HIS	ND1-CE1	14.80	1.47	1.32
1	A	118	THR	CB-CG2	14.80	2.01	1.52
1	A	14	TRP	C-N	-14.79	1.11	1.33
2	B	118	GLY	C-N	-14.78	1.08	1.33
2	D	59	VAL	C-O	14.77	1.41	1.24
2	D	101	ASN	CA-C	-14.77	1.32	1.52
2	B	71	THR	C-N	-14.76	1.13	1.33
1	C	83	LEU	C-O	14.76	1.42	1.24
2	B	99	PRO	C-O	14.75	1.44	1.24
1	C	138	SER	CA-C	-14.75	1.33	1.52
1	A	46	PHE	CG-CD2	-14.74	1.07	1.38
1	A	54	GLN	CA-CB	-14.74	1.30	1.53
1	A	83	LEU	CA-C	-14.74	1.31	1.52
2	D	62	HIS	C-N	14.71	1.54	1.33
2	D	142	HIS	N-CA	14.68	1.66	1.46
1	A	77	PRO	N-CD	-14.67	1.27	1.47
1	A	112	HIS	CB-CG	-14.67	1.29	1.50
2	D	55	ASN	C-O	14.67	1.41	1.24
2	D	104	LEU	CG-CD1	14.67	2.00	1.52
1	A	129	LEU	N-CA	14.61	1.64	1.46
1	C	27	GLN	C-O	-14.61	1.05	1.24
1	C	100	LEU	CA-C	-14.61	1.35	1.53
1	A	79	THR	CA-CB	14.59	1.76	1.53
1	A	23	ALA	CA-C	-14.58	1.34	1.53
1	A	9	ASN	CA-CB	-14.57	1.30	1.53
2	D	103	ARG	CZ-NH2	14.57	1.52	1.33
1	C	117	PHE	CD2-CE2	14.57	1.82	1.38
1	A	135	VAL	N-CA	-14.56	1.28	1.46
2	B	35	PRO	C-O	-14.56	1.05	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	HIS	CE1-NE2	14.56	1.47	1.32
2	D	145	HIS	CA-C	14.55	1.83	1.52
2	B	41	PHE	N-CA	14.54	1.66	1.47
2	D	14	TRP	C-O	-14.54	1.05	1.24
2	D	14	TRP	CE2-CZ2	-14.53	1.09	1.39
1	C	107	VAL	C-O	14.52	1.41	1.24
1	A	135	VAL	CB-CG2	14.51	2.00	1.52
1	A	35	SER	C-O	-14.50	1.05	1.24
1	C	24	TYR	CB-CG	14.49	1.83	1.51
1	C	125	LEU	CA-CB	-14.48	1.28	1.53
2	D	33	VAL	N-CA	-14.48	1.29	1.46
2	B	77	LEU	CA-C	-14.45	1.29	1.52
1	C	100	LEU	C-O	14.45	1.39	1.24
1	C	78	GLY	N-CA	14.44	1.66	1.45
1	C	99	LYS	CB-CG	-14.43	1.09	1.52
2	D	12	GLY	N-CA	14.43	1.68	1.45
2	B	54	MET	CB-CG	14.41	1.95	1.52
1	A	133	SER	C-O	-14.40	1.07	1.24
2	B	134	ALA	C-N	14.40	1.54	1.33
1	A	55	GLN	CA-C	14.39	1.73	1.52
1	A	45	HIS	C-N	-14.39	1.16	1.33
1	A	115	THR	CB-OG1	14.39	1.66	1.43
2	D	79	ASP	CG-OD1	-14.38	0.98	1.25
1	C	58	HIS	CA-C	14.36	1.71	1.52
1	A	122	HIS	C-N	-14.35	1.13	1.33
1	C	37	PRO	CG-CD	14.34	1.99	1.50
2	D	103	ARG	CZ-NH1	-14.33	1.12	1.32
1	A	83	LEU	C-O	14.33	1.42	1.24
2	D	99	PRO	CA-C	-14.32	1.32	1.52
2	B	94	LYS	C-N	14.32	1.53	1.33
2	D	2	LEU	C-N	-14.31	1.13	1.33
2	B	93	ASN	CG-ND2	14.30	1.63	1.33
1	A	81	SER	CA-CB	14.29	1.76	1.53
1	A	130	ALA	CA-C	14.29	1.72	1.52
2	B	40	PHE	N-CA	14.28	1.65	1.46
1	C	53	ALA	C-N	14.28	1.54	1.33
1	A	8	SER	N-CA	14.28	1.65	1.46
1	A	82	ASN	CA-C	14.27	1.71	1.52
1	A	64	ASN	CG-OD1	-14.27	0.96	1.23
1	C	89	HIS	CG-ND1	14.27	1.53	1.38
1	C	47	ASP	C-N	-14.25	1.13	1.33
2	D	16	LYS	CB-CG	14.24	1.95	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	SER	N-CA	-14.23	1.29	1.46
1	A	61	LYS	C-O	14.23	1.40	1.24
1	C	44	PRO	CG-CD	-14.22	1.02	1.50
1	C	60	GLN	C-N	-14.21	1.13	1.33
2	B	11	THR	CB-CG2	14.20	1.99	1.52
1	A	20	ASN	CB-CG	14.20	1.87	1.52
1	C	80	LEU	CA-C	14.19	1.75	1.52
1	A	130	ALA	C-N	14.19	1.52	1.33
2	B	134	ALA	C-O	-14.18	1.07	1.24
1	A	124	ASN	CB-CG	14.17	1.87	1.52
1	A	62	VAL	C-O	14.13	1.40	1.24
1	A	119	PRO	N-CA	14.13	1.66	1.47
2	B	124	ASN	CB-CG	-14.12	1.16	1.52
2	D	53	VAL	CB-CG2	14.10	1.99	1.52
1	A	141	ARG	C-OXT	-14.09	0.95	1.23
2	B	13	PHE	N-CA	14.09	1.65	1.46
2	B	11	THR	CA-C	14.08	1.71	1.52
1	A	82	ASN	CG-OD1	14.06	1.50	1.23
1	A	91	LEU	C-O	14.06	1.40	1.24
2	B	80	LEU	CB-CG	-14.06	1.25	1.53
1	C	34	LEU	CA-CB	-14.01	1.29	1.53
1	C	136	LEU	CA-CB	14.01	1.78	1.53
1	A	65	ALA	CA-CB	14.00	1.76	1.53
2	B	19	VAL	CA-C	-14.00	1.34	1.52
1	C	19	GLY	C-N	-13.99	1.16	1.33
1	C	75	ASP	CA-CB	13.99	1.77	1.53
1	A	76	LEU	CA-C	-13.98	1.36	1.52
2	B	33	VAL	C-N	-13.97	1.04	1.33
1	C	127	LYS	C-N	13.93	1.53	1.33
2	B	92	CYS	CB-SG	13.93	2.27	1.81
1	C	35	SER	N-CA	-13.93	1.28	1.46
1	C	74	ASN	CA-C	-13.92	1.34	1.52
2	D	67	LEU	N-CA	13.91	1.63	1.46
2	D	102	PHE	C-O	13.90	1.40	1.24
2	B	25	GLN	CB-CG	-13.88	1.10	1.52
2	D	65	ARG	N-CA	-13.88	1.27	1.46
2	B	90	LEU	CA-C	13.88	1.70	1.52
1	A	39	THR	C-O	13.87	1.40	1.24
1	A	31	ARG	CB-CG	-13.84	1.10	1.52
2	D	49	SER	C-N	13.84	1.51	1.33
2	B	57	PRO	CA-C	13.83	1.72	1.52
2	B	99	PRO	N-CD	-13.83	1.28	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	ALA	CA-C	-13.83	1.33	1.52
1	C	32	MET	C-N	13.82	1.52	1.33
1	A	117	PHE	CD1-CE1	-13.82	0.97	1.38
2	D	79	ASP	CG-OD2	13.82	1.51	1.25
2	D	121	PHE	CG-CD2	-13.82	1.09	1.38
1	A	86	LEU	C-O	-13.81	1.06	1.24
1	A	6	ASN	CG-OD1	13.81	1.49	1.23
1	C	89	HIS	C-O	-13.80	1.05	1.24
1	C	87	HIS	C-O	13.80	1.41	1.23
2	D	39	ARG	CA-C	13.80	1.71	1.52
2	D	42	GLN	CA-C	-13.79	1.34	1.52
1	A	2	LEU	N-CA	13.78	1.64	1.46
2	B	66	VAL	N-CA	-13.77	1.29	1.46
2	D	86	GLN	CA-CB	13.77	1.76	1.53
1	A	136	LEU	C-N	13.76	1.53	1.33
2	B	10	VAL	CA-CB	13.76	1.71	1.54
2	D	94	LYS	CD-CE	13.75	1.93	1.52
2	D	13	PHE	N-CA	13.75	1.62	1.46
1	C	103	HIS	ND1-CE1	-13.74	1.18	1.32
2	D	19	VAL	C-N	-13.73	1.14	1.33
1	A	58	HIS	N-CA	13.72	1.62	1.46
1	C	81	SER	N-CA	-13.71	1.29	1.46
1	A	117	PHE	CG-CD1	13.71	1.67	1.38
2	D	35	PRO	N-CA	13.70	1.65	1.47
1	C	55	GLN	CG-CD	13.70	1.86	1.52
2	B	67	LEU	N-CA	13.69	1.63	1.46
1	A	2	LEU	CA-CB	13.68	1.76	1.53
2	D	89	GLY	CA-C	13.68	1.71	1.51
2	B	90	LEU	C-O	-13.67	1.08	1.24
2	D	79	ASP	N-CA	-13.66	1.22	1.46
2	B	94	LYS	CE-NZ	13.65	1.90	1.49
2	D	60	LYS	CA-CB	-13.64	1.30	1.53
2	B	41	PHE	CE2-CZ	-13.63	0.97	1.38
1	A	10	VAL	N-CA	13.63	1.63	1.46
2	B	83	ALA	C-O	13.63	1.41	1.24
1	C	71	GLY	CA-C	13.62	1.76	1.52
2	D	36	TRP	CD1-NE1	13.62	1.66	1.37
2	B	26	ALA	CA-CB	-13.61	1.32	1.53
2	D	81	LYS	N-CA	13.61	1.63	1.46
2	D	47	LEU	C-O	-13.60	1.03	1.23
1	C	63	ALA	N-CA	-13.60	1.28	1.46
1	A	122	HIS	CD2-NE2	13.59	1.52	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	PHE	CA-C	13.59	1.71	1.52
1	A	132	ASP	N-CA	13.59	1.63	1.46
1	C	132	ASP	CB-CG	-13.58	1.18	1.52
2	B	88	SER	C-O	13.58	1.41	1.24
1	A	87	HIS	CE1-NE2	-13.57	1.19	1.32
1	A	15	GLY	C-N	13.56	1.52	1.33
1	C	134	THR	CA-C	-13.55	1.35	1.52
1	C	113	LEU	C-N	13.54	1.65	1.33
2	B	90	LEU	CA-CB	-13.53	1.32	1.53
1	C	96	VAL	CB-CG2	13.52	1.97	1.52
2	D	124	ASN	C-N	13.51	1.52	1.33
1	C	67	THR	N-CA	13.51	1.62	1.46
2	B	73	GLY	N-CA	13.50	1.65	1.45
1	C	137	THR	C-N	-13.50	1.14	1.33
1	C	58	HIS	N-CA	13.49	1.62	1.46
2	D	5	GLU	CD-OE2	13.48	1.50	1.25
1	C	23	ALA	CA-CB	13.47	1.75	1.53
2	D	68	ASP	CG-OD1	-13.47	0.99	1.25
2	B	58	LYS	CA-C	-13.46	1.35	1.52
2	B	32	VAL	CA-CB	-13.46	1.38	1.53
2	B	78	ASP	CB-CG	-13.46	1.18	1.52
2	B	41	PHE	CD1-CE1	-13.45	0.98	1.38
1	A	107	VAL	N-CA	13.45	1.63	1.46
1	C	13	ALA	C-N	-13.44	1.16	1.33
1	C	48	LEU	C-O	-13.45	1.07	1.24
2	B	76	HIS	C-O	13.44	1.41	1.24
2	B	99	PRO	CG-CD	13.43	1.96	1.50
2	B	145	HIS	CG-ND1	13.43	1.53	1.38
1	A	40	LYS	CA-C	-13.40	1.34	1.52
2	B	104	LEU	C-N	-13.40	1.15	1.33
1	A	64	ASN	C-N	13.39	1.53	1.33
1	A	132	ASP	C-N	-13.38	1.17	1.33
1	C	61	LYS	CD-CE	13.37	1.92	1.52
1	C	7	LYS	CE-NZ	13.36	1.89	1.49
1	A	70	GLN	CA-C	13.34	1.69	1.52
2	B	81	LYS	N-CA	-13.34	1.21	1.46
2	D	133	VAL	CA-CB	13.33	1.70	1.54
2	D	136	VAL	N-CA	-13.33	1.29	1.46
1	A	17	VAL	N-CA	-13.32	1.29	1.46
1	A	59	GLY	C-N	-13.31	1.15	1.33
1	C	105	LEU	C-O	13.30	1.40	1.24
1	A	134	THR	C-O	-13.29	1.08	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	98	ASN	N-CA	-13.29	1.27	1.46
1	C	39	THR	C-N	13.29	1.51	1.33
1	A	44	PRO	N-CD	-13.28	1.29	1.47
1	C	95	PRO	CA-C	-13.28	1.29	1.52
2	B	73	GLY	CA-C	-13.28	1.33	1.51
1	C	102	SER	CA-CB	-13.27	1.31	1.53
2	D	96	HIS	CB-CG	-13.26	1.31	1.50
1	C	129	LEU	C-O	-13.25	1.08	1.24
1	C	122	HIS	CA-CB	-13.23	1.31	1.53
2	B	16	LYS	CB-CG	-13.22	1.12	1.52
1	C	50	HIS	CD2-NE2	13.21	1.52	1.37
1	C	135	VAL	C-N	13.21	1.51	1.33
1	A	83	LEU	N-CA	-13.20	1.28	1.46
1	A	105	LEU	C-N	13.20	1.54	1.33
1	A	63	ALA	CA-CB	13.19	1.75	1.53
1	A	125	LEU	CB-CG	-13.17	1.27	1.53
2	B	133	VAL	CB-CG2	13.17	1.96	1.52
2	B	41	PHE	CE1-CZ	13.16	1.78	1.38
1	A	38	THR	N-CA	13.15	1.62	1.46
1	A	33	PHE	CA-C	13.15	1.70	1.52
1	A	112	HIS	N-CA	-13.14	1.29	1.46
1	C	129	LEU	C-N	-13.14	1.15	1.33
2	D	144	TYR	C-N	13.12	1.51	1.33
1	A	123	ALA	C-N	13.10	1.50	1.33
2	B	97	VAL	CB-CG2	13.10	1.95	1.52
1	C	20	ASN	CG-OD1	13.10	1.48	1.23
1	C	139	LYS	CB-CG	13.08	1.91	1.52
1	C	7	LYS	C-O	13.07	1.40	1.24
2	D	44	PHE	C-N	-13.06	1.14	1.33
1	C	16	LYS	CA-CB	-13.05	1.32	1.53
2	B	122	THR	C-O	13.03	1.49	1.23
2	D	31	LEU	C-O	13.02	1.39	1.24
1	A	99	LYS	CA-C	13.00	1.70	1.52
1	A	46	PHE	C-O	13.00	1.35	1.23
2	B	74	LEU	C-O	13.00	1.40	1.24
2	B	121	PHE	CE2-CZ	-12.98	0.99	1.38
2	B	91	HIS	CA-C	12.98	1.69	1.52
2	D	144	TYR	CG-CD2	12.97	1.66	1.39
2	D	27	LEU	C-N	12.97	1.52	1.33
2	D	124	ASN	CB-CG	12.96	1.84	1.52
1	C	98	PHE	N-CA	12.95	1.61	1.46
2	D	47	LEU	CB-CG	-12.94	1.27	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	PRO	N-CD	12.93	1.65	1.47
2	D	111	LEU	C-O	-12.93	1.08	1.23
2	B	119	GLY	N-CA	12.93	1.68	1.45
1	A	112	HIS	CG-CD2	-12.92	1.21	1.35
2	D	90	LEU	N-CA	12.91	1.62	1.46
2	D	18	ASP	C-N	12.91	1.51	1.33
1	C	47	ASP	CA-C	-12.90	1.36	1.52
1	A	132	ASP	C-O	12.90	1.40	1.24
1	A	47	ASP	CA-C	12.89	1.70	1.52
1	A	27	GLN	CA-CB	-12.89	1.33	1.53
1	A	118	THR	CA-C	12.88	1.69	1.52
1	A	93	VAL	CA-CB	-12.88	1.39	1.53
2	B	116	ASN	N-CA	-12.88	1.31	1.46
1	C	22	PRO	CA-C	-12.87	1.34	1.52
1	A	14	TRP	C-O	-12.84	1.07	1.24
2	B	143	LYS	C-N	-12.84	1.16	1.33
2	B	46	ASN	CG-ND2	-12.83	1.06	1.33
1	C	90	LYS	CD-CE	12.82	1.91	1.52
1	A	22	PRO	C-O	12.79	1.41	1.24
1	C	112	HIS	CA-C	12.78	1.67	1.52
1	C	114	PRO	CB-CG	12.78	2.13	1.49
2	B	61	ALA	CA-CB	-12.77	1.31	1.53
2	D	54	MET	CA-C	-12.75	1.36	1.52
1	C	24	TYR	CE2-CZ	12.74	1.68	1.38
2	B	37	THR	CA-CB	-12.73	1.30	1.53
1	A	122	HIS	CG-CD2	-12.73	1.21	1.35
2	B	137	ALA	CA-C	-12.73	1.35	1.52
2	D	32	VAL	N-CA	12.73	1.61	1.46
2	D	135	GLY	C-O	-12.72	1.08	1.23
1	A	21	ALA	CA-C	12.71	1.68	1.52
2	D	44	PHE	CB-CG	-12.71	1.21	1.50
2	D	14	TRP	CE3-CZ3	12.70	1.76	1.38
2	D	55	ASN	CG-ND2	12.70	1.59	1.33
2	D	36	TRP	C-N	12.69	1.50	1.33
1	A	64	ASN	C-O	-12.69	1.09	1.24
2	B	27	LEU	C-N	-12.66	1.15	1.33
1	C	39	THR	CA-CB	12.66	1.76	1.53
1	C	69	ALA	C-N	-12.65	1.12	1.34
2	D	143	LYS	CD-CE	12.65	1.90	1.52
1	A	140	TYR	CG-CD1	-12.65	1.12	1.39
2	D	54	MET	CG-SD	12.65	2.12	1.80
2	B	60	LYS	CA-C	12.64	1.69	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	SER	CA-CB	-12.64	1.32	1.53
1	A	140	TYR	CB-CG	12.63	1.79	1.51
2	D	131	LYS	CA-C	12.63	1.70	1.52
2	D	129	PHE	C-N	12.61	1.50	1.33
2	B	51	GLY	C-O	12.61	1.41	1.23
1	C	56	LYS	C-O	12.61	1.39	1.24
1	A	103	HIS	CA-C	12.60	1.68	1.52
2	B	53	VAL	N-CA	12.59	1.62	1.46
2	B	87	LEU	CG-CD1	12.59	1.94	1.52
2	B	84	PHE	C-N	12.58	1.51	1.33
2	B	70	PHE	CE1-CZ	12.57	1.76	1.38
2	B	103	ARG	CA-CB	-12.57	1.32	1.53
1	A	130	ALA	N-CA	12.56	1.60	1.46
1	C	112	HIS	CE1-NE2	-12.56	1.20	1.32
2	D	81	LYS	CA-CB	12.55	1.76	1.53
1	C	55	GLN	CD-OE1	12.54	1.47	1.23
1	A	53	ALA	N-CA	12.54	1.62	1.46
1	C	37	PRO	N-CA	12.54	1.63	1.47
2	B	55	ASN	CG-ND2	12.54	1.59	1.33
1	A	51	GLY	CA-C	12.52	1.69	1.51
1	C	92	ARG	NE-CZ	12.52	1.46	1.33
1	A	63	ALA	C-N	12.52	1.50	1.33
1	C	133	SER	CA-CB	12.51	1.74	1.53
2	D	36	TRP	CA-CB	-12.51	1.32	1.53
2	D	36	TRP	CZ2-CH2	-12.50	1.13	1.37
2	D	136	VAL	CA-C	12.48	1.70	1.52
2	D	1	MET	C-O	12.48	1.48	1.23
2	D	129	PHE	CA-C	-12.48	1.35	1.52
2	B	29	ARG	CA-C	-12.48	1.35	1.52
2	B	40	PHE	CG-CD2	-12.46	1.12	1.38
2	B	36	TRP	CD2-CE3	-12.45	1.20	1.40
2	B	56	ASN	C-N	12.45	1.62	1.33
2	B	134	ALA	CA-C	12.45	1.70	1.52
1	A	138	SER	CB-OG	12.44	1.67	1.42
1	C	37	PRO	CA-CB	12.44	1.71	1.53
1	C	32	MET	CA-CB	12.43	1.76	1.53
2	B	57	PRO	C-O	12.43	1.40	1.24
2	D	58	LYS	CE-NZ	12.42	1.86	1.49
1	A	87	HIS	CA-C	12.41	1.68	1.52
1	A	122	HIS	N-CA	-12.40	1.31	1.46
2	B	18	ASP	CB-CG	12.39	1.83	1.52
2	D	78	ASP	CB-CG	12.39	1.83	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	74	LEU	CG-CD1	12.39	1.93	1.52
2	B	56	ASN	CB-CG	-12.38	1.21	1.52
1	A	104	SER	N-CA	-12.38	1.31	1.46
1	C	108	THR	CA-CB	-12.38	1.37	1.53
2	D	55	ASN	CB-CG	-12.38	1.21	1.52
2	D	40	PHE	CD2-CE2	-12.37	1.01	1.38
1	A	3	SER	CA-CB	12.37	1.75	1.53
2	B	140	LEU	CG-CD2	12.36	1.93	1.52
2	D	122	THR	N-CA	12.36	1.63	1.46
2	D	77	LEU	N-CA	-12.36	1.30	1.46
1	A	61	LYS	N-CA	12.34	1.61	1.46
1	C	27	GLN	C-N	12.34	1.52	1.33
1	C	118	THR	CB-OG1	12.34	1.63	1.43
1	A	6	ASN	CB-CG	-12.33	1.21	1.52
1	A	116	ASN	C-O	-12.32	1.07	1.24
2	B	119	GLY	C-O	12.32	1.37	1.23
1	C	14	TRP	CA-C	12.31	1.69	1.52
1	A	141	ARG	N-CA	-12.30	1.22	1.46
2	B	41	PHE	CA-CB	12.28	1.72	1.52
1	C	17	VAL	CA-CB	-12.28	1.37	1.54
2	D	41	PHE	CD2-CE2	12.28	1.75	1.38
2	D	83	ALA	CA-CB	12.28	1.73	1.53
2	B	64	LYS	C-O	-12.26	1.08	1.24
2	B	35	PRO	C-N	12.25	1.51	1.33
2	D	60	LYS	CA-C	12.25	1.69	1.52
1	A	50	HIS	CA-C	-12.21	1.36	1.52
2	B	84	PHE	CA-CB	12.20	1.73	1.53
2	D	22	VAL	N-CA	-12.20	1.32	1.46
2	D	86	GLN	CD-OE1	12.20	1.46	1.23
2	D	70	PHE	CD2-CE2	-12.19	1.02	1.38
1	A	36	PHE	CB-CG	12.19	1.78	1.50
2	B	47	LEU	C-O	12.19	1.39	1.23
2	B	125	VAL	C-N	-12.18	1.16	1.33
1	A	128	PHE	CG-CD2	12.18	1.64	1.38
2	B	43	HIS	CA-C	12.16	1.78	1.52
1	A	27	GLN	CA-C	12.14	1.69	1.52
1	A	117	PHE	CG-CD2	12.14	1.64	1.38
2	D	111	LEU	CG-CD1	-12.13	1.12	1.52
1	A	71	GLY	CA-C	-12.13	1.34	1.51
1	C	30	GLN	CG-CD	12.13	1.82	1.52
1	A	7	LYS	CB-CG	-12.13	1.16	1.52
1	A	70	GLN	CA-CB	-12.13	1.34	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	TRP	CB-CG	-12.12	1.12	1.50
2	D	134	ALA	CA-C	12.12	1.69	1.52
1	C	6	ASN	CB-CG	-12.12	1.21	1.52
1	A	92	ARG	CA-CB	12.12	1.72	1.53
2	D	80	LEU	CG-CD2	-12.11	1.12	1.52
2	B	109	LEU	N-CA	12.11	1.60	1.46
2	D	64	LYS	N-CA	12.11	1.61	1.46
1	A	24	TYR	C-O	-12.10	1.13	1.23
1	C	117	PHE	CG-CD1	12.10	1.64	1.38
2	D	53	VAL	CA-C	12.10	1.65	1.52
1	A	126	ASN	CA-CB	-12.09	1.34	1.53
2	B	143	LYS	CG-CD	12.09	1.88	1.52
2	D	52	ALA	C-O	12.09	1.41	1.23
1	C	6	ASN	N-CA	-12.08	1.30	1.46
2	D	93	ASN	C-O	12.07	1.38	1.24
2	B	113	VAL	CB-CG1	12.06	1.92	1.52
2	D	141	ALA	C-O	12.06	1.39	1.24
1	C	82	ASN	CA-C	-12.04	1.36	1.52
1	A	20	ASN	C-O	-12.04	1.08	1.24
2	D	126	GLN	CG-CD	-12.04	1.22	1.52
2	D	71	THR	CB-CG2	12.04	1.92	1.52
1	A	14	TRP	CA-CB	12.02	1.73	1.53
2	D	109	LEU	C-N	-12.02	1.16	1.33
2	B	23	GLY	CA-C	-12.02	1.34	1.51
1	C	103	HIS	N-CA	-12.02	1.31	1.46
1	C	101	LEU	CB-CG	-12.01	1.29	1.53
1	A	6	ASN	CG-ND2	12.01	1.58	1.33
1	A	48	LEU	C-O	12.00	1.43	1.23
1	A	107	VAL	C-N	-12.00	1.16	1.33
1	C	16	LYS	CG-CD	12.00	1.88	1.52
2	D	118	GLY	C-O	12.00	1.40	1.23
2	B	70	PHE	CB-CG	-11.96	1.23	1.50
1	C	77	PRO	N-CA	11.96	1.63	1.47
2	D	20	ASP	CA-CB	-11.96	1.33	1.53
1	A	35	SER	CA-C	-11.95	1.36	1.52
1	A	95	PRO	N-CD	11.94	1.64	1.47
2	B	38	GLN	CA-C	11.94	2.00	1.52
2	B	9	ALA	CA-CB	-11.94	1.33	1.53
2	B	124	ASN	N-CA	-11.93	1.31	1.46
2	D	111	LEU	CA-C	11.93	1.68	1.53
1	C	7	LYS	N-CA	11.92	1.61	1.46
2	D	62	HIS	C-O	-11.91	1.08	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	41	PHE	N-CA	11.91	1.61	1.46
1	A	127	LYS	CA-C	11.90	1.68	1.52
1	A	29	LEU	CG-CD2	11.90	1.91	1.52
1	C	38	THR	N-CA	-11.90	1.30	1.46
1	C	140	TYR	CG-CD1	-11.90	1.14	1.39
2	B	47	LEU	CA-CB	-11.90	1.37	1.53
2	D	18	ASP	CA-CB	11.89	1.80	1.53
2	B	82	GLY	CA-C	-11.89	1.35	1.51
1	C	78	GLY	C-N	-11.88	1.18	1.33
1	A	11	LYS	CG-CD	-11.87	1.16	1.52
1	C	27	GLN	CG-CD	-11.87	1.22	1.52
1	C	76	LEU	CA-C	11.87	1.67	1.52
2	B	78	ASP	C-O	-11.87	0.99	1.23
1	C	49	SER	CB-OG	11.87	1.65	1.42
2	D	104	LEU	N-CA	-11.86	1.32	1.46
1	C	5	ALA	CA-C	11.86	1.67	1.52
1	A	49	SER	C-O	11.84	1.39	1.24
1	A	65	ALA	N-CA	-11.83	1.31	1.46
1	C	68	LYS	CA-C	11.82	1.68	1.52
2	D	63	GLY	CA-C	11.82	1.68	1.51
1	C	24	TYR	CZ-OH	-11.81	1.13	1.38
2	D	31	LEU	CG-CD1	-11.81	1.13	1.52
2	D	91	HIS	ND1-CE1	-11.81	1.20	1.32
2	D	102	PHE	CA-CB	-11.77	1.34	1.53
2	D	62	HIS	ND1-CE1	11.77	1.44	1.32
2	B	93	ASN	C-N	-11.76	1.14	1.33
1	C	125	LEU	CG-CD1	-11.75	1.13	1.52
2	B	132	VAL	CB-CG2	-11.73	1.13	1.52
1	C	68	LYS	C-O	-11.73	1.09	1.24
1	C	131	ASN	C-N	-11.73	1.18	1.33
2	B	27	LEU	CA-CB	-11.71	1.34	1.53
2	B	120	GLN	CD-OE1	11.70	1.45	1.23
2	D	89	GLY	C-O	-11.71	1.08	1.23
2	D	62	HIS	CA-CB	11.69	1.73	1.53
1	A	30	GLN	CA-CB	-11.69	1.33	1.53
2	D	129	PHE	C-O	-11.68	1.09	1.24
1	A	125	LEU	CA-C	11.68	1.69	1.52
1	C	66	LEU	CA-CB	11.68	1.72	1.53
1	C	42	TYR	C-O	11.67	1.39	1.24
1	C	133	SER	C-N	-11.67	1.19	1.33
2	D	99	PRO	N-CA	11.67	1.62	1.47
1	C	58	HIS	CA-CB	11.66	1.71	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	76	HIS	C-O	11.65	1.38	1.24
2	D	61	ALA	C-N	11.65	1.50	1.33
2	D	131	LYS	CE-NZ	11.65	1.84	1.49
2	D	2	LEU	CB-CG	11.64	1.76	1.53
1	A	90	LYS	N-CA	-11.64	1.32	1.46
1	A	86	LEU	N-CA	-11.63	1.31	1.46
2	D	96	HIS	CG-ND1	-11.63	1.25	1.38
2	B	87	LEU	C-O	11.63	1.39	1.24
2	D	67	LEU	C-O	11.63	1.37	1.24
2	D	108	VAL	CA-CB	11.63	1.68	1.54
1	C	50	HIS	C-N	11.62	1.43	1.33
1	C	140	TYR	CB-CG	11.61	1.77	1.51
1	C	10	VAL	CB-CG2	11.61	1.90	1.52
2	B	139	ALA	CA-C	-11.61	1.36	1.52
1	A	54	GLN	CD-NE2	11.60	1.57	1.33
1	C	80	LEU	N-CA	-11.60	1.33	1.46
2	B	75	LYS	CG-CD	11.59	1.87	1.52
2	B	14	TRP	CG-CD2	11.59	1.64	1.43
2	B	52	ALA	CA-C	11.59	1.68	1.52
1	A	75	ASP	N-CA	11.58	1.64	1.46
1	C	66	LEU	CA-C	-11.58	1.37	1.52
2	B	132	VAL	N-CA	-11.58	1.31	1.46
1	A	72	HIS	CG-CD2	11.58	1.48	1.35
2	D	70	PHE	CG-CD1	11.58	1.63	1.38
2	D	71	THR	N-CA	-11.57	1.24	1.46
1	A	74	ASN	C-N	-11.57	1.17	1.33
1	A	92	ARG	CD-NE	11.56	1.62	1.46
2	B	77	LEU	C-N	-11.56	1.17	1.33
1	C	8	SER	N-CA	11.55	1.61	1.46
1	A	9	ASN	C-O	-11.53	1.10	1.24
2	D	99	PRO	CG-CD	-11.53	1.11	1.50
1	C	79	THR	CB-OG1	-11.52	1.25	1.43
2	D	96	HIS	C-O	11.51	1.38	1.24
2	D	107	ASN	C-N	11.51	1.48	1.34
2	B	58	LYS	CB-CG	11.49	1.86	1.52
1	A	89	HIS	CB-CG	-11.48	1.34	1.50
1	A	48	LEU	CG-CD2	11.47	1.90	1.52
1	C	109	LEU	CA-CB	-11.47	1.34	1.53
1	C	48	LEU	CG-CD1	-11.46	1.14	1.52
1	C	73	LEU	CA-C	11.46	1.68	1.52
2	D	98	ASN	CG-ND2	-11.43	1.09	1.33
1	C	97	ASN	C-N	11.41	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	THR	C-N	-11.41	1.17	1.33
2	B	59	VAL	CA-CB	11.40	1.69	1.54
1	A	34	LEU	CB-CG	-11.40	1.30	1.53
2	B	20	ASP	N-CA	11.39	1.60	1.46
1	C	89	HIS	C-N	11.38	1.48	1.33
1	C	128	PHE	N-CA	-11.37	1.31	1.46
1	A	17	VAL	CB-CG1	-11.37	1.15	1.52
2	B	54	MET	CA-CB	11.36	1.71	1.53
1	C	106	LEU	CG-CD1	-11.36	1.15	1.52
1	C	46	PHE	CD1-CE1	11.35	1.72	1.38
2	B	109	LEU	CA-CB	-11.35	1.35	1.53
2	D	57	PRO	C-N	-11.35	1.17	1.33
1	A	38	THR	C-N	11.35	1.48	1.33
1	A	89	HIS	ND1-CE1	-11.34	1.21	1.32
1	C	135	VAL	CB-CG2	11.34	1.90	1.52
1	A	87	HIS	CG-CD2	-11.33	1.23	1.35
2	D	145	HIS	N-CA	-11.33	1.24	1.46
2	D	44	PHE	C-O	11.32	1.38	1.24
1	A	105	LEU	CB-CG	-11.32	1.30	1.53
1	A	89	HIS	CD2-NE2	-11.31	1.25	1.37
2	B	123	PRO	C-O	-11.31	1.11	1.24
2	B	11	THR	N-CA	-11.31	1.32	1.46
1	C	40	LYS	CA-CB	-11.31	1.32	1.53
1	A	74	ASN	N-CA	11.30	1.60	1.46
1	A	140	TYR	N-CA	-11.30	1.31	1.46
2	D	85	ALA	CA-C	-11.30	1.38	1.52
1	A	17	VAL	CB-CG2	11.30	1.89	1.52
1	A	73	LEU	N-CA	11.29	1.60	1.46
2	B	123	PRO	N-CD	11.29	1.63	1.47
2	B	125	VAL	CB-CG1	11.29	1.89	1.52
2	B	109	LEU	CG-CD1	-11.28	1.15	1.52
1	A	81	SER	CA-C	11.28	1.67	1.52
1	A	23	ALA	C-O	-11.27	1.10	1.23
1	C	117	PHE	CD1-CE1	-11.27	1.04	1.38
2	B	76	HIS	CB-CG	11.27	1.66	1.50
2	D	98	ASN	CA-C	11.26	1.67	1.52
1	C	22	PRO	CA-CB	11.24	1.69	1.53
1	A	130	ALA	CA-CB	-11.24	1.35	1.53
2	D	71	THR	C-N	-11.23	1.18	1.33
1	C	30	GLN	CD-OE1	11.23	1.44	1.23
1	C	113	LEU	C-O	11.23	1.37	1.24
2	D	142	HIS	CA-C	-11.22	1.38	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	65	ARG	CB-CG	-11.22	1.18	1.52
2	D	110	ALA	C-N	-11.22	1.18	1.33
2	B	24	ALA	C-O	11.21	1.37	1.24
1	C	105	LEU	CG-CD1	11.21	1.89	1.52
1	A	103	HIS	CB-CG	-11.20	1.34	1.50
2	B	60	LYS	CE-NZ	11.20	1.82	1.49
1	A	48	LEU	N-CA	-11.20	1.32	1.46
1	A	133	SER	CA-C	-11.19	1.38	1.52
1	C	21	ALA	CA-CB	11.19	1.71	1.53
1	C	13	ALA	CA-C	11.19	1.67	1.52
2	B	2	LEU	CG-CD2	11.18	1.89	1.52
1	A	58	HIS	CD2-NE2	-11.16	1.25	1.37
2	B	91	HIS	CE1-NE2	11.16	1.43	1.32
1	C	91	LEU	CB-CG	11.16	1.75	1.53
1	C	33	PHE	CA-CB	-11.14	1.35	1.53
1	A	28	ALA	CA-C	-11.13	1.37	1.52
2	B	114	ALA	C-O	-11.13	1.10	1.24
1	C	50	HIS	N-CA	11.13	1.67	1.46
1	C	42	TYR	CA-CB	11.12	1.73	1.53
2	D	4	ALA	CA-CB	-11.12	1.37	1.53
2	B	48	SER	C-O	11.12	1.38	1.23
2	B	128	LEU	CG-CD2	11.11	1.89	1.52
2	B	121	PHE	CB-CG	-11.11	1.25	1.50
1	A	119	PRO	CA-C	-11.11	1.35	1.52
1	C	97	ASN	N-CA	-11.10	1.32	1.46
2	D	132	VAL	CA-CB	-11.10	1.39	1.54
1	C	120	ALA	C-N	11.09	1.46	1.33
2	B	44	PHE	C-N	11.08	1.49	1.33
2	D	66	VAL	CA-CB	11.08	1.69	1.54
2	B	107	ASN	CA-C	-11.08	1.38	1.52
2	D	50	ALA	CA-CB	-11.08	1.35	1.53
1	A	74	ASN	CA-CB	-11.07	1.34	1.53
2	B	145	HIS	CB-CG	11.07	1.65	1.50
1	C	4	ALA	N-CA	11.06	1.59	1.46
2	D	29	ARG	CA-CB	-11.06	1.35	1.53
2	D	56	ASN	N-CA	-11.06	1.30	1.46
1	A	14	TRP	CD2-CE2	11.05	1.60	1.41
1	C	85	ASN	CB-CG	11.05	1.79	1.52
1	A	82	ASN	CA-CB	-11.05	1.34	1.53
2	D	109	LEU	CG-CD2	11.05	1.89	1.52
2	D	97	VAL	C-N	-11.04	1.10	1.33
1	A	66	LEU	N-CA	-11.04	1.31	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	66	VAL	CA-CB	-11.04	1.39	1.54
2	D	121	PHE	CB-CG	-11.03	1.25	1.50
1	C	136	LEU	C-O	11.03	1.38	1.24
2	D	117	PHE	CB-CG	-11.03	1.25	1.50
1	A	132	ASP	CA-C	11.02	1.67	1.52
2	D	59	VAL	N-CA	11.02	1.60	1.46
1	A	54	GLN	CD-OE1	-11.02	1.02	1.23
1	C	141	ARG	CA-CB	-11.01	1.31	1.53
2	B	84	PHE	CB-CG	11.01	1.75	1.50
1	C	26	ALA	CA-CB	11.01	1.71	1.53
1	A	36	PHE	C-N	11.01	1.59	1.33
1	A	11	LYS	N-CA	-11.00	1.32	1.46
1	A	2	LEU	C-O	11.00	1.37	1.24
2	D	140	LEU	CA-C	11.00	1.68	1.52
2	B	127	ALA	CA-CB	-10.99	1.34	1.53
2	B	6	GLU	CA-C	-10.97	1.38	1.52
1	C	104	SER	N-CA	-10.96	1.33	1.46
1	A	92	ARG	NE-CZ	10.96	1.45	1.33
1	A	106	LEU	CA-C	-10.95	1.33	1.52
2	B	93	ASN	CB-CG	10.95	1.79	1.52
1	A	77	PRO	C-O	10.91	1.38	1.24
2	B	6	GLU	CD-OE2	10.91	1.46	1.25
1	A	69	ALA	C-O	10.91	1.37	1.24
2	B	121	PHE	CA-C	-10.91	1.39	1.53
1	C	93	VAL	N-CA	10.91	1.59	1.46
1	A	131	ASN	C-O	10.90	1.36	1.24
1	C	23	ALA	CA-C	10.89	1.67	1.52
2	D	144	TYR	CG-CD1	10.88	1.62	1.39
1	A	110	ALA	CA-CB	10.87	1.71	1.53
2	D	42	GLN	CG-CD	-10.86	1.24	1.52
2	B	75	LYS	CA-CB	10.85	1.71	1.53
1	C	42	TYR	CE1-CZ	10.85	1.64	1.38
2	B	47	LEU	CG-CD2	-10.84	1.16	1.52
2	D	96	HIS	CA-CB	10.83	1.71	1.53
2	B	86	GLN	CD-OE1	10.79	1.44	1.23
1	C	36	PHE	CE1-CZ	10.78	1.71	1.38
2	B	89	GLY	C-N	-10.78	1.21	1.33
1	A	12	ALA	N-CA	10.77	1.60	1.46
1	C	86	LEU	C-N	10.77	1.48	1.33
2	B	57	PRO	CG-CD	10.77	1.87	1.50
1	A	54	GLN	C-N	10.76	1.48	1.33
1	A	89	HIS	N-CA	-10.76	1.25	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	80	LEU	N-CA	-10.76	1.25	1.46
2	B	96	HIS	CA-CB	10.76	1.71	1.53
2	B	129	PHE	C-N	10.74	1.47	1.33
1	C	36	PHE	CB-CG	-10.74	1.25	1.50
1	A	45	HIS	CG-CD2	10.73	1.47	1.35
2	B	13	PHE	CG-CD1	10.73	1.61	1.38
2	B	33	VAL	CA-C	10.73	1.66	1.52
2	B	41	PHE	CD2-CE2	-10.72	1.06	1.38
1	C	17	VAL	CB-CG2	10.72	1.88	1.52
2	B	79	ASP	CG-OD1	10.71	1.45	1.25
2	B	115	ARG	CD-NE	-10.71	1.31	1.46
1	C	11	LYS	C-N	10.71	1.48	1.33
2	B	25	GLN	CD-NE2	10.70	1.55	1.33
2	D	84	PHE	CE1-CZ	10.70	1.70	1.38
2	D	120	GLN	CG-CD	10.68	1.78	1.52
1	C	129	LEU	N-CA	-10.68	1.33	1.46
2	D	86	GLN	CB-CG	-10.67	1.20	1.52
2	B	131	LYS	N-CA	10.66	1.58	1.46
1	A	65	ALA	C-O	10.65	1.37	1.24
1	A	81	SER	C-O	-10.65	1.11	1.24
2	D	127	ALA	C-N	-10.64	1.18	1.33
1	C	71	GLY	C-O	-10.64	1.02	1.23
1	C	60	GLN	CD-OE1	10.64	1.43	1.23
1	C	89	HIS	CG-CD2	10.63	1.47	1.35
2	B	14	TRP	CZ2-CH2	-10.63	1.17	1.37
2	B	129	PHE	CA-CB	-10.62	1.36	1.53
2	B	74	LEU	CA-CB	10.60	1.71	1.53
1	A	87	HIS	C-O	-10.60	1.11	1.24
2	B	2	LEU	N-CA	-10.60	1.32	1.46
2	B	77	LEU	N-CA	-10.59	1.30	1.46
1	A	2	LEU	CB-CG	10.58	1.74	1.53
1	A	113	LEU	C-O	10.58	1.35	1.24
2	B	72	GLN	CA-CB	-10.58	1.35	1.53
1	C	116	ASN	N-CA	-10.58	1.33	1.46
2	D	44	PHE	CG-CD2	-10.58	1.16	1.38
1	C	19	GLY	N-CA	-10.57	1.28	1.45
1	C	134	THR	CB-OG1	-10.57	1.26	1.43
1	A	2	LEU	CG-CD1	10.56	1.87	1.52
2	B	50	ALA	C-N	10.56	1.49	1.33
2	D	35	PRO	C-N	-10.56	1.19	1.34
2	B	8	ALA	C-O	-10.56	1.10	1.24
2	B	143	LYS	CD-CE	10.55	1.84	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	65	ARG	CA-CB	10.54	1.70	1.53
2	B	124	ASN	C-O	10.54	1.36	1.24
2	B	38	GLN	CB-CG	-10.53	1.20	1.52
2	D	92	CYS	CB-SG	10.53	2.16	1.81
1	C	131	ASN	C-O	-10.53	1.09	1.23
2	B	137	ALA	CA-CB	-10.51	1.35	1.53
1	A	28	ALA	C-N	-10.50	1.19	1.33
2	D	21	VAL	CB-CG2	10.50	1.87	1.52
2	B	129	PHE	CB-CG	-10.49	1.26	1.50
2	B	43	HIS	C-N	10.48	1.48	1.33
1	A	90	LYS	C-N	-10.47	1.21	1.33
2	B	124	ASN	CA-CB	-10.47	1.36	1.53
1	C	62	VAL	C-N	-10.47	1.19	1.33
1	C	130	ALA	CA-CB	-10.47	1.35	1.53
2	D	85	ALA	C-N	-10.47	1.19	1.33
2	B	104	LEU	CA-CB	10.46	1.71	1.53
1	C	64	ASN	CA-C	10.46	1.66	1.52
2	B	91	HIS	CA-CB	-10.46	1.37	1.53
2	D	129	PHE	CG-CD1	10.44	1.60	1.38
2	B	3	THR	CB-OG1	10.43	1.60	1.43
1	C	67	THR	CB-CG2	10.43	1.86	1.52
2	D	68	ASP	CB-CG	10.41	1.78	1.52
2	B	67	LEU	C-N	-10.41	1.19	1.33
2	D	119	GLY	CA-C	-10.41	1.40	1.52
1	C	71	GLY	N-CA	-10.39	1.28	1.45
1	C	92	ARG	CA-C	10.39	1.67	1.53
1	C	97	ASN	CG-OD1	-10.39	1.03	1.23
1	A	100	LEU	CG-CD1	-10.39	1.18	1.52
1	A	109	LEU	C-N	-10.36	1.19	1.33
1	C	120	ALA	CA-CB	-10.36	1.36	1.53
2	B	22	VAL	CB-CG2	10.35	1.86	1.52
1	C	52	SER	CB-OG	-10.35	1.21	1.42
2	D	65	ARG	C-O	10.35	1.37	1.24
2	D	70	PHE	CD1-CE1	-10.35	1.07	1.38
1	A	137	THR	CB-CG2	10.35	1.86	1.52
2	D	21	VAL	C-O	10.34	1.36	1.24
1	C	36	PHE	C-O	-10.34	1.11	1.24
1	A	3	SER	C-N	-10.32	1.20	1.33
2	B	44	PHE	CG-CD2	-10.32	1.17	1.38
1	C	40	LYS	CA-C	10.31	1.67	1.52
1	C	123	ALA	C-O	-10.31	1.10	1.24
1	A	65	ALA	C-N	10.31	1.48	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	118	THR	C-O	10.31	1.37	1.24
1	A	14	TRP	N-CA	-10.31	1.32	1.46
1	C	65	ALA	CA-C	-10.30	1.39	1.52
2	B	129	PHE	CD1-CE1	10.29	1.69	1.38
2	D	123	PRO	CB-CG	-10.29	0.98	1.49
2	D	72	GLN	CA-C	-10.29	1.39	1.52
2	D	97	VAL	CB-CG2	-10.28	1.18	1.52
1	A	73	LEU	CG-CD1	10.28	1.86	1.52
1	A	60	GLN	N-CA	10.28	1.59	1.46
2	B	13	PHE	CA-CB	10.28	1.71	1.53
1	C	45	HIS	ND1-CE1	10.27	1.42	1.32
1	A	124	ASN	CG-OD1	10.27	1.43	1.23
2	B	57	PRO	N-CA	-10.27	1.34	1.47
1	C	53	ALA	C-O	10.27	1.37	1.24
1	A	118	THR	C-O	10.26	1.37	1.24
1	A	96	VAL	CB-CG2	-10.25	1.18	1.52
2	B	6	GLU	CD-OE1	10.24	1.44	1.25
1	A	43	PHE	CG-CD1	-10.24	1.17	1.38
1	C	47	ASP	CG-OD1	10.24	1.44	1.25
2	B	129	PHE	C-O	10.22	1.36	1.24
2	D	100	GLN	CB-CG	10.22	1.83	1.52
2	D	81	LYS	C-N	10.21	1.48	1.33
2	B	144	TYR	N-CA	10.21	1.59	1.46
1	A	114	PRO	N-CA	10.21	1.60	1.47
2	B	34	TYR	CG-CD1	10.20	1.60	1.39
2	D	126	GLN	CA-C	-10.20	1.40	1.52
1	A	56	LYS	CA-CB	-10.19	1.37	1.53
2	B	129	PHE	CG-CD2	-10.19	1.17	1.38
1	A	5	ALA	N-CA	10.19	1.59	1.46
1	A	28	ALA	C-O	10.18	1.36	1.24
1	A	90	LYS	CG-CD	-10.17	1.22	1.52
1	A	99	LYS	CE-NZ	10.17	1.79	1.49
2	B	68	ASP	CA-C	10.17	1.66	1.52
2	B	102	PHE	CE1-CZ	-10.16	1.08	1.38
2	D	44	PHE	CE2-CZ	-10.16	1.08	1.38
1	C	13	ALA	CA-CB	10.14	1.70	1.53
2	B	39	ARG	NE-CZ	-10.13	1.22	1.33
2	D	27	LEU	CB-CG	-10.13	1.33	1.53
2	B	34	TYR	CA-C	-10.13	1.40	1.52
2	B	131	LYS	CG-CD	10.12	1.82	1.52
1	C	46	PHE	CA-CB	10.12	1.69	1.53
2	B	48	SER	CA-C	10.12	1.66	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	ALA	C-N	10.11	1.47	1.33
2	B	86	GLN	C-N	10.11	1.49	1.33
2	D	66	VAL	C-N	-10.11	1.20	1.33
1	A	98	PHE	CE2-CZ	-10.11	1.08	1.38
1	A	106	LEU	CG-CD2	10.10	1.85	1.52
1	C	54	GLN	C-N	-10.10	1.20	1.33
2	B	84	PHE	CG-CD1	10.09	1.60	1.38
2	D	115	ARG	NE-CZ	10.08	1.44	1.33
1	C	108	THR	N-CA	-10.08	1.35	1.46
2	D	145	HIS	CE1-NE2	-10.08	1.22	1.32
2	D	144	TYR	CD1-CE1	10.08	1.68	1.38
1	A	32	MET	SD-CE	10.07	2.04	1.79
1	C	102	SER	C-O	-10.07	1.11	1.24
2	B	91	HIS	ND1-CE1	10.07	1.42	1.32
2	B	132	VAL	C-N	-10.07	1.21	1.33
2	D	126	GLN	CA-CB	-10.07	1.37	1.53
1	A	101	LEU	CB-CG	10.06	1.73	1.53
1	C	89	HIS	CB-CG	-10.06	1.36	1.50
1	C	47	ASP	CA-CB	10.06	1.66	1.53
1	C	113	LEU	CA-CB	10.05	1.66	1.53
1	A	31	ARG	CZ-NH1	-10.04	1.18	1.32
1	A	108	THR	C-N	10.04	1.47	1.33
1	C	52	SER	N-CA	10.04	1.58	1.46
1	C	139	LYS	N-CA	-10.04	1.33	1.46
1	A	131	ASN	C-N	-10.03	1.19	1.33
2	B	145	HIS	CA-C	-10.03	1.31	1.52
2	B	129	PHE	CG-CD1	10.02	1.59	1.38
2	B	55	ASN	CA-CB	-10.02	1.37	1.53
1	C	48	LEU	N-CA	-10.01	1.33	1.46
2	B	105	LEU	C-N	10.01	1.50	1.33
1	C	136	LEU	N-CA	10.01	1.59	1.46
1	A	53	ALA	CA-CB	10.00	1.70	1.53
2	B	95	LEU	CB-CG	9.99	1.73	1.53
1	C	98	PHE	CE2-CZ	-9.99	1.08	1.38
2	D	69	ALA	N-CA	-9.99	1.34	1.46
1	C	140	TYR	CG-CD2	-9.97	1.18	1.39
1	A	80	LEU	CG-CD2	9.97	1.85	1.52
2	B	33	VAL	N-CA	-9.96	1.33	1.46
2	B	117	PHE	CA-C	-9.96	1.40	1.52
2	B	117	PHE	N-CA	9.96	1.58	1.46
1	A	30	GLN	CD-OE1	-9.95	1.04	1.23
2	B	17	VAL	CB-CG1	-9.94	1.19	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	40	PHE	CA-CB	9.94	1.69	1.53
1	A	101	LEU	N-CA	9.94	1.58	1.46
2	B	37	THR	C-O	9.93	1.36	1.24
1	C	99	LYS	CG-CD	9.93	1.82	1.52
2	D	41	PHE	CE2-CZ	9.93	1.68	1.38
2	D	21	VAL	CB-CG1	-9.92	1.19	1.52
1	C	123	ALA	CA-C	9.92	1.66	1.52
2	D	13	PHE	CG-CD1	-9.91	1.18	1.38
1	C	47	ASP	CB-CG	9.91	1.76	1.52
1	A	91	LEU	C-N	-9.90	1.20	1.33
2	D	100	GLN	CD-NE2	9.90	1.54	1.33
1	C	89	HIS	CE1-NE2	9.89	1.42	1.32
1	A	37	PRO	CA-CB	-9.89	1.39	1.53
1	A	88	ALA	N-CA	-9.88	1.33	1.46
2	B	138	ASN	CG-OD1	9.88	1.42	1.23
1	C	68	LYS	CE-NZ	9.87	1.78	1.49
1	A	69	ALA	CA-CB	-9.85	1.37	1.53
1	C	72	HIS	C-O	-9.85	1.11	1.24
2	D	96	HIS	CE1-NE2	-9.85	1.22	1.32
2	D	127	ALA	CA-C	9.83	1.63	1.53
2	B	40	PHE	CE2-CZ	9.83	1.68	1.38
2	D	69	ALA	CA-CB	-9.83	1.38	1.53
2	D	72	GLN	CD-NE2	9.82	1.53	1.33
2	D	140	LEU	CG-CD1	9.82	1.84	1.52
2	B	31	LEU	C-O	-9.82	1.11	1.24
1	C	14	TRP	NE1-CE2	-9.82	1.26	1.37
1	C	125	LEU	C-O	9.81	1.36	1.24
1	A	113	LEU	CB-CG	-9.81	1.33	1.53
2	B	119	GLY	CA-C	-9.81	1.35	1.51
1	A	21	ALA	C-O	9.80	1.34	1.24
2	D	93	ASN	CB-CG	9.80	1.76	1.52
2	B	98	ASN	CA-C	-9.79	1.40	1.53
1	A	129	LEU	CA-C	-9.79	1.39	1.52
2	D	63	GLY	N-CA	-9.78	1.31	1.45
2	D	27	LEU	CG-CD1	9.78	1.84	1.52
2	D	124	ASN	C-O	9.77	1.36	1.24
1	A	133	SER	CB-OG	-9.77	1.22	1.42
1	C	42	TYR	CZ-OH	-9.77	1.17	1.38
1	A	45	HIS	CA-C	-9.77	1.38	1.52
2	D	57	PRO	CA-C	-9.76	1.38	1.52
1	A	86	LEU	CG-CD2	9.74	1.84	1.52
1	C	34	LEU	C-O	9.74	1.36	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	LEU	CG-CD2	9.74	1.84	1.52
2	B	7	LYS	C-N	-9.73	1.20	1.33
1	A	139	LYS	C-N	-9.73	1.20	1.33
2	B	139	ALA	N-CA	9.72	1.58	1.46
1	C	7	LYS	CA-C	9.71	1.65	1.52
2	B	112	VAL	CA-C	9.71	1.65	1.52
1	A	106	LEU	C-N	-9.70	1.20	1.33
2	B	52	ALA	C-O	9.70	1.36	1.24
1	C	32	MET	CA-C	9.69	1.66	1.52
2	B	66	VAL	CB-CG1	9.68	1.84	1.52
2	D	34	TYR	C-N	-9.68	1.19	1.33
1	C	46	PHE	N-CA	9.68	1.57	1.45
2	D	76	HIS	ND1-CE1	-9.68	1.22	1.32
2	B	127	ALA	CA-C	9.67	1.65	1.52
2	B	132	VAL	CA-CB	-9.67	1.41	1.54
2	B	99	PRO	N-CA	-9.67	1.34	1.47
2	D	84	PHE	CE2-CZ	-9.67	1.09	1.38
2	D	81	LYS	CA-C	-9.66	1.38	1.52
1	A	113	LEU	CA-CB	9.66	1.63	1.53
1	C	48	LEU	CB-CG	9.65	1.72	1.53
2	B	2	LEU	CA-C	9.65	1.65	1.52
1	A	44	PRO	C-O	9.64	1.36	1.24
2	D	14	TRP	CD1-NE1	-9.64	1.17	1.37
1	C	67	THR	CA-C	9.63	1.64	1.52
2	D	96	HIS	C-N	-9.63	1.21	1.33
2	D	113	VAL	N-CA	9.63	1.58	1.46
2	B	93	ASN	C-O	-9.63	1.11	1.24
1	C	54	GLN	CA-CB	-9.63	1.37	1.53
1	A	60	GLN	CD-NE2	9.62	1.53	1.33
1	C	105	LEU	CA-C	9.62	1.65	1.52
2	B	69	ALA	C-O	9.60	1.36	1.24
2	B	120	GLN	CA-C	-9.59	1.40	1.52
1	C	127	LYS	CG-CD	-9.59	1.23	1.52
2	D	40	PHE	CG-CD2	9.59	1.58	1.38
2	B	96	HIS	C-O	-9.59	1.11	1.24
1	C	68	LYS	N-CA	-9.58	1.33	1.46
2	D	29	ARG	CD-NE	-9.58	1.32	1.46
1	C	92	ARG	CZ-NH1	-9.57	1.19	1.32
1	A	97	ASN	C-N	-9.57	1.21	1.33
2	B	13	PHE	CB-CG	-9.56	1.28	1.50
2	B	88	SER	C-N	9.56	1.47	1.33
2	D	27	LEU	N-CA	-9.55	1.33	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	27	LEU	N-CA	9.55	1.57	1.46
1	C	90	LYS	C-O	-9.54	1.10	1.23
1	A	62	VAL	N-CA	-9.54	1.34	1.46
1	A	133	SER	C-N	9.53	1.46	1.33
2	B	20	ASP	C-O	9.53	1.35	1.24
1	C	64	ASN	CG-ND2	9.53	1.53	1.33
1	A	110	ALA	CA-C	9.52	1.65	1.52
2	B	131	LYS	CA-C	-9.52	1.41	1.52
1	C	14	TRP	CG-CD1	9.52	1.60	1.36
2	D	8	ALA	C-N	9.52	1.47	1.33
2	B	54	MET	C-O	9.52	1.35	1.24
1	A	136	LEU	CA-CB	9.52	1.69	1.53
1	C	14	TRP	CA-CB	9.51	1.68	1.53
1	A	87	HIS	N-CA	-9.51	1.34	1.46
2	B	20	ASP	C-N	-9.51	1.20	1.33
1	A	129	LEU	CB-CG	-9.51	1.34	1.53
2	B	88	SER	N-CA	-9.51	1.33	1.46
1	C	98	PHE	CA-CB	-9.51	1.38	1.53
2	D	141	ALA	N-CA	9.50	1.58	1.46
2	B	113	VAL	N-CA	9.49	1.58	1.46
1	A	79	THR	N-CA	-9.48	1.34	1.46
2	B	30	LEU	CG-CD1	-9.48	1.21	1.52
2	B	16	LYS	CD-CE	9.48	1.80	1.52
1	A	138	SER	CA-C	-9.47	1.40	1.52
2	D	72	GLN	CA-CB	-9.47	1.37	1.53
1	C	98	PHE	CA-C	9.46	1.66	1.52
2	D	106	GLY	N-CA	-9.46	1.34	1.45
1	A	69	ALA	C-N	9.46	1.46	1.33
2	B	8	ALA	C-N	9.46	1.47	1.33
2	B	116	ASN	CB-CG	-9.45	1.28	1.52
1	A	66	LEU	C-O	-9.44	1.12	1.24
1	A	115	THR	CA-CB	9.43	1.68	1.53
2	B	104	LEU	C-O	9.43	1.35	1.24
2	D	86	GLN	CD-NE2	9.43	1.53	1.33
2	B	56	ASN	CG-ND2	9.42	1.53	1.33
2	B	120	GLN	C-O	9.41	1.37	1.23
2	D	38	GLN	CG-CD	9.40	1.75	1.52
2	B	44	PHE	CG-CD1	9.40	1.58	1.38
2	B	8	ALA	N-CA	-9.40	1.34	1.46
1	C	80	LEU	CG-CD1	9.40	1.83	1.52
1	C	128	PHE	CE2-CZ	9.39	1.66	1.38
1	C	77	PRO	N-CD	9.39	1.60	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	128	PHE	CA-C	9.37	1.65	1.52
1	A	68	LYS	CA-C	-9.36	1.40	1.53
1	A	62	VAL	CB-CG1	9.35	1.83	1.52
2	B	133	VAL	CA-C	9.35	1.65	1.52
1	C	22	PRO	CG-CD	9.35	1.82	1.50
1	C	102	SER	N-CA	-9.35	1.34	1.46
2	B	27	LEU	CA-C	-9.34	1.41	1.52
2	D	136	VAL	C-N	9.34	1.51	1.34
1	C	56	LYS	C-N	9.33	1.46	1.33
2	D	54	MET	CA-CB	9.33	1.68	1.53
1	A	5	ALA	C-N	9.32	1.46	1.33
2	D	145	HIS	C-OXT	9.31	1.42	1.23
2	D	31	LEU	CG-CD2	-9.30	1.21	1.52
1	A	44	PRO	CA-C	9.29	1.65	1.52
1	C	118	THR	N-CA	9.28	1.59	1.46
2	D	130	GLN	N-CA	9.28	1.57	1.46
1	C	125	LEU	CA-C	-9.27	1.40	1.52
2	D	137	ALA	CA-C	-9.27	1.40	1.53
1	C	61	LYS	CA-C	9.27	1.65	1.52
1	A	11	LYS	CA-CB	9.27	1.68	1.53
2	D	70	PHE	CA-C	-9.27	1.41	1.53
1	C	115	THR	CA-CB	9.26	1.69	1.53
1	A	134	THR	N-CA	9.26	1.57	1.46
2	B	81	LYS	CA-CB	9.26	1.72	1.53
2	B	34	TYR	C-N	-9.23	1.12	1.33
2	D	43	HIS	C-N	9.23	1.46	1.33
2	D	125	VAL	C-N	9.23	1.46	1.33
1	C	77	PRO	CB-CG	9.23	1.95	1.49
2	D	41	PHE	CG-CD1	9.23	1.58	1.38
1	A	42	TYR	CG-CD1	9.22	1.58	1.39
2	B	24	ALA	C-N	9.22	1.45	1.33
1	A	136	LEU	N-CA	9.20	1.58	1.46
2	D	36	TRP	CG-CD2	9.19	1.60	1.43
2	B	73	GLY	C-N	-9.19	1.20	1.33
2	D	108	VAL	CB-CG2	-9.18	1.22	1.52
2	D	74	LEU	CA-CB	-9.17	1.39	1.53
1	C	50	HIS	CG-ND1	-9.17	1.28	1.38
1	A	7	LYS	CD-CE	9.16	1.79	1.52
1	C	50	HIS	CG-CD2	-9.16	1.25	1.35
1	A	114	PRO	CG-CD	9.15	1.81	1.50
2	B	83	ALA	N-CA	9.15	1.58	1.46
1	C	96	VAL	C-N	-9.15	1.21	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	PRO	C-N	9.15	1.46	1.33
1	A	93	VAL	CA-C	-9.12	1.44	1.52
1	C	1	VAL	N-CA	9.12	1.63	1.46
2	B	85	ALA	CA-C	-9.12	1.40	1.52
2	D	100	GLN	CA-C	9.11	1.64	1.52
1	A	95	PRO	CA-CB	9.11	1.67	1.53
2	D	19	VAL	N-CA	-9.11	1.34	1.46
2	D	29	ARG	NE-CZ	-9.11	1.23	1.33
1	A	109	LEU	N-CA	-9.10	1.34	1.46
2	B	59	VAL	CB-CG1	9.10	1.82	1.52
2	D	109	LEU	CA-CB	-9.09	1.38	1.53
1	A	18	GLY	C-N	-9.09	1.22	1.33
1	C	122	HIS	CG-CD2	9.09	1.45	1.35
1	C	80	LEU	C-N	-9.08	1.20	1.33
2	B	30	LEU	N-CA	-9.08	1.35	1.46
2	B	46	ASN	N-CA	9.08	1.57	1.46
1	C	109	LEU	CG-CD2	-9.07	1.22	1.52
1	A	35	SER	CB-OG	9.07	1.60	1.42
2	B	124	ASN	CA-C	-9.06	1.40	1.52
2	D	3	THR	C-O	9.06	1.35	1.24
1	C	96	VAL	N-CA	9.05	1.57	1.46
2	B	37	THR	CB-OG1	-9.04	1.29	1.43
2	D	29	ARG	CG-CD	-9.03	1.25	1.52
1	A	46	PHE	CE2-CZ	-9.03	1.11	1.38
1	C	67	THR	CA-CB	-9.03	1.39	1.53
2	B	70	PHE	C-O	-9.02	1.16	1.23
2	D	5	GLU	CA-CB	9.01	1.71	1.53
1	A	36	PHE	CE1-CZ	-9.00	1.11	1.38
2	B	68	ASP	CB-CG	8.99	1.74	1.52
1	A	47	ASP	N-CA	8.99	1.57	1.46
1	C	74	ASN	CA-CB	8.99	1.68	1.53
2	D	114	ALA	CA-CB	-8.99	1.39	1.53
2	B	138	ASN	CA-CB	8.98	1.67	1.53
1	A	116	ASN	CG-ND2	8.97	1.52	1.33
2	D	128	LEU	CA-CB	8.97	1.68	1.53
1	A	114	PRO	C-N	8.97	1.45	1.33
2	B	101	ASN	CG-OD1	-8.96	1.06	1.23
1	C	123	ALA	CA-CB	8.96	1.68	1.53
1	C	59	GLY	N-CA	-8.95	1.33	1.45
2	B	34	TYR	CE1-CZ	-8.95	1.16	1.38
2	B	114	ALA	CA-C	8.94	1.64	1.52
2	B	117	PHE	CE1-CZ	8.93	1.65	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	ARG	CA-CB	8.93	1.66	1.53
1	C	73	LEU	CG-CD1	-8.93	1.23	1.52
2	D	97	VAL	N-CA	-8.93	1.35	1.46
2	B	76	HIS	C-N	8.92	1.46	1.33
2	D	96	HIS	CG-CD2	8.92	1.45	1.35
1	C	85	ASN	CA-CB	-8.92	1.40	1.53
1	A	113	LEU	C-N	8.90	1.54	1.33
1	A	51	GLY	C-N	-8.89	1.21	1.33
1	C	65	ALA	N-CA	8.89	1.57	1.46
1	A	75	ASP	C-N	8.86	1.45	1.33
1	A	7	LYS	CA-CB	8.86	1.67	1.53
2	D	126	GLN	N-CA	8.86	1.56	1.46
2	D	74	LEU	C-O	8.85	1.34	1.24
1	A	45	HIS	ND1-CE1	-8.84	1.23	1.32
1	A	103	HIS	N-CA	-8.84	1.36	1.46
2	D	100	GLN	N-CA	8.84	1.56	1.46
1	C	66	LEU	CG-CD2	8.83	1.81	1.52
1	C	104	SER	C-O	-8.83	1.14	1.24
2	D	138	ASN	C-N	-8.83	1.21	1.33
2	D	33	VAL	CB-CG1	-8.82	1.23	1.52
2	D	131	LYS	CB-CG	8.82	1.78	1.52
2	D	7	LYS	N-CA	8.81	1.57	1.46
2	D	113	VAL	CB-CG2	8.81	1.81	1.52
2	B	58	LYS	CA-CB	-8.81	1.39	1.53
1	A	132	ASP	CG-OD1	8.80	1.42	1.25
1	C	76	LEU	CA-CB	-8.81	1.39	1.53
2	D	46	ASN	CG-OD1	8.80	1.40	1.23
1	A	127	LYS	CB-CG	8.80	1.78	1.52
2	D	120	GLN	CB-CG	8.80	1.78	1.52
1	C	92	ARG	CG-CD	8.80	1.78	1.52
2	D	38	GLN	CD-NE2	-8.80	1.14	1.33
2	B	61	ALA	C-O	-8.80	1.12	1.24
2	D	71	THR	C-O	-8.79	1.05	1.23
1	C	64	ASN	N-CA	-8.79	1.34	1.46
1	C	57	ALA	C-N	8.78	1.45	1.33
1	A	45	HIS	N-CA	-8.77	1.34	1.46
2	D	8	ALA	CA-C	-8.77	1.34	1.52
1	A	73	LEU	CG-CD2	8.76	1.81	1.52
2	D	78	ASP	C-O	-8.76	1.06	1.23
2	D	112	VAL	N-CA	-8.76	1.34	1.46
1	A	29	LEU	C-N	8.75	1.46	1.33
2	B	79	ASP	N-CA	8.75	1.57	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASN	CG-OD1	-8.75	1.06	1.23
1	C	136	LEU	CG-CD1	-8.74	1.23	1.52
2	B	80	LEU	CG-CD2	8.73	1.81	1.52
2	D	23	GLY	N-CA	8.72	1.57	1.45
1	C	18	GLY	CA-C	-8.71	1.39	1.51
2	D	11	THR	CA-CB	-8.71	1.40	1.53
2	D	80	LEU	C-N	8.71	1.45	1.33
1	C	138	SER	C-O	-8.71	1.13	1.24
2	D	2	LEU	N-CA	-8.70	1.34	1.46
1	A	82	ASN	CG-ND2	-8.69	1.15	1.33
2	B	43	HIS	N-CA	-8.68	1.29	1.46
1	A	84	SER	C-N	-8.68	1.21	1.33
1	C	76	LEU	CB-CG	8.68	1.70	1.53
1	A	24	TYR	CE1-CZ	-8.68	1.17	1.38
1	C	128	PHE	CG-CD2	-8.67	1.20	1.38
2	D	132	VAL	C-O	8.66	1.35	1.24
1	A	124	ASN	C-N	-8.64	1.23	1.33
2	B	57	PRO	CB-CG	-8.64	1.06	1.49
1	C	121	VAL	CA-C	8.63	1.64	1.52
2	D	143	LYS	CB-CG	-8.63	1.26	1.52
2	B	103	ARG	CB-CG	8.63	1.78	1.52
1	A	36	PHE	CD1-CE1	-8.62	1.12	1.38
1	C	20	ASN	CA-CB	-8.62	1.42	1.53
1	C	35	SER	C-N	-8.61	1.15	1.33
1	C	139	LYS	C-O	8.59	1.34	1.24
2	D	41	PHE	CE1-CZ	8.58	1.64	1.38
1	C	90	LYS	C-N	8.57	1.45	1.33
1	A	50	HIS	N-CA	-8.57	1.35	1.46
1	C	54	GLN	CD-OE1	-8.57	1.07	1.23
1	A	72	HIS	CD2-NE2	8.57	1.47	1.37
2	D	121	PHE	CG-CD1	-8.57	1.20	1.38
2	D	60	LYS	CD-CE	8.56	1.78	1.52
1	A	116	ASN	CB-CG	-8.55	1.30	1.52
2	B	88	SER	CA-CB	-8.55	1.39	1.53
2	D	14	TRP	CD2-CE2	8.55	1.55	1.41
2	D	66	VAL	CA-C	8.54	1.63	1.52
1	C	31	ARG	CA-CB	-8.54	1.39	1.53
2	D	64	LYS	CA-C	8.54	1.64	1.52
1	A	68	LYS	CD-CE	-8.54	1.26	1.52
1	C	77	PRO	C-N	8.54	1.46	1.33
2	B	26	ALA	N-CA	8.54	1.56	1.46
1	C	7	LYS	CG-CD	-8.54	1.26	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	HIS	N-CA	8.54	1.57	1.46
2	D	103	ARG	CA-C	8.54	1.64	1.52
1	C	3	SER	C-N	-8.53	1.20	1.33
2	D	75	LYS	N-CA	-8.53	1.35	1.46
1	C	32	MET	CB-CG	-8.53	1.26	1.52
1	C	98	PHE	CG-CD2	8.51	1.56	1.38
2	D	118	GLY	N-CA	8.51	1.57	1.45
2	D	56	ASN	CG-OD1	8.50	1.39	1.23
1	C	65	ALA	CA-CB	-8.49	1.40	1.53
1	C	81	SER	C-O	-8.49	1.13	1.24
2	D	60	LYS	N-CA	-8.48	1.35	1.46
2	B	14	TRP	CE3-CZ3	-8.48	1.13	1.38
1	A	98	PHE	C-O	8.47	1.33	1.24
1	C	71	GLY	C-N	8.47	1.45	1.33
2	D	91	HIS	C-N	-8.46	1.21	1.33
2	D	75	LYS	CA-C	-8.45	1.41	1.52
2	D	43	HIS	CG-ND1	8.44	1.47	1.38
2	D	48	SER	N-CA	8.43	1.57	1.46
1	A	125	LEU	CG-CD2	-8.42	1.24	1.52
1	C	49	SER	C-N	-8.42	1.21	1.33
2	B	117	PHE	CE2-CZ	8.41	1.63	1.38
2	D	96	HIS	CD2-NE2	8.41	1.47	1.37
1	A	140	TYR	CD1-CE1	8.40	1.63	1.38
1	A	14	TRP	CG-CD2	-8.39	1.28	1.43
1	C	4	ALA	C-N	-8.39	1.22	1.33
2	B	145	HIS	N-CA	8.38	1.62	1.46
1	A	102	SER	C-O	8.37	1.34	1.24
1	A	16	LYS	CD-CE	8.36	1.77	1.52
1	A	5	ALA	CA-C	8.36	1.64	1.52
2	D	76	HIS	CA-C	8.36	1.63	1.52
1	A	47	ASP	C-N	-8.35	1.22	1.33
2	B	117	PHE	CG-CD2	-8.35	1.21	1.38
1	C	62	VAL	N-CA	8.35	1.56	1.46
2	D	66	VAL	CB-CG2	-8.34	1.25	1.52
2	B	87	LEU	C-N	8.33	1.45	1.33
1	A	110	ALA	N-CA	8.32	1.56	1.46
1	C	44	PRO	CB-CG	8.32	1.91	1.49
2	D	123	PRO	N-CA	-8.31	1.36	1.47
2	B	5	GLU	CG-CD	8.31	1.72	1.52
2	D	89	GLY	N-CA	8.31	1.57	1.45
2	D	134	ALA	C-O	-8.31	1.13	1.24
2	D	15	GLY	CA-C	8.30	1.63	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	LYS	CD-CE	8.30	1.77	1.52
2	D	42	GLN	CD-NE2	8.30	1.50	1.33
2	D	94	LYS	CA-C	-8.29	1.45	1.53
1	A	91	LEU	CG-CD1	8.28	1.79	1.52
2	D	112	VAL	CB-CG1	8.28	1.79	1.52
2	D	123	PRO	C-N	8.28	1.45	1.33
2	B	53	VAL	CB-CG1	-8.28	1.25	1.52
2	D	5	GLU	CA-C	8.27	1.70	1.52
2	B	126	GLN	CD-NE2	8.27	1.50	1.33
1	A	93	VAL	CB-CG1	8.25	1.79	1.52
2	D	19	VAL	CA-C	-8.24	1.42	1.52
2	D	6	GLU	CG-CD	8.24	1.72	1.52
1	A	9	ASN	CA-C	-8.21	1.42	1.52
2	B	3	THR	CA-C	8.21	1.64	1.53
2	B	8	ALA	CA-C	8.21	1.63	1.52
2	B	10	VAL	CB-CG1	8.20	1.79	1.52
1	A	127	LYS	CD-CE	8.20	1.77	1.52
2	B	19	VAL	C-O	8.20	1.33	1.24
1	A	31	ARG	CD-NE	8.19	1.57	1.46
2	B	130	GLN	CB-CG	8.19	1.77	1.52
2	D	36	TRP	CE3-CZ3	-8.19	1.14	1.38
2	D	125	VAL	N-CA	8.19	1.56	1.46
2	D	99	PRO	C-N	-8.19	1.23	1.33
1	C	82	ASN	N-CA	-8.18	1.36	1.46
2	D	90	LEU	CA-CB	8.18	1.66	1.53
2	B	124	ASN	CG-OD1	8.18	1.39	1.23
1	C	87	HIS	C-N	8.18	1.45	1.33
1	C	7	LYS	CA-CB	-8.17	1.39	1.53
2	B	108	VAL	CA-CB	-8.17	1.44	1.54
1	C	72	HIS	CG-ND1	-8.17	1.29	1.38
1	A	17	VAL	CA-CB	-8.17	1.43	1.54
1	C	73	LEU	CB-CG	8.16	1.69	1.53
2	B	26	ALA	C-O	8.16	1.33	1.24
1	C	94	ASN	C-O	8.16	1.33	1.24
2	D	16	LYS	N-CA	-8.15	1.35	1.46
1	A	33	PHE	CD2-CE2	-8.12	1.14	1.38
1	C	49	SER	CA-CB	-8.12	1.37	1.53
1	C	93	VAL	CB-CG2	-8.12	1.25	1.52
2	B	44	PHE	CE2-CZ	-8.11	1.14	1.38
2	D	40	PHE	C-N	-8.10	1.23	1.33
1	A	128	PHE	CB-CG	-8.08	1.32	1.50
1	C	95	PRO	N-CA	8.08	1.58	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	TYR	CG-CD1	-8.08	1.22	1.39
1	C	91	LEU	CG-CD1	8.07	1.79	1.52
2	B	34	TYR	CA-CB	-8.07	1.40	1.53
2	D	140	LEU	CG-CD2	-8.07	1.25	1.52
2	D	33	VAL	C-O	-8.07	1.15	1.24
2	B	56	ASN	CA-CB	-8.06	1.40	1.53
1	C	103	HIS	CA-CB	8.06	1.67	1.53
2	D	72	GLN	N-CA	8.06	1.56	1.46
2	D	83	ALA	C-N	8.06	1.45	1.33
2	B	136	VAL	CB-CG2	-8.05	1.25	1.52
1	C	72	HIS	CB-CG	-8.04	1.38	1.50
1	C	97	ASN	CG-ND2	-8.05	1.16	1.33
2	B	6	GLU	CB-CG	-8.04	1.28	1.52
1	A	123	ALA	N-CA	-8.02	1.36	1.46
2	B	100	GLN	CD-NE2	8.01	1.50	1.33
1	A	106	LEU	CG-CD1	-8.01	1.26	1.52
1	C	131	ASN	CB-CG	8.01	1.72	1.52
1	A	136	LEU	CG-CD1	8.01	1.78	1.52
1	A	35	SER	C-N	8.00	1.50	1.33
1	A	141	ARG	CA-CB	8.00	1.69	1.53
2	B	81	LYS	C-N	-7.97	1.21	1.33
1	A	128	PHE	N-CA	-7.97	1.35	1.46
2	B	105	LEU	N-CA	-7.97	1.35	1.46
2	B	21	VAL	CB-CG1	-7.96	1.26	1.52
2	B	102	PHE	N-CA	7.96	1.56	1.46
1	C	29	LEU	CA-C	7.96	1.63	1.52
1	C	141	ARG	C-OXT	7.96	1.39	1.23
2	D	105	LEU	CB-CG	-7.96	1.37	1.53
1	A	13	ALA	CA-CB	7.96	1.67	1.53
1	C	60	GLN	CB-CG	7.96	1.76	1.52
1	A	55	GLN	CB-CG	-7.95	1.28	1.52
2	D	79	ASP	CA-C	7.95	1.63	1.53
1	A	44	PRO	CB-CG	-7.95	1.09	1.49
1	C	92	ARG	C-N	7.94	1.44	1.33
2	B	78	ASP	CG-OD1	-7.94	1.10	1.25
2	B	104	LEU	CB-CG	-7.94	1.37	1.53
1	C	54	GLN	CG-CD	-7.94	1.32	1.52
2	D	33	VAL	C-N	7.93	1.44	1.33
2	D	38	GLN	CA-CB	-7.93	1.40	1.53
2	D	106	GLY	C-O	-7.93	1.14	1.23
1	A	110	ALA	C-N	-7.92	1.22	1.33
2	D	31	LEU	N-CA	-7.91	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	ARG	CB-CG	-7.90	1.28	1.52
1	C	83	LEU	CG-CD2	7.90	1.78	1.52
2	B	126	GLN	C-N	-7.90	1.22	1.33
2	B	30	LEU	CA-C	7.89	1.64	1.52
1	A	7	LYS	N-CA	7.89	1.55	1.46
2	D	18	ASP	CA-C	-7.89	1.43	1.52
2	D	114	ALA	N-CA	7.89	1.63	1.46
1	A	43	PHE	C-O	-7.89	1.15	1.24
2	D	75	LYS	CG-CD	7.88	1.76	1.52
1	A	49	SER	N-CA	7.88	1.56	1.46
1	C	140	TYR	CD1-CE1	7.87	1.62	1.38
1	C	140	TYR	CZ-OH	-7.87	1.21	1.38
1	A	75	ASP	CA-C	7.87	1.64	1.52
2	D	6	GLU	CB-CG	-7.86	1.28	1.52
2	B	71	THR	CB-CG2	7.86	1.78	1.52
1	C	61	LYS	CG-CD	7.86	1.76	1.52
2	D	101	ASN	CA-CB	7.85	1.66	1.53
1	C	64	ASN	C-O	7.84	1.33	1.24
1	A	26	ALA	C-N	7.83	1.45	1.33
1	C	84	SER	N-CA	7.83	1.56	1.46
1	A	70	GLN	N-CA	7.83	1.55	1.46
2	B	72	GLN	CD-NE2	7.83	1.49	1.33
2	B	86	GLN	CB-CG	7.83	1.75	1.52
2	B	29	ARG	C-N	-7.82	1.24	1.33
1	A	112	HIS	CA-CB	7.80	1.66	1.53
2	B	64	LYS	CG-CD	7.80	1.75	1.52
1	C	114	PRO	CA-C	7.80	1.63	1.52
1	A	106	LEU	C-O	7.80	1.35	1.24
1	C	33	PHE	N-CA	-7.80	1.36	1.46
1	C	108	THR	CB-CG2	7.80	1.78	1.52
1	A	52	SER	CA-CB	7.79	1.65	1.53
1	C	17	VAL	CB-CG1	7.79	1.78	1.52
1	C	31	ARG	C-O	-7.79	1.14	1.24
2	D	52	ALA	CA-C	-7.79	1.42	1.52
2	B	130	GLN	CG-CD	7.78	1.71	1.52
2	B	9	ALA	C-N	-7.78	1.25	1.33
2	B	29	ARG	N-CA	-7.78	1.36	1.46
1	A	46	PHE	C-N	7.77	1.44	1.33
2	B	32	VAL	C-N	7.77	1.44	1.33
1	C	126	ASN	CB-CG	-7.76	1.32	1.52
1	A	75	ASP	CB-CG	7.76	1.71	1.52
2	B	49	SER	CA-CB	7.76	1.67	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	PHE	CA-C	-7.75	1.42	1.52
2	D	41	PHE	CG-CD2	-7.75	1.22	1.38
1	A	22	PRO	CA-CB	7.74	1.64	1.53
2	D	81	LYS	CD-CE	7.74	1.75	1.52
2	B	54	MET	C-N	7.74	1.44	1.33
1	C	76	LEU	CG-CD1	7.74	1.78	1.52
1	C	103	HIS	CG-ND1	7.74	1.46	1.38
1	A	97	ASN	CG-OD1	7.73	1.38	1.23
1	A	85	ASN	CG-ND2	7.73	1.49	1.33
1	C	27	GLN	CA-CB	7.73	1.67	1.53
1	C	70	GLN	C-N	-7.72	1.22	1.33
2	B	44	PHE	CA-C	7.72	1.63	1.52
1	C	21	ALA	CA-C	-7.72	1.43	1.52
1	A	91	LEU	CG-CD2	7.71	1.78	1.52
1	C	97	ASN	CA-CB	7.71	1.66	1.53
2	B	44	PHE	N-CA	7.71	1.56	1.46
2	B	116	ASN	CG-ND2	7.70	1.49	1.33
2	B	99	PRO	CA-C	-7.69	1.38	1.52
1	C	92	ARG	N-CA	7.69	1.58	1.46
2	B	133	VAL	N-CA	7.69	1.55	1.46
2	D	102	PHE	CD1-CE1	-7.68	1.15	1.38
2	B	107	ASN	CG-OD1	-7.68	1.08	1.23
1	A	24	TYR	CB-CG	-7.67	1.34	1.51
1	A	140	TYR	CA-C	-7.66	1.42	1.52
2	B	70	PHE	CG-CD1	-7.66	1.22	1.38
2	B	94	LYS	CG-CD	7.66	1.75	1.52
1	C	68	LYS	CB-CG	7.66	1.75	1.52
1	A	73	LEU	C-O	-7.66	1.14	1.24
1	C	126	ASN	C-O	7.66	1.32	1.24
1	C	7	LYS	CB-CG	7.66	1.75	1.52
1	C	124	ASN	C-O	7.66	1.33	1.24
2	D	59	VAL	CB-CG2	7.66	1.77	1.52
1	A	58	HIS	C-O	-7.65	1.14	1.24
2	B	32	VAL	CB-CG1	-7.64	1.27	1.52
2	D	108	VAL	CB-CG1	-7.64	1.27	1.52
1	C	115	THR	CB-CG2	7.63	1.77	1.52
1	C	85	ASN	C-N	-7.63	1.22	1.33
1	A	41	THR	CB-CG2	7.62	1.77	1.52
1	C	94	ASN	CB-CG	7.62	1.71	1.52
2	D	32	VAL	CB-CG2	-7.62	1.27	1.52
2	D	42	GLN	CA-CB	-7.62	1.42	1.54
2	B	143	LYS	N-CA	7.61	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	LEU	CB-CG	7.61	1.68	1.53
1	C	116	ASN	CB-CG	-7.60	1.33	1.52
2	B	115	ARG	N-CA	-7.60	1.35	1.46
1	C	109	LEU	CB-CG	-7.59	1.38	1.53
2	D	87	LEU	C-O	7.59	1.33	1.24
2	D	103	ARG	CG-CD	7.59	1.75	1.52
1	C	9	ASN	C-O	-7.59	1.14	1.24
1	A	11	LYS	CE-NZ	7.58	1.72	1.49
2	B	62	HIS	CA-C	-7.58	1.42	1.52
1	A	6	ASN	CA-C	7.57	1.62	1.52
1	C	112	HIS	CG-CD2	-7.57	1.27	1.35
2	D	37	THR	N-CA	-7.56	1.36	1.46
2	B	68	ASP	CG-OD2	7.55	1.39	1.25
2	D	117	PHE	CG-CD1	-7.55	1.23	1.38
1	A	31	ARG	CZ-NH2	7.54	1.43	1.33
2	B	71	THR	CA-C	7.54	1.61	1.53
2	D	58	LYS	C-N	7.54	1.43	1.33
1	C	91	LEU	C-N	7.52	1.44	1.33
1	C	62	VAL	CA-CB	-7.52	1.44	1.54
2	D	99	PRO	N-CD	7.51	1.58	1.47
1	C	54	GLN	CB-CG	7.51	1.75	1.52
1	A	125	LEU	N-CA	-7.49	1.37	1.46
1	C	56	LYS	CA-C	-7.49	1.42	1.52
2	B	26	ALA	C-N	-7.48	1.24	1.33
2	B	11	THR	C-N	-7.48	1.22	1.33
1	A	38	THR	CA-CB	7.48	1.66	1.53
2	B	85	ALA	N-CA	7.47	1.55	1.46
1	A	89	HIS	CA-CB	-7.46	1.38	1.53
2	D	75	LYS	CE-NZ	7.46	1.71	1.49
2	B	62	HIS	C-O	7.46	1.33	1.24
2	D	131	LYS	CG-CD	-7.46	1.30	1.52
1	A	139	LYS	CA-CB	-7.46	1.40	1.53
2	B	67	LEU	CG-CD2	-7.46	1.27	1.52
2	D	52	ALA	N-CA	-7.46	1.36	1.46
2	B	89	GLY	CA-C	7.46	1.62	1.51
2	B	82	GLY	N-CA	-7.45	1.34	1.45
1	C	110	ALA	CA-CB	-7.45	1.27	1.52
2	B	71	THR	CB-OG1	7.45	1.55	1.43
2	D	2	LEU	CG-CD2	-7.44	1.28	1.52
2	D	84	PHE	CA-C	7.43	1.63	1.52
1	A	140	TYR	CA-CB	-7.43	1.41	1.53
2	D	64	LYS	CG-CD	7.42	1.74	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	31	LEU	CG-CD1	7.41	1.77	1.52
1	C	74	ASN	CG-OD1	7.41	1.37	1.23
2	B	46	ASN	C-N	7.41	1.44	1.33
2	D	140	LEU	C-N	-7.40	1.23	1.33
1	C	46	PHE	C-N	7.40	1.44	1.33
1	C	137	THR	CA-C	7.38	1.62	1.52
2	D	65	ARG	NE-CZ	7.37	1.41	1.33
2	B	14	TRP	CD1-NE1	-7.37	1.22	1.37
2	D	14	TRP	CA-CB	7.36	1.66	1.53
1	C	14	TRP	C-O	7.36	1.32	1.24
1	C	21	ALA	N-CA	7.36	1.56	1.46
2	D	103	ARG	CD-NE	7.35	1.56	1.46
2	B	14	TRP	CA-C	-7.34	1.43	1.52
2	B	47	LEU	N-CA	7.34	1.54	1.46
1	C	94	ASN	C-N	7.34	1.43	1.34
1	A	31	ARG	CG-CD	7.34	1.74	1.52
1	A	72	HIS	C-N	-7.34	1.23	1.33
2	D	16	LYS	CD-CE	7.33	1.74	1.52
1	A	56	LYS	CE-NZ	7.33	1.71	1.49
2	D	130	GLN	CA-CB	-7.33	1.41	1.53
2	B	68	ASP	C-N	-7.33	1.23	1.33
1	C	16	LYS	CB-CG	7.32	1.74	1.52
2	D	43	HIS	N-CA	-7.32	1.36	1.46
2	B	101	ASN	CG-ND2	7.31	1.48	1.33
2	D	14	TRP	CG-CD2	7.31	1.56	1.43
1	C	104	SER	C-N	7.30	1.44	1.33
2	B	93	ASN	N-CA	-7.30	1.36	1.46
2	D	54	MET	SD-CE	7.30	1.97	1.79
2	D	105	LEU	CG-CD1	7.29	1.76	1.52
2	B	21	VAL	N-CA	7.27	1.55	1.46
2	D	105	LEU	N-CA	7.27	1.55	1.46
2	D	53	VAL	C-N	-7.26	1.23	1.33
2	B	86	GLN	N-CA	-7.25	1.32	1.46
1	A	27	GLN	C-N	-7.25	1.23	1.33
1	C	41	THR	CB-OG1	-7.25	1.32	1.43
1	A	131	ASN	CG-ND2	-7.24	1.18	1.33
2	D	126	GLN	C-O	-7.22	1.15	1.24
2	D	100	GLN	CD-OE1	-7.22	1.09	1.23
2	B	38	GLN	CD-NE2	-7.22	1.18	1.33
1	C	58	HIS	ND1-CE1	7.22	1.39	1.32
1	A	33	PHE	N-CA	-7.21	1.37	1.46
2	D	7	LYS	CD-CE	-7.21	1.30	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	84	PHE	CE1-CZ	7.20	1.60	1.38
1	C	27	GLN	CA-C	-7.20	1.42	1.52
2	D	124	ASN	N-CA	-7.20	1.36	1.46
2	D	134	ALA	C-N	-7.19	1.23	1.33
2	D	94	LYS	CA-CB	-7.19	1.44	1.53
2	D	133	VAL	CB-CG2	-7.18	1.28	1.52
2	D	136	VAL	CA-CB	-7.17	1.44	1.54
2	B	94	LYS	N-CA	7.17	1.55	1.45
2	D	44	PHE	CE1-CZ	7.17	1.60	1.38
1	C	117	PHE	CA-CB	7.17	1.61	1.52
1	C	57	ALA	N-CA	7.16	1.55	1.46
2	D	126	GLN	CB-CG	7.15	1.74	1.52
1	C	119	PRO	CB-CG	7.15	1.85	1.49
2	B	105	LEU	CG-CD2	-7.14	1.28	1.52
1	C	32	MET	N-CA	7.14	1.55	1.46
1	A	20	ASN	N-CA	-7.14	1.36	1.46
1	C	76	LEU	CG-CD2	7.14	1.76	1.52
2	B	42	GLN	N-CA	-7.13	1.36	1.46
1	A	105	LEU	CG-CD1	7.13	1.76	1.52
1	C	124	ASN	C-N	7.13	1.43	1.33
1	C	63	ALA	C-N	-7.12	1.23	1.33
1	C	24	TYR	CD1-CE1	-7.12	1.17	1.38
1	C	60	GLN	N-CA	-7.12	1.37	1.46
2	B	61	ALA	C-N	7.11	1.43	1.33
1	A	1	VAL	C-O	-7.10	1.09	1.23
2	D	65	ARG	CG-CD	7.10	1.73	1.52
1	C	141	ARG	NE-CZ	7.10	1.40	1.33
2	D	133	VAL	C-N	-7.10	1.23	1.33
2	B	80	LEU	CA-C	7.09	1.67	1.52
1	A	138	SER	CA-CB	-7.09	1.41	1.53
2	D	20	ASP	CG-OD1	7.09	1.38	1.25
1	C	114	PRO	CA-CB	-7.09	1.43	1.53
2	B	92	CYS	CA-C	7.08	1.62	1.52
1	C	82	ASN	CB-CG	-7.08	1.34	1.52
1	A	53	ALA	CA-C	-7.08	1.43	1.52
1	A	5	ALA	CA-CB	-7.07	1.42	1.53
1	C	129	LEU	CA-C	-7.06	1.44	1.52
1	C	93	VAL	CA-C	-7.05	1.43	1.52
1	C	72	HIS	CA-CB	-7.05	1.41	1.53
1	A	76	LEU	N-CA	-7.04	1.40	1.46
1	C	26	ALA	C-N	-7.04	1.24	1.33
1	C	37	PRO	C-N	7.04	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	30	LEU	CB-CG	-7.04	1.39	1.53
2	B	140	LEU	CG-CD1	7.03	1.75	1.52
1	C	2	LEU	CA-C	-7.03	1.44	1.52
2	B	48	SER	C-N	7.03	1.42	1.33
1	A	136	LEU	CG-CD2	-7.02	1.29	1.52
1	A	36	PHE	CD2-CE2	7.01	1.59	1.38
1	A	122	HIS	CB-CG	7.01	1.59	1.50
1	A	86	LEU	CA-C	-7.01	1.43	1.52
1	A	1	VAL	CB-CG1	7.00	1.75	1.52
2	D	83	ALA	N-CA	-6.99	1.38	1.46
2	B	100	GLN	C-N	6.99	1.43	1.33
2	D	115	ARG	CG-CD	-6.99	1.31	1.52
1	C	43	PHE	CE1-CZ	-6.99	1.17	1.38
1	C	90	LYS	CE-NZ	6.99	1.70	1.49
2	B	48	SER	N-CA	-6.99	1.38	1.46
1	C	86	LEU	CG-CD2	6.98	1.75	1.52
2	D	7	LYS	CB-CG	-6.98	1.31	1.52
2	B	35	PRO	CA-CB	6.98	1.63	1.53
2	D	123	PRO	CG-CD	6.97	1.74	1.50
1	C	124	ASN	CB-CG	-6.97	1.34	1.52
1	A	111	SER	CB-OG	-6.95	1.28	1.42
2	D	129	PHE	CB-CG	-6.95	1.34	1.50
1	A	18	GLY	CA-C	6.94	1.63	1.52
1	A	56	LYS	CA-C	-6.93	1.44	1.52
1	A	91	LEU	CB-CG	6.93	1.67	1.53
1	A	11	LYS	CD-CE	-6.92	1.31	1.52
2	D	9	ALA	C-N	-6.92	1.24	1.33
2	D	29	ARG	CB-CG	6.92	1.73	1.52
1	A	8	SER	CB-OG	6.91	1.55	1.42
1	A	72	HIS	CA-CB	-6.91	1.41	1.53
2	B	40	PHE	C-N	-6.89	1.23	1.33
1	C	26	ALA	C-O	-6.88	1.15	1.24
2	D	77	LEU	CA-C	6.88	1.61	1.52
1	C	44	PRO	C-N	6.88	1.43	1.33
1	C	126	ASN	N-CA	-6.87	1.38	1.46
1	A	57	ALA	CA-C	-6.86	1.45	1.53
1	A	76	LEU	CB-CG	-6.86	1.39	1.53
2	D	86	GLN	CG-CD	6.86	1.69	1.52
2	B	138	ASN	CB-CG	-6.85	1.34	1.52
2	D	117	PHE	N-CA	-6.84	1.37	1.46
1	A	94	ASN	CG-OD1	6.84	1.36	1.23
1	C	86	LEU	CG-CD1	6.84	1.75	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	LEU	CA-CB	-6.84	1.42	1.53
1	C	73	LEU	N-CA	6.84	1.55	1.46
2	D	34	TYR	CG-CD2	-6.84	1.25	1.39
1	C	75	ASP	C-N	6.84	1.47	1.33
2	D	102	PHE	CG-CD1	6.83	1.53	1.38
1	A	60	GLN	CB-CG	-6.83	1.31	1.52
1	C	131	ASN	CG-ND2	-6.83	1.19	1.33
1	A	24	TYR	CA-CB	-6.83	1.45	1.53
2	B	117	PHE	CA-CB	-6.82	1.42	1.53
1	C	28	ALA	C-O	-6.81	1.15	1.24
2	D	92	CYS	CA-CB	6.81	1.65	1.53
2	D	16	LYS	CG-CD	6.81	1.72	1.52
2	B	135	GLY	C-O	6.81	1.33	1.23
2	D	87	LEU	C-N	6.80	1.42	1.33
2	B	36	TRP	CZ2-CH2	6.80	1.50	1.37
1	A	89	HIS	CA-C	6.79	1.67	1.52
2	B	84	PHE	CA-C	-6.77	1.43	1.52
1	A	44	PRO	N-CA	-6.77	1.38	1.47
2	D	129	PHE	CE1-CZ	6.76	1.58	1.38
1	A	61	LYS	CD-CE	6.75	1.72	1.52
2	B	128	LEU	CG-CD1	6.75	1.74	1.52
2	B	39	ARG	CD-NE	-6.75	1.36	1.46
2	D	56	ASN	C-N	-6.75	1.18	1.33
2	B	107	ASN	CB-CG	-6.75	1.35	1.52
2	B	27	LEU	CG-CD1	-6.74	1.30	1.52
2	D	102	PHE	CG-CD2	6.74	1.53	1.38
1	A	9	ASN	CG-ND2	-6.74	1.19	1.33
1	A	33	PHE	CE2-CZ	-6.73	1.18	1.38
1	A	139	LYS	CE-NZ	6.73	1.69	1.49
1	C	6	ASN	CG-OD1	6.73	1.36	1.23
1	A	119	PRO	CB-CG	-6.73	1.16	1.49
2	D	107	ASN	CA-C	-6.72	1.44	1.52
2	D	126	GLN	C-N	6.72	1.42	1.33
1	A	36	PHE	CG-CD1	-6.71	1.24	1.38
1	A	33	PHE	C-N	-6.71	1.23	1.33
2	B	35	PRO	N-CA	-6.70	1.38	1.47
2	D	22	VAL	CB-CG1	6.70	1.74	1.52
1	C	49	SER	N-CA	-6.70	1.33	1.46
1	A	25	GLY	C-N	-6.70	1.25	1.33
2	B	51	GLY	CA-C	6.69	1.61	1.51
2	D	22	VAL	CB-CG2	6.69	1.74	1.52
1	A	93	VAL	CB-CG2	6.68	1.74	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	11	LYS	CB-CG	-6.68	1.32	1.52
1	C	34	LEU	N-CA	-6.68	1.37	1.46
1	A	38	THR	CB-OG1	-6.67	1.33	1.43
2	D	120	GLN	CA-C	-6.67	1.43	1.52
1	A	95	PRO	C-O	6.66	1.32	1.24
2	D	111	LEU	CA-CB	-6.66	1.42	1.53
2	B	5	GLU	CA-C	-6.64	1.43	1.52
2	D	13	PHE	CA-C	6.63	1.61	1.52
2	D	84	PHE	CG-CD2	-6.63	1.25	1.38
1	A	95	PRO	CB-CG	-6.63	1.16	1.49
2	B	60	LYS	CG-CD	-6.63	1.32	1.52
2	B	80	LEU	CA-CB	-6.63	1.40	1.53
1	C	105	LEU	CB-CG	-6.63	1.40	1.53
2	B	42	GLN	CA-C	-6.61	1.43	1.52
2	B	10	VAL	CA-C	-6.61	1.43	1.52
1	C	31	ARG	CG-CD	6.61	1.72	1.52
1	C	101	LEU	CG-CD2	-6.60	1.30	1.52
1	A	127	LYS	CA-CB	-6.59	1.42	1.53
1	C	60	GLN	C-O	6.57	1.32	1.24
1	C	90	LYS	CA-C	-6.57	1.46	1.52
2	B	111	LEU	N-CA	-6.57	1.38	1.46
1	A	108	THR	CA-C	6.56	1.61	1.52
2	B	78	ASP	N-CA	-6.56	1.33	1.46
2	B	42	GLN	C-O	6.55	1.32	1.23
1	A	112	HIS	CA-C	-6.55	1.43	1.52
1	C	105	LEU	CG-CD2	6.55	1.74	1.52
2	B	33	VAL	CB-CG1	6.55	1.74	1.52
1	C	30	GLN	C-N	6.55	1.42	1.33
2	D	115	ARG	N-CA	-6.54	1.38	1.46
1	C	56	LYS	CG-CD	6.54	1.72	1.52
1	C	136	LEU	CA-C	-6.54	1.43	1.52
2	D	56	ASN	CG-ND2	6.54	1.47	1.33
1	A	118	THR	N-CA	-6.52	1.36	1.46
1	A	113	LEU	N-CA	-6.52	1.40	1.46
2	B	121	PHE	CE1-CZ	-6.52	1.19	1.38
2	D	142	HIS	CG-CD2	6.52	1.43	1.35
2	B	111	LEU	C-N	6.51	1.42	1.33
1	A	42	TYR	CA-C	-6.51	1.44	1.52
2	B	127	ALA	N-CA	-6.51	1.37	1.46
2	D	18	ASP	CG-OD2	-6.51	1.12	1.25
1	A	91	LEU	CA-C	6.51	1.60	1.52
2	B	122	THR	N-CA	6.51	1.58	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	LYS	CA-CB	6.51	1.64	1.53
2	D	37	THR	CA-C	-6.51	1.43	1.52
2	D	74	LEU	C-N	-6.50	1.24	1.33
1	A	26	ALA	CA-C	-6.50	1.43	1.52
1	C	42	TYR	CA-C	6.50	1.61	1.52
2	D	118	GLY	C-N	-6.49	1.25	1.33
2	B	42	GLN	CA-CB	6.48	1.65	1.53
1	C	4	ALA	CA-C	6.47	1.61	1.53
1	A	104	SER	CA-C	-6.46	1.44	1.52
1	C	55	GLN	C-N	6.46	1.42	1.33
2	B	14	TRP	CZ3-CH2	-6.46	1.24	1.40
1	C	37	PRO	CB-CG	-6.46	1.17	1.49
2	D	77	LEU	C-O	6.46	1.31	1.24
2	B	4	ALA	CA-CB	-6.45	1.42	1.53
1	C	95	PRO	C-N	-6.45	1.24	1.33
1	C	135	VAL	CA-C	-6.45	1.43	1.52
2	D	5	GLU	CB-CG	-6.45	1.33	1.52
1	A	24	TYR	C-N	6.45	1.43	1.33
1	A	121	VAL	CA-C	-6.44	1.44	1.52
1	C	50	HIS	C-O	6.43	1.36	1.23
2	D	76	HIS	C-N	-6.43	1.24	1.33
2	B	13	PHE	CD1-CE1	6.43	1.57	1.38
2	D	47	LEU	CG-CD1	6.42	1.73	1.52
2	D	20	ASP	N-CA	-6.42	1.38	1.46
2	B	60	LYS	CA-CB	-6.42	1.42	1.53
1	C	38	THR	C-N	6.41	1.43	1.33
2	B	64	LYS	CB-CG	6.41	1.71	1.52
2	B	16	LYS	CA-CB	-6.40	1.42	1.53
1	C	9	ASN	CA-C	-6.39	1.44	1.52
1	A	38	THR	CA-C	6.38	1.61	1.52
2	B	142	HIS	C-O	6.38	1.32	1.24
2	D	42	GLN	C-O	6.38	1.32	1.24
2	D	104	LEU	CA-CB	6.37	1.63	1.53
1	A	141	ARG	CD-NE	6.37	1.55	1.46
1	C	23	ALA	C-N	6.37	1.42	1.33
2	B	28	GLY	C-N	6.36	1.42	1.34
1	A	54	GLN	CG-CD	6.36	1.68	1.52
1	A	89	HIS	C-N	-6.35	1.25	1.33
1	C	125	LEU	C-N	6.35	1.41	1.33
1	C	40	LYS	N-CA	6.35	1.54	1.46
1	C	73	LEU	CA-CB	6.34	1.64	1.53
1	C	118	THR	CA-CB	6.34	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	LEU	C-N	6.34	1.42	1.33
2	B	72	GLN	CA-C	6.33	1.61	1.52
1	A	75	ASP	CG-OD2	6.32	1.37	1.25
2	B	80	LEU	CG-CD1	6.32	1.73	1.52
2	B	81	LYS	CE-NZ	-6.31	1.30	1.49
1	C	139	LYS	CG-CD	-6.30	1.33	1.52
1	A	124	ASN	N-CA	-6.30	1.39	1.46
1	C	29	LEU	C-O	-6.30	1.16	1.24
1	A	43	PHE	CD1-CE1	-6.29	1.19	1.38
2	D	70	PHE	CG-CD2	6.29	1.52	1.38
2	D	122	THR	C-O	6.28	1.32	1.24
1	A	21	ALA	N-CA	6.26	1.52	1.46
2	D	116	ASN	CA-CB	-6.26	1.42	1.53
2	B	120	GLN	C-N	6.25	1.41	1.33
2	B	30	LEU	C-O	6.24	1.31	1.24
2	B	64	LYS	CE-NZ	6.24	1.68	1.49
2	B	95	LEU	C-O	6.24	1.31	1.24
1	C	109	LEU	C-O	6.24	1.31	1.24
2	D	122	THR	CB-CG2	6.24	1.73	1.52
1	A	103	HIS	C-O	6.22	1.31	1.24
1	C	103	HIS	C-N	-6.20	1.26	1.33
2	B	112	VAL	CB-CG1	-6.19	1.32	1.52
1	C	106	LEU	C-O	-6.19	1.16	1.24
1	C	133	SER	CB-OG	-6.19	1.29	1.42
2	D	29	ARG	CA-C	-6.19	1.44	1.52
1	A	63	ALA	N-CA	6.18	1.54	1.46
1	A	132	ASP	CB-CG	-6.18	1.36	1.52
2	D	30	LEU	CA-CB	6.18	1.63	1.53
2	D	53	VAL	CB-CG1	6.18	1.73	1.52
2	B	73	GLY	C-O	6.18	1.32	1.23
2	D	117	PHE	CA-C	-6.18	1.44	1.52
2	D	145	HIS	CA-CB	6.18	1.65	1.53
2	D	70	PHE	CA-CB	-6.17	1.43	1.53
2	D	116	ASN	CG-ND2	6.17	1.46	1.33
2	B	98	ASN	CB-CG	-6.16	1.36	1.52
2	B	112	VAL	CB-CG2	-6.16	1.32	1.52
1	A	58	HIS	CB-CG	-6.16	1.41	1.50
2	D	105	LEU	CA-CB	6.16	1.63	1.53
1	C	118	THR	C-N	-6.16	1.25	1.34
2	B	62	HIS	CA-CB	-6.15	1.43	1.53
2	D	22	VAL	C-O	-6.15	1.17	1.24
1	C	10	VAL	CB-CG1	6.14	1.72	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	28	ALA	CA-CB	-6.13	1.44	1.53
1	A	56	LYS	N-CA	-6.13	1.39	1.46
2	D	91	HIS	CG-CD2	-6.12	1.29	1.35
1	C	88	ALA	N-CA	-6.12	1.38	1.46
1	C	42	TYR	CD1-CE1	-6.12	1.20	1.38
1	A	128	PHE	CA-CB	6.12	1.63	1.53
1	A	37	PRO	CA-C	-6.12	1.43	1.52
1	A	90	LYS	CD-CE	6.12	1.70	1.52
1	A	15	GLY	C-O	-6.10	1.15	1.23
2	B	12	GLY	N-CA	6.10	1.54	1.45
2	B	16	LYS	CE-NZ	6.09	1.67	1.49
2	B	87	LEU	CG-CD2	-6.09	1.32	1.52
1	A	92	ARG	C-N	6.09	1.42	1.33
1	C	12	ALA	C-N	6.09	1.42	1.33
2	D	91	HIS	CE1-NE2	-6.08	1.26	1.32
1	A	129	LEU	CG-CD1	-6.08	1.32	1.52
1	C	36	PHE	CE2-CZ	-6.08	1.20	1.38
1	C	109	LEU	CA-C	-6.08	1.44	1.52
2	B	87	LEU	N-CA	-6.07	1.38	1.46
2	B	72	GLN	CG-CD	-6.07	1.36	1.52
1	C	141	ARG	CZ-NH1	6.07	1.41	1.32
1	A	31	ARG	NE-CZ	-6.06	1.26	1.33
2	D	10	VAL	N-CA	-6.06	1.38	1.46
2	D	94	LYS	CG-CD	6.06	1.70	1.52
2	B	65	ARG	CD-NE	6.06	1.54	1.46
2	B	77	LEU	CG-CD1	6.05	1.72	1.52
2	B	72	GLN	CD-OE1	6.05	1.35	1.23
2	B	60	LYS	CD-CE	6.04	1.70	1.52
1	C	92	ARG	CZ-NH2	6.04	1.41	1.33
2	B	21	VAL	C-N	6.03	1.41	1.33
2	B	123	PRO	CB-CG	6.03	1.79	1.49
1	A	74	ASN	CG-OD1	-6.02	1.12	1.23
2	D	82	GLY	C-N	6.02	1.41	1.33
2	D	91	HIS	CA-C	-6.01	1.45	1.53
1	C	8	SER	CA-C	6.01	1.60	1.52
2	D	70	PHE	CB-CG	6.01	1.64	1.50
2	D	131	LYS	N-CA	5.99	1.53	1.46
2	D	17	VAL	C-O	5.98	1.31	1.24
2	B	34	TYR	C-O	-5.97	1.16	1.24
2	D	97	VAL	CB-CG1	5.96	1.72	1.52
1	C	25	GLY	C-O	-5.96	1.16	1.23
1	C	77	PRO	CG-CD	-5.95	1.30	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	PHE	CE2-CZ	5.94	1.56	1.38
1	C	95	PRO	CA-CB	5.93	1.62	1.53
1	A	124	ASN	CA-C	-5.92	1.45	1.52
2	D	101	ASN	C-O	-5.92	1.16	1.24
1	C	62	VAL	CB-CG1	5.92	1.72	1.52
1	C	128	PHE	CA-CB	-5.91	1.43	1.53
1	A	98	PHE	CG-CD2	-5.90	1.26	1.38
2	D	54	MET	N-CA	-5.90	1.39	1.46
1	C	50	HIS	CA-CB	5.90	1.65	1.53
1	A	27	GLN	C-O	5.90	1.31	1.24
1	A	134	THR	CB-CG2	5.89	1.72	1.52
2	D	17	VAL	C-N	5.89	1.42	1.33
2	D	84	PHE	C-N	5.89	1.41	1.33
1	C	132	ASP	CA-C	5.89	1.60	1.52
2	D	20	ASP	CB-CG	5.88	1.66	1.52
1	A	35	SER	N-CA	5.88	1.54	1.45
1	C	21	ALA	C-O	5.88	1.31	1.24
1	C	133	SER	C-O	-5.87	1.16	1.24
2	D	57	PRO	CG-CD	5.87	1.70	1.50
1	A	99	LYS	CA-CB	-5.87	1.43	1.53
1	A	94	ASN	CA-C	-5.86	1.46	1.53
1	C	121	VAL	CA-CB	-5.86	1.46	1.54
2	D	21	VAL	C-N	5.86	1.41	1.33
1	C	103	HIS	CE1-NE2	-5.86	1.26	1.32
2	D	43	HIS	ND1-CE1	5.85	1.38	1.32
2	B	36	TRP	CE3-CZ3	-5.85	1.21	1.38
2	D	133	VAL	C-O	-5.85	1.17	1.24
1	A	58	HIS	CG-ND1	5.84	1.44	1.38
1	C	42	TYR	CB-CG	5.84	1.64	1.51
2	D	112	VAL	CB-CG2	-5.84	1.33	1.52
1	A	41	THR	C-N	-5.84	1.25	1.33
1	C	22	PRO	N-CD	5.82	1.55	1.47
2	B	54	MET	CG-SD	-5.82	1.66	1.80
2	D	143	LYS	CG-CD	-5.81	1.35	1.52
2	B	52	ALA	CA-CB	-5.81	1.43	1.53
1	A	115	THR	N-CA	5.80	1.53	1.46
2	B	119	GLY	C-N	-5.80	1.25	1.33
1	A	115	THR	CA-C	-5.80	1.45	1.52
1	C	33	PHE	CG-CD1	-5.80	1.26	1.38
1	C	87	HIS	CA-CB	5.79	1.63	1.53
1	C	129	LEU	CA-CB	-5.77	1.44	1.53
2	B	32	VAL	C-O	5.77	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	33	PHE	CE1-CZ	5.77	1.55	1.38
1	A	92	ARG	CG-CD	-5.76	1.35	1.52
1	C	31	ARG	CZ-NH2	5.76	1.41	1.33
2	D	17	VAL	CB-CG1	5.75	1.71	1.52
1	A	124	ASN	CG-ND2	-5.75	1.21	1.33
1	C	112	HIS	N-CA	5.75	1.53	1.46
2	D	121	PHE	CE1-CZ	5.75	1.55	1.38
2	B	97	VAL	N-CA	5.74	1.53	1.46
2	B	78	ASP	CA-C	5.74	1.65	1.52
2	D	126	GLN	CD-NE2	5.73	1.45	1.33
1	C	31	ARG	N-CA	5.72	1.53	1.46
2	B	9	ALA	C-O	5.72	1.31	1.24
1	A	22	PRO	CA-C	-5.72	1.42	1.52
1	A	111	SER	C-O	-5.72	1.16	1.24
1	C	86	LEU	CA-C	-5.71	1.41	1.52
1	A	38	THR	CB-CG2	5.70	1.71	1.52
2	D	15	GLY	C-O	-5.70	1.16	1.23
2	D	121	PHE	CA-C	-5.70	1.45	1.52
1	A	92	ARG	CA-C	-5.70	1.45	1.53
1	A	20	ASN	C-N	5.69	1.42	1.33
2	D	38	GLN	N-CA	-5.68	1.39	1.46
1	A	88	ALA	CA-CB	5.68	1.63	1.53
1	C	45	HIS	CG-CD2	5.68	1.42	1.35
1	A	80	LEU	CA-CB	5.68	1.62	1.53
1	A	117	PHE	CD2-CE2	-5.68	1.21	1.38
2	D	72	GLN	CB-CG	5.68	1.69	1.52
2	D	36	TRP	C-O	5.67	1.31	1.24
1	C	120	ALA	CA-C	5.67	1.60	1.52
2	B	14	TRP	NE1-CE2	5.65	1.43	1.37
2	B	86	GLN	C-O	-5.64	1.12	1.23
1	A	17	VAL	C-N	-5.64	1.24	1.33
1	C	101	LEU	CA-C	5.64	1.60	1.52
1	C	119	PRO	N-CD	5.63	1.55	1.47
2	B	12	GLY	C-N	5.63	1.41	1.33
1	A	21	ALA	CA-CB	-5.63	1.46	1.53
2	B	56	ASN	CG-OD1	5.63	1.34	1.23
1	C	55	GLN	CD-NE2	5.63	1.45	1.33
1	C	132	ASP	CA-CB	5.63	1.62	1.53
1	C	31	ARG	CZ-NH1	5.62	1.40	1.32
2	B	67	LEU	CB-CG	5.62	1.64	1.53
1	A	34	LEU	CG-CD2	5.61	1.71	1.52
2	D	23	GLY	C-O	5.61	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	THR	CA-CB	-5.60	1.44	1.53
2	B	98	ASN	C-N	5.60	1.40	1.34
1	C	89	HIS	CA-CB	5.59	1.62	1.53
2	B	78	ASP	C-N	-5.59	1.25	1.33
1	C	106	LEU	CA-CB	-5.59	1.43	1.53
1	C	39	THR	CA-C	5.59	1.60	1.52
2	D	124	ASN	CA-CB	5.59	1.62	1.53
1	A	1	VAL	C-N	-5.58	1.25	1.33
1	A	42	TYR	CZ-OH	-5.58	1.26	1.38
2	B	29	ARG	CG-CD	5.58	1.69	1.52
2	B	18	ASP	N-CA	-5.58	1.39	1.46
2	D	6	GLU	CD-OE1	5.58	1.35	1.25
1	C	33	PHE	CD2-CE2	5.56	1.55	1.38
1	A	30	GLN	C-O	-5.56	1.17	1.24
1	A	68	LYS	CE-NZ	5.56	1.66	1.49
2	D	77	LEU	CA-CB	-5.56	1.44	1.53
2	D	133	VAL	CA-C	-5.56	1.45	1.52
2	B	5	GLU	C-O	5.56	1.31	1.24
1	A	22	PRO	CB-CG	5.55	1.77	1.49
1	A	132	ASP	CA-CB	5.55	1.62	1.53
2	B	99	PRO	CA-CB	-5.55	1.44	1.53
2	D	14	TRP	CB-CG	-5.55	1.33	1.50
2	B	138	ASN	C-N	5.55	1.41	1.34
2	D	42	GLN	N-CA	-5.54	1.38	1.45
1	C	96	VAL	C-O	-5.54	1.17	1.24
2	B	65	ARG	CZ-NH1	5.54	1.40	1.32
1	A	101	LEU	CG-CD2	5.53	1.70	1.52
1	C	60	GLN	CA-C	5.53	1.60	1.52
2	B	7	LYS	CA-CB	5.53	1.62	1.53
2	D	30	LEU	C-O	5.53	1.30	1.24
1	A	55	GLN	CG-CD	5.52	1.65	1.52
2	B	111	LEU	CG-CD1	5.52	1.70	1.52
2	B	135	GLY	C-N	-5.52	1.26	1.33
2	D	117	PHE	CG-CD2	-5.51	1.27	1.38
1	A	66	LEU	CG-CD1	5.51	1.70	1.52
2	B	9	ALA	N-CA	-5.50	1.39	1.46
2	B	100	GLN	CD-OE1	5.50	1.34	1.23
2	B	7	LYS	CD-CE	5.49	1.69	1.52
2	B	107	ASN	C-N	-5.48	1.26	1.33
2	B	16	LYS	C-N	-5.48	1.26	1.33
2	B	27	LEU	CG-CD2	5.47	1.70	1.52
1	A	31	ARG	CA-CB	5.47	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	TYR	C-O	5.46	1.30	1.24
1	A	13	ALA	C-N	-5.46	1.26	1.33
2	B	74	LEU	CG-CD2	-5.46	1.34	1.52
2	B	135	GLY	CA-C	5.46	1.59	1.51
2	D	58	LYS	CA-C	-5.43	1.45	1.52
1	C	73	LEU	C-N	-5.43	1.26	1.33
1	A	98	PHE	CA-CB	-5.41	1.45	1.53
2	D	38	GLN	CB-CG	5.41	1.68	1.52
2	D	53	VAL	CA-CB	5.41	1.61	1.54
2	B	126	GLN	CB-CG	5.40	1.68	1.52
2	D	116	ASN	CG-OD1	-5.39	1.13	1.23
1	C	109	LEU	C-N	5.37	1.40	1.33
1	A	16	LYS	N-CA	-5.37	1.39	1.46
1	A	134	THR	CA-CB	-5.37	1.45	1.53
2	D	75	LYS	C-N	5.36	1.41	1.33
2	B	77	LEU	CG-CD2	5.36	1.70	1.52
1	A	36	PHE	N-CA	5.36	1.53	1.46
1	A	19	GLY	C-N	5.36	1.41	1.33
2	D	144	TYR	CE2-CZ	5.36	1.51	1.38
2	B	25	GLN	CG-CD	5.35	1.65	1.52
2	D	99	PRO	CB-CG	5.35	1.76	1.49
2	D	88	SER	C-O	5.35	1.30	1.23
1	C	32	MET	CG-SD	-5.35	1.67	1.80
2	B	91	HIS	CG-ND1	5.34	1.44	1.38
2	B	102	PHE	CD1-CE1	-5.34	1.22	1.38
1	A	101	LEU	C-O	-5.34	1.17	1.24
1	C	37	PRO	CA-C	-5.34	1.44	1.52
2	D	46	ASN	CB-CG	-5.32	1.38	1.52
2	D	72	GLN	C-O	-5.32	1.17	1.24
2	B	69	ALA	C-N	-5.31	1.25	1.33
2	B	37	THR	CA-C	5.31	1.60	1.52
2	D	61	ALA	C-O	-5.31	1.17	1.24
2	B	5	GLU	CA-CB	5.31	1.62	1.53
2	D	41	PHE	CA-CB	5.30	1.61	1.52
2	B	15	GLY	N-CA	-5.30	1.37	1.45
1	A	121	VAL	CA-CB	5.29	1.61	1.54
1	A	8	SER	C-N	-5.28	1.26	1.33
1	C	24	TYR	N-CA	-5.27	1.39	1.46
1	A	79	THR	CB-CG2	-5.26	1.35	1.52
1	A	96	VAL	CA-C	-5.26	1.46	1.52
2	D	11	THR	C-O	-5.26	1.13	1.23
1	A	33	PHE	C-O	-5.26	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	PHE	C-O	-5.26	1.18	1.24
1	C	20	ASN	CG-ND2	5.25	1.44	1.33
2	D	46	ASN	CA-C	-5.25	1.45	1.52
1	A	20	ASN	CA-C	-5.25	1.45	1.52
2	D	25	GLN	CA-CB	-5.24	1.44	1.53
1	C	89	HIS	CA-C	5.24	1.59	1.52
1	C	105	LEU	CA-CB	5.23	1.61	1.53
2	D	62	HIS	CB-CG	5.22	1.57	1.50
2	B	102	PHE	CA-CB	5.21	1.61	1.53
1	C	9	ASN	CA-CB	5.21	1.62	1.53
2	B	22	VAL	C-N	-5.20	1.25	1.33
2	B	144	TYR	CG-CD1	5.20	1.50	1.39
2	B	95	LEU	CG-CD1	5.19	1.69	1.52
2	D	67	LEU	CG-CD1	5.19	1.69	1.52
1	C	5	ALA	N-CA	5.18	1.52	1.45
2	D	81	LYS	CB-CG	-5.18	1.36	1.52
1	A	27	GLN	CG-CD	5.18	1.65	1.52
1	A	98	PHE	CD1-CE1	-5.18	1.23	1.38
1	C	116	ASN	CG-OD1	5.17	1.33	1.23
2	D	9	ALA	CA-C	5.17	1.59	1.52
2	D	6	GLU	N-CA	-5.17	1.39	1.46
1	A	122	HIS	CA-CB	-5.17	1.45	1.53
1	A	50	HIS	CG-ND1	5.16	1.44	1.38
1	A	88	ALA	C-N	-5.16	1.26	1.33
1	A	104	SER	C-O	5.15	1.30	1.24
2	B	43	HIS	C-O	5.15	1.33	1.23
1	A	37	PRO	N-CA	5.15	1.53	1.47
1	A	61	LYS	CB-CG	5.15	1.67	1.52
1	A	114	PRO	C-O	5.14	1.30	1.24
2	D	58	LYS	N-CA	-5.14	1.39	1.46
2	B	92	CYS	N-CA	5.14	1.52	1.46
1	C	131	ASN	CA-C	-5.12	1.46	1.52
2	D	46	ASN	CG-ND2	-5.12	1.22	1.33
2	B	5	GLU	CB-CG	5.12	1.67	1.52
2	D	116	ASN	CA-C	-5.11	1.46	1.52
1	C	83	LEU	CB-CG	-5.11	1.43	1.53
2	B	121	PHE	CD2-CE2	5.11	1.53	1.38
1	C	30	GLN	CA-C	-5.11	1.45	1.52
1	A	40	LYS	C-O	5.11	1.30	1.24
2	D	24	ALA	C-N	5.09	1.40	1.33
2	D	94	LYS	CB-CG	5.08	1.67	1.52
1	C	6	ASN	CG-ND2	-5.08	1.22	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	23	GLY	C-N	-5.08	1.26	1.33
2	B	49	SER	CB-OG	-5.08	1.31	1.42
2	D	103	ARG	N-CA	5.07	1.52	1.46
2	B	14	TRP	CD2-CE2	5.07	1.50	1.41
1	C	121	VAL	CB-CG2	-5.07	1.35	1.52
2	D	21	VAL	CA-C	-5.07	1.46	1.52
2	D	123	PRO	CA-CB	5.07	1.61	1.53
2	D	58	LYS	C-O	5.06	1.30	1.24
2	D	37	THR	CA-CB	-5.06	1.45	1.53
1	A	117	PHE	N-CA	-5.05	1.39	1.46
1	A	137	THR	CA-C	-5.05	1.46	1.52
2	B	45	GLY	CA-C	5.05	1.59	1.51
2	B	75	LYS	CE-NZ	-5.04	1.34	1.49
2	D	14	TRP	CZ2-CH2	-5.04	1.27	1.37
2	B	28	GLY	C-O	5.04	1.30	1.23
1	C	14	TRP	CZ3-CH2	5.03	1.53	1.40
2	D	29	ARG	C-N	5.02	1.40	1.33
2	B	131	LYS	CA-CB	5.01	1.61	1.53
1	A	120	ALA	CA-C	5.01	1.59	1.52
2	B	29	ARG	CA-CB	5.01	1.61	1.53
1	C	82	ASN	CA-CB	-5.01	1.45	1.53
1	A	77	PRO	CG-CD	-5.01	1.33	1.50
2	B	135	GLY	N-CA	-5.01	1.38	1.45

All (3877) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	7	LYS	O-C-N	-56.69	47.19	122.59
1	C	122	HIS	CA-CB-CG	55.70	169.50	113.80
2	D	100	GLN	OE1-CD-NE2	-51.06	71.54	122.60
2	D	11	THR	CB-CA-C	45.62	174.25	111.74
1	A	131	ASN	OD1-CG-ND2	-45.33	77.27	122.60
2	B	70	PHE	CA-C-O	45.08	170.30	120.71
1	C	112	HIS	ND1-CG-CD2	-43.76	62.34	106.10
1	C	85	ASN	CA-C-O	-43.60	70.78	120.92
2	D	18	ASP	CA-C-O	42.86	166.98	120.70
1	A	87	HIS	ND1-CG-CD2	42.77	148.87	106.10
2	D	3	THR	CA-C-N	-42.48	62.29	122.19
2	D	3	THR	C-N-CA	-42.48	62.29	122.19
1	A	94	ASN	OD1-CG-ND2	-41.56	81.04	122.60
1	C	112	HIS	CG-CD2-NE2	41.54	148.74	107.20
2	B	70	PHE	O-C-N	-41.47	77.59	122.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	ASN	CA-CB-CG	41.47	154.07	112.60
2	D	127	ALA	CA-C-O	-41.38	77.45	120.89
2	B	93	ASN	OD1-CG-ND2	-41.26	81.34	122.60
2	B	116	ASN	OD1-CG-ND2	-40.78	81.82	122.60
2	D	130	GLN	OE1-CD-NE2	40.43	163.03	122.60
2	D	70	PHE	CA-C-O	-40.11	70.17	120.31
2	D	126	GLN	OE1-CD-NE2	-39.68	82.92	122.60
1	A	29	LEU	O-C-N	-39.55	69.99	122.59
2	D	77	LEU	O-C-N	-39.24	71.22	122.23
1	A	116	ASN	OD1-CG-ND2	-39.18	83.42	122.60
1	C	6	ASN	OD1-CG-ND2	-38.86	83.74	122.60
1	C	103	HIS	ND1-CE1-NE2	38.62	147.03	108.40
2	D	11	THR	O-C-N	-38.25	64.52	122.67
1	C	126	ASN	OD1-CG-ND2	-38.19	84.41	122.60
1	C	124	ASN	OD1-CG-ND2	-38.16	84.44	122.60
1	A	81	SER	CA-C-O	-37.95	80.95	120.80
2	D	53	VAL	N-CA-C	-37.87	79.24	111.81
1	A	92	ARG	CA-C-N	37.76	168.62	122.93
1	A	92	ARG	C-N-CA	37.76	168.62	122.93
2	D	2	LEU	CA-C-O	-37.67	66.64	120.51
1	A	60	GLN	CB-CG-CD	37.51	176.37	112.60
2	D	72	GLN	OE1-CD-NE2	37.22	159.82	122.60
2	B	16	LYS	O-C-N	-36.89	73.53	122.59
2	B	77	LEU	CA-C-O	36.77	167.61	120.55
1	A	55	GLN	CA-C-N	36.76	170.63	120.63
1	A	55	GLN	C-N-CA	36.76	170.63	120.63
2	B	46	ASN	CA-CB-CG	-36.75	75.85	112.60
2	B	67	LEU	CA-C-O	-36.60	68.17	120.51
1	C	81	SER	CA-C-O	36.31	160.54	120.24
2	D	18	ASP	O-C-N	-36.15	76.24	123.23
1	C	108	THR	N-CA-CB	35.79	160.92	110.10
2	B	126	GLN	OE1-CD-NE2	-35.75	86.85	122.60
1	A	122	HIS	CA-CB-CG	35.54	149.34	113.80
1	C	112	HIS	CE1-NE2-CD2	-35.40	73.60	109.00
1	A	70	GLN	OE1-CD-NE2	-35.07	87.53	122.60
1	A	92	ARG	NE-CZ-NH2	-34.92	87.77	119.20
2	D	100	GLN	CG-CD-NE2	34.72	168.48	116.40
2	D	93	ASN	O-C-N	34.40	157.50	122.07
1	A	82	ASN	CA-CB-CG	34.34	146.94	112.60
1	A	94	ASN	CB-CG-ND2	34.29	167.84	116.40
1	C	85	ASN	O-C-N	-34.27	83.41	123.16
1	A	70	GLN	CB-CG-CD	34.13	170.63	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	SER	O-C-N	34.10	162.82	123.27
1	A	120	ALA	CA-C-O	-34.09	85.59	120.70
2	D	7	LYS	CA-C-O	33.89	168.97	120.51
2	D	96	HIS	ND1-CG-CD2	-33.85	72.25	106.10
2	B	79	ASP	CA-CB-CG	-33.77	78.83	112.60
1	C	46	PHE	CA-C-O	33.72	161.07	121.28
2	B	102	PHE	CA-CB-CG	33.49	147.29	113.80
2	D	65	ARG	NE-CZ-NH2	33.29	149.16	119.20
2	B	76	HIS	CA-C-N	33.28	174.53	122.61
2	B	76	HIS	C-N-CA	33.28	174.53	122.61
2	D	143	LYS	O-C-N	-33.11	78.56	122.59
2	B	138	ASN	CA-CB-CG	32.98	145.58	112.60
2	D	73	GLY	CA-C-N	32.88	164.34	120.28
2	D	73	GLY	C-N-CA	32.88	164.34	120.28
1	A	127	LYS	CA-C-O	-32.55	73.96	120.51
2	D	14	TRP	CG-CD2-CE3	-32.45	101.45	133.90
2	B	102	PHE	O-C-N	-32.39	87.79	122.12
1	A	85	ASN	CA-C-O	-32.36	74.24	120.51
1	C	55	GLN	OE1-CD-NE2	-32.33	90.27	122.60
1	A	97	ASN	CB-CG-ND2	31.84	164.16	116.40
1	A	55	GLN	OE1-CD-NE2	-31.75	90.85	122.60
2	B	95	LEU	N-CA-CB	-31.68	56.96	110.49
2	D	6	GLU	O-C-N	31.66	164.70	122.59
2	B	20	ASP	O-C-N	-31.58	80.59	122.59
1	A	132	ASP	CA-CB-CG	-31.56	81.04	112.60
1	A	87	HIS	CG-CD2-NE2	-31.31	75.89	107.20
1	A	126	ASN	OD1-CG-ND2	-31.27	91.33	122.60
2	B	65	ARG	NH1-CZ-NH2	-31.25	78.67	119.30
2	B	62	HIS	CA-CB-CG	-31.24	82.56	113.80
1	A	20	ASN	CB-CG-ND2	31.19	163.18	116.40
2	D	102	PHE	CA-C-O	-31.14	88.82	120.90
1	A	133	SER	O-C-N	-31.14	89.71	122.09
2	B	93	ASN	CA-CB-CG	-30.93	81.67	112.60
1	C	87	HIS	CA-C-O	-30.84	81.76	120.31
2	D	43	HIS	CA-CB-CG	30.77	144.57	113.80
2	D	70	PHE	CD1-CG-CD2	-30.77	72.45	118.60
1	C	109	LEU	CA-C-N	30.71	176.98	121.70
1	C	109	LEU	C-N-CA	30.71	176.98	121.70
2	B	65	ARG	CA-C-O	-30.65	87.93	120.42
2	D	91	HIS	CA-C-O	-30.57	82.10	120.31
1	A	102	SER	CA-C-N	30.44	160.83	120.65
1	A	102	SER	C-N-CA	30.44	160.83	120.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	43	HIS	CB-CG-CD2	-30.41	91.67	131.20
2	B	121	PHE	CA-C-N	30.39	176.40	121.70
2	B	121	PHE	C-N-CA	30.39	176.40	121.70
1	C	36	PHE	CG-CD2-CE2	30.39	172.36	120.70
2	D	19	VAL	CA-CB-CG1	30.38	162.05	110.40
2	D	103	ARG	CA-C-O	30.36	157.97	119.11
2	D	43	HIS	ND1-CG-CD2	-30.31	75.79	106.10
2	B	59	VAL	CA-C-O	-30.28	88.75	120.85
2	D	142	HIS	ND1-CE1-NE2	-30.25	78.15	108.40
2	D	70	PHE	CG-CD2-CE2	30.22	172.08	120.70
1	C	35	SER	CA-C-O	-30.18	82.97	119.49
2	B	54	MET	CA-C-N	30.05	162.97	120.29
2	B	54	MET	C-N-CA	30.05	162.97	120.29
1	C	37	PRO	CA-C-N	29.92	173.51	121.14
1	C	37	PRO	C-N-CA	29.92	173.51	121.14
2	D	67	LEU	CA-C-O	-29.92	88.84	120.55
2	D	135	GLY	CA-C-O	-29.75	91.64	120.80
2	D	34	TYR	CB-CA-C	29.69	141.53	110.65
2	D	70	PHE	CB-CG-CD2	29.68	171.15	120.70
1	C	49	SER	O-C-N	-29.67	75.53	123.00
1	A	141	ARG	NE-CZ-NH1	29.66	151.16	121.50
2	B	79	ASP	O-C-N	-29.65	83.15	122.59
2	D	22	VAL	O-C-N	-29.64	89.95	121.96
2	D	80	LEU	O-C-N	29.54	152.81	122.09
1	C	107	VAL	CA-C-N	29.44	165.05	120.89
1	C	107	VAL	C-N-CA	29.44	165.05	120.89
2	D	91	HIS	O-C-N	29.42	162.02	122.30
2	B	31	LEU	CA-C-N	-29.36	86.54	122.95
2	B	31	LEU	C-N-CA	-29.36	86.54	122.95
2	D	32	VAL	CA-C-O	-29.36	89.73	120.85
2	D	137	ALA	CA-C-N	29.23	167.19	122.17
2	D	137	ALA	C-N-CA	29.23	167.19	122.17
1	C	2	LEU	O-C-N	-29.22	89.12	123.31
1	C	82	ASN	O-C-N	29.12	152.37	122.09
1	A	40	LYS	O-C-N	-29.09	83.90	122.59
2	B	73	GLY	O-C-N	29.05	160.46	122.70
2	D	52	ALA	CA-C-N	29.01	156.59	122.35
2	D	52	ALA	C-N-CA	29.01	156.59	122.35
1	C	55	GLN	CG-CD-NE2	28.94	159.80	116.40
1	A	52	SER	CA-C-O	-28.91	89.37	120.30
2	D	43	HIS	CB-CG-ND1	28.89	166.03	122.70
2	D	144	TYR	CA-C-O	-28.84	79.27	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	PRO	O-C-N	28.83	161.56	122.64
1	A	72	HIS	ND1-CE1-NE2	-28.78	79.62	108.40
1	C	68	LYS	CA-C-N	28.77	162.39	120.38
1	C	68	LYS	C-N-CA	28.77	162.39	120.38
2	D	115	ARG	O-C-N	-28.57	88.48	122.19
2	D	128	LEU	O-C-N	28.52	160.52	122.59
2	D	113	VAL	N-CA-C	-28.48	84.82	110.74
2	D	72	GLN	CA-C-O	-28.45	79.82	120.51
2	B	106	GLY	CA-C-N	28.41	160.64	120.29
2	B	106	GLY	C-N-CA	28.41	160.64	120.29
2	D	124	ASN	OD1-CG-ND2	28.40	151.00	122.60
2	B	123	PRO	O-C-N	-28.25	84.14	122.27
2	D	50	ALA	CA-C-O	-28.20	90.17	120.63
1	C	139	LYS	CA-C-O	28.03	160.59	120.51
2	D	97	VAL	CA-C-O	-27.99	90.58	120.53
1	C	103	HIS	CE1-NE2-CD2	-27.90	81.10	109.00
1	A	116	ASN	CB-CG-ND2	27.87	158.20	116.40
1	C	47	ASP	CA-C-N	27.84	174.72	121.54
1	C	47	ASP	C-N-CA	27.84	174.72	121.54
2	D	77	LEU	CA-C-N	27.76	171.67	121.70
2	D	77	LEU	C-N-CA	27.76	171.67	121.70
2	D	4	ALA	CA-C-N	27.72	171.60	121.70
2	D	4	ALA	C-N-CA	27.72	171.60	121.70
2	B	100	GLN	OE1-CD-NE2	-27.71	94.89	122.60
1	C	112	HIS	CA-C-O	-27.67	81.40	120.13
2	B	14	TRP	CG-CD1-NE1	27.53	145.99	110.20
1	C	55	GLN	CA-C-O	-27.49	92.38	120.70
1	A	110	ALA	N-CA-CB	27.49	156.95	110.49
1	A	50	HIS	ND1-CG-CD2	27.49	133.59	106.10
2	B	37	THR	CA-C-O	27.44	152.69	119.49
1	A	140	TYR	CZ-CE2-CD2	27.41	168.94	119.60
2	D	57	PRO	N-CD-CG	-27.35	62.17	103.20
1	C	10	VAL	CA-C-O	27.33	154.94	120.78
2	D	61	ALA	CA-C-O	27.28	159.51	120.51
1	A	29	LEU	CA-C-N	27.24	173.57	121.54
1	A	29	LEU	C-N-CA	27.24	173.57	121.54
2	B	77	LEU	CA-C-N	27.20	170.66	121.70
2	B	77	LEU	C-N-CA	27.20	170.66	121.70
2	B	79	ASP	CA-C-O	27.13	159.31	120.51
2	D	70	PHE	CA-CB-CG	27.09	140.89	113.80
2	B	32	VAL	O-C-N	-27.05	84.98	122.59
2	D	11	THR	N-CA-CB	-27.02	79.27	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	134	THR	CA-C-O	-27.02	93.07	120.90
1	C	141	ARG	NE-CZ-NH1	-26.81	94.69	121.50
2	B	83	ALA	CA-C-N	26.80	161.01	120.82
2	B	83	ALA	C-N-CA	26.80	161.01	120.82
2	D	68	ASP	CA-C-N	26.79	156.01	120.65
2	D	68	ASP	C-N-CA	26.79	156.01	120.65
2	D	138	ASN	CA-C-O	-26.79	86.40	119.61
2	D	118	GLY	O-C-N	-26.74	96.92	122.86
1	A	16	LYS	CA-C-O	26.64	158.60	120.51
1	A	98	PHE	CA-CB-CG	26.53	140.33	113.80
1	A	92	ARG	NH1-CZ-NH2	26.51	153.76	119.30
1	A	44	PRO	CA-C-N	26.49	162.98	120.60
1	A	44	PRO	C-N-CA	26.49	162.98	120.60
2	B	65	ARG	NE-CZ-NH1	26.42	147.92	121.50
1	C	112	HIS	CB-CG-CD2	26.30	165.39	131.20
2	B	37	THR	O-C-N	-26.23	88.29	122.39
2	B	76	HIS	O-C-N	-26.18	87.77	122.59
2	D	119	GLY	O-C-N	-26.14	96.83	122.19
2	B	102	PHE	CD1-CG-CD2	-26.11	79.43	118.60
2	B	103	ARG	NE-CZ-NH2	-26.08	95.73	119.20
2	D	121	PHE	CG-CD1-CE1	26.06	165.00	120.70
2	D	19	VAL	CA-C-N	26.05	171.30	121.54
2	D	19	VAL	C-N-CA	26.05	171.30	121.54
1	C	84	SER	O-C-N	-26.04	87.96	122.59
1	C	115	THR	CA-CB-CG2	26.03	154.76	110.50
2	D	25	GLN	OE1-CD-NE2	25.95	148.55	122.60
2	B	92	CYS	CA-C-O	-25.93	89.20	119.79
1	C	110	ALA	N-CA-CB	25.93	149.29	110.40
2	D	5	GLU	CA-C-N	25.83	170.88	121.54
2	D	5	GLU	C-N-CA	25.83	170.88	121.54
2	D	99	PRO	CA-C-N	25.79	155.70	120.63
2	D	99	PRO	C-N-CA	25.79	155.70	120.63
1	C	5	ALA	CA-C-O	-25.76	91.40	118.97
2	D	110	ALA	N-CA-CB	25.75	154.02	110.49
2	D	21	VAL	CA-C-O	-25.75	94.17	120.95
1	C	83	LEU	CA-C-N	25.73	170.69	121.54
1	C	83	LEU	C-N-CA	25.73	170.69	121.54
2	B	38	GLN	CG-CD-NE2	25.73	154.99	116.40
1	A	81	SER	O-C-N	25.71	151.94	122.11
1	A	124	ASN	CA-CB-CG	25.71	138.31	112.60
2	D	65	ARG	O-C-N	25.68	156.59	122.43
1	C	92	ARG	NE-CZ-NH2	25.64	142.28	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	70	PHE	CZ-CE2-CD2	-25.60	73.93	120.00
1	C	100	LEU	CA-C-O	-25.58	89.61	120.56
2	B	42	GLN	O-C-N	-25.55	90.41	122.34
2	B	113	VAL	CA-CB-CG2	25.53	153.81	110.40
2	B	42	GLN	CA-C-N	25.51	167.62	121.70
2	B	42	GLN	C-N-CA	25.51	167.62	121.70
1	C	25	GLY	CA-C-O	-25.51	94.48	120.75
2	D	29	ARG	NE-CZ-NH2	25.50	142.15	119.20
1	C	98	PHE	CA-C-O	25.50	150.85	121.02
2	B	144	TYR	CA-C-O	25.41	154.78	120.47
1	A	138	SER	CA-C-O	-25.40	84.18	120.51
2	D	94	LYS	CA-C-O	-25.38	92.79	120.71
2	B	8	ALA	CA-C-N	25.34	169.95	121.54
2	B	8	ALA	C-N-CA	25.34	169.95	121.54
2	D	143	LYS	CA-C-N	25.27	169.81	121.54
2	D	143	LYS	C-N-CA	25.27	169.81	121.54
1	A	84	SER	CA-C-N	25.26	169.79	121.54
1	A	84	SER	C-N-CA	25.26	169.79	121.54
2	D	129	PHE	CA-CB-CG	-25.25	88.55	113.80
1	A	33	PHE	CA-CB-CG	25.25	139.05	113.80
2	D	1	MET	O-C-N	-25.25	82.60	123.00
2	B	115	ARG	CA-C-O	-25.24	85.65	119.47
2	D	7	LYS	CA-C-N	25.24	167.13	121.70
2	D	7	LYS	C-N-CA	25.24	167.13	121.70
2	D	115	ARG	NE-CZ-NH1	25.20	146.70	121.50
2	D	111	LEU	CA-C-O	-25.19	88.83	120.31
2	D	113	VAL	CG1-CB-CG2	-25.15	55.46	110.80
2	D	44	PHE	CB-CG-CD2	25.14	163.44	120.70
2	D	93	ASN	CA-C-O	-25.14	94.43	120.82
2	D	38	GLN	O-C-N	25.13	148.76	122.12
1	C	122	HIS	CB-CG-CD2	25.12	163.86	131.20
2	D	14	TRP	CB-CG-CD2	25.11	161.96	126.80
1	C	43	PHE	O-C-N	25.03	143.61	121.34
2	B	49	SER	CA-C-O	-25.02	94.31	121.33
2	B	68	ASP	CA-C-N	25.00	169.28	121.54
2	B	68	ASP	C-N-CA	25.00	169.28	121.54
2	D	103	ARG	N-CA-CB	24.97	152.35	110.41
2	D	107	ASN	OD1-CG-ND2	-24.94	97.66	122.60
2	D	129	PHE	CD1-CG-CD2	-24.94	81.19	118.60
1	C	115	THR	CA-C-N	24.94	159.97	122.56
1	C	115	THR	C-N-CA	24.94	159.97	122.56
2	D	84	PHE	CB-CG-CD1	-24.85	78.45	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	68	ASP	CA-CB-CG	-24.75	87.85	112.60
2	D	43	HIS	CG-ND1-CE1	24.75	151.38	109.30
1	A	89	HIS	CA-C-N	24.74	153.94	120.54
1	A	89	HIS	C-N-CA	24.74	153.94	120.54
1	C	106	LEU	CA-C-N	24.70	166.42	121.97
1	C	106	LEU	C-N-CA	24.70	166.42	121.97
2	D	79	ASP	CA-CB-CG	24.69	137.29	112.60
1	C	92	ARG	NH1-CZ-NH2	-24.69	87.21	119.30
1	C	34	LEU	CA-C-N	24.63	160.01	120.60
1	C	34	LEU	C-N-CA	24.63	160.01	120.60
2	B	1	MET	CB-CA-C	24.63	156.89	110.10
2	D	74	LEU	N-CA-C	-24.57	84.49	111.28
2	D	42	GLN	CA-CB-CG	-24.56	64.97	114.10
1	A	111	SER	CA-C-N	24.56	157.63	120.31
1	A	111	SER	C-N-CA	24.56	157.63	120.31
2	B	22	VAL	N-CA-C	-24.54	78.56	111.44
2	B	26	ALA	O-C-N	24.49	148.08	122.12
2	B	96	HIS	O-C-N	-24.46	90.05	122.59
2	D	9	ALA	CA-C-O	-24.43	85.58	120.51
2	D	102	PHE	N-CA-C	-24.42	83.92	111.03
2	D	125	VAL	CB-CA-C	24.42	151.34	111.29
2	D	14	TRP	CE2-CD2-CE3	24.36	143.16	118.80
1	C	46	PHE	CG-CD1-CE1	-24.34	79.32	120.70
1	C	80	LEU	N-CA-CB	-24.29	76.16	110.65
1	A	137	THR	CA-CB-OG1	-24.26	73.21	109.60
2	D	22	VAL	CA-C-O	24.23	146.61	121.41
2	D	68	ASP	O-C-N	-24.21	96.45	122.12
2	B	87	LEU	CA-C-O	-24.20	89.30	119.31
1	C	4	ALA	N-CA-CB	-24.17	73.69	111.39
2	D	76	HIS	CB-CG-CD2	-24.14	99.82	131.20
1	C	72	HIS	CA-C-O	24.10	154.98	120.51
2	D	39	ARG	CB-CG-CD	24.10	166.73	111.30
1	A	107	VAL	CA-C-N	24.09	167.56	121.54
1	A	107	VAL	C-N-CA	24.09	167.56	121.54
1	A	29	LEU	CB-CA-C	24.08	158.33	110.42
1	C	58	HIS	CA-CB-CG	24.07	137.87	113.80
1	C	139	LYS	O-C-N	-24.07	90.58	122.59
2	D	31	LEU	CA-C-O	-24.03	96.15	120.90
2	B	57	PRO	CA-N-CD	-24.01	78.39	112.00
1	C	46	PHE	CZ-CE2-CD2	-23.99	76.81	120.00
1	A	30	GLN	CA-C-N	23.99	167.36	121.54
1	A	30	GLN	C-N-CA	23.99	167.36	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	128	PHE	CA-CB-CG	23.97	137.77	113.80
1	C	137	THR	O-C-N	-23.95	90.74	122.59
1	C	5	ALA	N-CA-C	-23.93	83.34	113.97
2	B	129	PHE	N-CA-CB	23.92	145.56	110.16
2	B	79	ASP	OD1-CG-OD2	-23.88	65.58	122.90
2	B	87	LEU	N-CA-C	-23.86	83.30	112.89
1	C	128	PHE	CG-CD2-CE2	23.85	161.25	120.70
1	C	120	ALA	O-C-N	-23.78	89.64	122.46
2	B	71	THR	CA-C-N	23.77	166.94	121.54
2	B	71	THR	C-N-CA	23.77	166.94	121.54
1	C	31	ARG	NE-CZ-NH1	23.74	145.24	121.50
2	D	21	VAL	CA-CB-CG1	23.67	150.65	110.40
2	D	34	TYR	O-C-N	23.61	146.42	120.68
2	B	124	ASN	CA-C-O	-23.60	94.05	120.24
2	B	62	HIS	CG-CD2-NE2	-23.58	83.62	107.20
2	B	76	HIS	CA-CB-CG	23.58	137.38	113.80
1	C	127	LYS	CA-C-O	23.57	147.32	120.92
2	D	77	LEU	CA-C-O	23.52	146.34	120.24
1	C	89	HIS	CA-C-O	23.48	148.42	119.31
2	D	136	VAL	CA-C-N	-23.46	91.59	123.03
2	D	136	VAL	C-N-CA	-23.46	91.59	123.03
2	B	75	LYS	N-CA-CB	23.44	150.11	110.49
2	B	84	PHE	CB-CG-CD1	-23.36	80.99	120.70
2	B	25	GLN	N-CA-CB	23.36	143.27	110.10
2	D	11	THR	CA-CB-OG1	-23.31	74.63	109.60
1	A	84	SER	O-C-N	-23.25	93.67	122.27
2	D	99	PRO	O-C-N	-23.25	91.25	122.64
2	B	70	PHE	CG-CD2-CE2	23.21	160.16	120.70
2	D	20	ASP	CA-CB-CG	23.08	135.68	112.60
1	C	121	VAL	N-CA-C	-23.06	90.00	111.45
1	A	49	SER	CA-C-N	23.03	165.52	121.54
1	A	49	SER	C-N-CA	23.03	165.52	121.54
2	B	96	HIS	CE1-NE2-CD2	-23.02	85.98	109.00
1	C	47	ASP	O-C-N	-23.00	97.00	123.22
2	D	142	HIS	O-C-N	22.97	151.13	122.87
1	A	72	HIS	CA-CB-CG	-22.96	90.84	113.80
2	D	126	GLN	O-C-N	-22.91	97.35	122.09
1	C	50	HIS	ND1-CE1-NE2	-22.84	85.56	108.40
2	B	76	HIS	CB-CG-CD2	22.83	160.88	131.20
1	C	127	LYS	O-C-N	-22.82	95.87	122.11
2	D	1	MET	CA-C-O	22.82	159.60	120.80
1	A	34	LEU	CA-C-N	-22.81	86.42	122.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	LEU	C-N-CA	-22.81	86.42	122.23
1	A	74	ASN	CA-CB-CG	22.70	135.30	112.60
2	B	63	GLY	CA-C-N	22.68	164.86	121.54
2	B	63	GLY	C-N-CA	22.68	164.86	121.54
2	D	142	HIS	CA-C-N	22.59	164.69	121.54
2	D	142	HIS	C-N-CA	22.59	164.69	121.54
1	C	46	PHE	CG-CD2-CE2	22.58	159.09	120.70
2	D	143	LYS	CA-C-O	22.52	152.71	120.51
2	B	113	VAL	CA-C-O	-22.51	96.16	120.47
1	A	8	SER	CA-C-O	-22.47	79.97	120.42
2	D	115	ARG	CB-CG-CD	22.44	162.91	111.30
2	D	102	PHE	CB-CA-C	22.40	145.66	110.95
2	D	61	ALA	O-C-N	-22.39	92.81	122.59
2	B	128	LEU	CA-C-O	-22.38	93.39	119.79
2	D	72	GLN	CG-CD-OE1	-22.37	76.07	120.80
1	A	131	ASN	O-C-N	-22.36	97.94	122.09
2	D	84	PHE	CA-C-O	22.36	147.72	121.34
1	C	132	ASP	CA-CB-CG	-22.36	90.25	112.60
2	B	21	VAL	CB-CA-C	-22.35	74.63	111.29
2	B	55	ASN	O-C-N	22.35	147.62	122.15
1	C	103	HIS	CG-ND1-CE1	-22.33	71.33	109.30
1	A	121	VAL	N-CA-CB	22.33	148.08	111.23
2	B	6	GLU	CA-C-O	-22.32	88.59	120.51
2	D	128	LEU	CB-CA-C	22.31	154.81	110.42
2	D	82	GLY	CA-C-O	22.30	159.37	120.57
2	B	77	LEU	O-C-N	-22.29	79.98	122.11
2	B	14	TRP	CD2-CE2-CZ2	-22.28	100.12	122.40
2	D	113	VAL	CB-CA-C	22.27	141.34	111.94
1	A	39	THR	O-C-N	-22.26	98.53	122.12
2	B	123	PRO	N-CD-CG	-22.25	69.82	103.20
2	D	16	LYS	CB-CG-CD	-22.24	60.15	111.30
2	D	89	GLY	CA-C-N	22.23	158.59	120.58
2	D	89	GLY	C-N-CA	22.23	158.59	120.58
2	D	126	GLN	CB-CG-CD	-22.18	74.90	112.60
1	A	41	THR	CA-CB-OG1	22.14	142.81	109.60
2	D	84	PHE	N-CA-CB	-22.14	78.67	111.43
2	D	71	THR	CA-C-N	22.12	163.79	121.54
2	D	71	THR	C-N-CA	22.12	163.79	121.54
2	D	104	LEU	O-C-N	-22.11	98.21	122.09
2	D	115	ARG	CA-C-N	22.08	163.71	121.54
2	D	115	ARG	C-N-CA	22.08	163.71	121.54
1	A	87	HIS	CB-CG-CD2	-22.05	102.54	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	30	LEU	CA-C-O	22.04	145.61	120.92
2	B	51	GLY	CA-C-O	22.03	158.90	120.57
2	D	144	TYR	N-CA-CB	-22.02	73.28	110.49
2	D	51	GLY	O-C-N	-22.01	87.78	123.00
1	A	54	GLN	CG-CD-NE2	-22.00	83.39	116.40
1	C	117	PHE	CA-C-O	-22.00	92.95	122.44
1	C	33	PHE	CA-C-O	22.00	143.74	120.42
1	A	114	PRO	O-C-N	-21.95	93.01	122.64
2	B	32	VAL	CA-C-N	21.95	161.47	121.97
2	B	32	VAL	C-N-CA	21.95	161.47	121.97
2	D	30	LEU	N-CA-CB	21.94	141.88	110.07
2	B	102	PHE	CB-CG-CD2	21.89	157.90	120.70
2	D	107	ASN	CA-C-O	-21.87	98.17	120.70
1	C	45	HIS	O-C-N	-21.87	93.51	122.59
1	A	90	LYS	CA-C-N	21.86	149.50	120.65
1	A	90	LYS	C-N-CA	21.86	149.50	120.65
2	D	129	PHE	CA-C-O	21.84	144.66	120.20
2	B	114	ALA	N-CA-CB	21.84	143.85	110.22
1	A	61	LYS	CB-CG-CD	21.82	161.48	111.30
2	B	4	ALA	O-C-N	21.79	153.35	122.41
1	C	82	ASN	CA-C-O	-21.76	97.62	120.90
1	A	8	SER	CA-C-N	21.75	150.02	120.44
1	A	8	SER	C-N-CA	21.75	150.02	120.44
2	D	76	HIS	ND1-CG-CD2	21.74	127.84	106.10
2	B	142	HIS	CA-C-N	21.74	163.06	121.54
2	B	142	HIS	C-N-CA	21.74	163.06	121.54
2	B	13	PHE	CD1-CG-CD2	-21.73	86.00	118.60
2	D	36	TRP	N-CA-C	-21.73	86.72	111.71
2	B	34	TYR	CA-C-N	21.70	146.97	119.84
2	B	34	TYR	C-N-CA	21.70	146.97	119.84
2	D	42	GLN	CA-C-N	21.69	162.97	121.54
2	D	42	GLN	C-N-CA	21.69	162.97	121.54
2	D	21	VAL	CG1-CB-CG2	-21.68	63.10	110.80
2	B	112	VAL	CA-C-O	21.67	147.87	120.78
1	A	14	TRP	CA-C-N	21.66	163.86	121.41
1	A	14	TRP	C-N-CA	21.66	163.86	121.41
1	C	121	VAL	CA-C-O	-21.65	94.42	120.83
1	A	14	TRP	O-C-N	-21.63	93.83	122.59
2	B	133	VAL	CA-C-O	-21.59	97.96	120.85
2	B	102	PHE	CA-C-N	21.59	157.49	120.58
2	B	102	PHE	C-N-CA	21.59	157.49	120.58
1	A	61	LYS	O-C-N	21.55	145.37	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	121	PHE	CD1-CE1-CZ	-21.55	81.21	120.00
2	D	13	PHE	CA-CB-CG	21.52	135.32	113.80
2	B	40	PHE	CG-CD2-CE2	21.47	157.21	120.70
2	B	136	VAL	CA-C-O	-21.47	92.81	121.15
1	C	42	TYR	N-CA-C	-21.45	87.23	113.18
1	C	92	ARG	CA-C-O	21.44	147.57	120.98
1	A	70	GLN	O-C-N	-21.40	98.98	122.09
1	C	124	ASN	CB-CG-ND2	21.40	148.50	116.40
1	A	94	ASN	O-C-N	21.35	140.31	121.30
2	D	50	ALA	CA-C-N	21.35	160.12	121.70
2	D	50	ALA	C-N-CA	21.35	160.12	121.70
1	A	7	LYS	CB-CG-CD	21.34	160.39	111.30
2	D	144	TYR	CD1-CG-CD2	21.34	150.12	118.10
2	D	22	VAL	CB-CA-C	21.34	139.01	111.70
2	D	14	TRP	N-CA-CB	21.31	146.50	110.49
1	C	52	SER	CA-C-O	-21.29	97.36	120.36
1	A	93	VAL	N-CA-CB	21.28	137.30	112.40
2	D	142	HIS	N-CA-CB	21.27	145.49	110.39
2	D	35	PRO	O-C-N	21.26	147.89	122.17
1	C	80	LEU	N-CA-C	21.25	135.50	112.97
1	A	1	VAL	O-C-N	-21.25	89.00	123.00
1	A	27	GLN	OE1-CD-NE2	-21.23	101.36	122.60
2	D	70	PHE	CA-C-N	21.22	159.89	121.70
2	D	70	PHE	C-N-CA	21.22	159.89	121.70
2	D	62	HIS	ND1-CG-CD2	21.21	127.31	106.10
1	C	95	PRO	O-C-N	-21.19	93.48	122.30
2	D	93	ASN	CA-CB-CG	21.19	133.79	112.60
2	D	96	HIS	CE1-NE2-CD2	-21.14	87.86	109.00
2	B	78	ASP	CB-CA-C	21.14	150.26	110.10
2	B	143	LYS	CB-CA-C	21.12	152.45	110.42
1	A	28	ALA	CA-C-N	21.09	161.82	121.54
1	A	28	ALA	C-N-CA	21.09	161.82	121.54
2	D	144	TYR	CD1-CE1-CZ	-21.08	81.66	119.60
1	A	42	TYR	CA-C-N	-21.07	98.14	123.21
1	A	42	TYR	C-N-CA	-21.07	98.14	123.21
2	D	59	VAL	CA-C-O	-21.04	94.48	120.78
2	B	142	HIS	O-C-N	-21.02	93.46	122.46
2	D	118	GLY	CA-C-N	21.00	143.10	120.00
2	D	118	GLY	C-N-CA	21.00	143.10	120.00
1	A	46	PHE	CA-C-N	21.00	161.65	121.54
1	A	46	PHE	C-N-CA	21.00	161.65	121.54
2	D	69	ALA	O-C-N	20.98	143.85	122.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	VAL	CA-CB-CG2	20.98	146.07	110.40
2	B	98	ASN	CB-CA-C	-20.91	78.75	108.86
1	C	54	GLN	CA-C-O	-20.90	97.04	120.24
1	A	98	PHE	CB-CG-CD2	20.89	156.21	120.70
1	C	32	MET	CA-C-O	-20.88	94.97	119.61
1	A	118	THR	CA-CB-OG1	20.86	140.89	109.60
2	B	91	HIS	CG-CD2-NE2	20.86	128.06	107.20
2	B	33	VAL	CG1-CB-CG2	-20.84	64.95	110.80
2	B	69	ALA	CA-C-O	20.84	150.30	120.51
2	D	128	LEU	CA-C-O	-20.83	90.72	120.51
2	B	42	GLN	CA-C-O	20.82	143.71	119.35
1	C	132	ASP	O-C-N	-20.81	100.06	122.12
2	B	85	ALA	CA-C-N	20.81	159.15	121.70
2	B	85	ALA	C-N-CA	20.81	159.15	121.70
1	C	37	PRO	O-C-N	-20.79	94.57	122.64
2	D	55	ASN	OD1-CG-ND2	-20.78	101.82	122.60
1	C	81	SER	O-C-N	-20.75	95.25	122.23
1	A	41	THR	O-C-N	-20.75	97.37	122.48
1	A	51	GLY	CA-C-N	20.75	152.26	123.00
1	A	51	GLY	C-N-CA	20.75	152.26	123.00
2	B	94	LYS	CD-CE-NZ	20.70	178.14	111.90
1	C	23	ALA	O-C-N	20.70	146.44	122.22
1	C	11	LYS	CB-CG-CD	20.69	158.88	111.30
1	C	20	ASN	CB-CG-ND2	20.65	147.38	116.40
1	C	107	VAL	CA-C-O	-20.62	95.00	120.78
1	C	122	HIS	O-C-N	-20.61	98.71	122.20
2	B	81	LYS	N-CA-CB	-20.58	75.52	110.50
2	D	41	PHE	O-C-N	-20.51	93.58	122.29
2	D	44	PHE	CD1-CG-CD2	-20.50	87.84	118.60
1	C	122	HIS	ND1-CG-CD2	-20.47	85.63	106.10
2	B	62	HIS	ND1-CG-CD2	20.47	126.57	106.10
2	D	46	ASN	CA-CB-CG	20.45	133.05	112.60
1	A	15	GLY	CA-C-N	20.45	160.59	121.54
1	A	15	GLY	C-N-CA	20.45	160.59	121.54
2	B	47	LEU	CB-CA-C	20.44	144.04	111.13
1	C	36	PHE	CD1-CG-CD2	-20.41	87.98	118.60
2	D	10	VAL	CB-CA-C	-20.41	77.83	111.29
2	D	2	LEU	N-CA-C	-20.40	67.34	110.80
2	D	26	ALA	CA-C-O	-20.40	99.89	120.90
1	C	134	THR	O-C-N	-20.36	100.29	122.08
2	B	1	MET	CA-C-O	-20.35	86.20	120.80
2	D	116	ASN	OD1-CG-ND2	20.35	142.95	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	55	ASN	O-C-N	-20.30	100.92	122.03
1	A	130	ALA	CA-C-O	20.30	144.77	121.02
2	B	6	GLU	CG-CD-OE1	20.28	165.04	118.40
1	C	62	VAL	CA-C-N	20.26	160.23	121.54
1	C	62	VAL	C-N-CA	20.26	160.23	121.54
1	A	102	SER	O-C-N	-20.25	95.90	122.23
2	D	35	PRO	CA-C-O	-20.25	87.64	119.64
1	C	36	PHE	CB-CG-CD2	20.22	155.08	120.70
2	B	13	PHE	CG-CD2-CE2	20.21	155.06	120.70
1	C	105	LEU	CA-C-O	-20.20	97.81	120.24
1	C	103	HIS	CA-C-N	20.18	147.28	120.65
1	C	103	HIS	C-N-CA	20.18	147.28	120.65
1	A	126	ASN	O-C-N	20.17	143.07	122.09
2	D	99	PRO	CA-N-CD	-20.17	83.76	112.00
1	C	9	ASN	OD1-CG-ND2	-20.17	102.43	122.60
2	D	29	ARG	NH1-CZ-NH2	-20.16	93.09	119.30
1	A	73	LEU	N-CA-C	-20.14	77.45	108.67
1	A	22	PRO	CA-C-N	20.13	165.28	121.80
1	A	22	PRO	C-N-CA	20.13	165.28	121.80
1	A	38	THR	CA-CB-CG2	20.11	144.69	110.50
2	D	125	VAL	CA-CB-CG1	20.10	144.57	110.40
1	A	122	HIS	ND1-CE1-NE2	-20.09	88.31	108.40
1	A	76	LEU	CA-C-O	20.09	137.11	118.63
1	C	109	LEU	O-C-N	-20.09	95.87	122.59
1	C	67	THR	CA-C-O	-20.09	99.91	121.00
2	D	144	TYR	CE1-CZ-CE2	20.06	160.43	120.30
2	B	95	LEU	CA-C-N	20.06	159.85	121.54
2	B	95	LEU	C-N-CA	20.06	159.85	121.54
2	D	24	ALA	CA-C-N	20.05	159.83	121.54
2	D	24	ALA	C-N-CA	20.05	159.83	121.54
2	D	16	LYS	CA-C-N	20.05	158.05	121.97
2	D	16	LYS	C-N-CA	20.05	158.05	121.97
1	A	48	LEU	N-CA-C	-20.04	85.46	112.72
1	C	60	GLN	CA-C-N	20.00	159.73	121.54
1	C	60	GLN	C-N-CA	20.00	159.73	121.54
1	A	131	ASN	CB-CA-C	19.98	142.47	110.90
2	D	76	HIS	CG-CD2-NE2	-19.97	87.23	107.20
1	A	127	LYS	O-C-N	19.97	149.15	122.59
1	A	77	PRO	CA-C-N	-19.95	82.30	121.41
1	A	77	PRO	C-N-CA	-19.95	82.30	121.41
1	C	113	LEU	CA-C-O	19.94	147.75	120.83
1	C	128	PHE	N-CA-CB	19.94	144.19	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	8	ALA	CA-C-N	19.93	159.60	121.54
2	D	8	ALA	C-N-CA	19.93	159.60	121.54
1	C	100	LEU	O-C-N	19.92	145.23	122.32
2	D	123	PRO	N-CD-CG	-19.92	73.32	103.20
2	B	40	PHE	CB-CG-CD2	19.92	154.56	120.70
2	D	15	GLY	CA-C-N	19.89	159.53	121.54
2	D	15	GLY	C-N-CA	19.89	159.53	121.54
1	C	47	ASP	CA-C-O	19.89	141.64	120.36
1	A	27	GLN	CA-CB-CG	19.87	153.84	114.10
2	D	103	ARG	NE-CZ-NH1	19.87	141.37	121.50
2	B	28	GLY	O-C-N	19.86	148.52	122.70
1	C	26	ALA	O-C-N	-19.84	98.19	122.20
1	A	141	ARG	CG-CD-NE	-19.80	68.43	112.00
2	D	59	VAL	O-C-N	19.80	147.32	122.57
1	C	30	GLN	OE1-CD-NE2	19.79	142.39	122.60
2	B	84	PHE	CD1-CG-CD2	19.77	148.25	118.60
1	A	41	THR	CA-C-N	19.75	159.27	121.54
1	A	41	THR	C-N-CA	19.75	159.27	121.54
2	D	81	LYS	N-CA-CB	-19.75	74.64	110.18
1	A	82	ASN	OD1-CG-ND2	-19.72	102.88	122.60
1	C	132	ASP	CA-C-N	19.72	159.20	121.54
1	C	132	ASP	C-N-CA	19.72	159.20	121.54
1	C	44	PRO	CA-N-CD	-19.69	84.44	112.00
2	B	74	LEU	CA-C-O	-19.64	92.43	120.51
1	A	38	THR	CA-C-O	-19.64	98.21	120.20
2	D	44	PHE	CG-CD1-CE1	19.61	154.05	120.70
1	C	89	HIS	CG-CD2-NE2	-19.57	87.63	107.20
2	B	79	ASP	CB-CG-OD2	19.56	163.40	118.40
2	D	34	TYR	CA-C-O	-19.54	100.25	120.38
2	D	19	VAL	O-C-N	-19.53	98.16	122.57
2	D	119	GLY	CA-C-O	19.53	141.36	120.66
1	A	24	TYR	CA-C-O	-19.52	99.23	120.71
2	D	96	HIS	CG-ND1-CE1	19.50	142.44	109.30
2	B	96	HIS	CA-C-O	19.50	148.39	120.51
2	D	65	ARG	CA-C-O	-19.44	94.60	119.10
2	B	59	VAL	O-C-N	19.42	141.84	121.83
1	C	63	ALA	CA-C-O	-19.41	92.75	120.51
1	A	126	ASN	N-CA-CB	19.34	138.76	109.94
1	A	2	LEU	O-C-N	19.34	148.31	122.59
1	A	111	SER	CA-CB-OG	-19.34	72.43	111.10
2	B	68	ASP	CA-C-O	-19.32	92.88	120.51
2	B	107	ASN	CA-C-O	-19.31	99.95	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	129	LEU	CA-C-O	-19.30	100.53	120.80
2	D	126	GLN	CA-CB-CG	19.28	152.66	114.10
1	C	3	SER	CA-C-N	-19.27	91.37	122.79
1	C	3	SER	C-N-CA	-19.27	91.37	122.79
2	B	144	TYR	CB-CG-CD2	-19.26	91.91	120.80
2	D	113	VAL	CA-CB-CG2	19.23	143.10	110.40
1	A	80	LEU	CA-C-N	19.23	152.03	120.88
1	A	80	LEU	C-N-CA	19.23	152.03	120.88
1	A	139	LYS	N-CA-CB	19.23	142.98	110.49
2	B	129	PHE	CB-CG-CD1	-19.22	88.03	120.70
2	D	13	PHE	N-CA-CB	19.21	139.02	109.82
2	D	71	THR	CA-C-O	19.20	153.44	120.80
2	B	39	ARG	CA-C-O	19.20	141.75	119.67
1	A	31	ARG	CA-CB-CG	19.18	152.47	114.10
2	D	82	GLY	CA-C-N	19.18	151.68	121.19
2	D	82	GLY	C-N-CA	19.18	151.68	121.19
2	B	39	ARG	NE-CZ-NH1	-19.18	102.32	121.50
1	A	61	LYS	N-CA-C	19.15	131.82	111.14
1	A	94	ASN	CA-CB-CG	-19.14	93.45	112.60
1	A	62	VAL	CG1-CB-CG2	-19.14	68.68	110.80
2	B	76	HIS	CB-CG-ND1	-19.14	93.98	122.70
1	A	24	TYR	CB-CA-C	19.14	146.26	112.00
1	A	54	GLN	CB-CA-C	19.13	140.60	110.95
2	B	7	LYS	CA-CB-CG	19.11	152.32	114.10
2	B	118	GLY	CA-C-O	-19.09	87.34	120.57
1	C	54	GLN	CA-C-N	19.05	146.35	120.44
1	C	54	GLN	C-N-CA	19.05	146.35	120.44
2	D	72	GLN	CA-C-N	19.03	158.71	121.41
2	D	72	GLN	C-N-CA	19.03	158.71	121.41
1	A	60	GLN	CA-CB-CG	18.99	152.08	114.10
2	D	117	PHE	CA-C-O	-18.99	97.19	119.59
2	D	88	SER	O-C-N	-18.98	97.55	122.61
2	D	58	LYS	CB-CG-CD	18.98	154.94	111.30
2	D	100	GLN	CB-CA-C	18.96	140.34	110.95
2	B	96	HIS	CA-CB-CG	18.95	132.75	113.80
1	C	56	LYS	CB-CA-C	18.94	148.11	110.42
1	A	75	ASP	CB-CG-OD2	18.92	161.91	118.40
1	C	11	LYS	CA-C-O	-18.89	101.44	120.90
1	C	127	LYS	CA-C-N	18.89	157.62	121.54
1	C	127	LYS	C-N-CA	18.89	157.62	121.54
2	B	82	GLY	CA-C-N	18.89	157.61	121.54
2	B	82	GLY	C-N-CA	18.89	157.61	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	LEU	O-C-N	-18.88	102.62	121.31
2	D	130	GLN	N-CA-CB	18.87	137.86	110.12
2	B	103	ARG	CA-CB-CG	18.87	151.84	114.10
2	D	142	HIS	CE1-NE2-CD2	18.84	127.84	109.00
1	A	134	THR	N-CA-C	-18.84	90.12	111.03
1	C	94	ASN	O-C-N	-18.83	103.00	121.27
2	D	107	ASN	N-CA-C	-18.82	90.82	111.14
1	A	58	HIS	CA-C-N	18.79	140.66	120.00
1	A	58	HIS	C-N-CA	18.79	140.66	120.00
1	A	136	LEU	CA-C-O	18.78	147.37	120.51
1	C	104	SER	N-CA-CB	18.77	137.32	109.91
2	B	34	TYR	CB-CA-C	18.77	147.15	110.17
1	A	103	HIS	CB-CG-CD2	18.75	155.57	131.20
2	B	89	GLY	CA-C-N	18.70	146.78	120.79
2	B	89	GLY	C-N-CA	18.70	146.78	120.79
2	B	32	VAL	N-CA-CB	-18.70	89.17	111.60
2	D	14	TRP	CD2-CE3-CZ3	-18.69	94.31	118.60
2	B	13	PHE	CB-CG-CD2	18.68	152.46	120.70
2	B	121	PHE	CZ-CE2-CD2	18.68	153.62	120.00
1	A	50	HIS	ND1-CE1-NE2	-18.67	89.73	108.40
1	C	65	ALA	CA-C-O	-18.65	100.94	120.90
2	D	44	PHE	CD1-CE1-CZ	-18.64	86.45	120.00
1	A	59	GLY	N-CA-C	-18.61	88.94	112.77
2	B	92	CYS	O-C-N	18.61	147.27	122.33
1	C	56	LYS	O-C-N	-18.60	97.85	122.59
2	D	17	VAL	N-CA-CB	18.60	141.92	111.23
2	B	140	LEU	CA-C-O	18.60	142.25	119.38
1	C	108	THR	CA-C-O	-18.60	101.36	120.89
1	A	137	THR	OG1-CB-CG2	-18.59	72.11	109.30
2	B	14	TRP	CA-C-O	18.56	147.05	120.51
1	A	16	LYS	O-C-N	-18.55	97.92	122.59
2	D	129	PHE	CG-CD2-CE2	18.54	152.22	120.70
2	B	25	GLN	CB-CG-CD	18.53	144.09	112.60
2	B	62	HIS	CE1-NE2-CD2	18.51	127.51	109.00
2	D	90	LEU	O-C-N	18.49	146.27	122.23
2	B	16	LYS	CA-C-N	18.49	155.25	121.97
2	B	16	LYS	C-N-CA	18.49	155.25	121.97
1	A	42	TYR	CD1-CG-CD2	-18.48	90.38	118.10
2	B	16	LYS	CA-C-O	18.46	146.91	120.51
2	B	91	HIS	CE1-NE2-CD2	-18.43	90.57	109.00
1	A	140	TYR	CG-CD2-CE2	-18.43	93.56	121.20
2	B	132	VAL	N-CA-CB	18.41	141.61	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	PRO	N-CD-CG	-18.41	75.59	103.20
1	A	119	PRO	CA-C-O	-18.39	91.18	119.86
2	B	53	VAL	CA-C-N	-18.38	94.19	120.29
2	B	53	VAL	C-N-CA	-18.38	94.19	120.29
2	B	140	LEU	CA-C-N	-18.37	93.94	122.60
2	B	140	LEU	C-N-CA	-18.37	93.94	122.60
1	A	138	SER	CA-CB-OG	18.37	147.84	111.10
2	B	56	ASN	CA-C-N	18.37	142.80	119.84
2	B	56	ASN	C-N-CA	18.37	142.80	119.84
2	B	100	GLN	CB-CG-CD	18.36	143.80	112.60
1	C	47	ASP	CA-CB-CG	18.36	130.96	112.60
1	A	14	TRP	CD2-CE2-CZ2	-18.34	104.06	122.40
1	C	107	VAL	O-C-N	-18.32	99.67	122.57
2	D	112	VAL	CA-C-O	-18.29	97.45	119.58
2	D	145	HIS	ND1-CE1-NE2	18.29	126.69	108.40
1	A	97	ASN	CB-CG-OD1	-18.28	84.23	120.80
1	C	132	ASP	CA-C-O	18.28	139.93	120.55
1	A	65	ALA	O-C-N	-18.28	98.47	122.23
2	D	121	PHE	CB-CG-CD1	18.27	151.77	120.70
2	D	141	ALA	CA-C-N	-18.26	97.47	122.85
2	D	141	ALA	C-N-CA	-18.26	97.47	122.85
1	C	115	THR	CA-CB-OG1	-18.23	82.26	109.60
2	B	93	ASN	CA-C-N	-18.23	93.56	121.99
2	B	93	ASN	C-N-CA	-18.23	93.56	121.99
2	B	71	THR	O-C-N	-18.22	98.69	122.56
2	D	100	GLN	N-CA-C	-18.21	90.82	111.03
1	A	115	THR	CA-CB-OG1	-18.20	82.30	109.60
2	B	121	PHE	CB-CA-C	18.14	140.86	111.83
2	B	53	VAL	O-C-N	18.14	140.22	121.90
2	D	124	ASN	CA-CB-CG	-18.14	94.46	112.60
2	B	91	HIS	ND1-CG-CD2	-18.14	87.96	106.10
1	C	87	HIS	CA-CB-CG	18.13	131.93	113.80
2	D	138	ASN	CA-CB-CG	18.13	130.73	112.60
1	A	41	THR	CA-CB-CG2	-18.12	79.70	110.50
2	B	20	ASP	CA-C-N	18.11	154.56	121.97
2	B	20	ASP	C-N-CA	18.11	154.56	121.97
1	A	20	ASN	OD1-CG-ND2	-18.10	104.50	122.60
1	C	55	GLN	CB-CG-CD	-18.09	81.84	112.60
2	D	131	LYS	CA-C-N	-18.09	90.63	120.30
2	D	131	LYS	C-N-CA	-18.09	90.63	120.30
2	B	136	VAL	N-CA-C	-18.09	94.28	110.74
1	A	34	LEU	O-C-N	18.08	140.82	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	70	GLN	CG-CD-NE2	-18.08	89.29	116.40
1	C	134	THR	OG1-CB-CG2	18.07	145.44	109.30
1	A	128	PHE	CA-CB-CG	18.06	131.86	113.80
2	B	116	ASN	CA-C-N	18.05	144.99	120.44
2	B	116	ASN	C-N-CA	18.05	144.99	120.44
1	A	87	HIS	CG-ND1-CE1	-18.04	78.63	109.30
1	A	36	PHE	CG-CD1-CE1	18.04	151.37	120.70
1	A	13	ALA	CA-C-N	18.03	155.98	121.54
1	A	13	ALA	C-N-CA	18.03	155.98	121.54
2	B	145	HIS	N-CA-CB	-18.02	79.87	110.50
2	D	109	LEU	O-C-N	18.02	146.56	122.59
1	C	5	ALA	N-CA-CB	-18.02	85.63	110.67
2	B	13	PHE	CA-C-O	-18.01	97.22	119.38
1	A	39	THR	CA-C-N	18.01	155.93	121.54
1	A	39	THR	C-N-CA	18.01	155.93	121.54
1	C	14	TRP	CG-CD1-NE1	17.99	133.59	110.20
2	D	84	PHE	CB-CG-CD2	17.95	151.22	120.70
2	D	140	LEU	CA-C-O	-17.95	100.02	121.02
2	B	54	MET	N-CA-C	17.93	130.91	111.36
2	D	74	LEU	N-CA-CB	17.93	136.48	110.12
2	D	129	PHE	O-C-N	-17.92	101.77	122.20
1	C	72	HIS	ND1-CE1-NE2	17.91	126.31	108.40
2	D	144	TYR	CB-CG-CD1	-17.90	93.94	120.80
1	A	81	SER	N-CA-C	-17.90	88.15	111.24
2	D	86	GLN	CG-CD-NE2	17.89	143.23	116.40
2	B	14	TRP	CD2-CE3-CZ3	-17.88	95.35	118.60
2	B	59	VAL	N-CA-C	-17.88	92.66	110.72
1	A	12	ALA	CA-C-O	17.88	146.07	120.51
1	C	135	VAL	CA-CB-CG2	17.88	140.79	110.40
2	B	102	PHE	CG-CD2-CE2	17.87	151.08	120.70
1	A	110	ALA	CA-C-O	-17.86	94.96	120.51
2	D	96	HIS	CB-CG-ND1	17.86	149.49	122.70
1	A	49	SER	O-C-N	-17.85	98.86	122.59
2	D	105	LEU	N-CA-C	-17.83	91.12	113.23
2	D	37	THR	CA-C-N	17.83	144.81	120.38
2	D	37	THR	C-N-CA	17.83	144.81	120.38
2	B	26	ALA	CA-C-O	-17.82	101.66	120.55
1	A	46	PHE	CA-CB-CG	17.82	131.62	113.80
1	A	100	LEU	N-CA-CB	17.79	140.56	110.49
1	A	108	THR	CA-CB-OG1	17.79	136.29	109.60
1	C	59	GLY	CA-C-O	-17.79	101.19	120.40
1	C	36	PHE	CA-C-O	17.77	144.51	120.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	9	ASN	CA-CB-CG	-17.76	94.84	112.60
2	D	96	HIS	CG-CD2-NE2	17.76	124.96	107.20
2	B	64	LYS	O-C-N	-17.73	99.00	122.59
1	A	14	TRP	N-CA-CB	17.71	140.42	110.49
2	D	11	THR	CA-CB-CG2	17.71	140.61	110.50
1	C	115	THR	N-CA-C	-17.70	91.61	113.38
2	D	100	GLN	CA-CB-CG	-17.69	78.71	114.10
2	B	129	PHE	CE1-CZ-CE2	17.69	151.84	120.00
1	C	80	LEU	O-C-N	-17.68	98.37	122.06
2	B	29	ARG	CA-C-N	17.64	147.28	120.82
2	B	29	ARG	C-N-CA	17.64	147.28	120.82
2	B	54	MET	CA-CB-CG	-17.63	78.83	114.10
2	D	43	HIS	ND1-CE1-NE2	-17.62	90.78	108.40
1	C	1	VAL	O-C-N	-17.62	94.81	123.00
2	D	136	VAL	CA-CB-CG1	17.60	140.31	110.40
2	D	22	VAL	N-CA-CB	-17.60	92.14	110.62
2	B	58	LYS	O-C-N	-17.59	103.10	122.09
2	B	72	GLN	CB-CG-CD	17.57	142.46	112.60
2	D	137	ALA	CB-CA-C	17.56	137.67	111.85
1	A	34	LEU	N-CA-CB	17.54	134.13	110.98
1	A	43	PHE	CB-CG-CD1	17.53	150.50	120.70
2	D	82	GLY	O-C-N	-17.53	99.91	122.70
1	C	30	GLN	CG-CD-OE1	-17.51	85.77	120.80
2	B	59	VAL	CB-CA-C	-17.51	88.05	112.22
1	C	42	TYR	O-C-N	-17.51	96.87	122.43
1	A	87	HIS	N-CA-C	17.50	130.04	111.14
2	D	37	THR	CA-C-O	17.50	140.52	120.92
1	A	112	HIS	ND1-CE1-NE2	-17.50	90.91	108.40
2	B	14	TRP	CE2-CD2-CE3	17.48	136.28	118.80
2	B	80	LEU	O-C-N	-17.46	95.06	123.00
2	D	136	VAL	N-CA-CB	17.46	139.72	110.56
2	D	122	THR	OG1-CB-CG2	17.46	144.21	109.30
2	B	114	ALA	O-C-N	-17.45	101.80	122.22
2	B	46	ASN	CB-CG-OD1	-17.45	85.90	120.80
2	D	103	ARG	CB-CA-C	-17.45	75.22	109.95
2	D	115	ARG	CD-NE-CZ	17.45	148.83	124.40
1	A	70	GLN	CB-CA-C	17.43	138.44	110.90
1	A	50	HIS	CB-CG-ND1	-17.40	96.60	122.70
1	A	129	LEU	O-C-N	17.40	142.04	122.20
1	C	134	THR	CB-CA-C	17.40	138.58	110.92
2	D	7	LYS	CB-CA-C	-17.40	75.80	110.42
1	A	74	ASN	CB-CG-OD1	17.39	155.58	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	109	LEU	CA-C-O	-17.37	95.67	120.51
1	C	3	SER	CA-C-O	17.37	145.35	120.51
1	C	98	PHE	CD1-CE1-CZ	17.36	151.26	120.00
1	A	124	ASN	OD1-CG-ND2	17.32	139.92	122.60
1	C	26	ALA	CA-C-O	17.31	141.28	121.02
2	D	144	TYR	O-C-N	17.31	145.61	122.59
1	C	89	HIS	O-C-N	-17.30	98.59	122.46
1	A	67	THR	CA-CB-OG1	-17.29	83.66	109.60
1	A	61	LYS	CA-C-O	-17.29	102.89	120.70
1	C	23	ALA	N-CA-C	17.25	131.54	111.71
2	D	1	MET	N-CA-CB	17.25	139.82	110.50
1	A	40	LYS	CD-CE-NZ	17.25	167.09	111.90
1	C	70	GLN	N-CA-C	17.24	140.75	112.99
2	D	122	THR	CA-CB-OG1	-17.24	83.74	109.60
1	C	61	LYS	N-CA-CB	17.22	139.59	110.49
2	B	142	HIS	CA-C-O	17.20	140.63	119.31
1	A	53	ALA	CB-CA-C	17.17	144.59	110.42
1	A	31	ARG	N-CA-CB	17.17	139.51	110.49
2	B	138	ASN	OD1-CG-ND2	17.16	139.76	122.60
1	C	113	LEU	O-C-N	-17.16	105.93	121.37
2	B	112	VAL	N-CA-CB	17.16	139.54	111.23
1	A	114	PRO	N-CD-CG	-17.14	77.49	103.20
1	C	14	TRP	CD1-CG-CD2	-17.14	78.88	106.30
1	C	50	HIS	CA-C-O	-17.14	91.67	120.80
2	B	64	LYS	CA-C-O	17.13	145.01	120.51
1	A	141	ARG	NE-CZ-NH2	-17.09	103.82	119.20
1	A	39	THR	CB-CA-C	17.07	139.13	110.79
1	A	57	ALA	N-CA-CB	-17.07	85.86	110.10
1	C	14	TRP	O-C-N	17.06	140.21	122.12
2	D	118	GLY	CA-C-O	17.06	143.32	121.83
1	A	31	ARG	CB-CG-CD	17.05	150.52	111.30
2	D	121	PHE	CD1-CG-CD2	-17.05	93.02	118.60
1	C	95	PRO	CA-C-N	17.05	152.66	121.97
1	C	95	PRO	C-N-CA	17.05	152.66	121.97
1	C	1	VAL	CB-CA-C	17.05	143.79	111.40
1	C	112	HIS	O-C-N	17.05	144.52	122.19
2	D	133	VAL	CG1-CB-CG2	-17.05	73.30	110.80
1	A	43	PHE	O-C-N	17.04	138.18	121.31
2	D	25	GLN	CG-CD-OE1	-17.04	86.73	120.80
2	D	86	GLN	O-C-N	17.03	145.24	122.59
1	C	22	PRO	CA-N-CD	-17.02	88.18	112.00
1	A	74	ASN	CB-CG-ND2	-17.01	90.89	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	13	ALA	N-CA-CB	17.00	139.22	110.49
2	D	127	ALA	N-CA-CB	17.00	134.25	110.10
1	C	84	SER	CB-CA-C	-17.00	76.60	110.42
2	B	50	ALA	O-C-N	-16.99	99.36	122.30
1	A	23	ALA	CA-C-O	-16.99	99.08	120.31
2	B	100	GLN	N-CA-CB	16.99	135.04	110.07
1	A	60	GLN	OE1-CD-NE2	-16.98	105.62	122.60
1	C	49	SER	CA-C-O	16.97	149.65	120.80
1	A	103	HIS	ND1-CG-CD2	-16.96	89.14	106.10
1	C	19	GLY	CA-C-N	16.95	146.31	120.89
1	C	19	GLY	C-N-CA	16.95	146.31	120.89
2	D	139	ALA	N-CA-CB	16.94	139.12	110.49
1	A	109	LEU	CA-C-N	16.94	153.89	121.54
1	A	109	LEU	C-N-CA	16.94	153.89	121.54
2	D	62	HIS	CA-CB-CG	-16.92	96.88	113.80
1	C	14	TRP	N-CA-CB	16.92	135.44	110.06
2	B	65	ARG	CA-CB-CG	16.91	147.93	114.10
1	C	107	VAL	N-CA-CB	16.91	139.13	111.23
2	D	56	ASN	CA-C-O	-16.91	97.00	120.16
2	D	124	ASN	CB-CG-OD1	-16.90	87.00	120.80
2	D	76	HIS	CA-CB-CG	-16.88	96.92	113.80
1	A	140	TYR	CE1-CZ-CE2	-16.87	86.56	120.30
1	A	104	SER	CA-C-O	-16.85	102.69	120.55
2	D	26	ALA	O-C-N	16.85	140.23	122.03
2	B	115	ARG	CA-C-N	16.84	142.88	120.65
2	B	115	ARG	C-N-CA	16.84	142.88	120.65
2	D	38	GLN	CA-CB-CG	16.83	147.76	114.10
2	D	34	TYR	CB-CG-CD2	16.83	146.04	120.80
1	A	24	TYR	CA-CB-CG	16.82	144.18	113.90
1	C	37	PRO	N-CA-C	16.82	147.12	112.47
1	C	131	ASN	CA-CB-CG	-16.80	95.80	112.60
2	B	25	GLN	CA-C-N	16.79	142.78	120.28
2	B	25	GLN	C-N-CA	16.79	142.78	120.28
1	A	89	HIS	O-C-N	-16.79	96.14	123.00
2	D	37	THR	O-C-N	-16.78	102.81	122.11
2	D	99	PRO	CA-C-O	16.75	151.09	120.60
1	C	139	LYS	CA-C-N	16.74	151.17	122.37
1	C	139	LYS	C-N-CA	16.74	151.17	122.37
2	D	30	LEU	CB-CA-C	-16.74	84.45	110.90
2	D	130	GLN	CG-CD-OE1	-16.71	87.38	120.80
1	A	38	THR	O-C-N	16.71	141.25	122.20
1	A	106	LEU	O-C-N	-16.71	95.68	122.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	65	ALA	N-CA-C	-16.69	91.08	111.11
1	A	46	PHE	N-CA-CB	16.68	139.94	111.74
1	C	48	LEU	CA-C-O	16.68	144.37	120.51
1	A	141	ARG	CD-NE-CZ	-16.66	101.08	124.40
2	D	15	GLY	O-C-N	16.65	144.34	122.70
1	C	74	ASN	OD1-CG-ND2	-16.64	105.97	122.60
2	D	115	ARG	CA-C-O	16.60	144.99	120.42
2	B	101	ASN	CA-C-O	-16.60	98.97	119.38
2	B	33	VAL	CA-C-O	-16.59	100.04	120.78
2	D	14	TRP	CG-CD1-NE1	16.58	131.76	110.20
1	A	133	SER	CA-C-O	16.58	138.64	120.90
1	C	122	HIS	CG-CD2-NE2	16.57	123.77	107.20
1	C	28	ALA	CA-C-O	16.56	138.98	119.60
2	B	40	PHE	CD1-CG-CD2	-16.56	93.76	118.60
1	A	47	ASP	N-CA-CB	16.55	138.47	110.49
2	B	70	PHE	CA-C-N	16.55	147.71	122.23
2	B	70	PHE	C-N-CA	16.55	147.71	122.23
2	B	75	LYS	N-CA-C	-16.54	75.56	110.80
2	D	3	THR	N-CA-CB	16.54	138.45	110.49
1	A	28	ALA	O-C-N	-16.53	100.60	122.59
1	C	117	PHE	CA-C-N	16.53	162.14	121.80
1	C	117	PHE	C-N-CA	16.53	162.14	121.80
1	A	106	LEU	CA-C-N	16.52	151.70	121.97
1	A	106	LEU	C-N-CA	16.52	151.70	121.97
2	B	46	ASN	CB-CG-ND2	16.48	141.12	116.40
2	D	51	GLY	CA-C-O	16.48	155.40	120.80
1	C	53	ALA	N-CA-C	16.47	132.63	112.87
1	A	90	LYS	CA-C-O	-16.46	103.28	120.90
1	C	51	GLY	CA-C-N	-16.46	99.78	122.99
1	C	51	GLY	C-N-CA	-16.46	99.78	122.99
2	D	33	VAL	CA-CB-CG1	16.45	138.37	110.40
1	A	2	LEU	N-CA-CB	16.44	138.27	110.49
1	C	70	GLN	CB-CG-CD	-16.44	84.66	112.60
2	B	123	PRO	CA-C-N	16.44	148.69	120.58
2	B	123	PRO	C-N-CA	16.44	148.69	120.58
1	A	90	LYS	CG-CD-CE	16.43	149.09	111.30
1	A	21	ALA	N-CA-C	-16.43	90.41	112.75
2	B	72	GLN	OE1-CD-NE2	16.42	139.02	122.60
2	B	93	ASN	CB-CG-ND2	16.40	141.00	116.40
1	A	8	SER	O-C-N	-16.39	95.30	121.53
2	B	108	VAL	N-CA-CB	16.39	131.55	110.57
1	C	138	SER	N-CA-C	16.37	145.68	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	78	ASP	N-CA-CB	16.37	138.33	110.50
2	D	51	GLY	CA-C-N	-16.36	95.60	123.25
2	D	51	GLY	C-N-CA	-16.36	95.60	123.25
2	D	59	VAL	CA-CB-CG1	16.35	138.20	110.40
1	A	131	ASN	CB-CG-OD1	16.35	153.50	120.80
2	B	14	TRP	CE3-CZ3-CH2	16.34	142.35	121.10
1	A	16	LYS	CA-CB-CG	16.32	146.73	114.10
1	C	46	PHE	CD1-CE1-CZ	16.32	149.37	120.00
1	C	56	LYS	CA-CB-CG	-16.31	81.47	114.10
2	D	34	TYR	CD1-CG-CD2	-16.31	93.63	118.10
2	D	103	ARG	CD-NE-CZ	16.31	147.23	124.40
1	A	119	PRO	O-C-N	16.31	141.80	122.23
2	D	93	ASN	N-CA-CB	16.29	133.63	110.01
1	C	126	ASN	O-C-N	-16.28	104.66	122.08
1	C	3	SER	N-CA-CB	16.28	138.00	110.49
1	C	31	ARG	NH1-CZ-NH2	-16.27	98.15	119.30
1	A	92	ARG	CD-NE-CZ	16.25	147.15	124.40
1	A	8	SER	N-CA-C	-16.22	90.66	112.72
1	C	114	PRO	N-CA-CB	-16.22	86.22	103.25
1	C	61	LYS	CA-C-O	-16.21	97.33	120.51
1	A	117	PHE	N-CA-C	16.21	132.56	109.71
1	C	14	TRP	CB-CG-CD2	16.18	149.45	126.80
2	D	28	GLY	CA-C-N	16.16	148.22	120.58
2	D	28	GLY	C-N-CA	16.16	148.22	120.58
1	A	85	ASN	OD1-CG-ND2	16.16	138.76	122.60
1	C	27	GLN	OE1-CD-NE2	-16.15	106.45	122.60
2	D	55	ASN	CA-C-N	16.15	161.20	121.80
2	D	55	ASN	C-N-CA	16.15	161.20	121.80
2	D	138	ASN	CB-CA-C	16.14	138.06	111.26
1	C	87	HIS	CA-C-N	16.13	152.34	121.54
1	C	87	HIS	C-N-CA	16.13	152.34	121.54
1	A	42	TYR	CG-CD2-CE2	16.12	145.38	121.20
1	C	20	ASN	O-C-N	-16.11	103.10	122.11
2	B	31	LEU	CB-CG-CD1	16.11	159.03	110.70
1	A	75	ASP	OD1-CG-OD2	-16.11	84.25	122.90
2	B	12	GLY	CA-C-O	16.10	148.58	120.57
1	A	103	HIS	ND1-CE1-NE2	-16.09	92.31	108.40
1	C	19	GLY	O-C-N	-16.08	100.00	122.68
1	C	60	GLN	CG-CD-NE2	16.06	140.48	116.40
2	B	105	LEU	N-CA-CB	16.03	137.59	110.49
1	C	9	ASN	N-CA-CB	-16.03	83.40	110.49
1	C	135	VAL	O-C-N	-16.02	100.69	121.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	TYR	O-C-N	-16.01	105.08	122.38
2	B	70	PHE	CA-CB-CG	16.01	129.81	113.80
2	D	81	LYS	CA-C-N	16.00	152.77	121.41
2	D	81	LYS	C-N-CA	16.00	152.77	121.41
2	B	43	HIS	ND1-CE1-NE2	-16.00	92.40	108.40
2	D	80	LEU	CA-C-O	-15.98	103.80	120.90
1	C	29	LEU	CA-CB-CG	15.97	172.20	116.30
2	D	95	LEU	O-C-N	-15.96	99.75	122.41
2	B	38	GLN	OE1-CD-NE2	-15.95	106.65	122.60
1	C	102	SER	CA-C-N	-15.94	97.11	120.38
1	C	102	SER	C-N-CA	-15.94	97.11	120.38
2	B	14	TRP	O-C-N	-15.93	101.40	122.59
1	A	35	SER	N-CA-CB	15.93	132.86	110.88
1	A	122	HIS	N-CA-CB	15.93	133.53	110.12
2	D	25	GLN	N-CA-CB	15.91	137.38	110.49
2	D	57	PRO	CA-C-N	15.91	151.92	121.54
2	D	57	PRO	C-N-CA	15.91	151.92	121.54
2	B	84	PHE	CZ-CE2-CD2	15.91	148.63	120.00
2	D	75	LYS	CB-CG-CD	15.88	147.82	111.30
2	D	112	VAL	CA-C-N	15.88	140.25	120.88
2	D	112	VAL	C-N-CA	15.88	140.25	120.88
1	C	88	ALA	CA-C-O	-15.87	97.81	120.51
1	C	90	LYS	CA-C-O	-15.85	98.67	120.07
2	D	16	LYS	O-C-N	15.84	143.66	122.59
1	A	34	LEU	CA-C-O	-15.84	100.48	118.69
1	A	87	HIS	CB-CA-C	-15.83	85.88	110.90
1	C	82	ASN	CA-CB-CG	-15.82	96.78	112.60
1	C	66	LEU	CA-CB-CG	15.82	171.67	116.30
1	C	114	PRO	CB-CA-C	15.82	137.66	111.56
1	C	6	ASN	CB-CG-ND2	15.81	140.12	116.40
2	B	123	PRO	CA-N-CD	15.80	134.12	112.00
1	A	67	THR	CA-CB-CG2	15.79	137.34	110.50
1	A	132	ASP	CB-CA-C	15.77	141.80	110.42
1	A	50	HIS	CA-CB-CG	-15.75	98.05	113.80
1	C	29	LEU	CD1-CG-CD2	-15.75	76.16	110.80
2	B	29	ARG	NE-CZ-NH1	15.74	137.24	121.50
1	C	115	THR	N-CA-CB	15.74	133.99	110.53
2	D	14	TRP	O-C-N	15.72	143.50	122.59
1	C	20	ASN	CB-CA-C	15.72	136.38	111.39
2	B	65	ARG	NE-CZ-NH2	15.70	133.33	119.20
2	D	137	ALA	N-CA-C	-15.69	82.61	108.49
1	C	20	ASN	N-CA-C	-15.68	86.73	111.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	46	PHE	CB-CA-C	-15.68	83.00	109.50
2	B	28	GLY	CA-C-O	-15.68	93.29	120.57
1	C	78	GLY	CA-C-O	-15.68	93.29	120.57
1	A	49	SER	N-CA-CB	15.67	136.97	110.49
2	D	124	ASN	CA-C-O	-15.67	98.11	120.51
1	A	87	HIS	CA-CB-CG	-15.66	98.14	113.80
1	A	91	LEU	CD1-CG-CD2	-15.66	76.35	110.80
2	D	105	LEU	O-C-N	-15.65	101.02	122.46
1	C	10	VAL	O-C-N	-15.64	103.02	122.57
2	D	129	PHE	CA-C-N	15.64	141.23	120.28
2	D	129	PHE	C-N-CA	15.64	141.23	120.28
1	A	89	HIS	N-CA-CB	15.63	137.07	110.50
1	C	33	PHE	CG-CD1-CE1	15.62	147.26	120.70
2	D	101	ASN	N-CA-C	15.62	131.74	111.75
2	D	117	PHE	CZ-CE2-CD2	-15.62	91.89	120.00
1	C	86	LEU	O-C-N	-15.61	98.02	123.00
1	A	57	ALA	CA-C-O	-15.60	104.51	120.89
2	B	119	GLY	N-CA-C	15.60	134.65	115.31
1	C	108	THR	N-CA-C	-15.60	86.87	111.04
2	D	117	PHE	N-CA-CB	-15.59	86.56	110.73
1	A	68	LYS	CA-CB-CG	15.59	145.28	114.10
1	C	114	PRO	N-CD-CG	-15.58	79.82	103.20
2	D	22	VAL	CA-C-N	15.58	137.48	120.03
2	D	22	VAL	C-N-CA	15.58	137.48	120.03
2	D	85	ALA	CA-C-O	15.58	137.06	120.55
1	C	21	ALA	O-C-N	-15.57	103.41	121.32
1	A	2	LEU	CA-C-N	-15.57	97.81	122.87
1	A	2	LEU	C-N-CA	-15.57	97.81	122.87
1	A	9	ASN	CA-C-O	-15.57	104.67	120.70
2	B	125	VAL	CA-C-N	15.57	151.27	121.54
2	B	125	VAL	C-N-CA	15.57	151.27	121.54
1	C	32	MET	CA-CB-CG	15.55	145.20	114.10
1	C	45	HIS	N-CA-C	15.55	143.92	110.80
1	C	100	LEU	CA-C-N	-15.55	99.08	120.38
1	C	100	LEU	C-N-CA	-15.55	99.08	120.38
1	C	131	ASN	OD1-CG-ND2	15.55	138.15	122.60
2	D	140	LEU	N-CA-CB	15.55	136.15	109.72
2	D	128	LEU	CA-C-N	-15.54	97.70	120.38
2	D	128	LEU	C-N-CA	-15.54	97.70	120.38
2	D	142	HIS	ND1-CG-CD2	-15.53	90.57	106.10
2	B	25	GLN	CA-C-O	-15.53	104.59	120.89
1	A	15	GLY	CA-C-O	-15.53	93.55	120.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	87	HIS	N-CA-CB	15.52	132.57	110.07
1	C	127	LYS	CG-CD-CE	15.49	146.94	111.30
2	B	103	ARG	NE-CZ-NH1	15.49	136.99	121.50
2	B	79	ASP	N-CA-CB	-15.49	84.32	110.49
2	B	33	VAL	CA-CB-CG2	-15.48	84.09	110.40
2	B	99	PRO	N-CA-CB	-15.48	88.86	103.41
2	D	50	ALA	N-CA-C	-15.47	92.62	111.33
1	A	62	VAL	CA-CB-CG1	15.46	136.69	110.40
1	A	140	TYR	OH-CZ-CE2	15.46	166.29	119.90
2	B	91	HIS	CA-CB-CG	-15.46	98.34	113.80
2	D	100	GLN	O-C-N	15.46	138.73	122.03
2	B	108	VAL	CA-CB-CG1	15.45	136.67	110.40
2	B	133	VAL	CB-CA-C	15.44	133.53	112.22
2	B	43	HIS	CA-CB-CG	-15.44	98.36	113.80
1	A	44	PRO	N-CD-CG	15.42	126.33	103.20
2	B	40	PHE	CA-CB-CG	-15.41	98.39	113.80
2	B	14	TRP	CD1-NE1-CE2	-15.41	81.16	108.90
1	A	57	ALA	N-CA-C	-15.39	87.18	111.04
2	D	109	LEU	N-CA-CB	15.39	136.49	110.49
1	A	66	LEU	CA-C-N	15.38	146.40	120.72
1	A	66	LEU	C-N-CA	15.38	146.40	120.72
2	B	106	GLY	N-CA-C	15.37	133.71	113.27
1	C	87	HIS	N-CA-C	-15.36	89.92	112.04
2	D	111	LEU	O-C-N	15.36	143.04	122.30
1	A	82	ASN	CB-CA-C	15.35	140.97	110.42
2	B	10	VAL	CA-CB-CG2	15.34	136.47	110.40
1	C	99	LYS	CA-CB-CG	15.34	144.77	114.10
2	D	130	GLN	O-C-N	-15.34	105.86	122.12
2	B	38	GLN	CB-CG-CD	15.33	138.67	112.60
2	D	14	TRP	CA-C-O	-15.32	98.61	120.51
2	B	139	ALA	N-CA-CB	-15.31	85.94	110.14
1	C	68	LYS	O-C-N	-15.31	102.23	122.59
2	D	20	ASP	CB-CA-C	15.30	140.88	110.42
2	D	65	ARG	NE-CZ-NH1	-15.30	106.19	121.50
1	C	140	TYR	N-CA-C	15.30	135.07	109.06
2	B	139	ALA	CA-C-O	15.30	137.34	120.20
2	B	94	LYS	CA-CB-CG	15.29	144.69	114.10
2	B	129	PHE	CA-C-O	15.29	136.63	120.42
1	A	42	TYR	CB-CG-CD2	15.28	143.73	120.80
1	A	29	LEU	CA-C-O	-15.28	98.66	120.51
1	A	65	ALA	CA-C-N	15.27	150.70	121.54
1	A	65	ALA	C-N-CA	15.27	150.70	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	121	PHE	CE1-CZ-CE2	-15.25	92.55	120.00
2	D	35	PRO	N-CD-CG	-15.25	80.33	103.20
2	D	71	THR	CA-CB-OG1	15.23	132.45	109.60
1	C	44	PRO	CA-C-O	-15.23	92.88	120.60
2	B	78	ASP	CA-C-N	15.23	150.62	121.54
2	B	78	ASP	C-N-CA	15.23	150.62	121.54
2	B	56	ASN	CB-CG-ND2	15.22	139.23	116.40
1	C	42	TYR	CZ-CE2-CD2	15.22	147.00	119.60
1	A	117	PHE	CA-CB-CG	15.18	128.98	113.80
2	D	40	PHE	CD1-CG-CD2	15.18	141.37	118.60
1	A	132	ASP	CB-CG-OD2	-15.17	83.51	118.40
1	A	72	HIS	CG-CD2-NE2	-15.16	92.04	107.20
2	B	98	ASN	CB-CG-ND2	15.15	139.12	116.40
1	C	119	PRO	N-CA-CB	15.14	119.99	103.33
2	B	76	HIS	N-CA-CB	-15.14	84.90	110.49
1	A	45	HIS	CE1-NE2-CD2	-15.13	93.87	109.00
1	C	51	GLY	CA-C-O	15.12	132.85	120.30
1	A	140	TYR	CG-CD1-CE1	-15.12	98.52	121.20
2	D	70	PHE	O-C-N	15.12	142.71	122.30
2	D	47	LEU	CA-C-O	15.11	138.36	120.53
1	C	57	ALA	O-C-N	-15.10	102.50	122.59
1	A	120	ALA	O-C-N	-15.08	105.80	122.09
1	A	137	THR	CA-C-N	15.08	150.34	121.54
1	A	137	THR	C-N-CA	15.08	150.34	121.54
1	A	79	THR	O-C-N	-15.08	105.80	122.09
2	D	103	ARG	N-CA-C	15.07	131.41	113.18
1	A	31	ARG	CG-CD-NE	-15.05	78.89	112.00
2	D	107	ASN	N-CA-CB	-15.04	88.26	110.07
2	D	43	HIS	CA-C-N	15.04	150.26	121.54
2	D	43	HIS	C-N-CA	15.04	150.26	121.54
1	C	78	GLY	O-C-N	15.03	142.24	122.70
2	B	77	LEU	CB-CA-C	-15.01	87.61	111.48
2	B	64	LYS	CA-C-N	15.01	141.60	120.29
2	B	64	LYS	C-N-CA	15.01	141.60	120.29
2	B	125	VAL	CA-C-O	-15.01	104.26	120.47
1	C	133	SER	O-C-N	14.99	142.53	122.59
2	D	7	LYS	N-CA-CB	14.99	135.83	110.49
1	C	101	LEU	CA-C-N	14.98	150.16	121.54
1	C	101	LEU	C-N-CA	14.98	150.16	121.54
1	A	22	PRO	O-C-N	-14.96	104.07	122.17
2	B	142	HIS	CE1-NE2-CD2	14.96	123.96	109.00
1	C	27	GLN	CG-CD-NE2	14.96	138.84	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	128	LEU	CD1-CG-CD2	-14.95	77.92	110.80
2	B	12	GLY	O-C-N	-14.94	103.28	122.70
1	A	131	ASN	N-CA-C	-14.93	95.02	111.14
1	A	7	LYS	O-C-N	14.92	138.05	122.08
2	B	39	ARG	CG-CD-NE	14.92	144.82	112.00
1	C	48	LEU	CD1-CG-CD2	14.91	143.61	110.80
1	C	59	GLY	N-CA-C	-14.91	93.70	113.24
2	B	40	PHE	N-CA-C	-14.89	94.42	112.89
2	D	7	LYS	CA-CB-CG	14.89	143.88	114.10
2	B	11	THR	CA-CB-OG1	-14.89	87.27	109.60
2	B	35	PRO	O-C-N	-14.87	102.56	122.64
2	B	77	LEU	N-CA-C	14.86	130.90	112.47
1	C	141	ARG	NH1-CZ-NH2	14.85	138.61	119.30
2	B	84	PHE	CG-CD2-CE2	-14.84	95.48	120.70
2	D	59	VAL	CA-CB-CG2	-14.84	85.18	110.40
1	C	125	LEU	CA-C-O	-14.83	99.30	120.51
2	D	29	ARG	CA-C-N	14.83	140.61	120.44
2	D	29	ARG	C-N-CA	14.83	140.61	120.44
1	A	101	LEU	CA-C-N	14.82	145.93	120.58
1	A	101	LEU	C-N-CA	14.82	145.93	120.58
1	A	27	GLN	N-CA-C	-14.82	91.85	112.45
1	C	24	TYR	O-C-N	-14.82	102.89	122.59
1	A	77	PRO	CA-C-O	-14.81	93.64	120.60
2	D	125	VAL	O-C-N	-14.81	104.06	122.57
1	C	45	HIS	CA-C-N	14.80	147.80	122.64
1	C	45	HIS	C-N-CA	14.80	147.80	122.64
1	A	46	PHE	CE1-CZ-CE2	14.80	146.63	120.00
2	B	67	LEU	O-C-N	14.80	142.27	122.59
1	A	16	LYS	CD-CE-NZ	-14.77	64.64	111.90
1	A	132	ASP	CB-CG-OD1	14.74	152.30	118.40
1	A	72	HIS	CA-C-N	14.73	143.93	121.99
1	A	72	HIS	C-N-CA	14.73	143.93	121.99
2	B	47	LEU	N-CA-CB	-14.72	87.02	111.17
1	C	43	PHE	CE1-CZ-CE2	14.72	146.50	120.00
1	C	44	PRO	CA-C-N	-14.72	93.42	121.54
1	C	44	PRO	C-N-CA	-14.72	93.42	121.54
2	D	103	ARG	O-C-N	-14.70	100.97	122.43
1	A	20	ASN	CB-CG-OD1	-14.69	91.43	120.80
2	D	13	PHE	O-C-N	-14.69	106.37	122.08
2	B	102	PHE	CA-C-O	14.68	136.48	120.63
2	D	37	THR	CA-CB-CG2	14.67	135.44	110.50
1	C	12	ALA	CA-C-O	-14.66	100.00	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	52	SER	CA-CB-OG	14.65	140.41	111.10
2	B	22	VAL	CA-C-N	-14.65	92.69	121.41
2	B	22	VAL	C-N-CA	-14.65	92.69	121.41
1	A	108	THR	N-CA-CB	14.65	135.24	110.49
2	D	123	PRO	CB-CA-C	14.64	136.78	112.62
1	A	28	ALA	N-CA-CB	14.63	135.21	110.49
2	D	33	VAL	CA-CB-CG2	-14.63	85.53	110.40
1	C	112	HIS	CA-C-N	-14.62	105.17	123.16
1	C	112	HIS	C-N-CA	-14.62	105.17	123.16
1	A	10	VAL	N-CA-CB	14.62	135.35	111.23
1	C	132	ASP	CB-CA-C	14.61	135.05	110.79
1	A	105	LEU	CA-CB-CG	14.61	167.44	116.30
2	B	8	ALA	CA-C-O	-14.61	99.61	120.51
2	B	141	ALA	N-CA-CB	-14.61	88.09	110.73
1	A	68	LYS	CA-C-O	14.59	138.55	120.31
1	C	3	SER	O-C-N	-14.58	103.19	122.59
2	B	80	LEU	CB-CA-C	14.57	137.79	110.10
2	D	133	VAL	CA-C-N	14.57	149.37	121.54
2	D	133	VAL	C-N-CA	14.57	149.37	121.54
1	C	79	THR	CA-CB-CG2	14.57	135.26	110.50
2	D	42	GLN	CG-CD-NE2	-14.57	94.55	116.40
1	A	115	THR	CA-C-N	14.56	147.29	121.66
1	A	115	THR	C-N-CA	14.56	147.29	121.66
2	D	144	TYR	CG-CD2-CE2	-14.56	99.35	121.20
1	C	30	GLN	CB-CG-CD	-14.56	87.84	112.60
2	B	96	HIS	CA-C-N	14.56	141.77	120.95
2	B	96	HIS	C-N-CA	14.56	141.77	120.95
1	A	62	VAL	O-C-N	-14.56	104.38	122.57
2	D	131	LYS	CA-CB-CG	-14.55	85.01	114.10
2	B	81	LYS	CA-CB-CG	-14.53	85.05	114.10
2	B	57	PRO	CA-C-O	-14.52	94.17	120.60
1	C	135	VAL	N-CA-C	-14.52	95.17	111.00
2	B	103	ARG	CG-CD-NE	-14.51	80.07	112.00
2	D	117	PHE	CE1-CZ-CE2	14.51	146.11	120.00
1	C	50	HIS	CA-C-N	-14.50	107.93	120.98
1	C	50	HIS	C-N-CA	-14.50	107.93	120.98
1	C	117	PHE	CA-CB-CG	14.50	128.30	113.80
2	D	52	ALA	N-CA-CB	-14.50	89.97	111.43
1	A	62	VAL	CA-C-O	-14.49	102.66	120.78
2	B	122	THR	N-CA-CB	14.49	136.13	111.50
1	C	87	HIS	CG-CD2-NE2	14.48	121.68	107.20
2	B	126	GLN	N-CA-CB	14.48	134.96	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	PHE	CA-CB-CG	-14.47	99.33	113.80
2	D	124	ASN	N-CA-CB	14.47	134.95	110.49
2	D	137	ALA	O-C-N	-14.46	100.34	122.61
1	C	62	VAL	O-C-N	-14.46	104.50	122.57
1	C	85	ASN	CA-C-N	14.45	147.71	121.70
1	C	85	ASN	C-N-CA	14.45	147.71	121.70
1	A	20	ASN	CA-C-O	-14.44	102.71	119.60
2	D	134	ALA	CA-C-N	14.43	136.19	120.03
2	D	134	ALA	C-N-CA	14.43	136.19	120.03
2	D	39	ARG	CG-CD-NE	-14.43	80.25	112.00
1	C	108	THR	CA-C-N	14.43	149.09	121.54
1	C	108	THR	C-N-CA	14.43	149.09	121.54
1	A	46	PHE	CZ-CE2-CD2	-14.42	94.04	120.00
1	A	118	THR	CA-C-N	-14.42	103.04	119.05
1	A	118	THR	C-N-CA	-14.42	103.04	119.05
2	B	14	TRP	CB-CG-CD1	14.42	148.53	126.90
2	B	116	ASN	N-CA-CB	14.40	130.94	109.91
1	C	5	ALA	O-C-N	14.40	139.91	122.48
1	C	61	LYS	CG-CD-CE	14.38	144.36	111.30
2	D	129	PHE	CG-CD1-CE1	14.38	145.14	120.70
2	D	102	PHE	CB-CG-CD1	14.37	145.13	120.70
1	C	16	LYS	CA-CB-CG	-14.35	85.40	114.10
1	C	2	LEU	CA-C-N	14.35	148.94	121.54
1	C	2	LEU	C-N-CA	14.35	148.94	121.54
2	D	90	LEU	CD1-CG-CD2	14.34	142.36	110.80
2	D	103	ARG	CA-CB-CG	14.34	142.79	114.10
2	D	71	THR	N-CA-CB	-14.33	87.14	111.50
1	C	103	HIS	CB-CG-ND1	-14.33	101.21	122.70
2	D	90	LEU	CA-C-O	-14.32	104.35	120.24
1	C	27	GLN	O-C-N	14.31	140.99	122.39
1	C	47	ASP	N-CA-C	-14.30	85.42	108.73
1	C	95	PRO	N-CD-CG	14.30	124.66	103.20
1	C	13	ALA	CA-C-N	14.29	139.95	120.38
1	C	13	ALA	C-N-CA	14.29	139.95	120.38
2	D	72	GLN	CB-CG-CD	14.27	136.86	112.60
1	A	8	SER	CB-CA-C	14.26	128.76	111.22
2	B	83	ALA	O-C-N	-14.25	103.64	122.59
2	D	112	VAL	O-C-N	14.24	141.78	122.12
1	C	45	HIS	N-CA-CB	-14.24	86.42	110.49
2	D	46	ASN	OD1-CG-ND2	-14.24	108.36	122.60
1	A	54	GLN	CA-C-O	14.24	135.56	120.90
2	D	143	LYS	N-CA-C	14.23	141.11	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	103	HIS	CG-CD2-NE2	14.22	121.42	107.20
1	C	96	VAL	N-CA-CB	-14.21	87.78	111.23
1	C	42	TYR	CE1-CZ-CE2	-14.21	91.88	120.30
1	A	47	ASP	O-C-N	-14.19	103.72	122.59
2	B	94	LYS	N-CA-CB	14.18	131.37	110.95
1	C	46	PHE	CA-CB-CG	-14.18	99.62	113.80
1	C	116	ASN	OD1-CG-ND2	-14.18	108.42	122.60
2	D	19	VAL	CA-CB-CG2	-14.18	86.30	110.40
2	B	50	ALA	N-CA-C	-14.17	91.64	112.04
1	A	73	LEU	CB-CA-C	14.15	134.41	110.77
1	A	17	VAL	O-C-N	-14.15	104.89	122.57
1	A	54	GLN	N-CA-C	-14.14	95.33	111.03
1	C	128	PHE	CA-C-N	14.12	143.76	120.88
1	C	128	PHE	C-N-CA	14.12	143.76	120.88
2	B	128	LEU	CA-C-N	14.11	140.32	120.29
2	B	128	LEU	C-N-CA	14.11	140.32	120.29
1	C	120	ALA	N-CA-CB	14.11	133.40	110.40
1	A	19	GLY	CA-C-N	14.10	147.46	121.52
1	A	19	GLY	C-N-CA	14.10	147.46	121.52
1	A	133	SER	CA-C-N	14.09	139.79	120.63
1	A	133	SER	C-N-CA	14.09	139.79	120.63
2	B	129	PHE	CZ-CE2-CD2	-14.09	94.64	120.00
1	A	43	PHE	CB-CG-CD2	-14.08	96.76	120.70
1	A	50	HIS	CA-C-O	-14.07	100.39	120.51
1	C	62	VAL	CA-CB-CG1	14.07	134.32	110.40
1	A	11	LYS	CA-C-N	-14.07	94.67	121.54
1	A	11	LYS	C-N-CA	-14.07	94.67	121.54
2	D	117	PHE	CA-CB-CG	14.07	127.87	113.80
1	C	85	ASN	CA-CB-CG	14.06	126.67	112.60
2	D	130	GLN	N-CA-C	-14.06	95.95	111.28
1	C	110	ALA	CA-C-O	-14.06	96.90	120.80
2	D	14	TRP	CD1-CG-CD2	-14.05	83.82	106.30
1	C	40	LYS	CB-CG-CD	14.04	143.58	111.30
2	B	57	PRO	N-CD-CG	-14.03	82.15	103.20
2	B	78	ASP	CA-C-O	14.03	144.65	120.80
2	B	41	PHE	O-C-N	14.01	142.12	123.06
2	B	145	HIS	CB-CG-CD2	-14.01	112.98	131.20
1	C	23	ALA	CB-CA-C	-14.01	84.71	110.63
1	A	62	VAL	CA-C-N	14.00	140.44	120.28
1	A	62	VAL	C-N-CA	14.00	140.44	120.28
1	C	119	PRO	CA-C-N	14.00	145.64	121.14
1	C	119	PRO	C-N-CA	14.00	145.64	121.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	GLN	N-CA-C	-13.99	96.03	111.14
1	A	32	MET	CB-CA-C	13.98	136.56	109.72
1	A	52	SER	N-CA-C	13.96	131.17	108.41
1	C	79	THR	CA-CB-OG1	-13.96	88.66	109.60
1	A	124	ASN	CB-CG-OD1	-13.95	92.90	120.80
2	D	39	ARG	CD-NE-CZ	13.94	143.92	124.40
1	C	76	LEU	CD1-CG-CD2	13.94	141.47	110.80
2	D	116	ASN	N-CA-CB	13.94	134.04	110.49
1	A	46	PHE	CB-CG-CD2	13.93	144.39	120.70
2	D	39	ARG	CA-CB-CG	13.93	141.97	114.10
1	C	11	LYS	CA-CB-CG	-13.92	86.27	114.10
2	B	66	VAL	CA-CB-CG2	13.91	134.05	110.40
1	C	38	THR	N-CA-C	-13.90	95.66	112.89
2	D	119	GLY	N-CA-C	-13.88	95.00	112.77
1	C	49	SER	CA-CB-OG	13.88	138.86	111.10
1	A	70	GLN	CG-CD-NE2	13.88	137.22	116.40
2	B	80	LEU	CA-C-N	13.88	146.68	121.70
2	B	80	LEU	C-N-CA	13.88	146.68	121.70
2	D	68	ASP	CB-CA-C	-13.86	87.78	110.79
1	A	94	ASN	CB-CA-C	13.86	131.37	109.62
2	B	21	VAL	O-C-N	-13.86	105.25	122.57
2	B	14	TRP	CA-CB-CG	13.85	139.91	113.60
1	A	73	LEU	CA-C-N	13.84	147.98	121.54
1	A	73	LEU	C-N-CA	13.84	147.98	121.54
2	D	2	LEU	N-CA-CB	-13.84	87.09	110.49
1	A	45	HIS	CA-C-N	13.84	141.88	121.26
1	A	45	HIS	C-N-CA	13.84	141.88	121.26
1	A	117	PHE	CA-C-O	13.83	141.05	122.51
2	D	42	GLN	CB-CG-CD	-13.83	89.09	112.60
1	C	75	ASP	CA-C-O	13.83	140.28	120.51
2	D	55	ASN	N-CA-CB	13.83	130.10	109.91
1	C	29	LEU	N-CA-C	-13.82	96.29	111.36
1	C	23	ALA	CA-C-O	-13.82	104.48	120.10
1	C	69	ALA	CB-CA-C	-13.82	83.65	110.46
1	A	114	PRO	CA-N-CD	-13.80	92.68	112.00
1	A	11	LYS	O-C-N	13.79	140.16	122.23
1	C	134	THR	CA-C-N	13.79	142.62	120.55
1	C	134	THR	C-N-CA	13.79	142.62	120.55
1	A	117	PHE	CG-CD2-CE2	-13.79	97.26	120.70
1	A	98	PHE	CD1-CG-CD2	-13.78	97.93	118.60
2	D	30	LEU	CA-C-O	13.78	134.89	120.70
2	B	121	PHE	CD1-CG-CD2	-13.77	97.94	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	75	LYS	CA-CB-CG	-13.77	86.56	114.10
1	C	113	LEU	CA-C-N	-13.76	102.64	119.84
1	C	113	LEU	C-N-CA	-13.76	102.64	119.84
1	A	15	GLY	O-C-N	-13.74	104.83	122.70
2	B	63	GLY	O-C-N	-13.74	107.15	122.68
1	A	111	SER	CA-C-O	-13.74	100.86	120.51
2	B	24	ALA	CA-C-O	13.74	135.47	120.63
1	A	72	HIS	CG-ND1-CE1	13.73	132.65	109.30
1	C	89	HIS	ND1-CE1-NE2	13.72	122.12	108.40
1	A	74	ASN	O-C-N	-13.72	104.35	122.59
2	D	132	VAL	O-C-N	13.72	137.30	121.80
1	A	84	SER	CA-C-O	13.71	135.74	119.97
2	B	109	LEU	O-C-N	13.71	136.34	122.09
1	C	116	ASN	CA-C-O	-13.71	99.74	120.16
2	D	9	ALA	CB-CA-C	13.70	137.69	110.42
1	A	56	LYS	CA-C-N	13.69	141.43	120.89
1	A	56	LYS	C-N-CA	13.69	141.43	120.89
2	B	31	LEU	O-C-N	13.69	140.80	122.59
2	B	69	ALA	O-C-N	-13.69	104.38	122.59
1	A	113	LEU	CA-C-O	13.68	137.84	120.87
1	C	2	LEU	CA-C-O	13.68	135.51	120.32
1	C	12	ALA	N-CA-C	-13.68	96.60	113.01
1	C	129	LEU	N-CA-C	-13.67	93.60	111.24
2	D	59	VAL	N-CA-CB	13.67	133.78	111.23
2	B	104	LEU	CA-C-N	13.65	147.62	121.54
2	B	104	LEU	C-N-CA	13.65	147.62	121.54
2	D	67	LEU	O-C-N	13.65	136.59	122.12
1	C	63	ALA	N-CA-CB	13.65	133.56	110.49
2	D	13	PHE	CA-C-N	13.65	147.61	121.54
2	D	13	PHE	C-N-CA	13.65	147.61	121.54
1	C	14	TRP	CG-CD2-CE3	-13.64	120.25	133.90
1	C	60	GLN	CG-CD-OE1	-13.64	93.51	120.80
1	A	82	ASN	CB-CG-ND2	13.64	136.86	116.40
2	B	84	PHE	CA-CB-CG	-13.64	100.16	113.80
2	B	5	GLU	N-CA-C	-13.63	95.99	112.89
2	B	128	LEU	CB-CA-C	13.63	138.19	110.38
2	B	57	PRO	O-C-N	13.62	141.03	122.64
2	D	145	HIS	CB-CA-C	-13.61	84.24	110.10
2	D	44	PHE	CA-CB-CG	-13.60	100.20	113.80
1	C	112	HIS	CG-ND1-CE1	13.59	132.41	109.30
2	B	44	PHE	CD1-CG-CD2	-13.59	98.22	118.60
1	A	91	LEU	CB-CA-C	13.59	131.88	110.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	75	LYS	O-C-N	13.58	140.65	122.59
2	D	139	ALA	CA-C-N	13.57	142.76	121.19
2	D	139	ALA	C-N-CA	13.57	142.76	121.19
2	D	18	ASP	N-CA-CB	-13.56	87.23	110.83
2	B	96	HIS	CB-CG-ND1	-13.56	102.36	122.70
2	B	14	TRP	NE1-CE2-CD2	13.56	125.02	107.40
1	C	36	PHE	CZ-CE2-CD2	-13.55	95.61	120.00
1	C	39	THR	CA-CB-CG2	13.55	133.54	110.50
2	D	41	PHE	N-CA-CB	13.55	132.92	110.42
1	C	70	GLN	N-CA-CB	-13.55	81.70	111.10
1	C	92	ARG	CD-NE-CZ	-13.54	105.44	124.40
1	A	80	LEU	O-C-N	-13.53	100.63	122.42
2	D	127	ALA	CB-CA-C	-13.53	89.88	111.39
1	C	2	LEU	CD1-CG-CD2	13.52	140.55	110.80
2	D	31	LEU	N-CA-C	-13.52	96.02	111.03
2	D	2	LEU	CB-CG-CD1	-13.52	70.15	110.70
2	D	142	HIS	CB-CG-ND1	13.52	142.98	122.70
2	B	32	VAL	CA-CB-CG1	13.52	133.38	110.40
1	A	64	ASN	O-C-N	-13.51	107.80	122.12
1	A	85	ASN	CA-CB-CG	-13.51	99.09	112.60
2	B	6	GLU	OE1-CD-OE2	-13.51	90.49	122.90
2	B	14	TRP	N-CA-CB	13.50	133.31	110.49
1	C	24	TYR	N-CA-CB	13.49	133.29	110.49
1	A	6	ASN	CA-C-N	13.49	139.54	120.79
1	A	6	ASN	C-N-CA	13.49	139.54	120.79
1	A	120	ALA	CA-C-N	13.48	146.24	121.97
1	A	120	ALA	C-N-CA	13.48	146.24	121.97
1	A	133	SER	CA-CB-OG	13.48	138.06	111.10
1	A	77	PRO	CB-CA-C	13.46	133.78	111.56
1	C	135	VAL	CG1-CB-CG2	-13.46	81.18	110.80
2	D	136	VAL	CA-C-O	-13.44	106.33	120.71
2	B	96	HIS	ND1-CG-CD2	13.43	119.53	106.10
2	B	43	HIS	N-CA-CB	13.43	133.32	110.50
1	C	43	PHE	N-CA-C	13.42	132.56	108.94
1	C	36	PHE	CA-CB-CG	13.41	127.21	113.80
2	D	40	PHE	CA-C-O	-13.41	106.20	120.55
2	D	68	ASP	N-CA-CB	13.40	129.82	110.12
2	D	103	ARG	NE-CZ-NH2	-13.40	107.14	119.20
1	C	58	HIS	CE1-NE2-CD2	13.38	122.38	109.00
1	A	128	PHE	CA-C-O	13.38	139.64	120.51
2	D	127	ALA	N-CA-C	-13.37	90.31	111.04
2	D	44	PHE	CG-CD2-CE2	13.36	143.41	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	107	ASN	CB-CG-ND2	-13.36	96.37	116.40
2	D	10	VAL	N-CA-C	13.35	137.12	109.34
1	A	38	THR	CA-CB-OG1	-13.34	89.59	109.60
1	A	110	ALA	N-CA-C	-13.33	82.40	110.80
1	C	76	LEU	CA-C-O	-13.33	101.90	120.16
2	D	40	PHE	CA-CB-CG	13.32	127.12	113.80
2	B	113	VAL	CA-C-N	13.31	139.45	120.28
2	B	113	VAL	C-N-CA	13.31	139.45	120.28
1	A	126	ASN	CB-CG-ND2	13.31	136.36	116.40
2	B	5	GLU	N-CA-CB	-13.29	88.73	110.40
2	B	76	HIS	CE1-NE2-CD2	13.29	122.28	109.00
2	B	50	ALA	CA-C-N	13.28	147.44	121.41
2	B	50	ALA	C-N-CA	13.28	147.44	121.41
2	D	24	ALA	CA-C-O	-13.28	104.12	119.79
2	D	117	PHE	CD1-CE1-CZ	-13.28	96.10	120.00
1	A	137	THR	N-CA-CB	-13.27	92.23	110.67
2	B	127	ALA	N-CA-CB	13.26	132.91	110.49
2	D	57	PRO	N-CA-CB	-13.26	89.33	103.25
1	A	27	GLN	CA-C-O	-13.25	103.83	120.00
2	B	110	ALA	CA-C-O	13.25	135.08	120.10
1	A	33	PHE	CA-C-O	13.23	134.92	120.63
2	B	109	LEU	CA-C-O	-13.23	106.74	120.90
1	A	99	LYS	CA-C-N	13.23	146.81	121.54
1	A	99	LYS	C-N-CA	13.23	146.81	121.54
1	C	125	LEU	CA-C-N	13.23	139.18	120.79
1	C	125	LEU	C-N-CA	13.23	139.18	120.79
1	A	4	ALA	CA-C-N	-13.21	97.22	121.52
1	A	4	ALA	C-N-CA	-13.21	97.22	121.52
2	D	115	ARG	NE-CZ-NH2	-13.20	107.32	119.20
2	D	133	VAL	CA-CB-CG2	13.19	132.83	110.40
1	C	56	LYS	N-CA-C	-13.18	82.72	110.80
1	A	79	THR	CA-C-O	13.18	134.28	120.70
2	B	94	LYS	CA-C-O	13.17	133.92	119.03
1	C	72	HIS	CB-CG-CD2	-13.17	114.08	131.20
2	B	100	GLN	O-C-N	13.16	137.37	122.11
1	A	27	GLN	N-CA-CB	13.16	129.87	110.26
1	A	38	THR	N-CA-CB	-13.15	89.36	110.14
1	A	118	THR	CA-CB-CG2	-13.15	88.15	110.50
2	B	114	ALA	CA-C-O	13.14	134.95	120.10
1	A	18	GLY	CA-C-N	13.14	146.49	122.83
1	A	18	GLY	C-N-CA	13.14	146.49	122.83
1	A	16	LYS	CA-C-N	13.14	145.62	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	16	LYS	C-N-CA	13.14	145.62	121.97
1	C	9	ASN	CA-C-N	13.13	145.61	121.97
1	C	9	ASN	C-N-CA	13.13	145.61	121.97
1	A	33	PHE	CD1-CE1-CZ	-13.13	96.37	120.00
2	D	102	PHE	CA-CB-CG	13.12	126.92	113.80
2	D	140	LEU	CB-CG-CD2	13.12	150.06	110.70
2	D	18	ASP	N-CA-C	13.11	130.78	109.40
2	D	39	ARG	NH1-CZ-NH2	-13.11	102.26	119.30
2	D	102	PHE	CD1-CG-CD2	-13.11	98.94	118.60
1	C	46	PHE	CD1-CG-CD2	13.10	138.25	118.60
1	A	95	PRO	N-CA-CB	13.10	118.19	103.26
2	B	109	LEU	CB-CG-CD2	-13.09	71.42	110.70
1	C	39	THR	O-C-N	13.09	141.00	122.41
2	D	20	ASP	N-CA-C	-13.09	82.92	110.80
1	A	123	ALA	CA-C-O	13.09	134.77	120.24
2	B	44	PHE	CG-CD2-CE2	13.08	142.94	120.70
2	D	121	PHE	N-CA-C	13.06	138.63	110.80
2	B	48	SER	N-CA-C	-13.06	95.02	112.26
1	A	140	TYR	CD1-CE1-CZ	13.05	143.10	119.60
2	B	41	PHE	CZ-CE2-CD2	13.05	143.48	120.00
1	A	46	PHE	CG-CD2-CE2	13.04	142.88	120.70
1	C	19	GLY	CA-C-O	13.04	140.17	119.31
1	C	16	LYS	CG-CD-CE	13.03	141.28	111.30
2	B	62	HIS	CG-ND1-CE1	-13.02	87.16	109.30
1	A	114	PRO	CB-CG-CD	-13.01	64.45	106.10
2	B	129	PHE	CG-CD1-CE1	-13.00	98.61	120.70
1	C	137	THR	CA-C-O	-12.99	101.93	120.51
1	A	55	GLN	CG-CD-OE1	12.95	146.71	120.80
1	C	115	THR	CA-C-O	-12.95	104.38	119.15
1	A	3	SER	CA-C-O	12.95	135.80	121.16
2	B	59	VAL	CA-CB-CG1	-12.95	88.39	110.40
2	D	47	LEU	CA-CB-CG	12.93	161.56	116.30
2	D	93	ASN	OD1-CG-ND2	-12.93	109.67	122.60
1	C	102	SER	N-CA-CB	12.93	132.34	110.49
1	A	137	THR	CB-CA-C	12.93	130.78	109.07
1	C	2	LEU	CA-CB-CG	12.92	161.52	116.30
2	B	144	TYR	CG-CD2-CE2	-12.92	101.83	121.20
2	D	59	VAL	CG1-CB-CG2	-12.91	82.39	110.80
2	B	79	ASP	N-CA-C	-12.90	83.32	110.80
1	C	128	PHE	CE1-CZ-CE2	-12.90	96.79	120.00
2	D	129	PHE	N-CA-C	12.90	128.26	111.75
2	B	80	LEU	N-CA-CB	-12.88	88.60	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	103	ARG	CB-CG-CD	-12.86	81.73	111.30
2	D	37	THR	CB-CA-C	12.86	132.08	110.74
2	D	115	ARG	CB-CA-C	12.84	133.61	110.88
1	C	77	PRO	CA-CB-CG	-12.84	80.11	104.50
1	C	7	LYS	O-C-N	12.83	139.65	122.59
1	C	130	ALA	O-C-N	-12.83	105.53	122.59
2	D	57	PRO	O-C-N	-12.82	105.33	122.64
2	B	56	ASN	CB-CA-C	12.82	135.42	110.17
1	A	76	LEU	CA-CB-CG	12.80	161.12	116.30
1	A	130	ALA	N-CA-CB	12.80	131.48	109.72
1	A	9	ASN	N-CA-CB	-12.80	91.51	110.07
2	D	134	ALA	N-CA-C	-12.79	83.55	110.80
1	C	33	PHE	O-C-N	-12.79	107.57	122.15
2	D	101	ASN	O-C-N	12.79	136.78	122.20
2	B	40	PHE	CA-C-N	-12.79	101.91	122.76
2	B	40	PHE	C-N-CA	-12.79	101.91	122.76
1	C	93	VAL	CA-C-N	12.78	139.05	120.51
1	C	93	VAL	C-N-CA	12.78	139.05	120.51
1	A	31	ARG	NH1-CZ-NH2	-12.78	102.68	119.30
1	C	131	ASN	CA-C-N	12.78	137.41	120.28
1	C	131	ASN	C-N-CA	12.78	137.41	120.28
1	A	20	ASN	CA-CB-CG	-12.78	99.82	112.60
1	C	111	SER	CA-C-O	12.77	134.43	120.63
1	C	58	HIS	CG-CD2-NE2	-12.77	94.43	107.20
2	D	76	HIS	N-CA-CB	-12.76	89.92	110.21
1	C	10	VAL	CG1-CB-CG2	-12.76	82.73	110.80
1	C	129	LEU	O-C-N	-12.76	107.31	122.11
2	D	145	HIS	N-CA-C	12.72	146.62	111.00
1	C	74	ASN	O-C-N	-12.72	105.67	122.59
1	A	111	SER	O-C-N	-12.71	105.69	122.59
1	C	51	GLY	N-CA-C	-12.69	91.17	110.97
2	B	90	LEU	CB-CA-C	12.68	131.09	110.92
1	C	131	ASN	CB-CG-OD1	-12.68	95.43	120.80
2	B	126	GLN	N-CA-C	-12.68	83.79	110.80
1	A	80	LEU	N-CA-CB	-12.68	90.94	110.46
2	B	3	THR	O-C-N	-12.68	108.34	122.79
2	B	121	PHE	N-CA-C	-12.67	86.47	108.52
2	D	53	VAL	N-CA-CB	12.67	133.03	110.86
2	B	95	LEU	CA-CB-CG	-12.66	72.00	116.30
1	A	54	GLN	CG-CD-OE1	12.64	146.09	120.80
2	D	98	ASN	CA-C-O	-12.63	102.85	120.16
1	A	128	PHE	CE1-CZ-CE2	12.63	142.73	120.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	20	ASN	CB-CG-OD1	-12.61	95.57	120.80
1	C	129	LEU	CD1-CG-CD2	-12.61	83.06	110.80
1	A	9	ASN	CB-CG-ND2	12.61	135.31	116.40
2	B	6	GLU	CB-CG-CD	12.60	134.02	112.60
2	D	83	ALA	CA-C-N	-12.60	101.95	123.25
2	D	83	ALA	C-N-CA	-12.60	101.95	123.25
1	A	59	GLY	O-C-N	-12.59	109.98	122.19
2	B	93	ASN	CA-C-O	-12.58	102.52	120.51
1	C	97	ASN	CA-C-O	12.57	134.30	120.10
1	C	9	ASN	CB-CA-C	12.56	135.42	110.42
1	A	57	ALA	CB-CA-C	12.55	131.35	111.39
2	B	76	HIS	CB-CA-C	-12.54	85.45	110.42
1	C	57	ALA	CB-CA-C	12.54	135.38	110.42
2	D	81	LYS	N-CA-C	12.54	128.64	112.34
2	D	102	PHE	CG-CD1-CE1	12.54	142.01	120.70
1	C	112	HIS	ND1-CE1-NE2	12.53	120.93	108.40
2	D	34	TYR	CA-CB-CG	12.53	136.45	113.90
1	A	96	VAL	O-C-N	12.52	138.22	122.57
1	A	118	THR	O-C-N	12.51	135.71	121.32
1	C	3	SER	CB-CA-C	-12.51	85.52	110.42
1	A	20	ASN	O-C-N	12.49	140.10	122.36
1	A	50	HIS	CG-CD2-NE2	-12.49	94.71	107.20
2	D	26	ALA	N-CA-C	-12.49	97.17	111.03
2	D	101	ASN	CA-CB-CG	-12.49	100.11	112.60
1	C	50	HIS	CG-CD2-NE2	12.48	119.68	107.20
1	C	93	VAL	O-C-N	-12.47	106.98	122.57
2	D	54	MET	O-C-N	-12.45	107.10	122.17
2	B	36	TRP	CH2-CZ2-CE2	-12.43	101.34	117.50
2	B	101	ASN	OD1-CG-ND2	12.42	135.02	122.60
1	C	104	SER	CA-C-O	12.41	134.03	121.00
2	D	1	MET	N-CA-C	-12.40	76.28	111.00
1	C	137	THR	OG1-CB-CG2	12.39	134.07	109.30
2	D	51	GLY	N-CA-C	-12.38	77.39	113.30
1	C	135	VAL	CA-C-N	12.38	140.41	120.60
1	C	135	VAL	C-N-CA	12.38	140.41	120.60
1	C	138	SER	CA-CB-OG	-12.38	86.34	111.10
1	A	3	SER	CA-C-N	-12.37	100.81	120.60
1	A	3	SER	C-N-CA	-12.37	100.81	120.60
1	A	24	TYR	CD1-CG-CD2	-12.37	99.54	118.10
1	A	49	SER	CA-CB-OG	12.37	135.84	111.10
1	A	85	ASN	CB-CG-ND2	-12.37	97.84	116.40
1	A	45	HIS	CA-C-O	-12.37	104.53	119.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	SER	CA-C-O	12.36	138.19	120.51
2	D	25	GLN	CA-C-N	12.36	137.44	120.63
2	D	25	GLN	C-N-CA	12.36	137.44	120.63
1	A	69	ALA	N-CA-C	-12.36	97.89	111.36
2	B	77	LEU	N-CA-CB	-12.36	93.87	112.28
2	D	58	LYS	CA-C-N	12.35	144.20	121.97
2	D	58	LYS	C-N-CA	12.35	144.20	121.97
2	D	60	LYS	CB-CG-CD	12.35	139.69	111.30
1	A	102	SER	CA-C-O	-12.34	106.54	120.24
1	C	135	VAL	CA-CB-CG1	12.34	131.38	110.40
2	D	105	LEU	CB-CG-CD1	-12.34	73.67	110.70
1	A	18	GLY	O-C-N	-12.34	111.10	123.19
2	D	106	GLY	CA-C-N	12.34	137.22	120.44
2	D	106	GLY	C-N-CA	12.34	137.22	120.44
2	D	9	ALA	N-CA-CB	-12.32	89.67	110.49
2	D	129	PHE	CB-CG-CD1	12.32	141.65	120.70
2	B	138	ASN	N-CA-C	12.30	127.11	111.24
1	C	48	LEU	O-C-N	-12.30	106.23	122.59
1	C	122	HIS	ND1-CE1-NE2	-12.30	96.10	108.40
1	C	45	HIS	CG-CD2-NE2	-12.30	94.90	107.20
1	A	29	LEU	N-CA-C	-12.29	84.62	110.80
2	D	71	THR	CA-CB-CG2	-12.28	89.63	110.50
2	B	41	PHE	CA-CB-CG	12.28	126.08	113.80
1	C	33	PHE	CA-CB-CG	12.27	126.07	113.80
2	B	67	LEU	N-CA-CB	12.26	131.22	110.49
2	D	10	VAL	N-CA-CB	12.26	131.46	111.23
2	D	65	ARG	NH1-CZ-NH2	-12.26	103.36	119.30
1	C	76	LEU	CA-C-N	-12.26	105.25	119.47
1	C	76	LEU	C-N-CA	-12.26	105.25	119.47
1	A	18	GLY	CA-C-O	12.25	131.56	120.53
1	C	53	ALA	CA-C-O	12.25	134.54	119.10
1	A	66	LEU	O-C-N	-12.25	106.30	122.59
1	A	127	LYS	CD-CE-NZ	-12.25	72.71	111.90
1	C	103	HIS	ND1-CG-CD2	12.24	118.34	106.10
1	C	98	PHE	CD1-CG-CD2	-12.24	100.24	118.60
1	C	49	SER	N-CA-C	-12.24	76.74	111.00
1	A	33	PHE	CB-CG-CD2	12.23	141.49	120.70
2	D	128	LEU	CB-CG-CD2	12.22	147.38	110.70
2	B	37	THR	CA-CB-CG2	12.21	131.27	110.50
2	B	42	GLN	N-CA-CB	12.19	128.53	110.49
1	C	4	ALA	N-CA-C	-12.18	94.69	111.87
2	B	38	GLN	N-CA-C	-12.18	96.56	113.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	GLN	CB-CA-C	12.17	133.11	110.11
1	A	125	LEU	CA-C-N	12.16	136.96	120.54
1	A	125	LEU	C-N-CA	12.16	136.96	120.54
1	A	79	THR	CA-CB-CG2	-12.15	89.84	110.50
2	D	126	GLN	CG-CD-NE2	12.15	134.62	116.40
2	B	139	ALA	O-C-N	-12.14	108.36	122.20
1	C	14	TRP	CB-CA-C	-12.13	90.05	110.68
2	D	93	ASN	CB-CA-C	-12.12	91.84	110.88
2	D	70	PHE	CZ-CE2-CD2	-12.12	98.18	120.00
1	A	67	THR	OG1-CB-CG2	12.12	133.54	109.30
2	D	68	ASP	CA-C-O	12.12	133.40	120.55
1	C	80	LEU	CA-C-N	12.11	141.29	120.58
1	C	80	LEU	C-N-CA	12.11	141.29	120.58
1	C	96	VAL	CA-C-N	12.10	137.71	120.28
1	C	96	VAL	C-N-CA	12.10	137.71	120.28
2	D	85	ALA	O-C-N	-12.09	109.31	122.12
2	D	38	GLN	N-CA-C	12.07	125.94	111.33
2	B	142	HIS	N-CA-C	-12.07	97.93	112.89
1	C	110	ALA	O-C-N	12.05	142.29	123.00
1	C	116	ASN	CA-C-N	12.05	140.05	122.21
1	C	116	ASN	C-N-CA	12.05	140.05	122.21
2	B	122	THR	CA-C-N	12.05	131.96	119.19
2	B	122	THR	C-N-CA	12.05	131.96	119.19
1	A	66	LEU	CD1-CG-CD2	12.04	137.28	110.80
1	C	31	ARG	O-C-N	12.04	138.60	122.59
2	D	107	ASN	CB-CG-OD1	12.04	144.88	120.80
2	D	125	VAL	CG1-CB-CG2	-12.04	84.32	110.80
2	D	105	LEU	CA-C-O	-12.04	105.19	119.27
1	C	80	LEU	CB-CA-C	12.03	129.58	111.17
2	D	86	GLN	CG-CD-OE1	-12.02	96.75	120.80
2	B	138	ASN	O-C-N	-12.02	108.17	122.11
1	C	83	LEU	CA-C-O	-12.02	103.32	120.51
2	B	119	GLY	CA-C-N	12.01	145.58	122.53
2	B	119	GLY	C-N-CA	12.01	145.58	122.53
1	C	98	PHE	CB-CA-C	12.00	130.76	110.84
1	A	125	LEU	N-CA-C	12.00	131.17	111.37
2	B	47	LEU	CA-C-N	-12.00	104.50	122.86
2	B	47	LEU	C-N-CA	-12.00	104.50	122.86
2	B	95	LEU	CD1-CG-CD2	-12.00	84.40	110.80
2	D	108	VAL	CA-C-N	11.99	144.45	121.54
2	D	108	VAL	C-N-CA	11.99	144.45	121.54
2	B	124	ASN	CA-CB-CG	11.99	124.59	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	108	THR	CA-CB-CG2	11.99	130.88	110.50
2	D	46	ASN	CB-CG-ND2	11.98	134.37	116.40
1	C	28	ALA	N-CA-C	11.97	128.59	112.90
1	A	76	LEU	CB-CG-CD1	11.95	146.56	110.70
1	A	45	HIS	O-C-N	11.95	137.92	122.39
1	A	41	THR	CA-C-O	11.94	131.75	118.97
2	B	13	PHE	CD1-CE1-CZ	-11.92	98.55	120.00
2	D	30	LEU	CA-CB-CG	11.92	158.00	116.30
1	A	63	ALA	CA-C-O	-11.90	106.66	120.10
2	B	14	TRP	CE2-CD2-CG	-11.90	92.92	107.20
2	B	88	SER	CA-C-N	11.90	144.73	121.41
2	B	88	SER	C-N-CA	11.90	144.73	121.41
2	B	111	LEU	CA-C-N	11.90	143.38	121.97
2	B	111	LEU	C-N-CA	11.90	143.38	121.97
2	B	40	PHE	CZ-CE2-CD2	-11.89	98.60	120.00
1	C	117	PHE	CD1-CG-CD2	-11.88	100.78	118.60
1	C	67	THR	N-CA-C	-11.88	98.03	110.97
1	A	92	ARG	O-C-N	-11.87	108.61	122.86
1	A	88	ALA	O-C-N	-11.86	106.81	122.59
2	B	116	ASN	CB-CG-OD1	11.86	144.52	120.80
2	D	114	ALA	CA-C-N	11.86	140.81	122.42
2	D	114	ALA	C-N-CA	11.86	140.81	122.42
1	A	23	ALA	O-C-N	11.86	138.31	122.30
1	A	59	GLY	CA-C-N	11.86	144.19	121.54
1	A	59	GLY	C-N-CA	11.86	144.19	121.54
1	A	87	HIS	CA-C-O	11.86	132.91	120.70
2	B	13	PHE	CZ-CE2-CD2	-11.85	98.67	120.00
1	A	129	LEU	CA-C-O	-11.85	106.93	120.20
2	B	87	LEU	O-C-N	-11.84	106.13	122.46
2	D	94	LYS	N-CA-C	11.83	133.51	110.56
1	A	112	HIS	CB-CG-ND1	-11.83	104.95	122.70
2	D	80	LEU	CD1-CG-CD2	11.81	136.78	110.80
1	C	103	HIS	N-CA-C	11.80	126.86	111.75
2	B	108	VAL	CB-CA-C	-11.80	96.56	112.02
1	A	89	HIS	CB-CG-ND1	-11.80	105.00	122.70
1	A	136	LEU	O-C-N	-11.80	106.90	122.59
2	D	1	MET	CA-C-N	11.80	144.07	121.54
2	D	1	MET	C-N-CA	11.80	144.07	121.54
1	A	43	PHE	CG-CD1-CE1	11.79	140.74	120.70
2	B	39	ARG	NH1-CZ-NH2	11.79	134.63	119.30
1	A	88	ALA	CA-C-N	11.78	142.90	121.70
1	A	88	ALA	C-N-CA	11.78	142.90	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	57	ALA	N-CA-CB	-11.78	90.59	110.49
2	D	48	SER	N-CA-CB	11.78	130.39	110.49
2	D	40	PHE	CG-CD1-CE1	-11.77	100.69	120.70
1	C	101	LEU	N-CA-C	11.77	125.57	111.33
1	C	85	ASN	CB-CG-ND2	11.74	134.01	116.40
1	A	24	TYR	CA-C-N	11.73	144.40	121.41
1	A	24	TYR	C-N-CA	11.73	144.40	121.41
2	D	38	GLN	CA-C-N	-11.72	103.27	120.38
2	D	38	GLN	C-N-CA	-11.72	103.27	120.38
1	A	43	PHE	N-CA-C	11.72	130.88	110.02
2	B	38	GLN	CA-CB-CG	11.71	137.53	114.10
2	B	101	ASN	O-C-N	11.69	138.10	122.43
2	D	131	LYS	O-C-N	11.69	139.01	122.41
1	A	6	ASN	OD1-CG-ND2	-11.68	110.92	122.60
2	B	52	ALA	CB-CA-C	11.68	133.66	110.42
1	C	116	ASN	O-C-N	11.68	137.10	121.92
1	A	43	PHE	CA-C-N	-11.68	105.24	119.84
1	A	43	PHE	C-N-CA	-11.68	105.24	119.84
2	B	73	GLY	CA-C-O	-11.65	100.30	120.57
1	C	46	PHE	O-C-N	-11.64	109.71	123.10
2	D	44	PHE	N-CA-C	11.64	135.59	110.80
2	B	113	VAL	CA-CB-CG1	-11.61	90.66	110.40
2	D	44	PHE	O-C-N	-11.61	107.14	122.59
1	C	64	ASN	CB-CG-ND2	-11.61	98.98	116.40
2	D	40	PHE	O-C-N	11.61	136.22	122.17
2	B	143	LYS	N-CA-C	-11.60	86.09	110.80
2	B	44	PHE	CA-C-N	-11.59	98.69	121.41
2	B	44	PHE	C-N-CA	-11.59	98.69	121.41
1	C	86	LEU	CD1-CG-CD2	-11.59	85.29	110.80
2	D	85	ALA	CA-C-N	11.59	143.67	121.54
2	D	85	ALA	C-N-CA	11.59	143.67	121.54
1	A	107	VAL	N-CA-CB	11.59	130.35	111.23
2	B	123	PRO	N-CA-C	-11.59	98.39	113.57
1	A	115	THR	N-CA-CB	11.58	128.14	110.42
2	D	46	ASN	CA-C-O	-11.58	103.95	120.51
2	D	134	ALA	O-C-N	-11.57	107.20	122.59
2	B	80	LEU	CD1-CG-CD2	-11.57	85.34	110.80
1	A	138	SER	CB-CA-C	11.56	133.43	110.42
2	B	114	ALA	CB-CA-C	-11.56	89.24	110.63
1	C	33	PHE	N-CA-CB	-11.56	93.05	110.16
1	C	70	GLN	CA-C-N	11.55	142.49	121.70
1	C	70	GLN	C-N-CA	11.55	142.49	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	HIS	CE1-NE2-CD2	11.55	120.55	109.00
2	D	89	GLY	N-CA-C	-11.55	85.81	113.18
1	C	123	ALA	N-CA-CB	11.54	129.99	110.49
1	A	44	PRO	CB-CA-C	11.53	130.59	111.56
1	C	100	LEU	N-CA-CB	11.53	128.12	110.14
1	A	92	ARG	CA-C-O	11.53	135.64	122.27
2	D	26	ALA	N-CA-CB	11.52	126.69	109.98
1	A	141	ARG	NH1-CZ-NH2	-11.52	104.33	119.30
2	D	74	LEU	CA-C-N	11.51	143.53	121.54
2	D	74	LEU	C-N-CA	11.51	143.53	121.54
1	A	136	LEU	N-CA-C	11.51	135.31	110.80
1	A	107	VAL	O-C-N	-11.50	108.19	122.57
1	C	112	HIS	N-CA-C	-11.50	97.39	112.68
1	C	45	HIS	CA-C-O	11.50	136.95	120.51
2	D	49	SER	CA-C-N	11.50	136.13	120.38
2	D	49	SER	C-N-CA	11.50	136.13	120.38
2	B	44	PHE	CB-CG-CD2	11.49	140.24	120.70
2	B	129	PHE	CD1-CG-CD2	11.49	135.84	118.60
2	B	33	VAL	CA-CB-CG1	11.49	129.93	110.40
2	D	33	VAL	CG1-CB-CG2	11.49	136.07	110.80
2	B	25	GLN	CG-CD-NE2	-11.48	99.18	116.40
1	C	94	ASN	N-CA-C	-11.48	96.40	109.60
1	C	128	PHE	CA-C-O	-11.48	104.09	120.51
2	D	107	ASN	CA-CB-CG	11.47	124.07	112.60
1	A	32	MET	CB-CG-SD	11.47	147.10	112.70
1	C	76	LEU	O-C-N	11.46	134.50	121.32
2	D	97	VAL	CA-CB-CG2	11.45	129.87	110.40
2	D	3	THR	CA-C-O	11.44	136.88	120.51
2	D	123	PRO	CA-C-N	11.44	143.40	121.54
2	D	123	PRO	C-N-CA	11.44	143.40	121.54
2	B	84	PHE	CE1-CZ-CE2	-11.43	99.42	120.00
1	C	100	LEU	N-CA-C	-11.43	94.07	111.56
1	A	7	LYS	N-CA-C	-11.42	97.09	111.02
1	A	131	ASN	CA-C-N	11.42	143.35	121.54
1	A	131	ASN	C-N-CA	11.42	143.35	121.54
2	D	60	LYS	O-C-N	-11.41	107.41	122.59
1	A	118	THR	OG1-CB-CG2	-11.41	86.48	109.30
2	B	116	ASN	CB-CG-ND2	11.39	133.49	116.40
1	C	94	ASN	OD1-CG-ND2	-11.39	111.21	122.60
2	B	78	ASP	N-CA-CB	-11.38	91.15	110.50
1	C	9	ASN	CB-CG-ND2	11.38	133.48	116.40
1	A	107	VAL	CA-CB-CG1	11.38	129.75	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	67	THR	CA-CB-OG1	-11.38	92.54	109.60
2	D	2	LEU	CB-CA-C	-11.37	87.79	110.42
2	B	104	LEU	CA-C-O	-11.37	104.25	120.51
2	D	139	ALA	CB-CA-C	-11.37	87.80	110.42
1	A	105	LEU	CD1-CG-CD2	-11.36	85.80	110.80
1	C	3	SER	CA-CB-OG	-11.36	88.37	111.10
1	C	129	LEU	CB-CG-CD1	11.36	144.79	110.70
1	C	24	TYR	CE1-CZ-CE2	-11.36	97.59	120.30
1	A	108	THR	N-CA-C	-11.35	86.63	110.80
1	A	36	PHE	O-C-N	-11.34	108.28	121.32
2	B	42	GLN	CA-CB-CG	11.33	136.76	114.10
1	C	95	PRO	CA-N-CD	-11.33	96.14	112.00
2	D	143	LYS	CB-CG-CD	11.32	137.34	111.30
1	C	24	TYR	CG-CD1-CE1	11.32	138.18	121.20
1	C	49	SER	CB-CA-C	11.32	131.60	110.10
1	C	33	PHE	CB-CA-C	11.31	130.08	110.85
2	B	93	ASN	N-CA-C	11.31	134.89	110.80
2	B	29	ARG	N-CA-C	11.30	126.21	111.75
2	D	17	VAL	CA-CB-CG1	-11.29	91.20	110.40
1	C	37	PRO	CA-CB-CG	11.28	125.94	104.50
1	C	50	HIS	CG-ND1-CE1	11.28	128.48	109.30
1	C	24	TYR	CB-CG-CD1	11.28	137.71	120.80
2	B	139	ALA	N-CA-C	11.27	126.18	111.75
2	B	64	LYS	N-CA-C	-11.25	86.83	110.80
2	B	76	HIS	CA-C-O	-11.24	104.43	120.51
2	B	38	GLN	CG-CD-OE1	-11.22	98.36	120.80
1	C	1	VAL	CA-CB-CG2	11.22	129.47	110.40
1	A	124	ASN	CA-C-O	-11.21	109.22	121.00
2	D	132	VAL	CA-CB-CG2	11.21	129.45	110.40
1	C	4	ALA	O-C-N	-11.21	107.19	122.20
1	C	41	THR	CA-CB-CG2	11.19	129.53	110.50
1	C	49	SER	CA-C-N	11.18	141.83	121.70
1	C	49	SER	C-N-CA	11.18	141.83	121.70
2	B	122	THR	OG1-CB-CG2	11.18	131.66	109.30
2	B	62	HIS	CA-C-N	11.17	140.67	120.79
2	B	62	HIS	C-N-CA	11.17	140.67	120.79
2	B	120	GLN	N-CA-C	-11.16	99.16	113.12
2	D	75	LYS	CA-C-O	-11.16	104.55	120.51
1	C	10	VAL	CA-C-N	11.16	135.81	120.63
1	C	10	VAL	C-N-CA	11.16	135.81	120.63
2	B	13	PHE	CE1-CZ-CE2	11.16	140.09	120.00
1	C	41	THR	CB-CA-C	11.16	131.12	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	70	GLN	CG-CD-OE1	11.14	143.08	120.80
2	D	16	LYS	CA-C-O	-11.12	104.60	120.51
1	A	140	TYR	CB-CG-CD1	-11.12	104.12	120.80
1	C	124	ASN	CA-CB-CG	-11.12	101.48	112.60
1	A	36	PHE	CA-C-O	11.11	135.38	120.16
1	C	83	LEU	O-C-N	11.11	137.36	122.59
1	C	86	LEU	CB-CA-C	-11.11	89.00	110.10
2	B	121	PHE	CA-C-O	-11.10	108.97	122.41
2	B	88	SER	N-CA-CB	11.10	129.25	110.49
2	B	40	PHE	CB-CA-C	11.10	133.18	109.99
2	B	64	LYS	CB-CA-C	11.10	132.50	110.42
1	C	29	LEU	CA-C-O	-11.08	108.68	120.42
1	C	28	ALA	N-CA-CB	-11.07	93.72	110.33
2	B	35	PRO	CA-C-O	11.07	140.74	120.60
2	D	88	SER	CA-C-N	11.07	143.10	121.41
2	D	88	SER	C-N-CA	11.07	143.10	121.41
2	D	86	GLN	CA-C-O	-11.06	104.69	120.51
2	B	124	ASN	OD1-CG-ND2	-11.06	111.54	122.60
2	D	102	PHE	O-C-N	11.05	133.97	122.03
1	A	10	VAL	CA-CB-CG1	11.05	129.18	110.40
2	D	131	LYS	N-CA-CB	-11.04	93.12	110.46
1	A	64	ASN	CA-C-O	11.04	132.25	120.55
1	A	118	THR	N-CA-C	11.03	134.19	109.81
1	A	97	ASN	OD1-CG-ND2	-11.03	111.57	122.60
2	B	144	TYR	CB-CG-CD1	11.03	137.34	120.80
1	C	61	LYS	CA-C-N	11.03	141.82	121.97
1	C	61	LYS	C-N-CA	11.03	141.82	121.97
1	C	26	ALA	N-CA-CB	11.02	128.46	109.72
2	D	35	PRO	CB-CA-C	11.01	130.65	112.26
2	D	96	HIS	O-C-N	11.01	137.24	122.59
1	C	37	PRO	CA-C-O	11.01	140.64	120.60
2	B	77	LEU	CB-CG-CD1	-10.99	77.74	110.70
1	A	29	LEU	CB-CG-CD1	10.98	143.63	110.70
2	B	109	LEU	CA-C-N	-10.97	104.48	120.28
2	B	109	LEU	C-N-CA	-10.97	104.48	120.28
2	B	34	TYR	CA-C-O	-10.95	105.16	120.16
1	C	8	SER	N-CA-CB	10.94	128.99	110.49
1	C	141	ARG	N-CA-CB	10.94	129.10	110.50
2	D	22	VAL	CA-CB-CG2	10.94	129.00	110.40
1	A	40	LYS	CA-C-N	10.94	140.04	122.11
1	A	40	LYS	C-N-CA	10.94	140.04	122.11
2	D	94	LYS	O-C-N	10.93	134.19	122.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	89	HIS	CB-CG-CD2	-10.92	117.00	131.20
2	B	48	SER	CB-CA-C	10.92	128.71	111.13
1	C	50	HIS	ND1-CG-CD2	-10.92	95.18	106.10
2	D	13	PHE	CG-CD2-CE2	10.91	139.25	120.70
2	B	76	HIS	CG-ND1-CE1	-10.90	90.76	109.30
2	D	2	LEU	CB-CG-CD2	10.90	143.39	110.70
1	C	126	ASN	CA-C-N	10.89	137.16	120.82
1	C	126	ASN	C-N-CA	10.89	137.16	120.82
1	A	121	VAL	CA-C-N	10.89	134.87	120.28
1	A	121	VAL	C-N-CA	10.89	134.87	120.28
1	C	17	VAL	N-CA-CB	10.89	129.20	111.23
1	C	17	VAL	CA-CB-CG2	10.88	128.90	110.40
1	C	133	SER	N-CA-CB	10.88	128.88	110.49
1	C	117	PHE	O-C-N	10.88	136.97	122.61
1	C	107	VAL	N-CA-C	-10.87	86.72	109.34
1	A	112	HIS	CE1-NE2-CD2	10.87	119.87	109.00
1	C	117	PHE	CG-CD1-CE1	10.87	139.17	120.70
1	C	77	PRO	N-CD-CG	-10.86	86.91	103.20
1	A	76	LEU	CA-C-N	-10.85	106.28	119.84
1	A	76	LEU	C-N-CA	-10.85	106.28	119.84
2	B	2	LEU	N-CA-CB	10.85	128.82	110.49
2	B	126	GLN	CB-CG-CD	-10.84	94.17	112.60
1	C	90	LYS	O-C-N	10.84	136.77	122.03
2	B	54	MET	N-CA-CB	-10.84	94.12	110.16
1	A	122	HIS	CG-CD2-NE2	-10.84	96.36	107.20
1	C	33	PHE	N-CA-C	-10.83	99.55	111.36
1	A	24	TYR	CB-CG-CD2	10.83	137.04	120.80
1	A	17	VAL	N-CA-CB	10.82	129.09	111.23
1	A	77	PRO	N-CD-CG	-10.82	86.97	103.20
1	A	43	PHE	CA-C-O	10.81	134.28	120.87
1	A	109	LEU	N-CA-CB	10.81	128.76	110.49
2	D	69	ALA	N-CA-CB	10.81	125.69	109.91
2	D	39	ARG	O-C-N	10.81	134.52	122.20
2	B	55	ASN	N-CA-C	10.80	123.14	111.36
2	B	100	GLN	N-CA-C	-10.80	97.30	111.24
2	D	84	PHE	CA-C-N	-10.80	105.81	120.28
2	D	84	PHE	C-N-CA	-10.80	105.81	120.28
2	B	143	LYS	CA-C-O	-10.79	105.08	120.51
1	C	110	ALA	N-CA-C	-10.79	80.80	111.00
1	A	27	GLN	CG-CD-NE2	10.78	132.57	116.40
2	D	13	PHE	CZ-CE2-CD2	-10.78	100.60	120.00
1	C	46	PHE	CB-CG-CD1	-10.78	102.38	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	145	HIS	N-CA-CB	10.78	128.82	110.50
1	C	96	VAL	CA-CB-CG1	10.77	128.71	110.40
2	B	103	ARG	CB-CA-C	-10.77	91.00	110.70
2	B	121	PHE	CB-CG-CD2	10.76	139.00	120.70
1	C	139	LYS	CG-CD-CE	10.76	136.05	111.30
1	A	64	ASN	CA-CB-CG	10.75	123.35	112.60
2	B	45	GLY	N-CA-C	-10.75	87.71	113.18
1	A	103	HIS	CE1-NE2-CD2	10.73	119.73	109.00
1	C	128	PHE	CD1-CG-CD2	-10.73	102.50	118.60
1	A	44	PRO	N-CA-CB	-10.73	91.98	103.25
1	A	32	MET	O-C-N	10.71	137.62	122.41
2	B	14	TRP	CD1-CG-CD2	-10.71	89.17	106.30
2	B	120	GLN	O-C-N	-10.70	106.58	122.20
2	D	36	TRP	CB-CG-CD2	10.69	141.76	126.80
1	A	72	HIS	CE1-NE2-CD2	10.68	119.68	109.00
1	C	70	GLN	CB-CA-C	-10.68	80.55	110.14
2	B	98	ASN	CB-CG-OD1	-10.68	99.44	120.80
1	C	95	PRO	CB-CA-C	-10.67	96.10	111.68
2	D	95	LEU	CB-CA-C	-10.66	89.25	109.72
1	A	2	LEU	CD1-CG-CD2	-10.65	87.37	110.80
1	C	121	VAL	CA-C-N	-10.64	104.84	120.38
1	C	121	VAL	C-N-CA	-10.64	104.84	120.38
1	C	35	SER	CA-C-N	10.64	147.76	121.80
1	C	35	SER	C-N-CA	10.64	147.76	121.80
1	C	37	PRO	N-CA-CB	-10.63	92.08	103.25
2	B	87	LEU	CD1-CG-CD2	-10.62	87.43	110.80
2	B	29	ARG	CA-C-O	-10.61	108.31	120.20
1	A	104	SER	N-CA-CB	10.60	125.70	110.12
1	C	32	MET	CA-C-N	10.58	135.32	120.29
1	C	32	MET	C-N-CA	10.58	135.32	120.29
1	A	25	GLY	CA-C-N	-10.58	101.31	120.99
1	A	25	GLY	C-N-CA	-10.58	101.31	120.99
2	B	19	VAL	CA-C-O	-10.57	107.57	120.78
2	D	29	ARG	CA-CB-CG	10.57	135.24	114.10
2	D	62	HIS	CG-CD2-NE2	-10.57	96.63	107.20
1	A	6	ASN	O-C-N	10.56	136.64	122.59
1	C	84	SER	CA-CB-OG	-10.56	89.98	111.10
2	B	74	LEU	CB-CA-C	-10.56	89.41	110.42
2	B	133	VAL	O-C-N	10.55	132.70	121.83
1	C	62	VAL	CB-CA-C	10.55	128.59	111.29
1	A	103	HIS	O-C-N	-10.54	111.06	122.03
2	B	131	LYS	CA-C-O	10.54	132.07	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	81	LYS	CA-C-O	-10.54	102.88	120.80
2	D	94	LYS	CA-C-N	-10.53	102.47	122.06
2	D	94	LYS	C-N-CA	-10.53	102.47	122.06
1	A	112	HIS	CB-CG-CD2	10.53	144.89	131.20
1	C	132	ASP	N-CA-C	-10.53	99.80	111.28
2	B	90	LEU	CA-C-N	10.51	134.11	120.44
2	B	90	LEU	C-N-CA	10.51	134.11	120.44
1	C	54	GLN	O-C-N	10.50	135.88	122.23
1	A	123	ALA	N-CA-CB	-10.49	94.56	110.20
1	A	126	ASN	N-CA-C	-10.48	98.53	111.11
2	B	7	LYS	O-C-N	10.48	136.53	122.59
2	B	104	LEU	CB-CA-C	10.48	131.27	110.42
1	A	5	ALA	CA-C-N	10.48	141.55	121.54
1	A	5	ALA	C-N-CA	10.48	141.55	121.54
1	C	122	HIS	CA-C-N	10.48	141.55	121.54
1	C	122	HIS	C-N-CA	10.48	141.55	121.54
2	D	107	ASN	CB-CA-C	10.47	127.45	110.90
1	A	33	PHE	CG-CD1-CE1	10.47	138.50	120.70
2	B	36	TRP	O-C-N	10.47	135.84	122.23
2	D	53	VAL	CB-CA-C	-10.46	99.52	111.55
1	C	64	ASN	CA-C-N	10.46	134.66	120.54
1	C	64	ASN	C-N-CA	10.46	134.66	120.54
2	D	29	ARG	CB-CG-CD	10.46	135.35	111.30
2	B	13	PHE	CG-CD1-CE1	10.45	138.46	120.70
2	B	42	GLN	CG-CD-NE2	10.44	132.06	116.40
2	D	115	ARG	NH1-CZ-NH2	-10.44	105.73	119.30
2	D	91	HIS	N-CA-C	-10.43	97.02	112.04
1	C	77	PRO	N-CA-C	10.42	128.91	113.81
1	C	138	SER	CA-C-N	10.41	141.43	121.54
1	C	138	SER	C-N-CA	10.41	141.43	121.54
2	D	42	GLN	N-CA-C	10.41	127.26	113.72
2	D	126	GLN	CA-C-O	10.41	131.42	120.70
2	D	133	VAL	N-CA-C	10.40	122.48	110.62
1	C	92	ARG	N-CA-CB	10.40	128.79	112.46
2	D	60	LYS	CA-C-N	10.40	141.40	121.54
2	D	60	LYS	C-N-CA	10.40	141.40	121.54
1	A	99	LYS	O-C-N	-10.39	108.77	122.59
1	A	109	LEU	CA-CB-CG	10.39	152.68	116.30
1	C	140	TYR	CE1-CZ-CE2	-10.37	99.56	120.30
2	B	77	LEU	CD1-CG-CD2	10.37	133.61	110.80
1	A	46	PHE	CD1-CE1-CZ	-10.37	101.34	120.00
1	A	136	LEU	CB-CA-C	-10.36	89.81	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	87	LEU	O-C-N	-10.36	110.94	122.34
1	A	64	ASN	N-CA-CB	10.34	125.31	110.12
1	C	31	ARG	CA-C-O	-10.32	105.75	120.51
1	C	33	PHE	CE1-CZ-CE2	-10.32	101.43	120.00
2	D	9	ALA	CA-C-N	10.31	140.53	121.97
2	D	9	ALA	C-N-CA	10.31	140.53	121.97
2	B	106	GLY	CA-C-O	10.31	130.97	120.45
1	A	17	VAL	CA-C-O	10.31	133.66	120.78
1	A	50	HIS	CB-CA-C	10.30	130.93	110.42
2	B	115	ARG	N-CA-C	-10.30	99.47	113.18
1	C	72	HIS	CE1-NE2-CD2	-10.30	98.70	109.00
1	A	122	HIS	O-C-N	10.30	133.04	122.12
2	B	33	VAL	N-CA-CB	10.29	128.22	111.23
1	C	83	LEU	N-CA-C	10.28	132.69	110.80
2	D	76	HIS	CA-C-N	10.28	138.16	120.58
2	D	76	HIS	C-N-CA	10.28	138.16	120.58
1	A	45	HIS	N-CA-C	10.27	124.91	112.38
1	C	128	PHE	CB-CG-CD2	10.27	138.16	120.70
1	A	42	TYR	CE1-CZ-CE2	-10.27	99.76	120.30
2	D	41	PHE	CB-CG-CD2	-10.27	103.25	120.70
2	B	91	HIS	N-CA-CB	10.26	124.88	110.01
2	B	22	VAL	CA-C-O	-10.26	109.17	120.25
2	D	36	TRP	CD1-CG-CD2	-10.26	89.89	106.30
2	B	124	ASN	CB-CA-C	-10.25	91.94	110.70
1	A	106	LEU	CB-CG-CD1	10.24	141.42	110.70
2	B	133	VAL	N-CA-C	-10.24	100.38	110.72
2	D	119	GLY	CA-C-N	10.24	141.10	121.54
2	D	119	GLY	C-N-CA	10.24	141.10	121.54
1	C	72	HIS	CG-CD2-NE2	-10.23	96.97	107.20
2	B	145	HIS	ND1-CE1-NE2	10.23	118.63	108.40
1	C	62	VAL	CA-C-O	-10.23	107.99	120.78
2	D	50	ALA	N-CA-CB	10.23	125.40	110.06
2	B	44	PHE	CE1-CZ-CE2	-10.22	101.61	120.00
2	B	136	VAL	N-CA-CB	10.22	122.90	110.64
1	A	58	HIS	ND1-CE1-NE2	-10.21	98.19	108.40
2	B	83	ALA	N-CA-CB	-10.21	93.23	110.49
1	A	47	ASP	N-CA-C	-10.21	89.05	110.80
1	A	97	ASN	CA-CB-CG	-10.21	102.39	112.60
2	D	125	VAL	N-CA-CB	-10.21	94.39	111.23
2	B	48	SER	CA-CB-OG	-10.20	90.70	111.10
2	B	87	LEU	CA-C-N	10.20	141.02	121.54
2	B	87	LEU	C-N-CA	10.20	141.02	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	111	LEU	CA-C-O	-10.19	108.25	119.97
1	C	8	SER	CA-C-O	10.18	135.07	120.51
1	C	87	HIS	CG-ND1-CE1	-10.18	91.99	109.30
2	B	36	TRP	CZ3-CH2-CZ2	10.18	134.74	121.50
2	D	14	TRP	CZ3-CH2-CZ2	10.18	134.74	121.50
2	D	6	GLU	CA-C-O	-10.18	105.96	120.51
2	D	100	GLN	CA-C-N	-10.18	105.53	120.38
2	D	100	GLN	C-N-CA	-10.18	105.53	120.38
1	C	48	LEU	N-CA-C	-10.16	89.15	110.80
1	C	131	ASN	O-C-N	-10.16	107.36	122.20
2	D	110	ALA	CA-C-N	10.16	143.74	121.80
2	D	110	ALA	C-N-CA	10.16	143.74	121.80
1	A	20	ASN	CB-CA-C	10.16	130.09	109.67
2	B	100	GLN	CA-C-O	-10.16	110.14	120.80
1	C	104	SER	N-CA-C	-10.15	99.91	110.97
1	C	101	LEU	CB-CA-C	10.14	127.92	110.68
1	A	99	LYS	CA-CB-CG	-10.14	93.82	114.10
1	A	66	LEU	CA-C-O	10.14	135.00	120.51
1	C	4	ALA	CA-C-O	10.13	133.12	120.65
2	D	80	LEU	CA-C-N	-10.13	104.31	120.63
2	D	80	LEU	C-N-CA	-10.13	104.31	120.63
2	D	93	ASN	CA-C-N	-10.14	107.62	121.71
2	D	93	ASN	C-N-CA	-10.14	107.62	121.71
2	B	3	THR	N-CA-CB	-10.13	95.87	110.36
2	B	34	TYR	O-C-N	-10.13	109.67	121.32
1	A	27	GLN	CA-C-N	10.13	140.88	121.54
1	A	27	GLN	C-N-CA	10.13	140.88	121.54
2	B	46	ASN	OD1-CG-ND2	10.13	132.73	122.60
1	A	111	SER	N-CA-CB	10.12	127.60	110.49
1	A	33	PHE	CD1-CG-CD2	-10.12	103.42	118.60
1	C	118	THR	N-CA-CB	10.12	128.38	110.37
2	B	5	GLU	O-C-N	-10.11	108.51	122.46
1	C	67	THR	CB-CA-C	10.11	126.53	110.96
2	B	144	TYR	CG-CD1-CE1	10.10	136.35	121.20
1	C	126	ASN	CB-CG-ND2	10.10	131.55	116.40
2	B	109	LEU	CA-CB-CG	10.10	151.65	116.30
1	A	52	SER	CA-CB-OG	-10.10	90.91	111.10
2	B	17	VAL	N-CA-CB	10.09	127.88	111.23
2	D	17	VAL	O-C-N	-10.09	109.96	122.57
2	D	98	ASN	CA-CB-CG	-10.08	102.52	112.60
1	C	98	PHE	N-CA-CB	-10.07	92.60	109.72
1	C	116	ASN	CA-CB-CG	-10.07	102.53	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	13	ALA	CA-C-O	-10.06	106.12	120.51
2	D	36	TRP	NE1-CE2-CD2	10.06	120.48	107.40
1	C	11	LYS	CG-CD-CE	10.06	134.43	111.30
2	D	44	PHE	CE1-CZ-CE2	10.06	138.10	120.00
1	C	69	ALA	CA-C-O	10.05	131.46	120.20
1	A	24	TYR	N-CA-C	-10.05	91.07	110.56
1	A	44	PRO	CA-CB-CG	10.05	123.59	104.50
2	B	66	VAL	N-CA-CB	10.04	127.80	111.23
2	B	84	PHE	CA-C-O	-10.03	109.68	120.92
2	D	32	VAL	N-CA-C	-10.02	100.60	110.72
2	D	30	LEU	CD1-CG-CD2	10.02	132.83	110.80
1	A	87	HIS	CE1-NE2-CD2	10.01	119.01	109.00
1	A	45	HIS	CG-ND1-CE1	10.00	126.31	109.30
1	C	74	ASN	CB-CA-C	-10.00	90.52	110.42
1	C	50	HIS	O-C-N	9.99	138.99	123.00
2	D	103	ARG	CA-C-N	9.99	134.03	120.44
2	D	103	ARG	C-N-CA	9.99	134.03	120.44
1	A	74	ASN	OD1-CG-ND2	-9.99	112.61	122.60
2	B	66	VAL	CG1-CB-CG2	-9.97	88.86	110.80
1	A	3	SER	O-C-N	-9.96	110.61	123.16
1	C	58	HIS	CB-CG-CD2	-9.96	118.26	131.20
1	C	75	ASP	CA-CB-CG	9.95	122.55	112.60
1	A	36	PHE	CA-C-N	9.95	132.28	119.84
1	A	36	PHE	C-N-CA	9.95	132.28	119.84
2	B	126	GLN	CG-CD-OE1	9.95	140.70	120.80
1	C	82	ASN	CB-CG-ND2	9.95	131.33	116.40
1	A	106	LEU	N-CA-C	-9.95	101.35	113.19
2	D	29	ARG	CD-NE-CZ	-9.95	110.48	124.40
1	C	90	LYS	CA-C-N	-9.94	106.93	120.44
1	C	90	LYS	C-N-CA	-9.94	106.93	120.44
1	C	97	ASN	N-CA-C	9.94	123.14	111.71
1	A	9	ASN	CB-CG-OD1	-9.93	100.94	120.80
2	D	71	THR	OG1-CB-CG2	-9.93	89.43	109.30
1	C	69	ALA	O-C-N	-9.93	110.88	122.20
1	A	23	ALA	CA-C-N	9.93	135.51	121.71
1	A	23	ALA	C-N-CA	9.93	135.51	121.71
1	C	27	GLN	CA-C-N	-9.93	103.26	121.52
1	C	27	GLN	C-N-CA	-9.93	103.26	121.52
2	D	25	GLN	CA-CB-CG	-9.93	94.25	114.10
1	A	94	ASN	CB-CG-OD1	-9.92	100.96	120.80
2	D	109	LEU	CB-CG-CD1	9.92	140.46	110.70
2	B	47	LEU	CA-CB-CG	9.91	151.00	116.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	117	PHE	N-CA-CB	9.91	126.15	110.49
1	A	92	ARG	N-CA-C	9.91	125.14	111.17
1	A	34	LEU	CB-CG-CD1	-9.90	80.98	110.70
1	C	10	VAL	CA-CB-CG2	9.90	127.24	110.40
1	C	128	PHE	N-CA-C	-9.90	89.71	110.80
2	B	118	GLY	O-C-N	9.90	135.57	122.70
2	D	141	ALA	N-CA-C	-9.90	101.13	113.01
2	B	126	GLN	CA-C-N	9.90	140.45	121.54
2	B	126	GLN	C-N-CA	9.90	140.45	121.54
1	C	137	THR	CA-CB-CG2	9.89	127.31	110.50
2	D	22	VAL	N-CA-C	9.89	120.52	110.23
2	D	108	VAL	O-C-N	-9.89	112.20	121.89
1	C	90	LYS	N-CA-C	-9.88	99.79	112.93
2	D	59	VAL	CB-CA-C	-9.88	95.09	111.29
1	A	122	HIS	ND1-CG-CD2	9.87	115.97	106.10
1	A	67	THR	O-C-N	9.86	135.64	122.43
1	A	34	LEU	N-CA-C	-9.85	100.11	114.39
1	C	72	HIS	CB-CG-ND1	9.85	137.47	122.70
1	C	75	ASP	CB-CA-C	-9.85	90.82	110.42
2	D	34	TYR	N-CA-C	-9.83	87.43	108.66
1	C	54	GLN	CB-CG-CD	9.81	129.27	112.60
1	C	92	ARG	CB-CA-C	-9.81	98.29	111.63
1	A	79	THR	N-CA-C	9.81	121.73	111.14
1	A	45	HIS	ND1-CG-CD2	-9.80	96.30	106.10
2	B	53	VAL	CA-C-O	-9.80	109.96	120.64
2	D	57	PRO	CA-CB-CG	-9.80	85.88	104.50
1	C	34	LEU	CB-CG-CD1	9.79	140.09	110.70
2	B	94	LYS	CB-CG-CD	-9.79	88.78	111.30
2	D	63	GLY	CA-C-N	9.79	140.24	121.54
2	D	63	GLY	C-N-CA	9.79	140.24	121.54
1	C	47	ASP	OD1-CG-OD2	9.78	146.36	122.90
2	B	60	LYS	CD-CE-NZ	-9.77	80.63	111.90
1	C	98	PHE	CZ-CE2-CD2	9.77	137.59	120.00
2	D	142	HIS	CG-ND1-CE1	9.77	125.91	109.30
1	C	105	LEU	N-CA-C	-9.77	99.67	111.69
2	D	143	LYS	N-CA-CB	-9.76	93.99	110.49
2	D	20	ASP	CA-C-O	-9.75	106.57	120.51
1	C	117	PHE	CB-CA-C	9.75	126.72	111.91
2	D	34	TYR	CG-CD1-CE1	9.75	135.82	121.20
1	A	103	HIS	CG-ND1-CE1	9.73	125.85	109.30
2	B	30	LEU	N-CA-CB	9.73	125.65	109.78
2	D	145	HIS	CG-CD2-NE2	-9.73	97.47	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	ASN	CA-C-O	-9.72	107.89	119.27
2	B	13	PHE	N-CA-C	-9.72	100.68	112.54
1	A	46	PHE	CB-CG-CD1	-9.71	104.19	120.70
2	B	117	PHE	CE1-CZ-CE2	-9.71	102.51	120.00
1	C	78	GLY	N-CA-C	-9.72	90.15	113.18
2	B	4	ALA	CA-C-N	9.71	138.13	121.14
2	B	4	ALA	C-N-CA	9.71	138.13	121.14
1	A	46	PHE	O-C-N	-9.71	114.57	123.50
1	C	103	HIS	O-C-N	-9.70	111.14	122.20
2	B	26	ALA	N-CA-C	-9.70	100.70	111.28
1	C	74	ASN	CA-C-N	9.70	140.07	121.54
1	C	74	ASN	C-N-CA	9.70	140.07	121.54
2	B	72	GLN	N-CA-CB	9.70	126.88	110.49
1	A	41	THR	CB-CA-C	-9.70	92.78	109.07
2	B	81	LYS	CA-C-N	9.69	140.40	121.41
2	B	81	LYS	C-N-CA	9.69	140.40	121.41
2	B	82	GLY	O-C-N	9.69	135.30	122.70
1	C	45	HIS	CB-CG-CD2	-9.69	118.61	131.20
1	A	30	GLN	CA-C-O	9.69	134.36	120.51
1	A	62	VAL	N-CA-CB	9.68	127.21	111.23
2	B	55	ASN	CA-CB-CG	9.68	122.28	112.60
2	D	20	ASP	N-CA-CB	9.68	126.85	110.49
2	B	80	LEU	CB-CG-CD1	9.68	139.74	110.70
1	A	76	LEU	O-C-N	-9.68	111.36	120.55
1	A	26	ALA	N-CA-C	9.67	124.47	112.87
2	B	75	LYS	CG-CD-CE	-9.66	89.07	111.30
1	A	138	SER	N-CA-C	-9.66	90.22	110.80
1	C	83	LEU	CB-CG-CD1	9.65	139.66	110.70
2	B	133	VAL	CA-CB-CG2	9.65	126.81	110.40
1	A	3	SER	N-CA-CB	-9.64	95.42	110.85
1	A	129	LEU	CA-C-N	9.63	136.51	121.19
1	A	129	LEU	C-N-CA	9.63	136.51	121.19
1	A	112	HIS	N-CA-C	9.63	122.99	111.82
2	B	130	GLN	CB-CA-C	9.62	126.72	110.74
1	A	73	LEU	O-C-N	-9.62	110.31	122.82
1	C	130	ALA	CA-C-O	-9.62	106.76	120.51
1	A	98	PHE	CB-CG-CD1	-9.62	104.36	120.70
1	A	6	ASN	CB-CA-C	9.61	129.55	110.42
1	C	61	LYS	N-CA-C	-9.60	90.34	110.80
1	C	80	LEU	CA-CB-CG	9.60	149.90	116.30
2	B	43	HIS	N-CA-C	-9.60	84.12	111.00
2	D	131	LYS	CD-CE-NZ	-9.60	81.18	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	PHE	CD1-CG-CD2	-9.59	104.21	118.60
1	A	36	PHE	CE1-CZ-CE2	-9.59	102.73	120.00
2	B	62	HIS	O-C-N	-9.59	109.83	122.59
2	D	56	ASN	CB-CG-ND2	9.59	130.79	116.40
1	C	67	THR	OG1-CB-CG2	-9.58	90.13	109.30
2	D	84	PHE	N-CA-C	9.58	125.00	111.30
1	C	31	ARG	CB-CA-C	9.57	129.47	110.42
1	C	45	HIS	CE1-NE2-CD2	9.57	118.57	109.00
2	D	98	ASN	N-CA-C	9.56	130.95	109.81
2	D	7	LYS	CG-CD-CE	9.56	133.28	111.30
1	A	99	LYS	CD-CE-NZ	9.55	142.45	111.90
1	C	42	TYR	CA-C-O	-9.55	106.89	119.11
1	A	75	ASP	O-C-N	9.54	133.82	121.99
2	B	142	HIS	CG-CD2-NE2	-9.54	97.66	107.20
1	C	43	PHE	C-N-CD	9.54	164.12	125.00
2	D	12	GLY	CA-C-N	-9.53	107.54	120.79
2	D	12	GLY	C-N-CA	-9.53	107.54	120.79
2	B	124	ASN	CA-C-N	-9.53	104.67	120.30
2	B	124	ASN	C-N-CA	-9.53	104.67	120.30
1	C	30	GLN	CG-CD-NE2	9.53	130.69	116.40
1	C	40	LYS	CA-C-N	9.52	136.86	120.58
1	C	40	LYS	C-N-CA	9.52	136.86	120.58
2	B	58	LYS	N-CA-C	9.52	121.42	111.14
1	A	93	VAL	CA-CB-CG2	9.51	126.57	110.40
2	B	126	GLN	CG-CD-NE2	9.51	130.67	116.40
2	D	75	LYS	CB-CA-C	-9.50	91.51	110.42
1	C	41	THR	CA-C-N	9.49	140.09	121.58
1	C	41	THR	C-N-CA	9.49	140.09	121.58
2	D	133	VAL	CB-CA-C	9.49	124.47	112.04
1	A	47	ASP	CB-CG-OD1	9.48	140.20	118.40
1	A	12	ALA	N-CA-C	9.48	130.98	110.80
1	A	87	HIS	CB-CG-ND1	-9.47	108.49	122.70
1	C	113	LEU	CB-CA-C	9.47	129.48	111.29
1	C	86	LEU	CA-C-O	9.47	136.90	120.80
2	D	58	LYS	CB-CA-C	9.47	129.26	110.42
1	A	25	GLY	CA-C-O	9.47	137.04	120.57
2	B	60	LYS	CA-C-N	9.47	139.62	121.54
2	B	60	LYS	C-N-CA	9.47	139.62	121.54
1	A	68	LYS	CA-C-N	9.46	133.73	120.29
1	A	68	LYS	C-N-CA	9.46	133.73	120.29
1	C	43	PHE	CB-CG-CD2	9.46	136.78	120.70
1	C	122	HIS	CB-CG-ND1	-9.45	108.53	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	129	LEU	N-CA-CB	9.45	123.96	110.07
1	A	77	PRO	N-CA-C	-9.44	93.02	112.47
1	A	103	HIS	CA-C-N	9.43	132.92	120.28
1	A	103	HIS	C-N-CA	9.43	132.92	120.28
2	D	19	VAL	N-CA-CB	9.42	126.77	111.23
2	B	144	TYR	CA-CB-CG	-9.42	96.94	113.90
2	B	131	LYS	CD-CE-NZ	-9.42	81.76	111.90
2	B	133	VAL	CA-CB-CG1	9.42	126.41	110.40
2	D	116	ASN	CA-C-N	9.42	137.29	122.60
2	D	116	ASN	C-N-CA	9.42	137.29	122.60
2	D	122	THR	N-CA-C	9.42	130.62	109.81
1	A	113	LEU	N-CA-CB	-9.41	94.61	110.90
2	B	18	ASP	CA-C-O	-9.41	107.05	120.51
2	B	100	GLN	CG-CD-NE2	9.41	130.52	116.40
1	A	35	SER	O-C-N	-9.41	111.35	122.27
2	B	43	HIS	CA-C-O	-9.41	104.81	120.80
1	C	123	ALA	O-C-N	9.41	135.10	122.59
2	D	128	LEU	CA-CB-CG	9.40	149.21	116.30
1	C	102	SER	CA-CB-OG	-9.39	92.32	111.10
2	B	132	VAL	CA-CB-CG1	9.39	126.36	110.40
1	A	95	PRO	N-CD-CG	-9.38	89.13	103.20
2	B	35	PRO	CA-C-N	9.38	136.63	120.58
2	B	35	PRO	C-N-CA	9.38	136.63	120.58
2	D	112	VAL	CA-CB-CG2	9.38	126.35	110.40
1	A	4	ALA	N-CA-C	9.38	123.82	112.38
2	D	104	LEU	CA-C-N	9.38	138.16	121.66
2	D	104	LEU	C-N-CA	9.38	138.16	121.66
2	D	35	PRO	CA-C-N	9.38	133.78	120.28
2	D	35	PRO	C-N-CA	9.38	133.78	120.28
1	A	97	ASN	N-CA-CB	9.37	125.60	110.42
2	D	110	ALA	N-CA-C	-9.37	90.84	110.80
2	B	141	ALA	O-C-N	-9.36	111.12	122.25
1	C	11	LYS	CD-CE-NZ	9.35	141.83	111.90
2	B	58	LYS	CA-C-O	9.35	130.33	120.70
2	B	29	ARG	CD-NE-CZ	-9.35	111.31	124.40
2	D	46	ASN	CB-CA-C	9.34	129.01	110.42
2	D	117	PHE	O-C-N	-9.34	111.13	122.25
2	B	64	LYS	CG-CD-CE	-9.34	89.82	111.30
2	B	19	VAL	CG1-CB-CG2	9.34	131.34	110.80
1	A	124	ASN	CB-CA-C	9.33	125.33	110.96
2	B	4	ALA	CB-CA-C	9.33	127.63	109.72
2	B	62	HIS	CB-CG-CD2	-9.33	119.07	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	THR	N-CA-CB	9.33	125.87	110.39
1	C	20	ASN	N-CA-CB	9.33	123.34	110.10
2	D	23	GLY	CA-C-O	-9.33	111.66	120.80
1	C	58	HIS	CA-C-O	-9.32	110.54	120.42
2	D	15	GLY	N-CA-C	-9.32	91.08	113.18
1	C	42	TYR	CA-C-N	9.32	134.43	123.15
1	C	42	TYR	C-N-CA	9.32	134.43	123.15
1	A	8	SER	N-CA-CB	-9.32	95.03	110.22
2	B	63	GLY	N-CA-C	9.31	125.42	114.16
2	B	110	ALA	N-CA-C	9.31	122.42	111.71
1	A	123	ALA	O-C-N	-9.31	110.13	122.23
2	B	120	GLN	N-CA-CB	9.31	124.66	110.42
2	B	80	LEU	CA-C-O	9.30	136.61	120.80
2	D	11	THR	N-CA-C	-9.29	98.95	110.65
1	C	30	GLN	O-C-N	-9.28	109.89	122.33
2	D	56	ASN	N-CA-CB	9.28	126.88	110.37
1	A	30	GLN	CB-CA-C	9.27	128.87	110.42
2	B	99	PRO	CB-CA-C	-9.27	97.45	111.44
1	C	52	SER	O-C-N	9.26	134.32	123.30
1	C	124	ASN	CA-C-N	9.26	139.22	121.54
1	C	124	ASN	C-N-CA	9.26	139.22	121.54
2	D	115	ARG	N-CA-CB	-9.26	93.70	110.27
2	B	17	VAL	CG1-CB-CG2	9.26	131.16	110.80
1	A	104	SER	N-CA-C	-9.25	101.20	111.28
1	C	130	ALA	CA-C-N	9.25	140.28	122.53
1	C	130	ALA	C-N-CA	9.25	140.28	122.53
2	B	129	PHE	O-C-N	-9.24	111.61	122.15
2	D	123	PRO	CB-CG-CD	9.23	135.65	106.10
1	C	109	LEU	CA-C-O	9.23	133.71	120.51
2	D	1	MET	CA-CB-CG	9.23	132.56	114.10
2	D	58	LYS	CG-CD-CE	9.23	132.53	111.30
2	B	58	LYS	CA-C-N	9.23	133.52	120.42
2	B	58	LYS	C-N-CA	9.23	133.52	120.42
2	B	108	VAL	CA-CB-CG2	-9.23	94.72	110.40
2	B	6	GLU	CA-C-N	9.22	139.16	121.54
2	B	6	GLU	C-N-CA	9.22	139.16	121.54
1	A	116	ASN	CB-CA-C	9.22	128.26	109.55
1	A	48	LEU	CA-C-N	9.21	139.14	121.54
1	A	48	LEU	C-N-CA	9.21	139.14	121.54
1	A	98	PHE	CA-C-O	-9.21	109.42	120.56
2	B	78	ASP	CA-CB-CG	-9.21	103.39	112.60
1	A	40	LYS	CB-CA-C	-9.20	92.11	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	28	GLY	CA-C-O	-9.19	104.57	120.57
1	A	107	VAL	CA-CB-CG2	9.19	126.02	110.40
2	D	113	VAL	N-CA-CB	9.19	121.67	110.64
2	D	109	LEU	CA-C-N	9.19	139.08	121.54
2	D	109	LEU	C-N-CA	9.19	139.08	121.54
2	B	44	PHE	CB-CG-CD1	-9.18	105.09	120.70
2	D	124	ASN	O-C-N	9.18	134.80	122.59
1	A	1	VAL	CG1-CB-CG2	-9.18	90.61	110.80
2	D	84	PHE	CB-CA-C	-9.17	95.77	111.46
1	A	86	LEU	O-C-N	9.16	134.77	122.59
1	C	17	VAL	O-C-N	9.16	134.02	122.57
1	C	114	PRO	O-C-N	9.15	134.99	122.64
2	B	98	ASN	CA-C-O	9.14	128.83	120.60
1	C	128	PHE	CZ-CE2-CD2	-9.14	103.55	120.00
1	C	27	GLN	N-CA-C	9.13	123.52	112.38
2	D	29	ARG	N-CA-CB	-9.13	96.59	110.20
2	B	124	ASN	CB-CG-ND2	9.12	130.09	116.40
2	D	34	TYR	N-CA-CB	-9.12	95.15	110.38
1	C	82	ASN	CB-CG-OD1	-9.11	102.58	120.80
2	B	125	VAL	CA-CB-CG2	9.10	125.87	110.40
1	C	48	LEU	CB-CG-CD2	-9.09	83.44	110.70
2	D	34	TYR	CG-CD2-CE2	9.09	134.83	121.20
2	B	83	ALA	N-CA-C	-9.07	91.47	110.80
1	C	22	PRO	CB-CG-CD	-9.07	77.06	106.10
1	A	36	PHE	CB-CG-CD1	9.07	136.12	120.70
1	A	30	GLN	CB-CG-CD	9.07	128.01	112.60
2	B	90	LEU	O-C-N	9.07	131.78	122.08
1	C	68	LYS	CB-CA-C	-9.07	92.38	110.42
2	B	41	PHE	CE1-CZ-CE2	-9.06	103.69	120.00
1	C	130	ALA	N-CA-CB	-9.06	95.18	110.49
2	D	25	GLN	CB-CG-CD	-9.06	97.20	112.60
1	C	37	PRO	CA-N-CD	-9.05	99.32	112.00
2	B	107	ASN	CA-CB-CG	-9.05	103.55	112.60
2	B	136	VAL	CA-C-N	9.05	138.83	121.54
2	B	136	VAL	C-N-CA	9.05	138.83	121.54
2	B	33	VAL	N-CA-C	-9.04	90.53	109.34
2	D	95	LEU	CA-C-N	9.04	138.82	121.54
2	D	95	LEU	C-N-CA	9.04	138.82	121.54
1	A	45	HIS	CA-CB-CG	-9.04	104.76	113.80
2	B	128	LEU	O-C-N	9.04	134.44	122.33
1	A	96	VAL	CA-CB-CG1	-9.04	95.04	110.40
2	D	133	VAL	CA-C-O	9.03	130.44	121.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	THR	CA-C-O	9.03	130.71	119.78
2	B	11	THR	N-CA-C	9.03	121.12	111.28
1	C	67	THR	CA-C-N	9.03	138.78	121.54
1	C	67	THR	C-N-CA	9.03	138.78	121.54
1	C	68	LYS	CA-CB-CG	-9.03	96.04	114.10
2	D	67	LEU	CD1-CG-CD2	-9.03	90.94	110.80
2	D	47	LEU	CB-CA-C	9.02	125.26	111.18
2	D	135	GLY	CA-C-N	9.02	134.98	120.55
2	D	135	GLY	C-N-CA	9.02	134.98	120.55
2	B	34	TYR	CD1-CG-CD2	-9.01	104.58	118.10
1	A	138	SER	O-C-N	9.01	134.57	122.59
1	A	70	GLN	CA-C-O	9.01	129.97	120.70
2	B	86	GLN	CA-CB-CG	-9.00	96.10	114.10
2	D	77	LEU	CB-CA-C	9.00	127.17	110.70
2	B	20	ASP	CB-CG-OD1	-9.00	97.70	118.40
2	B	29	ARG	CB-CG-CD	9.00	132.00	111.30
1	C	50	HIS	CB-CG-CD2	9.00	142.89	131.20
2	B	128	LEU	N-CA-CB	-8.99	96.45	110.30
1	C	88	ALA	N-CA-CB	8.99	125.68	110.49
1	C	11	LYS	CB-CA-C	8.99	124.88	110.95
2	D	131	LYS	CB-CA-C	-8.99	92.47	109.72
1	C	38	THR	CA-C-N	8.98	138.77	122.06
1	C	38	THR	C-N-CA	8.98	138.77	122.06
1	C	56	LYS	CA-C-N	8.98	138.70	121.54
1	C	56	LYS	C-N-CA	8.98	138.70	121.54
1	C	64	ASN	N-CA-C	8.98	129.92	110.80
2	D	14	TRP	CA-CB-CG	-8.98	96.54	113.60
1	C	31	ARG	CA-C-N	-8.97	106.19	120.63
1	C	31	ARG	C-N-CA	-8.97	106.19	120.63
2	D	76	HIS	O-C-N	-8.97	112.17	122.93
2	D	52	ALA	CA-C-O	-8.96	110.76	121.34
1	C	125	LEU	N-CA-CB	8.96	125.63	110.49
2	B	42	GLN	CB-CG-CD	8.96	127.83	112.60
2	D	90	LEU	CB-CG-CD1	-8.95	83.84	110.70
2	B	56	ASN	CA-C-O	-8.95	107.89	120.16
1	C	97	ASN	N-CA-CB	8.95	124.01	110.22
1	C	137	THR	CA-C-N	8.95	138.63	121.54
1	C	137	THR	C-N-CA	8.95	138.63	121.54
2	D	79	ASP	CB-CA-C	-8.95	93.42	112.12
1	C	105	LEU	N-CA-CB	-8.94	96.88	110.20
1	C	118	THR	CA-CB-OG1	8.94	123.01	109.60
2	B	99	PRO	CA-C-N	8.94	135.36	120.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	99	PRO	C-N-CA	8.94	135.36	120.88
2	D	64	LYS	CA-C-O	8.94	133.29	120.51
1	C	11	LYS	O-C-N	-8.93	112.39	122.03
1	C	97	ASN	CB-CA-C	-8.93	94.12	110.63
1	A	33	PHE	CA-C-N	8.92	135.63	121.98
1	A	33	PHE	C-N-CA	8.92	135.63	121.98
2	B	71	THR	CA-C-O	8.92	133.79	122.64
2	D	91	HIS	CA-CB-CG	-8.92	104.88	113.80
2	D	39	ARG	N-CA-C	8.90	123.14	111.75
1	A	76	LEU	N-CA-CB	-8.89	93.27	110.08
1	A	110	ALA	CA-C-N	8.88	138.50	121.54
1	A	110	ALA	C-N-CA	8.88	138.50	121.54
2	B	34	TYR	CE1-CZ-CE2	8.88	138.05	120.30
2	B	134	ALA	CA-C-O	8.88	130.86	120.92
1	A	11	LYS	CG-CD-CE	8.87	131.71	111.30
1	C	137	THR	CA-CB-OG1	-8.87	96.29	109.60
2	D	136	VAL	N-CA-C	-8.87	101.33	111.00
1	C	89	HIS	N-CA-C	8.87	123.89	112.89
1	C	73	LEU	O-C-N	-8.86	110.80	122.59
1	C	90	LYS	CB-CG-CD	8.86	131.67	111.30
1	C	53	ALA	O-C-N	-8.85	110.66	122.43
2	B	52	ALA	CA-C-O	8.84	133.16	120.51
2	B	17	VAL	CB-CA-C	-8.84	96.79	111.29
2	B	74	LEU	N-CA-C	8.84	129.63	110.80
2	D	3	THR	O-C-N	8.84	134.35	122.59
2	D	96	HIS	CA-CB-CG	-8.84	104.96	113.80
1	A	96	VAL	CB-CA-C	-8.84	96.80	111.29
1	C	1	VAL	CA-C-N	-8.84	109.13	122.74
1	C	1	VAL	C-N-CA	-8.84	109.13	122.74
2	D	71	THR	N-CA-C	8.83	135.72	111.00
2	B	100	GLN	CA-C-N	-8.82	105.98	120.72
2	B	100	GLN	C-N-CA	-8.82	105.98	120.72
1	A	74	ASN	CA-C-N	-8.81	106.50	122.54
1	A	74	ASN	C-N-CA	-8.81	106.50	122.54
2	D	37	THR	N-CA-CB	-8.81	95.42	109.78
1	C	21	ALA	CA-C-N	-8.81	108.83	119.84
1	C	21	ALA	C-N-CA	-8.81	108.83	119.84
2	D	144	TYR	OH-CZ-CE2	-8.81	93.48	119.90
1	C	32	MET	N-CA-C	8.81	123.79	112.34
1	A	71	GLY	O-C-N	-8.80	111.26	122.70
1	A	119	PRO	CB-CG-CD	8.80	134.27	106.10
1	C	64	ASN	OD1-CG-ND2	8.80	131.40	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	87	LEU	CB-CG-CD1	8.79	137.08	110.70
1	A	92	ARG	CG-CD-NE	-8.79	92.66	112.00
2	D	13	PHE	CD1-CE1-CZ	-8.79	104.18	120.00
1	C	56	LYS	N-CA-CB	8.79	125.34	110.49
2	D	85	ALA	CB-CA-C	8.79	125.38	110.79
1	A	87	HIS	ND1-CE1-NE2	8.79	117.19	108.40
1	A	83	LEU	CA-CB-CG	8.78	147.03	116.30
2	D	69	ALA	CB-CA-C	-8.78	97.44	110.96
2	D	131	LYS	CG-CD-CE	-8.78	91.11	111.30
1	C	85	ASN	CB-CA-C	-8.77	95.06	109.53
1	A	85	ASN	CB-CA-C	-8.77	92.97	110.42
2	B	129	PHE	CB-CG-CD2	8.77	135.61	120.70
1	C	117	PHE	CB-CG-CD1	8.77	135.60	120.70
2	D	35	PRO	CA-CB-CG	-8.77	87.84	104.50
2	B	56	ASN	OD1-CG-ND2	-8.76	113.84	122.60
2	B	113	VAL	CG1-CB-CG2	-8.76	91.52	110.80
2	D	1	MET	CB-CG-SD	-8.76	86.42	112.70
2	D	14	TRP	CB-CG-CD1	-8.76	113.76	126.90
2	D	105	LEU	CB-CG-CD2	8.75	136.96	110.70
2	D	117	PHE	CD1-CG-CD2	8.75	131.72	118.60
1	C	140	TYR	N-CA-CB	-8.74	95.48	111.13
2	D	67	LEU	N-CA-CB	8.73	122.96	110.12
2	B	71	THR	N-CA-CB	-8.72	97.44	110.60
2	D	74	LEU	CB-CA-C	8.71	125.25	110.79
1	C	120	ALA	CA-C-O	8.71	130.10	119.31
1	A	48	LEU	CB-CG-CD2	8.70	136.79	110.70
1	A	69	ALA	O-C-N	-8.70	112.23	122.15
1	C	17	VAL	CG1-CB-CG2	-8.70	91.67	110.80
2	D	121	PHE	CA-C-O	8.69	132.94	120.51
2	D	42	GLN	CG-CD-OE1	8.68	138.16	120.80
2	B	11	THR	OG1-CB-CG2	-8.67	91.96	109.30
2	D	37	THR	N-CA-C	8.67	125.67	111.37
2	B	85	ALA	O-C-N	-8.66	111.06	122.59
2	B	2	LEU	CA-C-N	-8.66	105.21	120.97
2	B	2	LEU	C-N-CA	-8.66	105.21	120.97
2	D	62	HIS	CB-CG-ND1	-8.66	109.71	122.70
2	D	92	CYS	CA-CB-SG	-8.66	94.48	114.40
2	D	4	ALA	CA-C-O	8.66	130.32	120.54
2	D	56	ASN	CA-CB-CG	-8.65	103.95	112.60
2	B	95	LEU	N-CA-C	-8.65	92.37	110.80
2	D	43	HIS	CE1-NE2-CD2	8.65	117.65	109.00
2	B	94	LYS	N-CA-C	-8.64	100.23	113.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	143	LYS	O-C-N	-8.64	111.09	122.59
2	B	130	GLN	O-C-N	8.64	132.05	122.11
1	A	126	ASN	CB-CA-C	-8.64	96.99	110.81
1	C	14	TRP	CA-C-O	-8.64	111.30	120.63
1	C	85	ASN	CB-CG-OD1	-8.64	103.52	120.80
1	A	139	LYS	CG-CD-CE	8.62	131.13	111.30
1	C	40	LYS	N-CA-CB	8.62	126.01	110.32
1	A	84	SER	CB-CA-C	-8.61	94.13	110.67
1	A	11	LYS	CA-CB-CG	-8.61	96.88	114.10
2	B	36	TRP	CE2-CD2-CE3	8.61	127.41	118.80
1	A	121	VAL	CB-CA-C	-8.59	97.20	111.29
2	D	85	ALA	N-CA-CB	-8.59	97.49	110.12
1	C	31	ARG	CB-CG-CD	-8.58	91.57	111.30
1	A	81	SER	N-CA-CB	8.58	122.68	110.07
2	D	44	PHE	CB-CA-C	-8.58	93.35	110.42
1	A	75	ASP	CA-CB-CG	8.57	121.17	112.60
2	B	3	THR	CA-C-O	8.57	131.81	121.87
2	B	17	VAL	CA-CB-CG2	-8.57	95.83	110.40
2	B	96	HIS	CG-CD2-NE2	8.56	115.76	107.20
1	A	23	ALA	N-CA-CB	8.56	123.46	110.19
1	A	47	ASP	CB-CA-C	-8.56	93.38	110.42
1	A	48	LEU	N-CA-CB	8.56	124.18	110.22
1	C	97	ASN	O-C-N	8.56	132.24	122.22
1	A	4	ALA	CA-C-O	-8.55	109.14	119.49
1	C	89	HIS	ND1-CG-CD2	8.55	114.65	106.10
1	A	31	ARG	O-C-N	-8.55	111.22	122.59
1	C	96	VAL	CB-CA-C	8.55	125.31	111.29
1	A	96	VAL	CA-C-O	-8.54	110.11	120.78
2	B	127	ALA	O-C-N	8.54	133.94	122.59
1	C	75	ASP	N-CA-C	8.53	128.97	110.80
2	B	27	LEU	N-CA-CB	8.52	122.43	110.07
2	D	63	GLY	N-CA-C	-8.52	92.98	113.18
2	B	2	LEU	CA-C-O	-8.52	108.33	120.51
1	A	66	LEU	CB-CG-CD1	-8.51	85.18	110.70
2	B	122	THR	C-N-CD	-8.51	90.12	125.00
2	B	41	PHE	N-CA-C	8.50	124.97	107.37
2	D	55	ASN	CB-CA-C	-8.50	97.87	110.96
2	B	65	ARG	N-CA-C	-8.50	102.10	111.36
2	D	139	ALA	CA-C-O	-8.50	108.36	120.51
1	A	111	SER	CB-CA-C	-8.49	93.52	110.42
2	D	14	TRP	CH2-CZ2-CE2	-8.49	106.46	117.50
2	D	55	ASN	CB-CG-ND2	8.49	129.14	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	42	GLN	CB-CA-C	-8.49	95.28	109.55
1	A	32	MET	N-CA-C	-8.49	102.92	113.28
1	C	129	LEU	CB-CA-C	8.48	124.85	110.86
2	D	101	ASN	N-CA-CB	8.47	123.53	110.14
2	D	100	GLN	CB-CG-CD	8.47	127.00	112.60
1	A	58	HIS	CE1-NE2-CD2	8.47	117.47	109.00
2	D	84	PHE	CG-CD1-CE1	-8.47	106.31	120.70
2	B	108	VAL	N-CA-C	8.46	118.48	110.53
1	C	104	SER	CA-CB-OG	-8.45	94.19	111.10
1	A	21	ALA	O-C-N	-8.45	112.96	120.48
2	D	18	ASP	CA-C-N	-8.45	106.76	121.97
2	D	18	ASP	C-N-CA	-8.45	106.76	121.97
2	B	109	LEU	CD1-CG-CD2	8.45	129.39	110.80
1	C	112	HIS	CB-CA-C	8.45	124.35	110.24
2	B	107	ASN	OD1-CG-ND2	8.43	131.03	122.60
1	A	48	LEU	CB-CG-CD1	-8.43	85.42	110.70
1	C	93	VAL	CA-CB-CG2	8.43	124.73	110.40
1	C	133	SER	CA-C-O	-8.43	108.46	120.51
2	D	68	ASP	CB-CG-OD1	8.43	137.79	118.40
1	A	60	GLN	CA-C-O	8.43	132.56	120.51
2	D	70	PHE	CG-CD1-CE1	8.42	135.02	120.70
1	C	69	ALA	N-CA-CB	8.42	123.45	110.14
1	A	33	PHE	CB-CA-C	8.42	124.99	110.68
2	B	145	HIS	CG-ND1-CE1	-8.41	95.00	109.30
1	C	79	THR	CB-CA-C	-8.41	96.83	110.79
2	D	62	HIS	CA-C-N	8.40	137.88	121.41
2	D	62	HIS	C-N-CA	8.40	137.88	121.41
1	A	29	LEU	N-CA-CB	-8.40	96.29	110.49
1	A	22	PRO	N-CA-C	8.40	125.98	113.81
2	B	51	GLY	N-CA-C	-8.39	93.30	113.18
2	B	43	HIS	CA-C-N	-8.38	105.53	121.54
2	B	43	HIS	C-N-CA	-8.38	105.53	121.54
1	C	72	HIS	CA-CB-CG	-8.38	105.42	113.80
2	B	126	GLN	CA-CB-CG	8.38	130.85	114.10
1	C	24	TYR	CD1-CE1-CZ	8.38	134.68	119.60
2	D	102	PHE	CE1-CZ-CE2	8.38	135.07	120.00
2	D	126	GLN	CG-CD-OE1	8.38	137.55	120.80
1	A	89	HIS	CB-CG-CD2	8.37	142.09	131.20
1	A	31	ARG	NE-CZ-NH2	8.37	126.73	119.20
1	A	131	ASN	CA-C-O	-8.37	112.08	120.70
2	B	95	LEU	O-C-N	-8.37	111.46	122.59
1	C	36	PHE	N-CA-C	8.37	128.30	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	126	ASN	CB-CG-OD1	8.36	137.51	120.80
2	B	101	ASN	CB-CG-ND2	-8.34	103.88	116.40
2	D	97	VAL	CA-CB-CG1	8.34	124.58	110.40
1	A	74	ASN	N-CA-C	-8.34	93.04	110.80
2	B	68	ASP	N-CA-CB	8.34	124.58	110.49
2	B	79	ASP	CB-CA-C	8.33	127.00	110.42
2	B	104	LEU	O-C-N	8.33	133.67	122.59
1	C	95	PRO	CA-CB-CG	8.33	120.33	104.50
2	B	60	LYS	O-C-N	-8.32	111.52	122.59
2	B	34	TYR	CG-CD2-CE2	8.32	133.69	121.20
2	D	121	PHE	CG-CD2-CE2	8.32	134.85	120.70
2	B	16	LYS	CA-CB-CG	8.31	130.73	114.10
1	A	73	LEU	CD1-CG-CD2	-8.31	92.52	110.80
2	B	29	ARG	O-C-N	-8.30	112.74	122.20
1	C	68	LYS	N-CA-CB	8.30	124.52	110.49
1	A	19	GLY	CA-C-O	8.30	129.55	119.10
2	B	22	VAL	N-CA-CB	8.29	126.63	110.95
1	A	68	LYS	N-CA-CB	-8.29	97.35	110.19
2	D	46	ASN	CA-C-N	-8.28	107.42	122.50
2	D	46	ASN	C-N-CA	-8.28	107.42	122.50
1	A	37	PRO	CA-N-CD	-8.27	100.43	112.00
1	C	44	PRO	N-CA-CB	8.26	111.92	103.25
1	A	39	THR	CA-CB-CG2	8.24	124.51	110.50
2	B	38	GLN	N-CA-CB	8.24	127.82	110.67
1	A	42	TYR	CD1-CE1-CZ	8.23	134.41	119.60
1	C	115	THR	O-C-N	8.23	133.20	122.42
1	C	73	LEU	CB-CG-CD2	-8.23	86.02	110.70
2	B	90	LEU	CB-CG-CD1	8.22	135.37	110.70
1	C	137	THR	N-CA-C	-8.22	93.29	110.80
1	A	95	PRO	CA-N-CD	-8.21	100.50	112.00
2	D	73	GLY	O-C-N	-8.21	112.02	122.70
1	C	93	VAL	CA-CB-CG1	-8.21	96.45	110.40
1	A	74	ASN	CB-CA-C	8.21	126.75	110.42
2	B	72	GLN	CG-CD-OE1	-8.21	104.39	120.80
1	C	17	VAL	CA-C-O	-8.21	110.52	120.78
2	B	86	GLN	CG-CD-NE2	-8.20	104.09	116.40
2	B	129	PHE	CD1-CE1-CZ	-8.20	105.23	120.00
1	C	136	LEU	N-CA-C	-8.20	102.38	112.38
2	D	135	GLY	N-CA-C	-8.20	102.82	112.83
2	B	69	ALA	N-CA-C	8.20	128.26	110.80
2	B	71	THR	OG1-CB-CG2	8.20	125.70	109.30
2	D	68	ASP	OD1-CG-OD2	-8.20	103.22	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	ASN	CA-CB-CG	8.20	120.80	112.60
1	C	101	LEU	N-CA-CB	-8.20	97.77	110.06
1	C	76	LEU	CB-CA-C	-8.19	94.03	110.17
1	A	32	MET	CA-C-O	-8.19	109.43	119.18
1	A	98	PHE	CB-CA-C	8.19	126.35	111.03
2	D	100	GLN	CG-CD-OE1	-8.19	104.42	120.80
2	B	50	ALA	N-CA-CB	8.19	122.88	110.19
1	C	134	THR	CA-CB-CG2	-8.18	96.59	110.50
2	D	138	ASN	CA-C-N	8.17	137.15	121.54
2	D	138	ASN	C-N-CA	8.17	137.15	121.54
1	A	114	PRO	N-CA-CB	-8.17	94.67	103.25
1	C	32	MET	CB-CG-SD	8.16	137.19	112.70
2	B	122	THR	O-C-N	-8.16	109.94	123.00
1	A	135	VAL	O-C-N	8.16	132.77	122.57
1	A	91	LEU	CB-CG-CD1	8.16	135.17	110.70
1	A	107	VAL	CB-CA-C	8.15	124.66	111.29
1	C	58	HIS	N-CA-CB	8.15	122.22	110.16
2	B	114	ALA	CA-C-N	8.15	145.21	122.15
2	B	114	ALA	C-N-CA	8.15	145.21	122.15
2	B	46	ASN	N-CA-C	8.14	128.13	110.80
2	D	36	TRP	CD2-CE2-CZ2	-8.14	114.26	122.40
1	A	60	GLN	CB-CA-C	8.13	126.61	110.42
2	B	57	PRO	CB-CG-CD	-8.12	80.10	106.10
2	B	81	LYS	N-CA-C	-8.12	88.26	111.00
2	B	87	LEU	N-CA-CB	8.12	123.64	110.40
1	C	48	LEU	N-CA-CB	8.12	124.20	110.49
2	B	127	ALA	CA-C-O	-8.11	108.91	120.51
1	C	106	LEU	O-C-N	-8.11	111.56	122.43
1	A	109	LEU	CA-C-O	8.11	132.10	120.51
2	D	40	PHE	CD1-CE1-CZ	8.11	134.59	120.00
1	C	114	PRO	CA-C-O	-8.10	105.86	120.60
1	C	127	LYS	N-CA-CB	8.09	122.97	109.78
1	A	82	ASN	O-C-N	8.09	133.35	122.59
2	B	125	VAL	O-C-N	8.09	130.94	121.80
2	B	2	LEU	O-C-N	8.09	133.35	122.59
2	B	123	PRO	CA-C-O	8.09	131.22	119.34
1	A	47	ASP	OD1-CG-OD2	-8.08	103.50	122.90
1	A	97	ASN	O-C-N	-8.08	110.43	122.39
2	B	82	GLY	N-CA-C	-8.08	94.03	113.18
2	D	117	PHE	CB-CA-C	8.07	124.36	110.72
1	A	46	PHE	CB-CA-C	-8.07	100.37	111.51
1	A	17	VAL	CA-CB-CG1	8.06	124.11	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	132	VAL	O-C-N	-8.05	112.50	122.57
2	D	22	VAL	CG1-CB-CG2	-8.05	93.08	110.80
2	D	40	PHE	N-CA-CB	8.05	122.05	110.13
2	B	27	LEU	CA-C-N	8.05	137.18	121.41
2	B	27	LEU	C-N-CA	8.05	137.18	121.41
2	D	44	PHE	CZ-CE2-CD2	-8.05	105.52	120.00
1	C	98	PHE	CG-CD1-CE1	-8.04	107.02	120.70
2	D	38	GLN	CA-C-O	-8.04	111.95	120.63
1	C	99	LYS	CA-C-O	-8.03	109.50	119.38
1	A	29	LEU	CD1-CG-CD2	-8.03	93.14	110.80
1	A	137	THR	CA-C-O	-8.02	110.39	118.97
2	D	84	PHE	CE1-CZ-CE2	8.02	134.44	120.00
2	B	35	PRO	CB-CA-C	-8.00	98.36	111.56
2	D	41	PHE	CA-CB-CG	-8.00	105.80	113.80
1	C	18	GLY	O-C-N	8.00	133.10	122.70
2	B	89	GLY	O-C-N	7.99	133.09	122.70
2	B	90	LEU	CA-C-O	-7.99	112.28	121.07
1	C	38	THR	OG1-CB-CG2	-7.99	93.32	109.30
2	B	145	HIS	CB-CG-ND1	7.98	134.67	122.70
1	C	124	ASN	CB-CA-C	7.98	126.30	110.42
2	B	1	MET	N-CA-C	-7.98	88.66	111.00
2	B	43	HIS	O-C-N	7.98	135.76	123.00
2	D	62	HIS	CG-ND1-CE1	-7.97	95.74	109.30
2	B	63	GLY	CA-C-O	7.97	128.91	119.50
2	B	132	VAL	CA-C-N	7.97	131.74	120.42
2	B	132	VAL	C-N-CA	7.97	131.74	120.42
1	C	31	ARG	CD-NE-CZ	7.96	135.55	124.40
2	D	142	HIS	CA-CB-CG	7.96	121.76	113.80
1	C	73	LEU	N-CA-CB	7.96	123.95	110.49
2	D	40	PHE	CG-CD2-CE2	-7.96	107.16	120.70
1	C	77	PRO	CA-C-N	-7.96	105.81	121.41
1	C	77	PRO	C-N-CA	-7.96	105.81	121.41
2	D	96	HIS	CA-C-O	-7.96	109.13	120.51
2	B	133	VAL	N-CA-CB	-7.95	98.65	110.58
1	A	55	GLN	N-CA-C	7.95	122.08	112.38
2	B	31	LEU	N-CA-CB	7.95	123.93	110.49
2	D	34	TYR	CD1-CE1-CZ	-7.95	105.30	119.60
1	A	140	TYR	CB-CA-C	7.94	126.22	110.42
1	C	55	GLN	CA-C-N	7.94	136.71	121.54
1	C	55	GLN	C-N-CA	7.94	136.71	121.54
2	B	25	GLN	CG-CD-OE1	7.94	136.68	120.80
2	D	16	LYS	CA-CB-CG	-7.93	98.24	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	83	ALA	O-C-N	7.93	131.79	122.20
1	C	55	GLN	CB-CA-C	7.92	123.42	110.90
1	C	38	THR	CA-CB-CG2	7.92	123.97	110.50
1	A	93	VAL	CA-C-O	7.92	133.79	121.36
2	B	4	ALA	N-CA-C	-7.92	103.62	113.28
2	B	49	SER	N-CA-CB	7.92	124.88	111.66
1	A	9	ASN	O-C-N	7.91	130.63	122.09
2	D	38	GLN	CG-CD-NE2	7.91	128.26	116.40
1	C	115	THR	CB-CA-C	7.90	123.39	109.65
2	B	54	MET	CA-C-O	-7.90	112.05	120.42
2	B	56	ASN	CB-CG-OD1	-7.89	105.01	120.80
1	C	81	SER	N-CA-C	-7.89	101.98	111.69
1	A	117	PHE	CB-CG-CD2	-7.89	107.29	120.70
1	A	9	ASN	N-CA-C	-7.89	102.62	111.14
1	A	118	THR	CA-C-O	-7.88	109.36	120.16
2	D	3	THR	N-CA-C	-7.88	94.01	110.80
1	C	47	ASP	CB-CG-OD1	-7.88	100.28	118.40
1	C	7	LYS	CB-CG-CD	7.88	129.41	111.30
2	D	70	PHE	N-CA-CB	-7.87	97.99	110.19
2	D	73	GLY	CA-C-O	-7.87	106.87	120.57
1	A	116	ASN	N-CA-C	-7.87	103.47	113.23
2	D	130	GLN	CA-C-O	7.87	128.89	120.55
2	B	25	GLN	N-CA-C	-7.87	98.85	111.04
1	C	125	LEU	CA-CB-CG	7.86	143.81	116.30
2	B	65	ARG	CD-NE-CZ	-7.85	113.41	124.40
2	B	52	ALA	O-C-N	7.84	133.02	122.59
1	C	58	HIS	CA-C-N	7.84	129.94	120.14
1	C	58	HIS	C-N-CA	7.84	129.94	120.14
2	D	40	PHE	CB-CG-CD1	-7.84	107.37	120.70
1	A	95	PRO	CA-CB-CG	-7.83	89.62	104.50
1	A	21	ALA	CA-C-O	7.83	126.40	118.73
2	B	93	ASN	CB-CG-OD1	7.82	136.43	120.80
1	A	42	TYR	N-CA-CB	7.82	123.70	110.49
1	A	14	TRP	NE1-CE2-CZ2	7.81	141.82	130.10
2	D	87	LEU	CA-C-O	7.81	127.44	118.77
1	A	105	LEU	CA-C-O	7.81	128.95	119.97
1	A	91	LEU	CB-CG-CD2	7.80	134.09	110.70
2	B	116	ASN	CA-C-O	-7.79	112.82	121.00
1	C	78	GLY	CA-C-N	-7.79	109.84	120.28
1	C	78	GLY	C-N-CA	-7.79	109.84	120.28
1	C	43	PHE	CB-CG-CD1	-7.78	107.47	120.70
1	A	62	VAL	N-CA-C	-7.78	93.15	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	ALA	N-CA-C	-7.78	100.83	112.04
1	C	24	TYR	CA-C-N	7.78	128.62	119.98
1	C	24	TYR	C-N-CA	7.78	128.62	119.98
1	C	104	SER	CA-C-N	7.78	133.88	120.58
1	C	104	SER	C-N-CA	7.78	133.88	120.58
1	A	98	PHE	CG-CD2-CE2	7.78	133.92	120.70
2	B	59	VAL	N-CA-CB	7.78	122.25	110.58
1	C	43	PHE	CA-CB-CG	7.77	121.57	113.80
2	D	33	VAL	N-CA-C	7.77	117.84	110.53
2	D	75	LYS	CA-CB-CG	7.77	129.64	114.10
2	B	34	TYR	CZ-CE2-CD2	-7.76	105.63	119.60
2	B	134	ALA	O-C-N	-7.76	113.18	122.11
1	A	140	TYR	CA-C-O	7.76	131.61	120.51
2	D	107	ASN	O-C-N	7.75	130.46	122.09
1	A	72	HIS	ND1-CG-CD2	7.75	113.85	106.10
2	B	2	LEU	CB-CA-C	-7.75	95.01	110.42
1	A	2	LEU	CB-CG-CD2	7.74	133.91	110.70
1	C	23	ALA	CA-C-N	7.74	136.31	121.54
1	C	23	ALA	C-N-CA	7.74	136.31	121.54
2	D	95	LEU	CB-CG-CD1	-7.73	87.52	110.70
1	C	76	LEU	N-CA-CB	7.73	124.12	110.37
2	B	16	LYS	CB-CG-CD	7.72	129.06	111.30
2	D	73	GLY	N-CA-C	-7.72	94.88	113.18
2	B	22	VAL	CA-CB-CG1	7.72	123.53	110.40
1	C	52	SER	N-CA-CB	7.72	123.65	110.68
1	C	98	PHE	N-CA-C	7.71	124.02	111.37
2	D	9	ALA	O-C-N	-7.71	112.34	122.59
1	C	133	SER	N-CA-C	-7.70	94.39	110.80
2	D	145	HIS	ND1-CG-CD2	7.70	113.80	106.10
2	B	121	PHE	O-C-N	-7.70	112.22	122.38
2	D	112	VAL	N-CA-CB	7.70	128.58	111.50
1	C	136	LEU	CA-C-N	7.69	136.23	121.54
1	C	136	LEU	C-N-CA	7.69	136.23	121.54
1	A	14	TRP	CA-C-O	7.69	131.50	120.51
1	A	56	LYS	CA-CB-CG	7.69	129.48	114.10
2	B	102	PHE	CB-CA-C	7.68	123.74	110.68
2	D	41	PHE	CD1-CG-CD2	7.68	130.13	118.60
2	D	106	GLY	CA-C-O	7.68	128.81	120.66
1	C	24	TYR	CB-CG-CD2	-7.68	109.28	120.80
1	A	44	PRO	N-CA-C	7.68	128.29	112.47
1	A	100	LEU	CB-CG-CD2	-7.68	87.66	110.70
1	C	74	ASN	CA-C-O	7.68	131.49	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	51	GLY	O-C-N	-7.68	112.72	122.70
2	B	24	ALA	CB-CA-C	7.66	123.71	110.68
2	B	72	GLN	CA-C-N	7.66	136.43	121.41
2	B	72	GLN	C-N-CA	7.66	136.43	121.41
1	C	46	PHE	N-CA-C	7.66	122.50	110.17
2	D	78	ASP	N-CA-C	-7.66	89.55	111.00
2	B	42	GLN	CB-CA-C	-7.65	97.31	110.09
2	B	7	LYS	N-CA-C	7.64	127.07	110.80
2	D	105	LEU	N-CA-CB	7.64	122.36	110.44
1	A	5	ALA	N-CA-CB	-7.64	98.87	110.33
2	D	99	PRO	N-CD-CG	-7.64	91.74	103.20
1	C	113	LEU	N-CA-CB	-7.63	99.99	111.21
2	B	3	THR	CA-C-N	-7.63	107.86	122.06
2	B	3	THR	C-N-CA	-7.63	107.86	122.06
2	D	79	ASP	OD1-CG-OD2	7.63	141.21	122.90
1	C	119	PRO	CB-CA-C	-7.62	100.04	112.62
2	B	22	VAL	O-C-N	7.62	132.25	121.82
1	A	105	LEU	CB-CG-CD2	7.61	133.53	110.70
2	B	133	VAL	CG1-CB-CG2	-7.61	94.06	110.80
2	D	78	ASP	O-C-N	7.61	135.18	123.00
1	C	125	LEU	O-C-N	-7.61	112.47	122.59
1	A	117	PHE	CB-CA-C	-7.60	100.82	112.07
2	B	130	GLN	CG-CD-NE2	-7.59	105.01	116.40
2	D	62	HIS	O-C-N	-7.59	112.49	122.59
2	D	99	PRO	N-CA-CB	-7.59	95.28	103.25
2	D	59	VAL	N-CA-C	-7.59	93.55	109.34
2	B	129	PHE	CA-CB-CG	7.59	121.39	113.80
2	D	5	GLU	CA-CB-CG	7.58	129.27	114.10
1	C	122	HIS	CE1-NE2-CD2	7.58	116.58	109.00
2	B	118	GLY	N-CA-C	7.58	131.14	113.18
2	D	84	PHE	CD1-CG-CD2	7.58	129.97	118.60
2	D	116	ASN	CB-CG-ND2	-7.57	105.05	116.40
1	C	103	HIS	N-CA-CB	-7.57	98.18	110.14
1	C	127	LYS	CB-CA-C	-7.57	98.18	110.74
1	C	104	SER	CB-CA-C	-7.57	99.31	110.96
1	A	53	ALA	CA-C-O	-7.56	109.69	120.51
1	C	32	MET	CG-SD-CE	7.55	117.52	100.90
1	C	106	LEU	CB-CG-CD2	-7.55	88.05	110.70
2	D	82	GLY	N-CA-C	-7.55	95.29	113.18
2	B	80	LEU	CA-CB-CG	7.54	142.71	116.30
2	D	54	MET	N-CA-C	-7.54	102.20	111.40
1	A	91	LEU	CA-C-O	-7.54	113.09	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	17	VAL	CA-C-N	7.53	128.39	121.31
1	A	17	VAL	C-N-CA	7.53	128.39	121.31
1	C	6	ASN	CB-CG-OD1	7.53	135.86	120.80
2	D	67	LEU	N-CA-C	-7.53	103.07	111.28
2	D	60	LYS	CG-CD-CE	7.53	128.62	111.30
2	D	124	ASN	CB-CA-C	-7.53	95.44	110.42
2	D	88	SER	N-CA-C	-7.53	99.03	110.70
1	A	128	PHE	CB-CG-CD1	-7.51	107.92	120.70
2	D	84	PHE	CA-CB-CG	-7.51	106.28	113.80
2	D	83	ALA	N-CA-C	-7.51	99.05	111.37
2	D	78	ASP	CB-CA-C	7.51	124.36	110.10
1	A	52	SER	CA-C-N	-7.50	107.21	121.54
1	A	52	SER	C-N-CA	-7.50	107.21	121.54
1	A	128	PHE	CB-CG-CD2	7.50	133.46	120.70
2	D	40	PHE	N-CA-C	7.50	120.55	111.40
1	C	34	LEU	O-C-N	-7.49	112.63	122.59
1	A	98	PHE	CA-C-N	7.49	135.84	121.54
1	A	98	PHE	C-N-CA	7.49	135.84	121.54
1	C	77	PRO	CA-C-O	7.48	131.46	119.64
1	C	2	LEU	CB-CG-CD2	-7.48	88.27	110.70
2	B	58	LYS	CB-CA-C	7.47	122.71	110.90
1	C	79	THR	CA-C-N	-7.47	110.48	122.66
1	C	79	THR	C-N-CA	-7.47	110.48	122.66
1	A	108	THR	CB-CA-C	7.47	125.29	110.42
1	C	93	VAL	CA-C-O	7.47	130.12	120.78
1	A	37	PRO	CA-C-O	-7.47	107.00	120.60
2	B	91	HIS	CG-ND1-CE1	7.47	122.00	109.30
1	C	57	ALA	CA-C-N	7.47	130.90	120.29
1	C	57	ALA	C-N-CA	7.47	130.90	120.29
2	D	120	GLN	CA-C-O	-7.47	109.83	120.51
1	C	52	SER	CA-C-N	-7.47	107.10	120.99
1	C	52	SER	C-N-CA	-7.47	107.10	120.99
2	B	50	ALA	CA-C-O	7.46	129.64	120.31
1	C	22	PRO	CB-CA-C	7.46	123.88	111.56
1	A	61	LYS	CG-CD-CE	7.46	128.46	111.30
2	D	48	SER	CA-CB-OG	7.46	126.02	111.10
2	B	64	LYS	CA-CB-CG	-7.45	99.19	114.10
2	D	116	ASN	CB-CG-OD1	-7.44	105.93	120.80
1	C	138	SER	N-CA-CB	-7.43	97.93	110.49
1	A	35	SER	CA-CB-OG	-7.43	96.24	111.10
1	A	87	HIS	O-C-N	7.41	130.09	122.09
2	B	65	ARG	CB-CA-C	-7.41	98.26	110.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	51	GLY	O-C-N	7.41	127.88	122.62
1	C	89	HIS	CA-C-N	-7.40	110.20	122.79
1	C	89	HIS	C-N-CA	-7.40	110.20	122.79
1	C	92	ARG	CG-CD-NE	-7.40	95.72	112.00
2	D	81	LYS	CB-CA-C	7.40	126.76	110.18
2	D	67	LEU	CA-C-N	7.39	130.19	120.28
2	D	67	LEU	C-N-CA	7.39	130.19	120.28
1	C	117	PHE	CD1-CE1-CZ	7.39	133.30	120.00
2	B	138	ASN	CB-CG-OD1	-7.39	106.03	120.80
1	C	16	LYS	CB-CA-C	7.38	124.21	110.70
1	A	119	PRO	N-CA-C	-7.38	103.27	113.53
2	B	37	THR	CA-C-N	7.38	147.43	122.20
2	B	37	THR	C-N-CA	7.38	147.43	122.20
2	B	3	THR	N-CA-C	-7.38	100.80	110.53
1	A	6	ASN	N-CA-C	-7.37	95.09	110.80
1	A	6	ASN	N-CA-CB	7.37	122.94	110.49
2	B	94	LYS	CG-CD-CE	-7.37	94.35	111.30
2	B	66	VAL	CA-C-N	7.37	135.61	121.54
2	B	66	VAL	C-N-CA	7.37	135.61	121.54
2	D	13	PHE	CA-C-O	-7.37	112.97	121.07
2	B	110	ALA	O-C-N	-7.36	113.60	122.22
1	C	65	ALA	N-CA-CB	7.36	120.91	109.94
1	C	101	LEU	O-C-N	-7.36	114.31	122.12
1	C	44	PRO	N-CD-CG	7.36	114.24	103.20
1	A	75	ASP	N-CA-CB	-7.35	101.36	111.65
2	D	27	LEU	CD1-CG-CD2	-7.34	94.64	110.80
2	D	145	HIS	CG-ND1-CE1	-7.34	96.82	109.30
1	A	135	VAL	CG1-CB-CG2	-7.34	94.65	110.80
1	C	131	ASN	CB-CA-C	-7.34	97.45	109.56
2	D	53	VAL	O-C-N	-7.34	110.57	122.16
2	B	97	VAL	CA-C-O	-7.33	113.11	121.98
2	B	1	MET	CG-SD-CE	-7.33	84.77	100.90
2	B	120	GLN	CA-CB-CG	-7.33	99.43	114.10
1	C	71	GLY	N-CA-C	-7.33	92.05	113.30
1	A	75	ASP	CA-C-O	-7.31	113.59	121.20
1	A	104	SER	CA-CB-OG	-7.29	96.51	111.10
2	B	14	TRP	CB-CG-CD2	-7.29	116.59	126.80
1	C	140	TYR	CA-C-O	7.29	129.35	120.60
2	D	111	LEU	CA-C-N	7.29	132.59	120.64
2	D	111	LEU	C-N-CA	7.29	132.59	120.64
1	C	75	ASP	CB-CG-OD1	-7.29	101.64	118.40
1	C	20	ASN	OD1-CG-ND2	-7.29	115.31	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	109	LEU	N-CA-CB	7.28	122.80	110.49
1	A	122	HIS	CA-C-O	-7.27	112.84	120.55
2	D	142	HIS	N-CA-C	-7.27	94.22	107.75
2	B	48	SER	N-CA-CB	7.27	123.09	111.17
1	A	125	LEU	CD1-CG-CD2	-7.27	94.81	110.80
2	D	104	LEU	N-CA-C	-7.27	103.29	111.14
2	D	137	ALA	CA-C-O	7.26	135.59	121.35
2	B	67	LEU	CB-CA-C	-7.26	95.97	110.42
2	B	144	TYR	OH-CZ-CE2	-7.26	98.12	119.90
1	C	87	HIS	CE1-NE2-CD2	-7.26	101.74	109.00
2	B	116	ASN	N-CA-C	-7.25	103.07	110.97
1	A	112	HIS	N-CA-CB	-7.24	99.05	110.28
2	B	47	LEU	CA-C-O	7.23	129.30	120.55
2	D	103	ARG	NH1-CZ-NH2	-7.23	109.90	119.30
2	D	134	ALA	N-CA-CB	7.23	122.70	110.49
1	C	40	LYS	CB-CA-C	-7.22	94.39	110.21
1	C	134	THR	N-CA-CB	-7.22	98.85	109.82
1	C	37	PRO	CB-CG-CD	-7.22	83.00	106.10
1	A	7	LYS	CA-C-O	-7.22	113.13	121.07
1	C	60	GLN	CA-CB-CG	-7.21	99.67	114.10
1	C	65	ALA	CB-CA-C	7.21	122.35	110.81
2	D	128	LEU	N-CA-CB	-7.21	98.30	110.49
2	B	30	LEU	CA-CB-CG	7.21	141.54	116.30
2	D	62	HIS	CB-CG-CD2	-7.21	121.83	131.20
2	B	22	VAL	CB-CA-C	7.21	123.91	112.16
2	B	35	PRO	N-CA-CB	7.21	110.82	103.25
2	D	19	VAL	CG1-CB-CG2	-7.21	94.94	110.80
1	A	101	LEU	CB-CG-CD2	-7.21	89.08	110.70
1	A	141	ARG	CA-CB-CG	-7.20	99.70	114.10
2	B	29	ARG	NH1-CZ-NH2	-7.20	109.94	119.30
1	A	1	VAL	CA-CB-CG2	-7.20	98.16	110.40
1	C	91	LEU	CB-CG-CD2	7.20	132.29	110.70
1	A	128	PHE	CD1-CE1-CZ	-7.19	107.05	120.00
2	D	44	PHE	CA-C-O	-7.19	110.23	120.51
2	D	140	LEU	CA-CB-CG	7.19	141.46	116.30
2	D	104	LEU	CA-C-O	7.18	128.10	120.70
1	A	90	LYS	N-CA-CB	7.18	120.64	109.94
2	D	14	TRP	CE3-CZ3-CH2	-7.18	111.76	121.10
2	B	19	VAL	CA-CB-CG2	-7.18	98.19	110.40
2	B	124	ASN	N-CA-CB	7.17	120.89	110.20
1	A	127	LYS	CA-CB-CG	7.17	128.45	114.10
1	A	68	LYS	CG-CD-CE	-7.17	94.82	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	83	ALA	CB-CA-C	-7.17	98.94	110.84
1	C	7	LYS	N-CA-C	7.16	126.04	110.80
2	B	103	ARG	O-C-N	-7.15	112.94	122.23
1	A	54	GLN	OE1-CD-NE2	7.15	129.75	122.60
2	B	25	GLN	CB-CA-C	-7.15	100.03	111.39
1	C	55	GLN	O-C-N	-7.15	114.37	122.09
1	A	30	GLN	O-C-N	-7.14	113.09	122.59
2	B	92	CYS	N-CA-C	-7.14	103.23	112.23
1	A	70	GLN	CG-CD-OE1	7.14	135.07	120.80
1	A	91	LEU	CA-C-N	7.14	132.96	122.82
1	A	91	LEU	C-N-CA	7.14	132.96	122.82
2	B	102	PHE	N-CA-C	7.13	119.96	111.33
1	A	119	PRO	CA-C-N	-7.13	110.74	120.44
1	A	119	PRO	C-N-CA	-7.13	110.74	120.44
2	D	72	GLN	CA-CB-CG	7.13	128.36	114.10
1	C	121	VAL	CA-CB-CG2	-7.12	98.29	110.40
1	A	81	SER	CB-CA-C	7.12	122.61	110.86
1	C	69	ALA	N-CA-C	-7.12	102.64	111.75
1	A	45	HIS	CB-CA-C	-7.12	95.30	110.32
2	D	136	VAL	O-C-N	-7.11	112.45	121.84
1	A	79	THR	OG1-CB-CG2	7.11	123.52	109.30
2	B	29	ARG	NE-CZ-NH2	-7.11	112.80	119.20
1	C	114	PRO	CA-C-N	-7.11	109.96	122.26
1	C	114	PRO	C-N-CA	-7.11	109.96	122.26
2	D	4	ALA	CB-CA-C	-7.11	98.14	109.80
2	B	36	TRP	CE3-CZ3-CH2	-7.11	111.86	121.10
1	C	42	TYR	CG-CD2-CE2	-7.11	110.54	121.20
1	A	33	PHE	CZ-CE2-CD2	7.11	132.79	120.00
1	C	35	SER	N-CA-C	-7.11	103.71	112.38
1	C	140	TYR	CA-C-N	7.11	134.49	121.70
1	C	140	TYR	C-N-CA	7.11	134.49	121.70
2	B	78	ASP	O-C-N	-7.10	111.64	123.00
2	D	53	VAL	CA-C-N	7.10	132.56	120.71
2	D	53	VAL	C-N-CA	7.10	132.56	120.71
1	A	20	ASN	CA-C-N	7.10	129.77	120.26
1	A	20	ASN	C-N-CA	7.10	129.77	120.26
2	D	140	LEU	CB-CG-CD1	-7.09	89.42	110.70
2	D	122	THR	N-CA-CB	-7.09	97.75	110.37
1	C	33	PHE	CA-C-N	7.07	135.05	121.54
1	C	33	PHE	C-N-CA	7.07	135.05	121.54
1	C	103	HIS	CB-CG-CD2	7.07	140.39	131.20
1	A	74	ASN	CA-C-O	-7.07	110.41	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	125	VAL	N-CA-C	7.06	119.92	111.09
1	C	103	HIS	CA-C-O	-7.06	112.30	120.20
1	A	72	HIS	N-CA-CB	7.05	122.41	110.49
2	B	134	ALA	N-CA-CB	7.05	121.28	109.78
1	A	107	VAL	CG1-CB-CG2	-7.05	95.29	110.80
2	D	44	PHE	CB-CG-CD1	-7.05	108.72	120.70
2	D	69	ALA	CA-C-N	-7.05	106.58	121.80
2	D	69	ALA	C-N-CA	-7.05	106.58	121.80
2	B	32	VAL	CB-CA-C	7.04	121.46	111.81
2	B	42	GLN	N-CA-C	-7.04	104.30	113.17
2	B	36	TRP	CD2-CE2-CZ2	7.04	129.44	122.40
1	C	6	ASN	N-CA-CB	7.03	122.37	110.49
2	B	65	ARG	O-C-N	-7.03	114.14	122.15
2	D	95	LEU	CA-C-O	7.03	127.54	119.18
1	A	69	ALA	CA-C-N	7.02	129.99	120.44
1	A	69	ALA	C-N-CA	7.02	129.99	120.44
1	A	86	LEU	CA-C-O	-7.02	110.47	120.51
1	A	121	VAL	CA-CB-CG1	7.02	122.33	110.40
2	B	32	VAL	N-CA-C	-7.02	96.21	106.88
1	A	99	LYS	CB-CG-CD	-7.02	95.16	111.30
2	B	44	PHE	CZ-CE2-CD2	7.01	132.62	120.00
2	D	141	ALA	CA-C-O	7.01	128.16	119.05
1	A	123	ALA	CA-C-N	7.00	129.89	120.65
1	A	123	ALA	C-N-CA	7.00	129.89	120.65
2	B	11	THR	O-C-N	7.00	129.54	122.12
1	C	5	ALA	CA-C-N	7.00	134.90	121.54
1	C	5	ALA	C-N-CA	7.00	134.90	121.54
1	C	42	TYR	CA-CB-CG	-7.00	101.31	113.90
1	A	24	TYR	CG-CD1-CE1	6.99	131.69	121.20
2	B	81	LYS	CB-CG-CD	6.99	127.37	111.30
1	C	70	GLN	CA-C-O	-6.99	111.74	119.08
1	A	113	LEU	CB-CG-CD1	-6.98	89.75	110.70
2	B	16	LYS	N-CA-CB	-6.98	98.69	110.49
1	A	50	HIS	O-C-N	6.97	131.87	122.59
2	B	116	ASN	CA-CB-CG	-6.97	105.63	112.60
2	D	25	GLN	CB-CA-C	-6.97	96.54	110.42
1	C	16	LYS	CD-CE-NZ	-6.97	89.59	111.90
2	B	54	MET	CG-SD-CE	-6.97	85.57	100.90
1	C	38	THR	O-C-N	-6.96	112.85	122.46
1	C	113	LEU	CB-CG-CD1	-6.96	89.81	110.70
1	A	101	LEU	CD1-CG-CD2	-6.96	95.49	110.80
1	A	69	ALA	N-CA-CB	6.96	120.45	110.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	LYS	CA-C-O	6.95	130.46	120.51
2	D	10	VAL	CA-CB-CG1	6.95	122.22	110.40
2	B	50	ALA	CB-CA-C	6.95	123.27	110.56
1	C	38	THR	CA-C-O	-6.95	110.70	119.31
1	A	22	PRO	CA-C-O	6.94	130.61	119.64
1	C	18	GLY	CA-C-N	6.94	137.44	121.34
1	C	18	GLY	C-N-CA	6.94	137.44	121.34
1	C	71	GLY	CA-C-O	6.94	135.37	120.80
2	D	39	ARG	NE-CZ-NH2	6.94	125.45	119.20
2	D	105	LEU	CD1-CG-CD2	-6.94	95.54	110.80
1	A	105	LEU	N-CA-CB	-6.93	99.53	110.28
2	D	31	LEU	CB-CA-C	6.93	121.70	110.95
1	A	128	PHE	CZ-CE2-CD2	-6.93	107.53	120.00
1	C	17	VAL	CA-CB-CG1	6.93	122.18	110.40
2	D	27	LEU	N-CA-C	6.93	120.83	112.38
1	C	24	TYR	CE1-CZ-OH	6.92	140.66	119.90
2	B	5	GLU	CA-C-N	6.92	134.75	121.54
2	B	5	GLU	C-N-CA	6.92	134.75	121.54
1	C	95	PRO	CA-C-O	-6.91	109.32	119.00
2	D	22	VAL	CA-CB-CG1	6.91	122.15	110.40
2	D	74	LEU	CA-C-O	-6.91	113.23	120.55
2	B	34	TYR	CD1-CE1-CZ	-6.90	107.17	119.60
2	B	52	ALA	N-CA-CB	-6.90	98.82	110.49
2	D	140	LEU	CD1-CG-CD2	-6.90	95.61	110.80
1	A	124	ASN	CB-CG-ND2	6.90	126.75	116.40
2	B	33	VAL	CA-C-N	6.90	138.63	121.80
2	B	33	VAL	C-N-CA	6.90	138.63	121.80
2	D	108	VAL	CB-CA-C	6.90	121.08	112.04
2	B	27	LEU	CA-CB-CG	6.89	140.43	116.30
2	D	75	LYS	CD-CE-NZ	-6.88	89.87	111.90
2	D	136	VAL	CG1-CB-CG2	-6.88	95.65	110.80
2	D	102	PHE	CD1-CE1-CZ	-6.88	107.62	120.00
1	A	9	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	100	LEU	CA-C-N	-6.88	110.34	120.38
1	A	100	LEU	C-N-CA	-6.88	110.34	120.38
1	C	73	LEU	N-CA-C	-6.88	96.15	110.80
1	A	31	ARG	NE-CZ-NH1	6.88	128.38	121.50
2	D	131	LYS	CA-C-O	-6.88	111.00	119.18
1	C	105	LEU	CB-CG-CD1	6.87	131.32	110.70
1	C	42	TYR	N-CA-CB	-6.87	98.87	110.41
1	C	64	ASN	O-C-N	6.87	131.72	122.59
1	C	98	PHE	CB-CG-CD1	6.87	132.38	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	64	ASN	CA-C-O	-6.87	110.69	120.51
2	D	134	ALA	CB-CA-C	6.87	124.08	110.42
1	C	15	GLY	CA-C-O	6.86	127.55	119.45
1	A	101	LEU	CB-CG-CD1	6.86	131.28	110.70
1	C	17	VAL	CB-CA-C	6.86	122.54	111.29
2	B	127	ALA	CA-C-N	6.86	132.34	120.68
2	B	127	ALA	C-N-CA	6.86	132.34	120.68
2	B	131	LYS	N-CA-CB	6.86	119.92	109.91
1	A	135	VAL	N-CA-CB	6.85	122.54	111.23
1	C	59	GLY	O-C-N	6.85	129.50	122.24
1	C	97	ASN	CB-CG-OD1	-6.85	107.09	120.80
1	A	58	HIS	CB-CA-C	6.85	122.21	110.84
1	C	120	ALA	CA-C-N	6.85	131.79	121.65
1	C	120	ALA	C-N-CA	6.85	131.79	121.65
1	A	48	LEU	O-C-N	-6.84	110.58	121.53
2	B	53	VAL	N-CA-C	-6.84	101.72	111.17
2	B	21	VAL	CA-C-O	-6.84	112.23	120.78
2	D	87	LEU	CB-CG-CD1	6.83	131.19	110.70
1	A	89	HIS	N-CA-C	-6.83	91.89	111.00
2	D	103	ARG	CG-CD-NE	-6.83	96.98	112.00
1	A	84	SER	N-CA-CB	6.82	120.85	110.28
2	D	14	TRP	CE2-CD2-CG	6.82	115.38	107.20
2	D	110	ALA	CB-CA-C	-6.82	96.86	110.42
1	A	103	HIS	N-CA-C	-6.81	103.54	110.97
1	C	54	GLN	CG-CD-OE1	-6.81	107.18	120.80
2	B	55	ASN	CA-C-O	6.80	127.63	120.42
2	B	57	PRO	N-CA-CB	6.80	110.40	103.25
2	D	3	THR	CA-CB-CG2	-6.80	98.93	110.50
1	A	11	LYS	CB-CA-C	6.80	123.15	110.70
1	A	89	HIS	ND1-CG-CD2	6.80	112.90	106.10
1	A	94	ASN	CA-C-O	-6.80	113.36	119.75
1	C	41	THR	O-C-N	-6.79	113.40	122.23
2	D	122	THR	CB-CA-C	6.79	123.55	110.17
1	A	51	GLY	N-CA-C	-6.79	97.09	113.18
2	B	144	TYR	CD1-CE1-CZ	-6.79	107.39	119.60
2	D	133	VAL	O-C-N	-6.79	115.24	121.89
1	C	97	ASN	CA-CB-CG	-6.78	105.82	112.60
2	D	136	VAL	CA-CB-CG2	-6.78	98.87	110.40
2	D	57	PRO	CA-N-CD	-6.78	102.51	112.00
2	D	97	VAL	N-CA-CB	6.78	120.00	111.46
1	A	8	SER	CA-CB-OG	6.77	124.63	111.10
1	C	106	LEU	CB-CG-CD1	6.77	131.00	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	45	HIS	N-CA-CB	6.76	121.82	110.32
1	C	128	PHE	CG-CD1-CE1	6.76	132.20	120.70
2	D	80	LEU	N-CA-C	6.76	119.22	111.11
1	A	65	ALA	CB-CA-C	-6.76	98.33	110.70
2	D	108	VAL	N-CA-C	6.76	118.32	110.62
2	B	86	GLN	N-CA-CB	6.75	121.98	110.50
2	D	54	MET	CA-C-O	-6.75	113.33	120.55
2	B	117	PHE	CA-C-N	6.75	134.63	121.41
2	B	117	PHE	C-N-CA	6.75	134.63	121.41
2	B	102	PHE	CG-CD1-CE1	6.74	132.16	120.70
2	D	96	HIS	N-CA-C	-6.74	96.44	110.80
2	B	84	PHE	CB-CA-C	6.74	121.92	110.74
1	C	67	THR	O-C-N	6.74	129.04	122.03
1	A	42	TYR	CE1-CZ-OH	6.74	140.11	119.90
1	A	134	THR	OG1-CB-CG2	-6.74	95.83	109.30
1	A	91	LEU	N-CA-C	-6.73	103.63	110.97
1	C	61	LYS	CA-CB-CG	-6.73	100.63	114.10
1	A	89	HIS	ND1-CE1-NE2	-6.73	101.67	108.40
1	C	141	ARG	CB-CG-CD	-6.73	95.82	111.30
2	D	45	GLY	O-C-N	6.73	131.45	122.70
1	C	43	PHE	CA-C-N	-6.73	111.43	119.84
1	C	43	PHE	C-N-CA	-6.73	111.43	119.84
2	D	66	VAL	O-C-N	6.73	130.98	122.57
1	A	80	LEU	CB-CA-C	6.72	122.80	110.36
2	B	94	LYS	CB-CA-C	-6.72	98.19	109.75
1	A	5	ALA	N-CA-C	-6.71	104.10	112.90
1	A	26	ALA	CA-C-O	-6.71	110.64	119.10
2	D	49	SER	N-CA-C	-6.71	96.51	110.80
2	D	63	GLY	CA-C-O	-6.70	108.91	120.57
2	D	110	ALA	CA-C-O	-6.70	110.92	120.51
1	C	54	GLN	OE1-CD-NE2	6.70	129.30	122.60
2	B	74	LEU	O-C-N	-6.70	113.69	122.59
2	B	39	ARG	CD-NE-CZ	-6.69	115.03	124.40
2	D	92	CYS	CA-C-O	-6.69	110.94	120.51
2	D	144	TYR	CB-CA-C	-6.69	97.10	110.42
2	D	74	LEU	CA-CB-CG	6.69	139.71	116.30
1	A	100	LEU	CB-CG-CD1	-6.69	90.64	110.70
2	D	97	VAL	CB-CA-C	6.68	120.71	110.96
2	D	33	VAL	CA-C-O	-6.67	113.64	121.05
2	B	31	LEU	CB-CA-C	6.67	123.69	110.42
2	D	138	ASN	CB-CG-ND2	6.67	126.40	116.40
1	C	131	ASN	CB-CG-ND2	6.66	126.39	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	69	ALA	CA-C-O	-6.66	114.01	121.00
2	B	99	PRO	CB-CG-CD	-6.66	84.81	106.10
2	D	41	PHE	CB-CA-C	6.65	122.41	111.50
2	D	111	LEU	CD1-CG-CD2	6.65	125.44	110.80
1	C	17	VAL	CA-C-N	-6.65	108.38	121.41
1	C	17	VAL	C-N-CA	-6.65	108.38	121.41
2	D	37	THR	CA-CB-OG1	-6.64	99.64	109.60
1	A	67	THR	N-CA-C	6.64	120.64	112.54
1	A	7	LYS	CG-CD-CE	6.64	126.57	111.30
1	C	42	TYR	CD1-CE1-CZ	6.63	131.54	119.60
1	C	56	LYS	CB-CG-CD	-6.63	96.05	111.30
1	A	100	LEU	CA-C-O	6.63	129.99	120.51
1	A	101	LEU	CA-C-O	6.63	127.62	120.20
1	C	94	ASN	CA-C-N	-6.62	112.87	119.56
1	C	94	ASN	C-N-CA	-6.62	112.87	119.56
1	A	3	SER	CB-CA-C	-6.62	97.25	109.37
1	C	99	LYS	N-CA-C	-6.62	104.46	112.54
1	C	81	SER	N-CA-CB	-6.62	100.34	110.20
1	A	44	PRO	CA-N-CD	-6.62	102.74	112.00
2	B	105	LEU	CA-C-O	-6.61	111.05	120.51
1	C	87	HIS	N-CA-CB	6.61	120.44	110.19
2	D	38	GLN	CG-CD-OE1	-6.61	107.59	120.80
1	A	117	PHE	O-C-N	-6.60	114.18	122.83
2	B	91	HIS	CB-CG-CD2	6.60	139.78	131.20
1	A	83	LEU	O-C-N	-6.60	113.66	122.43
1	C	111	SER	CA-C-N	-6.60	110.20	122.60
1	C	111	SER	C-N-CA	-6.60	110.20	122.60
1	A	140	TYR	CD1-CG-CD2	6.59	127.99	118.10
1	C	17	VAL	N-CA-C	-6.59	95.62	109.34
1	C	76	LEU	N-CA-C	6.59	124.38	109.81
1	A	43	PHE	C-N-CD	6.58	151.99	125.00
2	B	145	HIS	CE1-NE2-CD2	-6.58	102.42	109.00
2	D	45	GLY	CA-C-N	-6.58	108.97	121.54
2	D	45	GLY	C-N-CA	-6.58	108.97	121.54
2	B	48	SER	CA-C-N	-6.58	110.37	121.75
2	B	48	SER	C-N-CA	-6.58	110.37	121.75
1	A	35	SER	CA-C-N	6.57	137.84	121.80
1	A	35	SER	C-N-CA	6.57	137.84	121.80
2	B	108	VAL	O-C-N	6.57	128.73	121.90
2	D	36	TRP	CG-CD2-CE3	-6.57	127.33	133.90
1	C	52	SER	N-CA-C	6.57	119.61	108.90
1	C	73	LEU	CD1-CG-CD2	-6.57	96.36	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	141	ARG	NE-CZ-NH2	6.56	125.11	119.20
2	D	76	HIS	CE1-NE2-CD2	-6.56	102.44	109.00
1	A	80	LEU	CB-CG-CD2	6.56	130.37	110.70
2	B	56	ASN	CA-CB-CG	-6.55	106.05	112.60
2	D	140	LEU	CA-C-N	6.55	134.16	121.18
2	D	140	LEU	C-N-CA	6.55	134.16	121.18
2	B	4	ALA	N-CA-CB	6.55	120.75	110.46
2	B	84	PHE	N-CA-C	-6.55	100.56	111.37
1	A	103	HIS	N-CA-CB	6.55	119.47	109.91
2	B	44	PHE	CA-CB-CG	-6.55	107.25	113.80
2	B	14	TRP	CA-C-N	6.54	134.24	121.41
2	B	14	TRP	C-N-CA	6.54	134.24	121.41
2	B	134	ALA	CA-C-N	6.54	134.23	121.41
2	B	134	ALA	C-N-CA	6.54	134.23	121.41
1	A	52	SER	CB-CA-C	6.54	121.01	110.16
1	C	90	LYS	CB-CA-C	6.53	120.33	110.08
2	B	10	VAL	CA-CB-CG1	-6.53	99.31	110.40
1	A	79	THR	N-CA-CB	6.52	119.53	110.07
2	D	128	LEU	N-CA-C	-6.52	96.91	110.80
2	B	18	ASP	N-CA-CB	-6.51	99.50	110.49
1	C	5	ALA	CB-CA-C	6.51	120.00	109.07
1	A	2	LEU	CA-C-O	-6.50	111.21	120.51
1	A	95	PRO	N-CA-C	6.50	123.44	113.75
1	A	108	THR	O-C-N	-6.50	113.95	122.59
1	C	42	TYR	CB-CG-CD1	-6.49	111.06	120.80
2	B	112	VAL	CG1-CB-CG2	6.49	125.08	110.80
1	A	97	ASN	CA-C-O	-6.49	110.62	119.12
2	D	67	LEU	CB-CG-CD2	-6.48	91.25	110.70
2	D	14	TRP	CA-C-N	6.48	134.11	121.41
2	D	14	TRP	C-N-CA	6.48	134.11	121.41
2	B	68	ASP	CA-CB-CG	-6.48	106.12	112.60
2	D	54	MET	CA-C-N	6.48	129.20	120.65
2	D	54	MET	C-N-CA	6.48	129.20	120.65
2	D	133	VAL	N-CA-CB	-6.48	102.37	110.47
1	A	44	PRO	CB-CG-CD	-6.48	85.38	106.10
2	B	84	PHE	O-C-N	-6.47	114.67	122.11
1	C	12	ALA	O-C-N	-6.47	113.53	122.46
1	C	18	GLY	CA-C-O	-6.46	109.33	120.57
2	D	89	GLY	O-C-N	-6.46	114.30	122.70
1	C	109	LEU	CA-CB-CG	6.46	138.90	116.30
2	B	33	VAL	CB-CA-C	6.45	121.87	111.29
1	A	10	VAL	CB-CA-C	-6.45	100.71	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	LYS	CA-CB-CG	6.45	127.00	114.10
1	A	108	THR	CA-C-N	6.45	133.86	121.54
1	A	108	THR	C-N-CA	6.45	133.86	121.54
1	A	107	VAL	N-CA-C	-6.45	95.93	109.34
2	D	142	HIS	CG-CD2-NE2	6.44	113.64	107.20
1	A	17	VAL	CB-CA-C	6.44	121.85	111.29
1	A	105	LEU	CA-C-N	-6.44	106.46	121.52
1	A	105	LEU	C-N-CA	-6.44	106.46	121.52
1	C	91	LEU	N-CA-CB	-6.44	100.74	110.07
1	C	24	TYR	CZ-CE2-CD2	-6.43	108.02	119.60
2	D	32	VAL	CA-CB-CG2	6.43	121.33	110.40
2	B	34	TYR	OH-CZ-CE2	-6.43	100.61	119.90
1	C	33	PHE	CZ-CE2-CD2	6.43	131.57	120.00
1	C	111	SER	O-C-N	-6.43	115.30	122.12
2	B	115	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	C	101	LEU	CD1-CG-CD2	6.42	124.93	110.80
2	B	87	LEU	CB-CG-CD2	6.42	129.96	110.70
1	C	102	SER	N-CA-C	-6.42	97.13	110.80
1	C	31	ARG	CG-CD-NE	6.41	126.10	112.00
2	B	131	LYS	CA-C-N	6.41	133.51	121.97
2	B	131	LYS	C-N-CA	6.41	133.51	121.97
1	A	16	LYS	CB-CA-C	6.40	123.16	110.42
2	B	62	HIS	CB-CG-ND1	-6.40	113.10	122.70
2	D	65	ARG	CA-CB-CG	6.40	126.90	114.10
1	C	21	ALA	CB-CA-C	6.39	122.77	110.17
1	A	131	ASN	CB-CG-ND2	6.39	125.99	116.40
1	A	108	THR	CA-C-O	6.38	129.63	120.51
1	C	112	HIS	CB-CG-ND1	6.38	132.27	122.70
1	C	124	ASN	O-C-N	-6.37	114.12	122.59
2	B	55	ASN	CB-CA-C	6.37	121.67	110.85
1	A	14	TRP	CD2-CE3-CZ3	6.36	126.87	118.60
2	B	36	TRP	CD1-NE1-CE2	6.36	120.35	108.90
2	B	83	ALA	CB-CA-C	6.36	123.07	110.42
2	D	124	ASN	N-CA-C	-6.36	97.26	110.80
2	D	104	LEU	CB-CA-C	6.35	120.94	110.90
2	D	129	PHE	CB-CG-CD2	6.35	131.50	120.70
2	D	31	LEU	O-C-N	6.35	128.88	122.03
2	D	141	ALA	O-C-N	6.35	131.22	122.46
1	A	60	GLN	CG-CD-OE1	6.34	133.48	120.80
2	B	135	GLY	CA-C-N	6.34	128.62	120.88
2	B	135	GLY	C-N-CA	6.34	128.62	120.88
2	B	84	PHE	N-CA-CB	-6.34	99.45	109.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	12	ALA	N-CA-CB	-6.34	99.30	110.39
1	C	94	ASN	C-N-CD	6.33	150.95	125.00
2	D	21	VAL	CA-C-N	6.33	129.06	120.77
2	D	21	VAL	C-N-CA	6.33	129.06	120.77
1	C	33	PHE	CB-CG-CD1	6.32	131.45	120.70
2	B	43	HIS	CB-CG-ND1	-6.32	113.22	122.70
2	D	120	GLN	N-CA-CB	6.32	121.17	110.49
2	D	136	VAL	CB-CA-C	-6.32	103.77	112.24
2	D	57	PRO	CB-CG-CD	-6.32	85.88	106.10
2	D	99	PRO	CA-CB-CG	-6.32	92.49	104.50
2	D	111	LEU	CA-CB-CG	6.31	138.40	116.30
2	B	55	ASN	CB-CG-OD1	-6.31	108.17	120.80
2	D	144	TYR	CA-C-N	-6.31	110.34	121.70
2	D	144	TYR	C-N-CA	-6.31	110.34	121.70
1	A	128	PHE	O-C-N	-6.31	114.20	122.59
2	B	22	VAL	CA-CB-CG2	6.30	121.11	110.40
2	B	42	GLN	CG-CD-OE1	-6.29	108.21	120.80
1	A	63	ALA	N-CA-CB	6.29	119.91	110.22
2	D	106	GLY	O-C-N	-6.29	116.09	122.19
1	A	61	LYS	CD-CE-NZ	-6.28	91.82	111.90
2	D	67	LEU	CB-CA-C	6.28	121.21	110.79
2	B	20	ASP	N-CA-C	6.27	124.16	110.80
1	C	118	THR	OG1-CB-CG2	-6.27	96.76	109.30
2	B	52	ALA	CA-C-N	-6.26	110.36	120.62
2	B	52	ALA	C-N-CA	-6.26	110.36	120.62
2	B	84	PHE	CG-CD1-CE1	-6.25	110.07	120.70
2	B	91	HIS	CB-CG-ND1	6.25	132.08	122.70
1	A	43	PHE	CD1-CG-CD2	-6.25	109.22	118.60
2	D	81	LYS	CA-CB-CG	6.25	126.61	114.10
2	D	86	GLN	CB-CA-C	6.25	122.86	110.42
1	A	108	THR	CA-CB-CG2	6.25	121.12	110.50
2	B	30	LEU	CB-CG-CD1	6.25	129.45	110.70
1	A	124	ASN	O-C-N	-6.25	115.53	122.03
1	C	92	ARG	N-CA-C	6.25	120.29	111.92
2	B	129	PHE	CA-C-N	6.24	130.19	120.82
2	B	129	PHE	C-N-CA	6.24	130.19	120.82
1	C	11	LYS	N-CA-C	6.24	117.96	111.03
1	C	10	VAL	N-CA-CB	6.24	121.53	111.23
1	A	7	LYS	N-CA-CB	6.24	119.30	109.82
2	B	71	THR	CA-CB-OG1	6.24	118.95	109.60
1	C	14	TRP	CE2-CD2-CG	6.23	114.68	107.20
1	C	15	GLY	N-CA-C	-6.23	106.93	114.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	ASN	O-C-N	6.23	130.87	122.59
2	B	136	VAL	O-C-N	-6.22	114.35	121.94
2	B	41	PHE	CA-C-N	-6.22	112.27	122.54
2	B	41	PHE	C-N-CA	-6.22	112.27	122.54
2	D	41	PHE	CD1-CE1-CZ	-6.21	108.81	120.00
2	B	99	PRO	CA-CB-CG	6.21	116.30	104.50
2	B	29	ARG	N-CA-CB	-6.21	100.33	110.14
2	D	20	ASP	OD1-CG-OD2	6.21	137.80	122.90
2	B	23	GLY	CA-C-O	-6.21	109.77	120.57
1	C	40	LYS	CA-CB-CG	6.21	126.52	114.10
1	C	71	GLY	O-C-N	-6.20	113.08	123.00
2	B	10	VAL	N-CA-C	6.19	121.11	112.50
1	C	40	LYS	N-CA-C	6.19	120.30	112.87
1	C	97	ASN	CB-CG-ND2	6.18	125.67	116.40
1	C	132	ASP	N-CA-CB	-6.17	101.05	110.12
2	B	78	ASP	OD1-CG-OD2	-6.16	108.12	122.90
2	D	36	TRP	CD2-CE3-CZ3	-6.15	110.60	118.60
2	B	123	PRO	CB-CG-CD	6.15	125.78	106.10
2	D	47	LEU	CA-C-N	6.14	133.27	121.54
2	D	47	LEU	C-N-CA	6.14	133.27	121.54
2	D	6	GLU	CG-CD-OE2	-6.14	104.27	118.40
2	D	17	VAL	CG1-CB-CG2	6.14	124.31	110.80
2	D	120	GLN	CA-CB-CG	-6.14	101.81	114.10
1	C	45	HIS	ND1-CE1-NE2	-6.14	102.26	108.40
1	A	133	SER	CB-CA-C	6.14	120.63	110.81
2	B	129	PHE	N-CA-C	-6.14	104.67	111.36
2	B	106	GLY	O-C-N	-6.13	115.87	122.19
1	C	39	THR	CA-C-N	-6.13	109.58	120.99
1	C	39	THR	C-N-CA	-6.13	109.58	120.99
2	B	126	GLN	O-C-N	6.13	130.74	122.59
2	B	133	VAL	CA-C-N	6.13	130.01	120.82
2	B	133	VAL	C-N-CA	6.13	130.01	120.82
1	C	85	ASN	N-CA-C	-6.13	99.67	109.96
1	A	12	ALA	CA-C-N	6.12	133.24	121.54
1	A	12	ALA	C-N-CA	6.12	133.24	121.54
2	D	93	ASN	CB-CG-OD1	6.12	133.05	120.80
2	D	121	PHE	O-C-N	-6.12	114.45	122.59
1	C	72	HIS	N-CA-C	6.12	123.83	110.80
2	D	121	PHE	CB-CA-C	-6.12	98.25	110.42
2	D	117	PHE	CG-CD2-CE2	6.12	131.10	120.70
2	D	29	ARG	CB-CA-C	6.11	121.89	110.70
1	C	97	ASN	CA-C-N	-6.11	111.47	121.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	97	ASN	C-N-CA	-6.11	111.47	121.19
1	C	55	GLN	N-CA-CB	6.11	118.93	110.07
2	B	89	GLY	N-CA-C	-6.11	98.71	113.18
1	C	111	SER	CA-CB-OG	6.09	123.29	111.10
1	A	141	ARG	N-CA-C	6.09	128.06	111.00
1	C	70	GLN	CA-CB-CG	6.09	126.28	114.10
2	D	96	HIS	CA-C-N	-6.09	115.20	123.12
2	D	96	HIS	C-N-CA	-6.09	115.20	123.12
2	B	6	GLU	CG-CD-OE2	-6.09	104.39	118.40
1	C	73	LEU	CB-CG-CD1	6.09	128.97	110.70
2	B	96	HIS	ND1-CE1-NE2	6.08	114.48	108.40
1	A	38	THR	CA-C-N	6.08	128.43	120.28
1	A	38	THR	C-N-CA	6.08	128.43	120.28
1	A	51	GLY	CA-C-O	-6.08	109.99	120.57
1	C	105	LEU	CB-CA-C	6.08	121.82	110.70
2	D	47	LEU	CD1-CG-CD2	6.08	124.17	110.80
1	A	10	VAL	CA-C-O	-6.07	113.19	120.78
2	B	66	VAL	O-C-N	-6.07	114.98	122.57
1	C	87	HIS	CB-CG-ND1	-6.07	113.60	122.70
1	A	9	ASN	CA-C-N	6.06	132.88	121.97
1	A	9	ASN	C-N-CA	6.06	132.88	121.97
1	C	139	LYS	CD-CE-NZ	-6.06	92.50	111.90
2	B	144	TYR	CE1-CZ-OH	6.06	138.08	119.90
2	B	126	GLN	CB-CA-C	6.05	122.46	110.42
2	B	18	ASP	CB-CA-C	6.05	122.46	110.42
1	C	82	ASN	N-CA-CB	6.05	118.95	109.94
2	B	31	LEU	CD1-CG-CD2	-6.04	97.50	110.80
1	C	26	ALA	CA-C-N	6.04	130.27	120.60
1	C	26	ALA	C-N-CA	6.04	130.27	120.60
2	D	98	ASN	O-C-N	6.04	128.27	121.32
2	D	144	TYR	CA-CB-CG	6.04	124.78	113.90
1	C	117	PHE	CG-CD2-CE2	-6.04	110.43	120.70
2	B	103	ARG	NH1-CZ-NH2	6.04	127.14	119.30
1	A	93	VAL	CB-CA-C	6.03	118.58	111.59
1	A	104	SER	CB-CA-C	-6.02	100.80	110.79
1	A	22	PRO	CB-CA-C	-6.02	102.21	112.26
1	C	29	LEU	CB-CG-CD1	6.02	128.75	110.70
2	D	117	PHE	CB-CG-CD2	-6.02	110.47	120.70
1	C	118	THR	CA-C-N	-6.01	112.37	119.05
1	C	118	THR	C-N-CA	-6.01	112.37	119.05
2	B	43	HIS	CG-ND1-CE1	6.01	119.52	109.30
2	B	21	VAL	CA-CB-CG1	6.01	120.61	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	THR	CA-CB-CG2	6.01	120.71	110.50
2	B	123	PRO	N-CA-CB	6.01	109.89	103.52
2	D	123	PRO	CA-CB-CG	6.01	115.91	104.50
1	A	78	GLY	CA-C-O	-6.00	110.12	120.57
2	B	43	HIS	CB-CG-CD2	6.00	139.01	131.20
2	B	138	ASN	CB-CA-C	-6.00	100.96	110.86
1	C	106	LEU	N-CA-C	6.00	119.86	112.54
2	D	102	PHE	N-CA-CB	-6.00	101.29	109.98
1	A	40	LYS	CA-C-O	5.99	129.08	120.51
2	B	37	THR	OG1-CB-CG2	-5.99	97.32	109.30
1	A	134	THR	CA-CB-OG1	5.99	118.58	109.60
2	B	60	LYS	CB-CG-CD	-5.99	97.53	111.30
1	A	94	ASN	N-CA-CB	-5.98	99.02	109.73
1	A	119	PRO	CA-CB-CG	-5.97	93.15	104.50
1	C	32	MET	N-CA-CB	-5.97	99.44	110.18
1	A	60	GLN	O-C-N	5.96	130.52	122.59
2	B	15	GLY	CA-C-N	-5.96	110.15	121.54
2	B	15	GLY	C-N-CA	-5.96	110.15	121.54
2	D	56	ASN	CB-CG-OD1	-5.96	108.88	120.80
2	D	76	HIS	CA-C-O	-5.96	114.20	120.58
2	B	92	CYS	N-CA-CB	-5.95	101.14	110.30
1	A	97	ASN	CB-CA-C	5.94	121.40	110.11
2	B	80	LEU	CB-CG-CD2	-5.94	92.87	110.70
1	A	40	LYS	N-CA-CB	5.94	120.53	110.49
1	C	35	SER	CB-CA-C	5.94	122.86	110.32
1	C	80	LEU	CB-CG-CD1	-5.94	92.88	110.70
2	D	97	VAL	CG1-CB-CG2	-5.93	97.75	110.80
2	B	82	GLY	CA-C-O	-5.93	110.25	120.57
1	A	60	GLN	CA-C-N	-5.93	112.38	120.44
1	A	60	GLN	C-N-CA	-5.93	112.38	120.44
2	B	39	ARG	CB-CG-CD	-5.93	97.67	111.30
2	D	77	LEU	CB-CG-CD2	5.93	128.48	110.70
2	B	115	ARG	CB-CA-C	-5.92	99.80	110.23
2	B	34	TYR	N-CA-C	-5.92	96.72	109.81
1	C	106	LEU	CA-C-O	-5.92	112.09	119.38
2	B	40	PHE	CE1-CZ-CE2	-5.92	109.34	120.00
1	C	14	TRP	CA-C-N	-5.92	110.43	120.79
1	C	14	TRP	C-N-CA	-5.92	110.43	120.79
2	D	17	VAL	CA-C-N	5.92	131.82	122.94
2	D	17	VAL	C-N-CA	5.92	131.82	122.94
1	C	90	LYS	N-CA-CB	-5.91	100.05	110.34
2	B	36	TRP	CD1-CG-CD2	-5.91	96.85	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	120	ALA	N-CA-C	-5.91	105.56	112.89
2	D	60	LYS	CA-C-O	-5.91	112.06	120.51
1	A	54	GLN	CA-CB-CG	-5.90	102.30	114.10
1	C	9	ASN	N-CA-C	5.90	123.37	110.80
1	C	105	LEU	O-C-N	5.90	129.90	122.23
2	D	138	ASN	O-C-N	-5.90	115.05	121.95
1	A	135	VAL	CA-C-N	-5.90	110.28	121.54
1	A	135	VAL	C-N-CA	-5.90	110.28	121.54
1	C	127	LYS	CB-CG-CD	5.90	124.86	111.30
2	B	125	VAL	N-CA-CB	5.89	121.43	110.77
1	A	88	ALA	CA-C-O	5.88	128.92	120.51
1	A	67	THR	CA-C-O	-5.88	112.15	119.38
1	C	82	ASN	CB-CA-C	5.88	120.22	110.81
1	A	76	LEU	CB-CA-C	5.87	125.12	112.38
2	D	33	VAL	O-C-N	5.87	128.01	121.90
2	B	35	PRO	CA-CB-CG	-5.87	93.35	104.50
1	C	136	LEU	CB-CG-CD1	5.87	128.31	110.70
2	B	11	THR	CA-CB-CG2	5.87	120.47	110.50
2	B	57	PRO	N-CA-C	-5.87	100.39	112.47
1	A	101	LEU	O-C-N	-5.86	115.52	122.20
2	B	19	VAL	CB-CA-C	-5.86	101.67	111.29
2	B	99	PRO	CA-C-O	5.86	126.95	118.86
2	B	21	VAL	N-CA-C	-5.86	97.15	109.34
1	C	68	LYS	CD-CE-NZ	-5.86	93.14	111.90
2	D	36	TRP	CE3-CZ3-CH2	5.86	128.72	121.10
2	B	107	ASN	CB-CG-OD1	5.86	132.52	120.80
1	A	118	THR	N-CA-CB	-5.86	99.95	110.37
2	D	77	LEU	N-CA-CB	-5.86	101.48	110.20
2	B	20	ASP	OD1-CG-OD2	5.85	136.94	122.90
2	B	26	ALA	CB-CA-C	5.85	120.51	110.79
2	B	52	ALA	N-CA-C	-5.84	98.35	110.80
1	C	29	LEU	CB-CA-C	5.84	120.79	110.85
2	D	58	LYS	N-CA-C	-5.84	98.35	110.80
2	D	123	PRO	CA-C-O	5.84	128.98	119.86
1	A	66	LEU	N-CA-CB	5.84	120.36	110.49
1	C	8	SER	O-C-N	5.84	130.36	122.59
1	C	107	VAL	CG1-CB-CG2	5.84	123.64	110.80
1	C	22	PRO	CA-C-O	-5.83	109.98	120.60
2	D	109	LEU	CA-CB-CG	5.83	136.72	116.30
2	B	67	LEU	CB-CG-CD1	-5.83	93.20	110.70
2	D	55	ASN	CA-CB-CG	-5.83	106.77	112.60
2	D	88	SER	CA-CB-OG	5.83	122.76	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	97	ASN	N-CA-C	-5.83	106.14	113.20
2	D	87	LEU	N-CA-C	-5.83	106.79	114.31
2	D	122	THR	CA-CB-CG2	5.83	120.41	110.50
1	A	83	LEU	CA-C-N	-5.82	111.46	120.31
1	A	83	LEU	C-N-CA	-5.82	111.46	120.31
2	D	104	LEU	CB-CG-CD2	5.82	128.16	110.70
1	A	40	LYS	CG-CD-CE	5.81	124.67	111.30
2	B	86	GLN	OE1-CD-NE2	5.81	128.41	122.60
2	D	104	LEU	CB-CG-CD1	-5.81	93.28	110.70
2	B	113	VAL	CB-CA-C	5.80	121.66	112.26
2	D	44	PHE	N-CA-CB	5.80	120.29	110.49
1	C	14	TRP	CE2-CD2-CE3	5.80	124.60	118.80
2	B	39	ARG	N-CA-CB	5.80	118.81	110.40
2	B	65	ARG	CA-C-N	5.80	132.41	121.97
2	B	65	ARG	C-N-CA	5.80	132.41	121.97
2	D	11	THR	CA-C-O	5.79	131.29	122.20
2	B	30	LEU	CA-C-N	5.79	132.60	121.54
2	B	30	LEU	C-N-CA	5.79	132.60	121.54
1	C	74	ASN	N-CA-C	-5.79	98.47	110.80
2	B	72	GLN	CA-C-O	-5.79	112.24	120.51
2	D	98	ASN	CB-CA-C	-5.78	98.78	110.17
1	C	99	LYS	CB-CG-CD	5.78	124.59	111.30
2	D	64	LYS	CB-CG-CD	5.78	124.58	111.30
1	C	100	LEU	CB-CA-C	5.77	121.82	111.03
1	C	87	HIS	ND1-CE1-NE2	5.76	114.16	108.40
1	C	102	SER	CB-CA-C	5.75	121.87	110.42
1	A	14	TRP	CZ3-CH2-CZ2	5.75	128.97	121.50
2	B	131	LYS	CB-CG-CD	5.75	124.52	111.30
2	B	131	LYS	N-CA-C	5.75	117.23	110.97
2	D	29	ARG	CA-C-O	-5.74	113.87	120.24
1	A	56	LYS	CG-CD-CE	5.74	124.50	111.30
2	D	78	ASP	CB-CG-OD1	5.72	131.56	118.40
2	D	53	VAL	CA-CB-CG2	5.72	120.12	110.40
2	D	79	ASP	O-C-N	5.72	132.15	121.63
1	C	41	THR	CA-C-O	-5.71	113.90	120.24
1	A	87	HIS	CA-C-N	5.71	132.45	121.54
1	A	87	HIS	C-N-CA	5.71	132.45	121.54
2	D	40	PHE	CB-CG-CD2	-5.71	110.99	120.70
2	B	128	LEU	CD1-CG-CD2	5.71	123.36	110.80
1	A	22	PRO	N-CA-CB	-5.71	96.91	103.30
1	A	98	PHE	N-CA-C	-5.71	102.83	111.56
2	B	5	GLU	CA-CB-CG	-5.70	102.70	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	140	LEU	CD1-CG-CD2	-5.70	98.26	110.80
2	B	100	GLN	CB-CA-C	5.69	120.25	110.86
2	B	145	HIS	ND1-CG-CD2	5.69	111.79	106.10
1	C	74	ASN	CB-CG-ND2	5.69	124.93	116.40
1	A	4	ALA	N-CA-CB	-5.68	100.66	110.32
2	B	99	PRO	O-C-N	5.68	130.30	122.35
2	D	120	GLN	N-CA-C	-5.68	98.70	110.80
2	B	115	ARG	CB-CG-CD	5.67	124.35	111.30
2	B	9	ALA	O-C-N	5.67	130.13	122.59
2	D	41	PHE	CG-CD1-CE1	5.66	130.33	120.70
1	C	55	GLN	N-CA-C	-5.66	105.03	111.14
1	C	45	HIS	CB-CG-ND1	5.65	131.18	122.70
1	A	43	PHE	CZ-CE2-CD2	-5.65	109.83	120.00
1	C	122	HIS	CA-C-O	5.65	126.53	120.20
1	A	53	ALA	CA-C-N	-5.65	112.95	120.63
1	A	53	ALA	C-N-CA	-5.65	112.95	120.63
2	B	122	THR	CA-CB-CG2	-5.63	100.93	110.50
2	B	27	LEU	CB-CG-CD1	5.63	127.58	110.70
2	B	98	ASN	C-N-CD	-5.63	101.93	125.00
2	B	107	ASN	O-C-N	5.62	128.56	122.15
1	A	47	ASP	CA-C-O	5.61	128.54	120.51
1	A	63	ALA	N-CA-C	5.60	118.15	111.71
1	A	46	PHE	CD1-CG-CD2	-5.60	110.20	118.60
2	B	124	ASN	O-C-N	-5.59	114.96	122.23
1	C	55	GLN	CG-CD-OE1	-5.59	109.61	120.80
1	C	141	ARG	CD-NE-CZ	5.59	132.23	124.40
2	D	10	VAL	CG1-CB-CG2	5.59	123.10	110.80
2	D	76	HIS	CB-CG-ND1	5.59	131.09	122.70
1	C	58	HIS	O-C-N	-5.59	115.78	122.15
2	D	96	HIS	N-CA-CB	5.59	119.94	110.49
1	C	7	LYS	CA-CB-CG	5.58	125.27	114.10
1	A	113	LEU	CD1-CG-CD2	-5.58	98.53	110.80
2	D	92	CYS	N-CA-CB	5.58	119.91	110.49
2	B	38	GLN	CA-C-N	5.57	132.71	122.79
2	B	38	GLN	C-N-CA	5.57	132.71	122.79
2	B	24	ALA	N-CA-CB	5.57	118.41	110.06
2	D	57	PRO	CB-CA-C	5.57	120.75	111.56
1	A	48	LEU	CD1-CG-CD2	-5.57	98.56	110.80
2	B	90	LEU	N-CA-C	-5.57	104.23	111.02
1	A	32	MET	CA-C-N	5.56	128.00	120.38
1	A	32	MET	C-N-CA	5.56	128.00	120.38
2	D	24	ALA	N-CA-C	-5.56	105.22	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	109	LEU	CB-CG-CD2	5.56	127.37	110.70
2	D	54	MET	CB-CA-C	5.56	120.12	110.79
2	B	8	ALA	CB-CA-C	5.55	121.47	110.42
2	B	101	ASN	CA-CB-CG	5.55	118.15	112.60
2	D	12	GLY	O-C-N	5.55	131.88	123.00
1	A	59	GLY	CA-C-O	5.54	126.53	120.66
2	D	43	HIS	N-CA-CB	-5.54	101.12	110.49
1	A	132	ASP	O-C-N	5.54	129.96	122.59
2	B	62	HIS	ND1-CE1-NE2	5.54	113.94	108.40
1	C	94	ASN	CA-CB-CG	-5.54	107.06	112.60
1	C	20	ASN	CA-C-N	5.54	135.31	121.80
1	C	20	ASN	C-N-CA	5.54	135.31	121.80
2	B	36	TRP	CG-CD1-NE1	5.53	117.39	110.20
1	A	39	THR	N-CA-C	-5.53	105.25	111.28
2	B	115	ARG	CA-CB-CG	-5.53	103.04	114.10
1	A	68	LYS	CD-CE-NZ	5.53	129.58	111.90
2	B	9	ALA	CA-C-N	-5.52	111.59	120.64
2	B	9	ALA	C-N-CA	-5.52	111.59	120.64
2	B	99	PRO	N-CD-CG	-5.52	94.92	103.20
1	C	20	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	113	LEU	CA-CB-CG	5.51	135.58	116.30
2	B	136	VAL	CA-CB-CG2	5.51	119.77	110.40
1	C	12	ALA	CA-C-N	5.49	132.03	121.54
1	C	12	ALA	C-N-CA	5.49	132.03	121.54
2	B	78	ASP	CB-CG-OD1	5.49	131.03	118.40
1	C	75	ASP	N-CA-CB	-5.49	101.22	110.49
1	A	96	VAL	CA-CB-CG2	5.48	119.72	110.40
1	A	113	LEU	CB-CA-C	5.47	118.24	110.96
2	B	103	ARG	CA-C-O	-5.47	114.16	120.24
2	D	75	LYS	N-CA-C	-5.47	99.14	110.80
1	A	18	GLY	N-CA-C	-5.46	103.10	111.24
1	C	54	GLN	N-CA-CB	5.46	118.34	110.20
1	C	63	ALA	CB-CA-C	-5.46	99.55	110.42
2	D	34	TYR	CE1-CZ-OH	-5.46	103.50	119.90
1	C	22	PRO	N-CD-CG	5.46	111.39	103.20
2	B	85	ALA	N-CA-C	5.46	122.43	110.80
2	D	130	GLN	CA-CB-CG	5.46	125.01	114.10
2	B	138	ASN	CA-C-N	-5.45	112.42	120.38
2	B	138	ASN	C-N-CA	-5.45	112.42	120.38
1	C	92	ARG	NE-CZ-NH1	5.45	126.95	121.50
1	A	71	GLY	CA-C-O	5.45	130.05	120.57
2	B	30	LEU	CB-CG-CD2	5.45	127.04	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	PHE	CE1-CZ-CE2	-5.44	110.21	120.00
1	A	31	ARG	CA-C-N	-5.43	111.95	122.06
1	A	31	ARG	C-N-CA	-5.43	111.95	122.06
1	A	94	ASN	N-CA-C	-5.43	101.65	109.48
1	A	117	PHE	CZ-CE2-CD2	5.43	129.78	120.00
2	D	95	LEU	N-CA-CB	-5.43	101.93	110.46
1	A	122	HIS	CG-ND1-CE1	5.43	118.53	109.30
2	D	91	HIS	CB-CA-C	5.43	120.49	110.56
1	A	113	LEU	CB-CG-CD2	5.43	126.98	110.70
1	C	127	LYS	CD-CE-NZ	5.42	129.25	111.90
2	D	13	PHE	CG-CD1-CE1	5.42	129.91	120.70
2	D	87	LEU	CD1-CG-CD2	5.42	122.72	110.80
1	C	16	LYS	CA-C-N	5.42	131.72	121.97
1	C	16	LYS	C-N-CA	5.42	131.72	121.97
1	A	114	PRO	CB-CA-C	5.41	120.49	111.56
1	A	90	LYS	CB-CA-C	-5.41	102.15	110.81
2	D	96	HIS	CB-CG-CD2	5.41	138.23	131.20
2	B	40	PHE	CG-CD1-CE1	5.39	129.87	120.70
1	A	20	ASN	N-CA-C	-5.39	105.84	112.90
2	B	105	LEU	CD1-CG-CD2	-5.39	98.95	110.80
2	D	14	TRP	CD1-NE1-CE2	-5.39	99.20	108.90
2	B	36	TRP	CA-CB-CG	5.38	123.83	113.60
2	B	40	PHE	CB-CG-CD1	-5.38	111.55	120.70
2	D	76	HIS	ND1-CE1-NE2	5.38	113.78	108.40
2	D	130	GLN	CB-CA-C	5.38	119.72	110.79
1	A	33	PHE	N-CA-C	5.38	117.84	111.33
1	C	40	LYS	CA-C-O	5.37	125.87	119.10
2	D	36	TRP	N-CA-CB	5.37	118.49	110.22
1	A	85	ASN	N-CA-CB	5.37	119.57	110.49
1	A	89	HIS	CA-C-O	-5.37	111.67	120.80
1	A	101	LEU	N-CA-CB	5.37	118.62	110.14
2	D	56	ASN	CA-C-N	5.37	126.55	119.84
2	D	56	ASN	C-N-CA	5.37	126.55	119.84
2	B	39	ARG	CB-CA-C	-5.36	101.03	109.34
1	A	6	ASN	CA-CB-CG	-5.36	107.24	112.60
2	B	72	GLN	CA-CB-CG	5.35	124.81	114.10
2	B	60	LYS	CA-C-O	5.35	128.16	120.51
1	C	110	ALA	CB-CA-C	-5.35	102.47	110.50
1	C	98	PHE	CG-CD2-CE2	-5.35	111.61	120.70
2	B	141	ALA	N-CA-C	5.35	119.78	112.88
2	B	129	PHE	CG-CD2-CE2	5.34	129.78	120.70
2	B	75	LYS	CA-C-N	-5.34	111.34	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	75	LYS	C-N-CA	-5.34	111.34	121.54
2	D	140	LEU	N-CA-C	-5.34	102.61	111.37
2	B	34	TYR	C-N-CD	-5.34	103.12	125.00
1	A	68	LYS	CB-CA-C	5.33	120.32	110.56
2	B	47	LEU	CB-CG-CD2	5.33	126.71	110.70
1	A	39	THR	OG1-CB-CG2	-5.33	98.63	109.30
2	B	29	ARG	CB-CA-C	-5.33	100.12	110.46
2	B	36	TRP	CB-CG-CD2	5.33	134.26	126.80
2	B	141	ALA	CA-C-O	5.33	125.88	119.59
2	D	6	GLU	CG-CD-OE1	5.32	130.64	118.40
2	D	132	VAL	CB-CA-C	5.32	120.88	112.26
2	B	33	VAL	O-C-N	-5.32	115.93	122.57
2	D	12	GLY	N-CA-C	-5.31	97.90	113.30
2	B	99	PRO	CA-N-CD	5.31	119.43	112.00
1	C	99	LYS	CD-CE-NZ	5.31	128.88	111.90
1	A	95	PRO	O-C-N	-5.30	116.14	122.24
2	D	141	ALA	CB-CA-C	5.30	120.98	110.17
1	A	34	LEU	CB-CG-CD2	-5.30	94.80	110.70
2	D	20	ASP	CB-CG-OD1	-5.30	106.21	118.40
2	D	58	LYS	CD-CE-NZ	5.30	128.86	111.90
2	B	58	LYS	N-CA-CB	-5.30	102.39	110.07
2	B	122	THR	CB-CA-C	-5.29	97.45	109.10
1	A	92	ARG	CA-CB-CG	-5.29	103.51	114.10
2	B	58	LYS	CD-CE-NZ	-5.28	95.00	111.90
1	A	5	ALA	CB-CA-C	5.28	120.28	109.67
2	B	105	LEU	N-CA-C	-5.28	99.55	110.80
2	D	112	VAL	CG1-CB-CG2	5.28	122.41	110.80
2	B	93	ASN	CB-CA-C	-5.28	99.92	110.42
2	D	2	LEU	CA-C-N	5.28	131.61	121.54
2	D	2	LEU	C-N-CA	5.28	131.61	121.54
1	C	41	THR	N-CA-C	-5.27	105.20	111.69
1	A	90	LYS	CA-CB-CG	5.27	124.64	114.10
2	D	36	TRP	CA-C-N	-5.27	112.91	120.82
2	D	36	TRP	C-N-CA	-5.27	112.91	120.82
2	B	132	VAL	CB-CA-C	-5.27	102.65	111.29
1	A	12	ALA	CB-CA-C	-5.26	99.96	110.42
1	C	134	THR	N-CA-C	-5.25	104.61	111.02
1	A	66	LEU	CB-CA-C	5.25	120.87	110.42
2	B	128	LEU	CB-CG-CD2	5.25	126.45	110.70
2	D	139	ALA	O-C-N	5.25	129.57	122.59
2	D	81	LYS	O-C-N	5.24	129.15	122.33
1	A	75	ASP	N-CA-C	-5.24	104.06	110.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	26	ALA	N-CA-CB	5.24	117.82	110.12
2	B	127	ALA	CB-CA-C	-5.24	99.99	110.42
2	D	127	ALA	CA-C-N	5.23	131.54	121.54
2	D	127	ALA	C-N-CA	5.23	131.54	121.54
2	D	43	HIS	CB-CA-C	5.23	120.83	110.42
1	A	117	PHE	CD1-CE1-CZ	-5.23	110.58	120.00
1	C	21	ALA	C-N-CD	5.23	146.44	125.00
1	A	67	THR	CA-C-N	5.23	133.09	121.80
1	A	67	THR	C-N-CA	5.23	133.09	121.80
2	B	120	GLN	OE1-CD-NE2	5.22	127.82	122.60
2	D	120	GLN	CG-CD-NE2	-5.21	108.58	116.40
1	A	126	ASN	CB-CG-OD1	5.21	131.22	120.80
2	B	59	VAL	CA-CB-CG2	5.21	119.26	110.40
2	B	65	ARG	CG-CD-NE	-5.21	100.54	112.00
2	B	16	LYS	CD-CE-NZ	5.21	128.56	111.90
2	B	49	SER	CA-C-N	5.20	133.03	121.80
2	B	49	SER	C-N-CA	5.20	133.03	121.80
1	C	29	LEU	CA-C-N	5.20	129.52	120.68
1	C	29	LEU	C-N-CA	5.20	129.52	120.68
2	B	87	LEU	CA-CB-CG	5.20	134.49	116.30
1	C	83	LEU	CB-CG-CD2	-5.20	95.11	110.70
1	A	72	HIS	CB-CG-CD2	-5.20	124.45	131.20
2	B	40	PHE	N-CA-CB	-5.20	101.93	110.40
2	B	59	VAL	CA-C-N	-5.20	111.62	121.54
2	B	59	VAL	C-N-CA	-5.20	111.62	121.54
2	B	88	SER	CA-CB-OG	5.19	121.49	111.10
2	B	47	LEU	N-CA-C	-5.19	105.41	112.26
2	B	140	LEU	CA-CB-CG	5.19	134.46	116.30
1	C	14	TRP	NE1-CE2-CZ2	5.19	137.89	130.10
1	C	50	HIS	CE1-NE2-CD2	-5.19	103.81	109.00
2	D	65	ARG	CA-C-N	-5.19	112.64	121.97
2	D	65	ARG	C-N-CA	-5.19	112.64	121.97
1	A	63	ALA	O-C-N	-5.18	116.16	122.22
2	B	117	PHE	CZ-CE2-CD2	5.18	129.33	120.00
1	A	10	VAL	CA-CB-CG2	-5.18	101.59	110.40
1	C	66	LEU	N-CA-C	5.18	118.06	111.69
2	D	69	ALA	N-CA-C	5.18	116.61	110.97
1	A	138	SER	CA-C-N	5.17	131.42	121.54
1	A	138	SER	C-N-CA	5.17	131.42	121.54
1	A	24	TYR	CE1-CZ-CE2	-5.17	109.96	120.30
1	A	128	PHE	N-CA-CB	5.17	119.23	110.49
1	C	108	THR	CB-CA-C	-5.17	103.17	111.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	117	PHE	CA-C-N	-5.17	112.69	120.65
2	D	117	PHE	C-N-CA	-5.17	112.69	120.65
1	C	58	HIS	N-CA-C	5.17	116.99	111.36
1	C	111	SER	N-CA-CB	-5.16	102.31	110.06
1	C	42	TYR	OH-CZ-CE2	5.16	135.38	119.90
2	B	119	GLY	O-C-N	-5.16	115.57	122.48
2	B	86	GLN	CB-CA-C	5.15	119.89	110.10
1	C	66	LEU	CA-C-O	5.15	125.96	120.24
1	C	84	SER	CA-C-O	-5.15	113.15	120.51
1	A	48	LEU	CB-CA-C	5.15	117.55	111.22
1	C	90	LYS	CG-CD-CE	5.15	123.14	111.30
2	B	93	ASN	N-CA-CB	5.15	119.19	110.49
1	A	19	GLY	O-C-N	-5.15	116.40	122.27
1	C	140	TYR	O-C-N	5.15	129.56	123.33
1	C	115	THR	OG1-CB-CG2	-5.14	99.01	109.30
1	A	39	THR	N-CA-CB	-5.14	102.56	110.12
2	D	41	PHE	CG-CD2-CE2	-5.14	111.97	120.70
1	A	120	ALA	CB-CA-C	5.13	119.00	110.90
1	A	22	PRO	CA-N-CD	-5.12	104.83	112.00
1	A	14	TRP	NE1-CE2-CD2	5.12	114.06	107.40
1	A	43	PHE	CG-CD2-CE2	-5.12	111.99	120.70
1	C	93	VAL	N-CA-CB	-5.12	102.78	111.23
1	C	35	SER	N-CA-CB	5.12	119.03	110.32
2	B	14	TRP	CB-CA-C	-5.12	100.23	110.42
1	A	80	LEU	CA-CB-CG	-5.11	98.41	116.30
2	B	62	HIS	N-CA-C	-5.11	99.92	110.80
1	C	62	VAL	CA-CB-CG2	5.11	119.08	110.40
2	B	130	GLN	CA-C-O	-5.10	115.20	120.92
2	D	17	VAL	CB-CA-C	-5.10	102.92	111.29
2	D	33	VAL	CB-CA-C	5.10	118.70	112.02
1	C	7	LYS	N-CA-CB	-5.10	101.88	110.49
2	D	112	VAL	N-CA-C	-5.09	105.42	112.50
2	B	19	VAL	N-CA-C	5.09	119.93	109.34
2	D	18	ASP	CB-CA-C	5.09	119.09	109.37
1	A	69	ALA	CB-CA-C	5.09	119.50	110.85
1	C	99	LYS	N-CA-CB	-5.09	101.95	110.39
2	B	23	GLY	N-CA-C	-5.08	101.14	113.18
2	D	11	THR	OG1-CB-CG2	-5.08	99.14	109.30
2	D	62	HIS	N-CA-C	5.08	121.61	110.80
2	D	14	TRP	CD2-CE2-CZ2	5.07	127.47	122.40
1	A	104	SER	O-C-N	5.07	127.49	122.12
1	A	127	LYS	N-CA-CB	5.07	119.06	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	32	VAL	CA-C-O	-5.07	114.94	120.97
2	D	114	ALA	CA-C-O	-5.06	101.06	118.58
1	A	2	LEU	CA-CB-CG	-5.06	98.58	116.30
2	D	120	GLN	CA-C-N	5.06	131.21	121.54
2	D	120	GLN	C-N-CA	5.06	131.21	121.54
1	A	112	HIS	CA-C-N	-5.06	117.19	123.21
1	A	112	HIS	C-N-CA	-5.06	117.19	123.21
1	A	127	LYS	CB-CA-C	-5.06	100.35	110.42
1	C	73	LEU	CA-C-O	5.06	127.74	120.51
2	D	122	THR	CA-C-O	-5.06	113.23	120.16
1	C	14	TRP	CD2-CE2-CZ2	-5.05	117.35	122.40
2	D	80	LEU	CA-CB-CG	5.05	133.97	116.30
2	D	102	PHE	CB-CG-CD2	-5.05	112.12	120.70
1	A	79	THR	CB-CA-C	-5.05	102.93	110.90
1	A	129	LEU	N-CA-CB	5.04	118.10	110.14
2	B	30	LEU	O-C-N	-5.04	116.32	122.11
2	D	14	TRP	CB-CA-C	-5.03	100.41	110.42
2	D	66	VAL	CA-CB-CG1	5.03	118.96	110.40
1	A	140	TYR	O-C-N	-5.03	115.90	122.59
2	B	66	VAL	CA-C-O	-5.03	114.49	120.78
2	D	98	ASN	C-N-CD	5.03	145.62	125.00
2	B	85	ALA	N-CA-CB	-5.03	101.99	110.49
2	D	21	VAL	N-CA-C	5.03	115.75	110.62
2	D	64	LYS	CA-CB-CG	-5.03	104.04	114.10
1	C	89	HIS	CA-CB-CG	-5.03	108.77	113.80
1	C	75	ASP	CA-C-N	-5.02	109.54	121.80
1	C	75	ASP	C-N-CA	-5.02	109.54	121.80
2	B	121	PHE	CG-CD1-CE1	5.02	129.24	120.70
2	B	122	THR	N-CA-C	-5.01	96.96	111.00
2	D	49	SER	CA-CB-OG	5.01	121.13	111.10
2	B	121	PHE	CD1-CE1-CZ	5.01	129.02	120.00
1	C	141	ARG	CA-C-O	-5.01	105.96	121.00
2	D	62	HIS	CB-CA-C	-5.01	100.45	110.42
2	B	30	LEU	CD1-CG-CD2	-5.01	99.78	110.80
1	C	1	VAL	N-CA-C	-5.00	96.99	111.00
1	C	14	TRP	CA-CB-CG	-5.00	104.09	113.60
1	C	30	GLN	N-CA-C	-5.00	105.92	112.23
1	C	45	HIS	CA-CB-CG	5.00	118.80	113.80
1	A	119	PRO	CA-N-CD	5.00	119.00	112.00
1	C	140	TYR	OH-CZ-CE2	5.00	134.91	119.90

All (19) chirality outliers are listed below:

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

All (184) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Peptide,Mainchain
1	A	100	LEU	Mainchain
1	A	102	SER	Mainchain
1	A	103	HIS	Mainchain
1	A	104	SER	Mainchain
1	A	106	LEU	Mainchain
1	A	107	VAL	Peptide
1	A	111	SER	Mainchain
1	A	117	PHE	Sidechain
1	A	127	LYS	Mainchain
1	A	131	ASN	Mainchain
1	A	132	ASP	Sidechain
1	A	138	SER	Mainchain
1	A	15	GLY	Peptide
1	A	22	PRO	Mainchain
1	A	24	TYR	Sidechain
1	A	26	ALA	Mainchain
1	A	28	ALA	Peptide,Mainchain
1	A	29	LEU	Mainchain
1	A	3	SER	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	30	GLN	Peptide
1	A	31	ARG	Sidechain
1	A	33	PHE	Sidechain
1	A	37	PRO	Mainchain
1	A	40	LYS	Mainchain
1	A	41	THR	Peptide
1	A	42	TYR	Sidechain
1	A	45	HIS	Peptide
1	A	46	PHE	Peptide,Mainchain
1	A	49	SER	Peptide,Mainchain
1	A	50	HIS	Mainchain
1	A	51	GLY	Mainchain
1	A	55	GLN	Mainchain
1	A	70	GLN	Mainchain
1	A	74	ASN	Mainchain
1	A	8	SER	Peptide,Mainchain
1	A	80	LEU	Peptide
1	A	85	ASN	Mainchain,Sidechain
1	A	89	HIS	Mainchain,Sidechain
1	A	92	ARG	Peptide,Sidechain
1	A	97	ASN	Mainchain
1	A	98	PHE	Mainchain,Sidechain
1	A	99	LYS	Mainchain
2	B	1	MET	Mainchain
2	B	10	VAL	Mainchain
2	B	100	GLN	Sidechain
2	B	101	ASN	Mainchain
2	B	102	PHE	Sidechain
2	B	103	ARG	Mainchain,Sidechain
2	B	115	ARG	Sidechain
2	B	118	GLY	Mainchain
2	B	121	PHE	Sidechain
2	B	129	PHE	Sidechain
2	B	13	PHE	Mainchain
2	B	136	VAL	Mainchain
2	B	137	ALA	Mainchain
2	B	144	TYR	Sidechain
2	B	16	LYS	Mainchain
2	B	18	ASP	Sidechain
2	B	21	VAL	Mainchain
2	B	29	ARG	Sidechain
2	B	32	VAL	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	39	ARG	Sidechain
2	B	43	HIS	Sidechain
2	B	44	PHE	Sidechain
2	B	46	ASN	Mainchain
2	B	5	GLU	Mainchain
2	B	55	ASN	Sidechain
2	B	59	VAL	Mainchain
2	B	6	GLU	Mainchain
2	B	65	ARG	Sidechain
2	B	67	LEU	Mainchain
2	B	68	ASP	Peptide
2	B	71	THR	Mainchain
2	B	72	GLN	Mainchain
2	B	74	LEU	Mainchain
2	B	76	HIS	Sidechain
2	B	82	GLY	Peptide
2	B	84	PHE	Mainchain
2	B	87	LEU	Mainchain
2	B	95	LEU	Mainchain
2	B	96	HIS	Sidechain
1	C	1	VAL	Mainchain
1	C	103	HIS	Mainchain
1	C	11	LYS	Mainchain
1	C	111	SER	Mainchain
1	C	115	THR	Mainchain
1	C	117	PHE	Peptide
1	C	12	ALA	Mainchain
1	C	120	ALA	Mainchain
1	C	125	LEU	Mainchain
1	C	126	ASN	Sidechain
1	C	131	ASN	Mainchain
1	C	135	VAL	Mainchain
1	C	137	THR	Mainchain
1	C	139	LYS	Peptide
1	C	140	TYR	Mainchain
1	C	16	LYS	Mainchain
1	C	2	LEU	Mainchain
1	C	24	TYR	Sidechain
1	C	35	SER	Mainchain
1	C	38	THR	Mainchain
1	C	42	TYR	Mainchain,Sidechain
1	C	47	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	49	SER	Mainchain
1	C	50	HIS	Sidechain
1	C	54	GLN	Mainchain
1	C	55	GLN	Mainchain
1	C	57	ALA	Mainchain
1	C	58	HIS	Sidechain
1	C	62	VAL	Peptide
1	C	72	HIS	Sidechain
1	C	79	THR	Mainchain
1	C	80	LEU	Mainchain
1	C	82	ASN	Sidechain
1	C	83	LEU	Peptide
1	C	84	SER	Peptide,Mainchain
1	C	85	ASN	Mainchain
1	C	91	LEU	Mainchain
1	C	92	ARG	Sidechain
1	C	93	VAL	Mainchain
2	D	10	VAL	Mainchain
2	D	102	PHE	Sidechain
2	D	103	ARG	Sidechain
2	D	105	LEU	Mainchain
2	D	114	ALA	Mainchain
2	D	115	ARG	Sidechain
2	D	116	ASN	Sidechain
2	D	117	PHE	Peptide,Mainchain,Sidechain
2	D	12	GLY	Mainchain
2	D	124	ASN	Mainchain
2	D	126	GLN	Sidechain
2	D	127	ALA	Mainchain
2	D	129	PHE	Sidechain
2	D	133	VAL	Mainchain
2	D	135	GLY	Mainchain
2	D	137	ALA	Peptide
2	D	138	ASN	Peptide,Mainchain
2	D	142	HIS	Peptide,Sidechain
2	D	143	LYS	Mainchain
2	D	144	TYR	Sidechain
2	D	17	VAL	Mainchain
2	D	18	ASP	Sidechain
2	D	2	LEU	Mainchain
2	D	28	GLY	Mainchain
2	D	29	ARG	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	D	34	TYR	Sidechain
2	D	39	ARG	Sidechain
2	D	42	GLN	Peptide
2	D	44	PHE	Sidechain
2	D	5	GLU	Peptide,Mainchain
2	D	53	VAL	Mainchain
2	D	55	ASN	Sidechain
2	D	65	ARG	Sidechain
2	D	67	LEU	Mainchain
2	D	69	ALA	Mainchain
2	D	71	THR	Peptide
2	D	72	GLN	Mainchain
2	D	73	GLY	Peptide
2	D	76	HIS	Mainchain,Sidechain
2	D	77	LEU	Mainchain
2	D	8	ALA	Peptide
2	D	88	SER	Mainchain
2	D	89	GLY	Peptide
2	D	9	ALA	Mainchain
2	D	99	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1076	0	1041	839	80
1	C	1076	0	1038	826	3
2	B	1116	0	1081	1146	0
2	D	1116	0	1079	947	77
3	A	43	0	30	49	0
3	B	43	0	30	56	0
3	C	43	0	30	42	0
3	D	43	0	30	29	0
All	All	4556	0	4359	3772	80

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 423.

All (3772) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:TYR:CZ	2:B:34:TYR:CE2	1.79	1.70
2:B:144:TYR:CD2	2:B:144:TYR:CG	1.76	1.69
3:A:142:HEM:CMA	3:A:142:HEM:C3A	1.75	1.67
1:C:140:TYR:CB	1:C:140:TYR:CG	1.77	1.67
2:D:14:TRP:CE3	2:D:14:TRP:CZ3	1.76	1.66
1:C:103:HIS:CB	1:C:103:HIS:CG	1.78	1.66
2:D:22:VAL:CB	2:D:22:VAL:CG1	1.74	1.65
2:B:84:PHE:CB	2:B:84:PHE:CG	1.76	1.65
1:A:14:TRP:CZ2	1:A:14:TRP:CH2	1.79	1.65
1:C:91:LEU:CB	1:C:91:LEU:CG	1.75	1.65
3:C:142:HEM:CAB	3:C:142:HEM:C3B	1.80	1.65
1:C:86:LEU:CD1	1:C:86:LEU:CG	1.75	1.64
1:A:36:PHE:CB	1:A:36:PHE:CG	1.78	1.64
2:B:70:PHE:CZ	2:B:70:PHE:CE2	1.84	1.64
2:D:123:PRO:CG	2:D:123:PRO:CD	1.74	1.64
1:A:2:LEU:CA	1:A:2:LEU:CB	1.76	1.64
2:B:70:PHE:CZ	2:B:70:PHE:CE1	1.76	1.64
1:A:140:TYR:CB	1:A:140:TYR:CG	1.79	1.64
1:C:7:LYS:CB	1:C:7:LYS:CG	1.75	1.63
2:D:41:PHE:CD2	2:D:41:PHE:CE2	1.75	1.63
1:A:63:ALA:CA	1:A:63:ALA:CB	1.75	1.63
1:A:81:SER:CA	1:A:81:SER:CB	1.76	1.63
3:A:142:HEM:CAA	3:A:142:HEM:CBA	1.75	1.62
3:A:142:HEM:CAD	3:A:142:HEM:CBD	1.74	1.62
2:B:41:PHE:CZ	2:B:41:PHE:CE1	1.78	1.62
2:B:64:LYS:CG	2:B:64:LYS:CD	1.75	1.62
1:C:23:ALA:CB	1:C:23:ALA:CA	1.75	1.62
1:C:24:TYR:CB	1:C:24:TYR:CG	1.83	1.62
2:D:2:LEU:CB	2:D:2:LEU:CG	1.76	1.62
2:D:60:LYS:CD	2:D:60:LYS:CE	1.78	1.62
3:D:146:HEM:CAA	3:D:146:HEM:CBA	1.77	1.61
3:B:146:HEM:CAD	3:B:146:HEM:C3D	1.77	1.61
1:C:92:ARG:CD	1:C:92:ARG:CG	1.78	1.61
3:A:142:HEM:C1D	3:A:142:HEM:C2D	1.78	1.61
2:B:102:PHE:CD1	2:B:102:PHE:CG	1.89	1.61
2:D:81:LYS:CB	2:D:81:LYS:CA	1.76	1.61
2:B:36:TRP:CD2	2:B:36:TRP:CG	1.85	1.61
2:D:120:GLN:CG	2:D:120:GLN:CB	1.78	1.61
1:C:117:PHE:CD2	1:C:117:PHE:CE2	1.82	1.61
2:B:11:THR:CA	2:B:11:THR:CB	1.79	1.60
1:C:54:GLN:CG	1:C:54:GLN:CB	1.75	1.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LEU:CA	1:C:136:LEU:CB	1.78	1.60
2:D:17:VAL:C	2:D:17:VAL:CA	1.75	1.60
2:D:59:VAL:CB	2:D:59:VAL:CG2	1.77	1.60
2:D:84:PHE:CG	2:D:84:PHE:CD1	1.84	1.60
1:A:22:PRO:CB	1:A:22:PRO:CG	1.77	1.60
1:A:93:VAL:CG1	1:A:93:VAL:CB	1.79	1.60
1:A:137:THR:CA	1:A:137:THR:CB	1.79	1.60
2:B:10:VAL:CG1	2:B:10:VAL:CB	1.79	1.60
1:C:24:TYR:CD2	1:C:24:TYR:CE2	1.89	1.60
1:C:3:SER:C	1:C:3:SER:CA	1.74	1.60
2:D:22:VAL:CB	2:D:22:VAL:CG2	1.74	1.60
2:B:117:PHE:CG	2:B:117:PHE:CD1	1.81	1.60
1:C:68:LYS:CG	1:C:68:LYS:CB	1.75	1.60
2:B:16:LYS:CD	2:B:16:LYS:CE	1.80	1.59
2:B:21:VAL:CA	2:B:21:VAL:CB	1.77	1.59
2:B:68:ASP:CG	2:B:68:ASP:CB	1.74	1.59
2:B:77:LEU:CB	2:B:77:LEU:CA	1.79	1.59
1:C:128:PHE:CE1	1:C:128:PHE:CZ	1.84	1.59
3:D:146:HEM:C2B	3:D:146:HEM:CMB	1.80	1.59
1:A:2:LEU:CB	1:A:2:LEU:CG	1.74	1.59
1:A:16:LYS:CD	1:A:16:LYS:CE	1.77	1.59
1:A:41:THR:CA	1:A:41:THR:CB	1.80	1.59
1:A:79:THR:CA	1:A:79:THR:CB	1.76	1.59
1:C:60:GLN:CB	1:C:60:GLN:CG	1.76	1.59
1:C:80:LEU:CA	1:C:80:LEU:C	1.75	1.59
2:B:4:ALA:C	2:B:4:ALA:CA	1.75	1.59
1:C:61:LYS:CG	1:C:61:LYS:CD	1.76	1.59
2:D:86:GLN:CA	2:D:86:GLN:CB	1.76	1.59
1:A:91:LEU:CD2	1:A:91:LEU:CG	1.78	1.59
1:A:127:LYS:CE	1:A:127:LYS:CD	1.77	1.59
2:B:10:VAL:HG11	2:B:128:LEU:CD2	1.17	1.59
2:B:103:ARG:CB	2:B:103:ARG:CG	1.78	1.59
1:A:1:VAL:CB	1:A:1:VAL:CG1	1.75	1.59
1:A:12:ALA:CA	1:A:12:ALA:CB	1.81	1.59
1:C:17:VAL:CG1	1:C:17:VAL:CB	1.78	1.58
1:C:32:MET:CB	1:C:32:MET:CA	1.76	1.58
1:C:75:ASP:CA	1:C:75:ASP:CB	1.77	1.58
1:C:76:LEU:CD1	1:C:76:LEU:CG	1.78	1.58
1:C:91:LEU:CG	1:C:91:LEU:CD1	1.79	1.58
2:D:6:GLU:CA	2:D:6:GLU:CB	1.79	1.58
2:D:47:LEU:CA	2:D:47:LEU:CB	1.77	1.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:LYS:CG	2:D:75:LYS:CD	1.76	1.58
1:A:3:SER:CA	1:A:3:SER:CB	1.75	1.58
1:A:65:ALA:CA	1:A:65:ALA:CB	1.76	1.58
1:A:73:LEU:CD2	1:A:73:LEU:CG	1.81	1.58
2:B:26:ALA:C	2:B:26:ALA:CA	1.74	1.58
2:B:31:LEU:CG	2:B:31:LEU:CD1	1.77	1.58
2:B:94:LYS:C	2:B:94:LYS:CA	1.74	1.58
3:B:146:HEM:C2B	3:B:146:HEM:CMB	1.84	1.58
1:C:54:GLN:CA	1:C:54:GLN:C	1.76	1.58
2:D:76:HIS:CG	2:D:76:HIS:CB	1.86	1.58
1:A:55:GLN:CA	1:A:55:GLN:CB	1.81	1.58
1:A:93:VAL:CB	1:A:93:VAL:CG2	1.74	1.58
2:B:97:VAL:CA	2:B:97:VAL:CB	1.75	1.58
2:D:10:VAL:CA	2:D:10:VAL:C	1.77	1.58
1:A:31:ARG:CG	1:A:31:ARG:CD	1.74	1.58
1:A:41:THR:CB	1:A:41:THR:CG2	1.77	1.58
1:A:128:PHE:CD1	1:A:128:PHE:CE1	1.83	1.58
2:B:68:ASP:CA	2:B:71:THR:CG2	1.75	1.58
1:C:116:ASN:CA	1:C:116:ASN:C	1.77	1.58
1:A:10:VAL:CA	1:A:10:VAL:C	1.76	1.58
2:B:87:LEU:CA	2:B:87:LEU:C	1.76	1.58
1:C:133:SER:CA	1:C:133:SER:C	1.77	1.58
1:C:138:SER:CA	1:C:138:SER:CB	1.82	1.58
2:D:73:GLY:CA	2:D:73:GLY:C	1.75	1.58
2:B:16:LYS:CE	2:B:16:LYS:NZ	1.67	1.57
1:C:83:LEU:CD2	1:C:83:LEU:CG	1.78	1.57
2:D:14:TRP:CA	2:D:14:TRP:C	1.77	1.57
1:A:127:LYS:CB	1:A:127:LYS:CG	1.78	1.57
2:B:128:LEU:CA	2:B:128:LEU:C	1.75	1.57
1:A:139:LYS:CE	1:A:139:LYS:CD	1.77	1.57
1:C:66:LEU:CG	1:C:66:LEU:CD2	1.81	1.57
1:C:71:GLY:C	1:C:71:GLY:CA	1.76	1.57
1:A:104:SER:CB	1:A:104:SER:CA	1.78	1.57
2:B:1:MET:HG2	2:B:77:LEU:CD1	1.29	1.57
2:B:128:LEU:CG	2:B:128:LEU:CD1	1.74	1.57
1:A:7:LYS:CD	1:A:7:LYS:CE	1.79	1.57
1:A:43:PHE:CB	1:A:43:PHE:CA	1.77	1.57
2:B:43:HIS:CA	2:B:43:HIS:C	1.78	1.57
2:B:86:GLN:CG	2:B:86:GLN:CB	1.75	1.57
2:D:64:LYS:CG	2:D:64:LYS:CD	1.74	1.57
1:C:22:PRO:CG	1:C:22:PRO:CD	1.82	1.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:THR:CB	1:C:108:THR:CG2	1.78	1.56
2:D:121:PHE:CA	2:D:121:PHE:CB	1.83	1.56
1:A:97:ASN:N	1:A:97:ASN:CA	1.69	1.56
1:A:136:LEU:CD1	1:A:136:LEU:CG	1.79	1.56
3:A:142:HEM:NB	3:A:142:HEM:C4B	1.67	1.56
2:B:94:LYS:CG	2:B:94:LYS:CD	1.75	1.56
2:D:31:LEU:CA	2:D:31:LEU:CB	1.81	1.56
2:D:43:HIS:CA	2:D:43:HIS:CB	1.84	1.56
1:A:43:PHE:CD2	1:A:43:PHE:CG	1.86	1.56
1:A:57:ALA:CA	1:A:57:ALA:CB	1.74	1.56
1:A:85:ASN:C	1:A:85:ASN:CA	1.76	1.56
2:B:3:THR:HG23	2:B:5:GLU:CB	1.12	1.56
2:B:17:VAL:C	2:B:17:VAL:CA	1.76	1.56
2:B:64:LYS:NZ	2:B:64:LYS:CE	1.68	1.56
1:C:80:LEU:CG	1:C:80:LEU:CD1	1.83	1.56
2:D:103:ARG:CG	2:D:103:ARG:CD	1.75	1.56
2:B:116:ASN:CA	2:B:116:ASN:CB	1.77	1.56
1:A:50:HIS:CG	1:A:50:HIS:CB	1.87	1.56
2:B:140:LEU:CD1	2:B:140:LEU:CG	1.75	1.56
1:C:28:ALA:N	1:C:28:ALA:CA	1.69	1.56
1:C:76:LEU:CG	1:C:76:LEU:CD2	1.76	1.56
1:C:133:SER:CA	1:C:133:SER:CB	1.74	1.56
2:D:12:GLY:N	2:D:12:GLY:CA	1.68	1.56
2:D:93:ASN:CB	2:D:93:ASN:CG	1.76	1.56
2:D:144:TYR:CE1	2:D:144:TYR:CZ	1.94	1.56
1:A:62:VAL:CG1	1:A:62:VAL:CB	1.83	1.55
1:A:105:LEU:CD1	1:A:105:LEU:CG	1.76	1.55
2:B:45:GLY:N	2:B:45:GLY:CA	1.67	1.55
1:C:29:LEU:CA	1:C:29:LEU:CB	1.77	1.55
1:C:36:PHE:CA	1:C:36:PHE:CB	1.84	1.55
1:C:101:LEU:CA	1:C:101:LEU:CB	1.77	1.55
2:D:65:ARG:CA	2:D:65:ARG:C	1.75	1.55
2:D:81:LYS:CD	2:D:81:LYS:CE	1.75	1.55
2:B:13:PHE:CA	2:B:13:PHE:C	1.79	1.55
2:B:128:LEU:CA	2:B:128:LEU:CB	1.82	1.55
2:D:69:ALA:C	2:D:69:ALA:CA	1.74	1.55
2:D:105:LEU:CD1	2:D:105:LEU:CG	1.76	1.55
2:B:16:LYS:N	2:B:16:LYS:CA	1.68	1.55
1:C:47:ASP:CB	1:C:47:ASP:CG	1.76	1.55
2:D:11:THR:C	2:D:11:THR:CA	1.79	1.55
2:D:62:HIS:CG	2:D:62:HIS:ND1	1.70	1.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:HIS:NE2	2:D:62:HIS:CE1	1.68	1.55
2:D:120:GLN:CG	2:D:120:GLN:CD	1.78	1.55
1:A:60:GLN:CA	1:A:60:GLN:C	1.77	1.55
2:B:37:THR:N	2:B:37:THR:CA	1.69	1.55
2:B:40:PHE:C	2:B:40:PHE:CA	1.79	1.55
1:A:35:SER:CA	1:A:35:SER:CB	1.79	1.55
1:A:58:HIS:CA	1:A:58:HIS:CB	1.85	1.55
1:A:119:PRO:CB	1:A:119:PRO:CA	1.81	1.55
1:C:15:GLY:N	1:C:15:GLY:CA	1.69	1.55
1:C:53:ALA:N	1:C:53:ALA:CA	1.70	1.55
1:C:72:HIS:CD2	1:C:72:HIS:CG	1.85	1.55
1:C:86:LEU:CG	1:C:86:LEU:CD2	1.75	1.55
2:D:40:PHE:CZ	2:D:40:PHE:CE2	1.90	1.55
1:A:91:LEU:CG	1:A:91:LEU:CD1	1.79	1.54
3:A:142:HEM:C4D	3:A:142:HEM:CHA	1.89	1.54
2:B:143:LYS:CE	2:B:143:LYS:CD	1.84	1.54
1:C:55:GLN:CB	1:C:55:GLN:CA	1.84	1.54
2:D:2:LEU:CB	2:D:2:LEU:CA	1.81	1.54
1:A:139:LYS:CE	1:A:139:LYS:NZ	1.69	1.54
2:B:141:ALA:N	2:B:141:ALA:CA	1.69	1.54
2:D:18:ASP:CA	2:D:18:ASP:CB	1.81	1.54
2:D:90:LEU:CB	2:D:90:LEU:CG	1.84	1.54
2:B:64:LYS:N	2:B:64:LYS:CA	1.67	1.54
1:A:108:THR:CA	1:A:108:THR:CB	1.82	1.54
2:B:19:VAL:CA	2:B:19:VAL:CB	1.81	1.54
2:B:130:GLN:CB	2:B:130:GLN:CG	1.77	1.54
1:C:114:PRO:N	1:C:114:PRO:CA	1.67	1.54
2:D:36:TRP:CA	2:D:36:TRP:C	1.79	1.54
2:D:68:ASP:CB	2:D:68:ASP:CG	1.78	1.54
2:D:131:LYS:CB	2:D:131:LYS:CG	1.78	1.54
1:A:86:LEU:CD2	1:A:86:LEU:CG	1.84	1.54
1:A:122:HIS:CA	1:A:122:HIS:C	1.74	1.54
2:B:71:THR:CG2	2:B:71:THR:CB	1.78	1.54
3:B:146:HEM:NA	3:B:146:HEM:C4A	1.68	1.54
1:C:39:THR:CA	1:C:39:THR:CB	1.76	1.54
1:C:43:PHE:CA	1:C:43:PHE:CB	1.83	1.54
1:C:64:ASN:CB	1:C:64:ASN:CA	1.82	1.54
1:C:126:ASN:CA	1:C:126:ASN:C	1.76	1.54
1:C:141:ARG:NE	1:C:141:ARG:CD	1.71	1.54
2:D:110:ALA:N	2:D:110:ALA:CA	1.69	1.54
1:A:137:THR:CB	1:A:137:THR:CG2	1.86	1.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:GLY:C	2:B:106:GLY:CA	1.80	1.53
2:B:123:PRO:CG	2:B:123:PRO:CB	1.79	1.53
1:C:113:LEU:CD2	1:C:113:LEU:CG	1.84	1.53
1:C:115:THR:CB	1:C:115:THR:CG2	1.77	1.53
1:A:45:HIS:CA	1:A:45:HIS:CB	1.85	1.53
1:A:88:ALA:C	1:A:88:ALA:CA	1.76	1.53
2:B:4:ALA:CA	2:B:4:ALA:N	1.69	1.53
2:B:49:SER:CA	2:B:49:SER:C	1.75	1.53
1:C:19:GLY:C	1:C:19:GLY:CA	1.79	1.53
1:C:45:HIS:CA	1:C:45:HIS:CB	1.81	1.53
2:D:38:GLN:CG	2:D:38:GLN:CD	1.75	1.53
1:A:114:PRO:CD	1:A:114:PRO:CG	1.81	1.53
1:A:135:VAL:CA	1:A:135:VAL:C	1.77	1.53
2:B:66:VAL:CG1	2:B:66:VAL:CB	1.84	1.53
1:C:83:LEU:CB	1:C:83:LEU:CA	1.79	1.53
2:D:16:LYS:CD	2:D:16:LYS:CB	1.85	1.53
1:A:19:GLY:C	1:A:19:GLY:CA	1.79	1.53
1:A:106:LEU:CD2	1:A:106:LEU:CG	1.85	1.53
1:C:43:PHE:CD1	1:C:43:PHE:CG	1.96	1.53
1:C:99:LYS:CG	1:C:99:LYS:CD	1.82	1.53
2:D:101:ASN:N	2:D:101:ASN:CA	1.68	1.53
1:A:56:LYS:NZ	1:A:56:LYS:CE	1.71	1.53
1:A:116:ASN:N	1:A:116:ASN:CA	1.69	1.53
1:C:114:PRO:N	1:C:114:PRO:CD	1.71	1.53
2:D:61:ALA:CB	2:D:61:ALA:CA	1.84	1.53
2:D:127:ALA:CA	2:D:127:ALA:CB	1.81	1.53
1:A:11:LYS:NZ	1:A:11:LYS:CE	1.72	1.52
1:C:134:THR:N	1:C:134:THR:CA	1.70	1.52
1:C:137:THR:N	1:C:137:THR:CA	1.71	1.52
2:D:107:ASN:N	2:D:107:ASN:CA	1.69	1.52
2:D:112:VAL:CG1	2:D:112:VAL:CB	1.79	1.52
2:D:119:GLY:N	2:D:119:GLY:CA	1.72	1.52
1:A:136:LEU:CA	1:A:136:LEU:C	1.80	1.52
2:B:59:VAL:CB	2:B:59:VAL:CG1	1.82	1.52
2:B:131:LYS:CD	2:B:131:LYS:CG	1.82	1.52
2:B:141:ALA:C	2:B:142:HIS:N	1.68	1.52
2:B:24:ALA:N	2:B:24:ALA:CA	1.68	1.52
2:B:58:LYS:CB	2:B:58:LYS:CG	1.86	1.52
2:B:65:ARG:N	2:B:65:ARG:CA	1.72	1.52
2:B:80:LEU:CD2	2:B:80:LEU:CG	1.81	1.52
1:C:17:VAL:CB	1:C:17:VAL:CG2	1.87	1.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LYS:NZ	1:C:90:LYS:CE	1.70	1.52
2:D:100:GLN:CB	2:D:100:GLN:CG	1.83	1.52
1:A:86:LEU:C	1:A:87:HIS:N	1.68	1.52
2:B:18:ASP:CB	2:B:18:ASP:CG	1.83	1.52
2:D:27:LEU:CG	2:D:27:LEU:CD1	1.84	1.52
2:D:43:HIS:NE2	2:D:43:HIS:CD2	1.75	1.52
1:A:67:THR:C	1:A:67:THR:CA	1.82	1.51
1:C:131:ASN:CA	1:C:131:ASN:CB	1.81	1.51
2:D:16:LYS:CB	2:D:16:LYS:HD3	1.38	1.51
2:D:34:TYR:N	2:D:34:TYR:CA	1.73	1.51
2:D:140:LEU:CD1	2:D:140:LEU:CG	1.85	1.51
1:A:126:ASN:C	1:A:126:ASN:CA	1.79	1.51
2:B:25:GLN:N	2:B:25:GLN:CA	1.68	1.51
2:B:130:GLN:CB	2:B:130:GLN:CA	1.84	1.51
1:C:81:SER:CA	1:C:81:SER:CB	1.88	1.51
2:D:68:ASP:CA	2:D:68:ASP:C	1.82	1.51
1:A:100:LEU:CG	1:A:100:LEU:CB	1.86	1.51
2:B:8:ALA:CA	2:B:8:ALA:CB	1.82	1.51
2:B:43:HIS:CG	2:B:43:HIS:ND1	1.75	1.51
2:B:93:ASN:CG	2:B:93:ASN:CB	1.79	1.51
2:B:119:GLY:N	2:B:119:GLY:CA	1.67	1.51
2:D:75:LYS:CA	2:D:75:LYS:CB	1.85	1.51
1:A:73:LEU:CG	1:A:73:LEU:CD1	1.86	1.51
2:B:22:VAL:CB	2:B:22:VAL:CG2	1.86	1.51
1:C:16:LYS:CG	1:C:16:LYS:CD	1.88	1.51
2:D:52:ALA:CA	2:D:52:ALA:CB	1.83	1.51
2:B:2:LEU:CB	2:B:2:LEU:CA	1.88	1.51
1:C:30:GLN:CG	1:C:30:GLN:CD	1.82	1.51
1:C:79:THR:N	1:C:79:THR:CA	1.69	1.51
2:B:74:LEU:CB	2:B:74:LEU:CG	1.83	1.50
2:B:125:VAL:CG1	2:B:125:VAL:CB	1.89	1.50
1:C:20:ASN:N	1:C:20:ASN:CA	1.71	1.50
1:C:85:ASN:CB	1:C:85:ASN:CG	1.79	1.50
1:C:104:SER:CA	1:C:104:SER:C	1.77	1.50
2:D:59:VAL:C	2:D:59:VAL:CA	1.84	1.50
2:D:86:GLN:CA	2:D:86:GLN:C	1.84	1.50
2:D:145:HIS:CA	2:D:145:HIS:C	1.83	1.50
2:B:2:LEU:CD2	2:B:2:LEU:CG	1.89	1.50
2:B:104:LEU:N	2:B:104:LEU:CA	1.74	1.50
2:B:138:ASN:ND2	2:B:138:ASN:CG	1.70	1.50
2:D:100:GLN:CB	2:D:100:GLN:CA	1.82	1.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:CG	1:A:2:LEU:CD1	1.87	1.50
3:A:142:HEM:C2D	3:A:142:HEM:C4D	1.98	1.50
1:A:48:LEU:CA	1:A:48:LEU:CB	1.86	1.50
1:A:64:ASN:C	1:A:64:ASN:CA	1.81	1.50
1:A:80:LEU:CD2	1:A:80:LEU:CG	1.85	1.50
2:B:57:PRO:CD	2:B:57:PRO:N	1.74	1.50
1:C:105:LEU:CG	1:C:105:LEU:CD1	1.89	1.50
2:D:39:ARG:NE	2:D:39:ARG:CD	1.70	1.50
2:D:124:ASN:CB	2:D:124:ASN:CG	1.84	1.50
2:B:137:ALA:N	2:B:137:ALA:CA	1.71	1.50
1:C:108:THR:CA	1:C:108:THR:C	1.85	1.50
2:D:46:ASN:N	2:D:46:ASN:CA	1.68	1.50
2:D:109:LEU:CD2	2:D:109:LEU:CG	1.89	1.50
1:A:119:PRO:C	1:A:120:ALA:N	1.69	1.50
2:B:3:THR:CG2	2:B:5:GLU:HB3	1.39	1.50
2:B:83:ALA:CA	2:B:83:ALA:CB	1.86	1.50
1:C:97:ASN:CA	1:C:97:ASN:C	1.76	1.50
2:D:44:PHE:CB	2:D:44:PHE:CA	1.86	1.50
2:D:78:ASP:CA	2:D:78:ASP:C	1.85	1.50
2:B:24:ALA:CA	2:B:24:ALA:CB	1.85	1.50
2:B:143:LYS:CD	2:B:143:LYS:CG	1.88	1.50
1:C:129:LEU:CB	1:C:129:LEU:CG	1.87	1.50
2:D:75:LYS:NZ	2:D:75:LYS:CE	1.71	1.50
1:A:11:LYS:C	1:A:12:ALA:N	1.69	1.49
1:A:48:LEU:CD2	1:A:48:LEU:CG	1.90	1.49
2:B:43:HIS:CD2	2:B:43:HIS:NE2	1.79	1.49
2:B:101:ASN:CA	2:B:101:ASN:C	1.85	1.49
2:D:93:ASN:CA	2:D:93:ASN:C	1.80	1.49
1:A:78:GLY:C	1:A:78:GLY:CA	1.81	1.49
1:A:114:PRO:CD	1:A:114:PRO:CB	1.89	1.49
2:B:75:LYS:CG	2:B:75:LYS:CD	1.87	1.49
2:B:86:GLN:CD	2:B:86:GLN:NE2	1.70	1.49
2:B:110:ALA:CA	2:B:110:ALA:CB	1.90	1.49
1:C:44:PRO:CG	1:C:44:PRO:CB	1.91	1.49
1:C:67:THR:CB	1:C:67:THR:CG2	1.87	1.49
1:C:85:ASN:CA	1:C:85:ASN:C	1.83	1.49
2:D:124:ASN:C	2:D:124:ASN:CA	1.83	1.49
2:D:129:PHE:N	2:D:129:PHE:CA	1.76	1.49
1:A:105:LEU:N	1:A:105:LEU:CA	1.73	1.49
2:B:6:GLU:CB	2:B:6:GLU:CA	1.87	1.49
1:C:11:LYS:N	1:C:11:LYS:CA	1.73	1.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:LEU:N	1:C:91:LEU:CA	1.69	1.49
2:D:78:ASP:CG	2:D:78:ASP:CB	1.83	1.49
2:D:88:SER:CB	2:D:88:SER:CA	1.85	1.49
2:D:142:HIS:CA	2:D:142:HIS:CB	1.87	1.49
2:B:42:GLN:CD	2:B:42:GLN:NE2	1.69	1.49
2:B:62:HIS:CG	2:B:62:HIS:ND1	1.68	1.49
1:C:135:VAL:CB	1:C:135:VAL:CG2	1.90	1.49
2:D:67:LEU:CA	2:D:67:LEU:C	1.86	1.49
2:D:96:HIS:CA	2:D:96:HIS:C	1.84	1.49
2:B:128:LEU:CD2	2:B:128:LEU:CG	1.89	1.49
2:D:31:LEU:CA	2:D:31:LEU:C	1.81	1.49
2:D:67:LEU:CA	2:D:67:LEU:CB	1.84	1.49
2:D:76:HIS:N	2:D:76:HIS:CA	1.72	1.49
2:D:141:ALA:C	2:D:142:HIS:N	1.71	1.49
1:A:61:LYS:CA	1:A:61:LYS:CB	1.88	1.48
1:A:103:HIS:CA	1:A:103:HIS:CB	1.88	1.48
2:B:62:HIS:N	2:B:62:HIS:CA	1.74	1.48
2:B:72:GLN:N	2:B:72:GLN:CA	1.70	1.48
2:D:132:VAL:N	2:D:132:VAL:CA	1.72	1.48
2:B:54:MET:N	2:B:54:MET:CA	1.72	1.48
2:B:57:PRO:CD	2:B:57:PRO:CG	1.87	1.48
1:A:29:LEU:CD2	1:A:29:LEU:CG	1.91	1.48
1:C:69:ALA:CA	1:C:69:ALA:C	1.83	1.48
2:B:124:ASN:C	2:B:125:VAL:N	1.68	1.48
2:B:136:VAL:C	2:B:136:VAL:CA	1.81	1.48
1:A:20:ASN:CB	1:A:20:ASN:CG	1.87	1.48
2:B:41:PHE:C	2:B:41:PHE:CA	1.85	1.48
2:B:52:ALA:N	2:B:52:ALA:CA	1.75	1.48
1:C:10:VAL:CB	1:C:10:VAL:CG2	1.90	1.48
2:D:128:LEU:N	2:D:128:LEU:CA	1.72	1.48
3:B:146:HEM:CMA	3:B:146:HEM:C3A	1.95	1.47
1:C:84:SER:CA	1:C:84:SER:C	1.87	1.47
1:C:126:ASN:CG	1:C:126:ASN:ND2	1.70	1.47
3:D:146:HEM:CHA	3:D:146:HEM:C1A	1.94	1.47
1:A:94:ASN:N	1:A:94:ASN:CA	1.75	1.47
2:B:76:HIS:N	2:B:76:HIS:CA	1.74	1.47
1:C:25:GLY:N	1:C:25:GLY:CA	1.75	1.47
1:A:141:ARG:CZ	1:A:141:ARG:NH2	1.76	1.47
1:C:46:PHE:CZ	1:C:46:PHE:CE2	2.01	1.47
1:C:90:LYS:CE	1:C:90:LYS:CD	1.90	1.47
2:D:143:LYS:CD	2:D:143:LYS:CE	1.90	1.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:CB	1:A:29:LEU:CA	1.92	1.47
1:A:124:ASN:CB	1:A:124:ASN:CG	1.87	1.47
2:D:104:LEU:CG	2:D:104:LEU:CB	1.91	1.47
2:D:108:VAL:O	2:D:108:VAL:CA	1.63	1.47
2:B:1:MET:CG	2:B:77:LEU:CD1	1.91	1.47
2:B:98:ASN:CG	2:B:98:ASN:ND2	1.73	1.47
1:C:17:VAL:CA	1:C:17:VAL:C	1.86	1.46
2:D:120:GLN:CD	2:D:120:GLN:NE2	1.72	1.46
1:A:25:GLY:CA	1:A:25:GLY:C	1.87	1.46
2:B:58:LYS:C	2:B:59:VAL:N	1.71	1.46
2:B:80:LEU:C	2:B:81:LYS:N	1.71	1.46
2:B:95:LEU:CA	2:B:95:LEU:CB	1.90	1.46
2:D:115:ARG:CA	2:D:115:ARG:CB	1.93	1.46
2:B:110:ALA:C	2:B:111:LEU:N	1.74	1.46
2:B:140:LEU:CG	2:B:140:LEU:CD2	1.93	1.46
2:D:105:LEU:CD1	2:D:105:LEU:CB	1.90	1.46
2:D:142:HIS:CE1	2:D:142:HIS:ND1	1.68	1.46
1:A:1:VAL:CA	1:A:1:VAL:C	1.87	1.46
1:A:32:MET:C	1:A:33:PHE:N	1.69	1.46
2:B:34:TYR:N	2:B:34:TYR:CA	1.77	1.46
2:B:70:PHE:CZ	2:B:70:PHE:CD2	2.04	1.46
1:C:55:GLN:CG	1:C:55:GLN:CD	1.86	1.46
1:C:139:LYS:CB	1:C:139:LYS:CG	1.91	1.46
2:D:20:ASP:C	2:D:21:VAL:N	1.70	1.46
1:A:17:VAL:CB	1:A:17:VAL:CG2	1.89	1.46
1:A:55:GLN:NE2	1:A:55:GLN:CD	1.73	1.46
1:A:77:PRO:C	1:A:78:GLY:N	1.68	1.46
1:C:111:SER:CA	1:C:111:SER:C	1.86	1.46
1:C:118:THR:OG1	1:C:118:THR:CB	1.63	1.46
2:D:94:LYS:CD	2:D:94:LYS:CE	1.93	1.46
2:B:95:LEU:CB	2:B:95:LEU:N	1.77	1.45
1:C:61:LYS:CD	1:C:61:LYS:CE	1.92	1.45
1:A:69:ALA:N	1:A:69:ALA:CA	1.76	1.45
2:B:126:GLN:CA	2:B:126:GLN:C	1.89	1.45
1:C:20:ASN:C	1:C:21:ALA:N	1.71	1.45
1:A:16:LYS:CD	1:A:16:LYS:NZ	1.74	1.45
2:B:74:LEU:CG	2:B:74:LEU:CD1	1.93	1.45
2:B:113:VAL:CG1	2:B:113:VAL:CB	1.92	1.45
2:D:1:MET:N	2:D:1:MET:CA	1.80	1.45
2:D:71:THR:CB	2:D:71:THR:CG2	1.92	1.45
2:D:92:CYS:C	2:D:92:CYS:CA	1.88	1.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PRO:CA	1:A:44:PRO:CB	1.76	1.45
1:C:3:SER:CA	1:C:3:SER:CB	1.94	1.45
2:D:87:LEU:CB	2:D:87:LEU:CA	1.92	1.45
2:D:131:LYS:CB	2:D:131:LYS:CA	1.94	1.45
3:D:146:HEM:C3C	3:D:146:HEM:C4C	1.83	1.45
1:A:58:HIS:C	1:A:59:GLY:N	1.71	1.45
1:A:91:LEU:N	1:A:91:LEU:CA	1.78	1.45
2:D:42:GLN:CA	2:D:42:GLN:CG	1.93	1.45
2:B:96:HIS:NE2	2:B:96:HIS:CE1	1.68	1.44
2:B:105:LEU:CA	2:B:105:LEU:C	1.87	1.44
2:D:141:ALA:C	2:D:141:ALA:CA	1.86	1.44
1:A:20:ASN:CG	1:A:20:ASN:ND2	1.75	1.44
1:A:32:MET:CE	1:A:32:MET:SD	2.04	1.44
2:B:133:VAL:CB	2:B:133:VAL:CG2	1.96	1.44
1:C:68:LYS:NZ	1:C:68:LYS:CE	1.78	1.44
2:D:123:PRO:CA	2:D:123:PRO:C	1.89	1.44
1:A:12:ALA:CA	1:A:12:ALA:C	1.89	1.44
2:B:6:GLU:CA	2:B:6:GLU:N	1.79	1.44
1:C:18:GLY:N	1:C:18:GLY:CA	1.77	1.44
2:D:36:TRP:CA	2:D:36:TRP:N	1.80	1.44
2:D:116:ASN:C	2:D:117:PHE:N	1.71	1.44
2:B:54:MET:CG	2:B:54:MET:CB	1.95	1.44
2:B:95:LEU:CA	2:B:95:LEU:N	1.81	1.44
1:C:121:VAL:C	1:C:122:HIS:N	1.74	1.44
2:D:77:LEU:CG	2:D:77:LEU:CB	1.93	1.44
1:A:9:ASN:N	1:A:9:ASN:CA	1.82	1.43
2:D:99:PRO:CB	2:D:99:PRO:CG	1.76	1.43
1:A:62:VAL:CG1	1:A:62:VAL:CG2	1.93	1.43
2:B:43:HIS:NE2	2:B:43:HIS:CE1	1.84	1.43
1:C:96:VAL:CB	1:C:96:VAL:CG2	1.97	1.43
2:D:26:ALA:CA	2:D:26:ALA:C	1.90	1.43
2:B:107:ASN:ND2	2:B:107:ASN:CG	1.72	1.43
1:C:79:THR:CA	1:C:79:THR:CB	1.94	1.43
1:C:85:ASN:CG	1:C:85:ASN:ND2	1.75	1.43
2:D:3:THR:N	2:D:3:THR:CA	1.81	1.43
2:B:21:VAL:CB	2:B:21:VAL:C	1.90	1.43
2:B:144:TYR:OH	2:B:144:TYR:CZ	1.70	1.43
1:C:36:PHE:C	1:C:37:PRO:N	1.76	1.43
2:D:83:ALA:CA	2:D:83:ALA:C	1.90	1.43
2:D:96:HIS:CA	2:D:96:HIS:N	1.80	1.43
2:B:46:ASN:CA	2:B:46:ASN:CB	1.97	1.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LEU:CG	2:B:87:LEU:CD1	1.94	1.43
2:B:125:VAL:C	2:B:125:VAL:CA	1.89	1.43
1:C:6:ASN:C	1:C:7:LYS:N	1.75	1.43
1:A:16:LYS:C	1:A:17:VAL:N	1.76	1.42
1:A:42:TYR:C	1:A:43:PHE:N	1.73	1.42
2:B:69:ALA:CB	2:B:69:ALA:N	1.68	1.42
2:B:97:VAL:CB	2:B:97:VAL:CG2	1.95	1.42
1:C:115:THR:C	1:C:115:THR:CA	1.90	1.42
1:C:117:PHE:C	1:C:117:PHE:CA	1.88	1.42
2:D:57:PRO:CA	2:D:57:PRO:CB	1.97	1.42
2:D:138:ASN:N	2:D:138:ASN:CA	1.82	1.42
1:A:34:LEU:CA	1:A:34:LEU:CB	1.94	1.42
1:C:59:GLY:CA	1:C:59:GLY:C	1.92	1.42
1:A:99:LYS:NZ	1:A:99:LYS:CE	1.79	1.42
1:A:138:SER:OG	1:A:138:SER:CB	1.67	1.42
1:C:4:ALA:CB	1:C:4:ALA:CA	1.94	1.42
2:B:57:PRO:CD	2:B:57:PRO:CA	1.97	1.42
3:D:146:HEM:CBA	3:D:146:HEM:CGA	1.98	1.42
1:A:70:GLN:CD	1:A:70:GLN:NE2	1.75	1.42
2:D:16:LYS:CB	2:D:16:LYS:CG	1.95	1.42
1:A:43:PHE:C	1:A:44:PRO:N	1.78	1.41
2:B:10:VAL:CG1	2:B:128:LEU:CD2	1.76	1.41
2:B:131:LYS:CD	2:B:131:LYS:CE	1.97	1.41
1:A:7:LYS:CA	1:A:7:LYS:C	1.90	1.41
1:A:70:GLN:CD	1:A:70:GLN:CG	1.92	1.41
1:A:126:ASN:ND2	1:A:126:ASN:CG	1.77	1.41
3:A:142:HEM:CAD	3:A:142:HEM:C2D	2.02	1.41
2:D:50:ALA:CA	2:D:50:ALA:C	1.91	1.41
2:B:103:ARG:NH2	2:B:103:ARG:CZ	1.83	1.41
1:C:45:HIS:CA	1:C:45:HIS:N	1.81	1.41
1:C:100:LEU:N	1:C:100:LEU:CA	1.82	1.41
1:C:119:PRO:CA	1:C:119:PRO:C	1.93	1.41
2:D:6:GLU:O	2:D:6:GLU:C	1.63	1.41
1:A:31:ARG:C	1:A:31:ARG:O	1.64	1.41
2:B:10:VAL:N	2:B:10:VAL:CA	1.83	1.41
2:B:11:THR:CB	2:B:11:THR:CG2	1.99	1.41
2:B:117:PHE:C	2:B:118:GLY:CA	1.90	1.41
2:D:79:ASP:CA	2:D:79:ASP:CB	1.97	1.41
2:D:103:ARG:CA	2:D:103:ARG:CB	1.96	1.41
1:A:115:THR:CB	1:A:115:THR:OG1	1.66	1.41
1:C:22:PRO:CA	1:C:22:PRO:N	1.81	1.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:LEU:C	2:D:109:LEU:CA	1.91	1.41
1:A:54:GLN:C	1:A:54:GLN:O	1.65	1.40
2:B:3:THR:HG22	2:B:6:GLU:N	1.24	1.40
2:B:10:VAL:CG1	2:B:128:LEU:HD21	0.93	1.40
2:B:11:THR:CB	2:B:11:THR:OG1	1.68	1.40
2:B:36:TRP:CE2	2:B:36:TRP:CH2	1.89	1.40
2:B:145:HIS:CE1	2:B:145:HIS:NE2	1.79	1.40
3:B:146:HEM:C3D	3:B:146:HEM:C4D	1.96	1.40
2:D:14:TRP:CD1	2:D:14:TRP:CG	1.81	1.40
2:D:53:VAL:CB	2:D:53:VAL:CG2	1.99	1.40
1:A:127:LYS:C	1:A:128:PHE:CA	1.95	1.40
1:C:46:PHE:CB	1:C:46:PHE:CG	2.04	1.40
1:C:49:SER:OG	1:C:49:SER:CB	1.65	1.40
1:A:106:LEU:N	1:A:106:LEU:CA	1.83	1.40
1:C:16:LYS:N	1:C:16:LYS:CA	1.83	1.40
2:D:2:LEU:CB	2:D:2:LEU:CD1	1.98	1.40
1:A:80:LEU:CG	1:A:80:LEU:CB	1.98	1.40
2:B:68:ASP:HA	2:B:71:THR:CG2	0.92	1.40
1:C:1:VAL:C	1:C:1:VAL:CA	1.94	1.40
1:C:70:GLN:CA	1:C:70:GLN:CB	2.00	1.40
1:C:102:SER:C	1:C:103:HIS:N	1.78	1.40
1:C:131:ASN:OD1	1:C:131:ASN:CG	1.65	1.40
2:D:100:GLN:C	2:D:101:ASN:HA	1.43	1.40
2:D:101:ASN:N	2:D:101:ASN:HA	1.26	1.39
1:A:127:LYS:C	1:A:127:LYS:O	1.63	1.39
2:B:60:LYS:NZ	2:B:60:LYS:CE	1.83	1.39
2:D:138:ASN:CG	2:D:138:ASN:OD1	1.66	1.39
1:A:94:ASN:CA	1:A:94:ASN:CB	2.00	1.39
2:B:145:HIS:CA	2:B:145:HIS:CB	2.00	1.39
1:A:8:SER:C	1:A:8:SER:O	1.64	1.39
1:C:100:LEU:CG	1:C:100:LEU:CB	1.98	1.39
2:D:35:PRO:CD	2:D:35:PRO:N	1.80	1.39
2:D:81:LYS:CD	2:D:81:LYS:CG	2.00	1.39
2:D:143:LYS:CB	2:D:143:LYS:CA	1.99	1.39
1:A:82:ASN:N	1:A:82:ASN:CA	1.86	1.39
2:B:65:ARG:NH2	2:B:65:ARG:CZ	1.84	1.39
2:B:109:LEU:CB	2:B:109:LEU:CG	1.97	1.39
1:C:53:ALA:CA	1:C:53:ALA:CB	1.99	1.39
2:D:11:THR:CA	2:D:11:THR:N	1.83	1.39
1:A:135:VAL:CB	1:A:135:VAL:CG2	2.00	1.38
2:B:139:ALA:C	2:B:139:ALA:O	1.66	1.38

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:PRO:CD	1:C:44:PRO:N	1.85	1.38
1:C:98:PHE:CD1	1:C:98:PHE:CG	1.79	1.38
2:D:84:PHE:CA	2:D:84:PHE:CB	1.99	1.38
1:A:74:ASN:CB	1:A:74:ASN:CG	1.95	1.38
1:A:141:ARG:CA	1:A:141:ARG:C	1.95	1.38
2:B:78:ASP:CG	2:B:78:ASP:OD2	1.65	1.38
1:C:116:ASN:CG	1:C:116:ASN:ND2	1.82	1.38
2:D:58:LYS:NZ	2:D:58:LYS:CE	1.86	1.38
1:A:56:LYS:C	1:A:56:LYS:O	1.63	1.38
2:B:57:PRO:CD	2:B:57:PRO:CB	1.98	1.38
2:B:143:LYS:CG	2:B:143:LYS:CB	2.00	1.38
1:C:124:ASN:CG	1:C:124:ASN:ND2	1.79	1.38
2:D:30:LEU:CA	2:D:30:LEU:C	1.94	1.38
1:A:32:MET:N	1:A:32:MET:CA	1.86	1.38
2:B:23:GLY:N	2:B:23:GLY:CA	1.84	1.38
2:B:144:TYR:CZ	2:B:144:TYR:CE2	2.11	1.38
1:C:61:LYS:CA	1:C:61:LYS:CB	2.00	1.38
1:C:93:VAL:CA	1:C:93:VAL:CB	2.00	1.38
1:C:122:HIS:CG	1:C:122:HIS:ND1	1.70	1.38
1:C:135:VAL:C	1:C:135:VAL:O	1.65	1.38
2:D:65:ARG:CB	2:D:65:ARG:CG	2.00	1.38
2:D:104:LEU:CG	2:D:104:LEU:CD1	2.01	1.38
2:B:46:ASN:CB	2:B:46:ASN:CG	1.96	1.38
2:B:55:ASN:C	2:B:56:ASN:N	1.78	1.38
2:B:113:VAL:CB	2:B:113:VAL:CG2	2.01	1.38
1:C:37:PRO:CG	1:C:37:PRO:CD	1.99	1.38
2:D:54:MET:CG	2:D:54:MET:SD	2.12	1.38
2:D:56:ASN:C	2:D:56:ASN:O	1.66	1.38
2:B:43:HIS:ND1	2:B:43:HIS:CE1	1.92	1.37
1:C:74:ASN:N	1:C:74:ASN:CA	1.86	1.37
1:C:130:ALA:C	1:C:130:ALA:O	1.64	1.37
1:C:134:THR:CA	1:C:134:THR:CB	1.99	1.37
1:A:29:LEU:CG	1:A:29:LEU:CB	2.03	1.37
2:B:22:VAL:CA	2:B:22:VAL:C	1.93	1.37
1:C:44:PRO:N	1:C:44:PRO:CA	1.86	1.37
2:D:131:LYS:NZ	2:D:131:LYS:CE	1.84	1.37
2:B:69:ALA:CB	2:B:69:ALA:C	1.93	1.37
2:D:44:PHE:CA	2:D:44:PHE:C	1.97	1.37
1:A:31:ARG:C	1:A:32:MET:N	1.81	1.37
1:A:53:ALA:O	1:A:53:ALA:C	1.68	1.36
1:A:118:THR:CB	1:A:118:THR:CG2	2.01	1.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:THR:C	1:C:115:THR:O	1.66	1.36
2:D:130:GLN:CG	2:D:130:GLN:CA	2.02	1.36
2:B:68:ASP:CG	2:B:71:THR:HG23	1.47	1.36
2:B:126:GLN:CG	2:B:126:GLN:CD	1.99	1.36
2:D:41:PHE:C	2:D:42:GLN:N	1.83	1.36
2:D:108:VAL:CA	2:D:108:VAL:N	1.86	1.36
1:C:41:THR:CB	1:C:41:THR:CG2	2.03	1.36
1:A:85:ASN:C	1:A:85:ASN:O	1.69	1.36
1:C:7:LYS:NZ	1:C:7:LYS:CE	1.89	1.36
2:D:6:GLU:CD	2:D:6:GLU:OE2	1.67	1.36
2:D:57:PRO:N	2:D:57:PRO:CG	1.89	1.36
2:B:32:VAL:N	2:B:32:VAL:CA	1.89	1.35
2:B:103:ARG:CG	2:B:103:ARG:CD	2.01	1.35
1:C:30:GLN:CD	1:C:30:GLN:NE2	1.83	1.35
1:C:31:ARG:CA	1:C:31:ARG:C	1.99	1.35
2:D:42:GLN:CG	2:D:42:GLN:CB	2.04	1.35
2:D:65:ARG:NH1	2:D:65:ARG:CZ	1.90	1.35
2:B:39:ARG:CB	2:B:39:ARG:CG	2.04	1.35
2:B:110:ALA:CA	2:B:110:ALA:N	1.87	1.35
1:C:12:ALA:C	1:C:12:ALA:O	1.66	1.35
1:C:74:ASN:C	1:C:75:ASP:N	1.84	1.35
1:A:22:PRO:CD	1:A:22:PRO:N	1.87	1.35
1:A:84:SER:N	1:A:84:SER:CA	1.86	1.35
2:B:109:LEU:CB	2:B:109:LEU:CD2	2.02	1.35
1:A:50:HIS:NE2	1:A:50:HIS:CE1	1.89	1.35
1:C:84:SER:C	1:C:84:SER:CB	2.00	1.35
2:D:102:PHE:N	2:D:102:PHE:CA	1.90	1.35
1:A:3:SER:O	1:A:3:SER:C	1.67	1.34
1:C:33:PHE:O	1:C:33:PHE:C	1.68	1.34
1:C:35:SER:CB	1:C:35:SER:OG	1.75	1.34
1:C:130:ALA:N	1:C:130:ALA:CA	1.91	1.34
2:D:16:LYS:CB	2:D:16:LYS:CA	2.05	1.34
2:B:68:ASP:CA	2:B:71:THR:HG22	1.37	1.34
2:B:98:ASN:CG	2:B:98:ASN:OD1	1.67	1.34
2:B:99:PRO:CG	2:B:99:PRO:CD	1.96	1.34
2:D:124:ASN:CG	2:D:124:ASN:OD1	1.70	1.34
1:C:94:ASN:OD1	1:C:94:ASN:CG	1.69	1.34
2:D:25:GLN:CG	2:D:25:GLN:CD	1.99	1.34
1:A:37:PRO:CD	1:A:37:PRO:N	1.77	1.34
2:D:92:CYS:SG	2:D:92:CYS:CB	2.16	1.34
2:B:55:ASN:O	2:B:60:LYS:NZ	1.60	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:GLN:CA	2:B:38:GLN:C	2.00	1.33
1:A:45:HIS:NE2	1:A:45:HIS:CD2	1.84	1.33
2:B:59:VAL:C	2:B:59:VAL:O	1.70	1.33
2:B:65:ARG:NH1	3:B:146:HEM:O2D	1.61	1.33
2:B:71:THR:CB	2:B:71:THR:CA	2.06	1.33
2:D:59:VAL:CG2	2:D:59:VAL:HA	1.57	1.33
2:B:7:LYS:C	2:B:7:LYS:CA	2.01	1.33
2:B:41:PHE:C	2:B:42:GLN:N	1.85	1.33
2:D:130:GLN:CG	2:D:130:GLN:CD	2.01	1.33
2:B:94:LYS:NZ	2:B:94:LYS:CE	1.90	1.33
1:C:119:PRO:CG	1:C:119:PRO:CB	1.85	1.33
2:D:111:LEU:C	2:D:112:VAL:CA	2.01	1.33
2:D:2:LEU:HD22	2:D:3:THR:O	1.23	1.33
2:B:115:ARG:CA	2:B:115:ARG:CB	2.08	1.32
1:A:124:ASN:CB	1:A:124:ASN:N	1.92	1.32
2:B:39:ARG:NH1	2:B:40:PHE:CZ	1.97	1.32
1:C:11:LYS:CD	1:C:11:LYS:CE	2.07	1.32
1:C:90:LYS:N	1:C:90:LYS:CA	1.90	1.32
2:D:70:PHE:HA	2:D:70:PHE:O	1.26	1.32
1:A:78:GLY:CA	1:A:78:GLY:N	1.91	1.32
1:A:114:PRO:CD	1:A:114:PRO:N	1.90	1.32
2:B:20:ASP:OD1	2:B:20:ASP:CG	1.72	1.32
2:D:54:MET:O	2:D:54:MET:C	1.73	1.32
1:A:26:ALA:CB	1:A:26:ALA:CA	2.07	1.31
2:B:4:ALA:N	2:B:5:GLU:H	1.26	1.31
2:D:110:ALA:CA	2:D:110:ALA:C	2.02	1.31
1:A:74:ASN:CG	1:A:74:ASN:ND2	1.86	1.31
2:B:45:GLY:O	2:B:45:GLY:C	1.69	1.31
2:D:42:GLN:CG	2:D:42:GLN:HA	1.57	1.31
2:D:95:LEU:CB	2:D:95:LEU:CG	2.07	1.31
1:C:137:THR:O	1:C:137:THR:C	1.71	1.31
1:C:8:SER:C	1:C:8:SER:O	1.72	1.31
2:D:144:TYR:CZ	2:D:144:TYR:OH	1.82	1.31
2:D:55:ASN:OD1	2:D:55:ASN:CG	1.73	1.31
1:C:22:PRO:CD	1:C:22:PRO:CB	2.09	1.30
1:C:75:ASP:CA	1:C:75:ASP:C	2.04	1.30
3:C:142:HEM:CHD	3:C:142:HEM:C3C	2.13	1.30
2:D:51:GLY:C	2:D:52:ALA:N	1.87	1.30
1:A:2:LEU:CA	1:A:2:LEU:C	2.05	1.30
2:B:108:VAL:CB	2:B:108:VAL:CG2	2.07	1.30
2:D:57:PRO:N	2:D:57:PRO:CD	1.93	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:HIS:C	2:D:145:HIS:O	1.75	1.30
2:D:59:VAL:CG2	2:D:59:VAL:CA	2.09	1.30
1:A:9:ASN:OD1	1:A:9:ASN:CG	1.71	1.30
2:D:11:THR:OG1	2:D:11:THR:CB	1.78	1.30
2:B:5:GLU:N	2:B:5:GLU:CA	1.93	1.30
1:C:9:ASN:CB	1:C:9:ASN:CG	2.03	1.30
1:C:38:THR:CB	1:C:38:THR:CG2	2.09	1.30
1:C:86:LEU:CA	1:C:86:LEU:CB	2.10	1.30
2:D:4:ALA:C	2:D:4:ALA:CA	2.04	1.30
2:D:5:GLU:CG	2:D:5:GLU:CD	2.04	1.30
2:D:19:VAL:CB	2:D:19:VAL:CG2	2.10	1.30
2:D:105:LEU:CD1	2:D:105:LEU:CD2	2.10	1.29
3:D:146:HEM:CBD	3:D:146:HEM:CGD	2.10	1.29
2:B:1:MET:CG	2:B:77:LEU:HD13	1.57	1.29
2:B:79:ASP:C	2:B:79:ASP:O	1.76	1.29
2:B:95:LEU:CB	2:B:95:LEU:H	1.35	1.29
2:B:64:LYS:CD	2:B:64:LYS:CE	2.09	1.29
2:B:68:ASP:CB	2:B:71:THR:HG23	1.60	1.29
1:C:141:ARG:CD	1:C:141:ARG:CG	2.10	1.29
3:C:142:HEM:C4C	3:C:142:HEM:C1D	2.18	1.29
3:C:142:HEM:CGD	3:C:142:HEM:O1D	1.80	1.29
3:A:142:HEM:CBD	3:A:142:HEM:CGD	2.12	1.28
2:B:49:SER:C	2:B:49:SER:O	1.75	1.28
1:A:124:ASN:C	1:A:124:ASN:O	1.76	1.28
1:A:127:LYS:CD	1:A:127:LYS:NZ	1.94	1.28
2:D:71:THR:CB	2:D:71:THR:OG1	1.78	1.28
1:A:40:LYS:CB	1:A:40:LYS:CG	2.10	1.28
2:B:39:ARG:NH1	2:B:40:PHE:HZ	1.27	1.28
1:C:56:LYS:NZ	1:C:56:LYS:CE	1.96	1.28
1:A:4:ALA:N	1:A:4:ALA:CA	1.97	1.27
2:B:34:TYR:CZ	2:B:34:TYR:CD2	2.22	1.27
2:B:81:LYS:HZ2	2:B:142:HIS:CG	1.51	1.27
1:A:87:HIS:CG	1:A:87:HIS:CB	2.16	1.27
1:C:80:LEU:C	1:C:80:LEU:O	1.73	1.27
2:D:14:TRP:CZ3	2:D:14:TRP:CD2	2.16	1.27
2:D:1:MET:CE	2:D:1:MET:SD	2.22	1.27
2:B:68:ASP:N	2:B:71:THR:CG2	1.94	1.27
1:C:77:PRO:CB	1:C:77:PRO:CG	1.95	1.27
2:D:7:LYS:O	2:D:8:ALA:CA	1.80	1.27
1:A:52:SER:OG	1:A:52:SER:CB	1.82	1.27
2:B:55:ASN:C	2:B:55:ASN:CA	2.07	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TRP:CZ2	2:B:36:TRP:NE1	2.03	1.26
2:B:133:VAL:O	2:B:134:ALA:N	1.68	1.26
2:D:10:VAL:C	2:D:10:VAL:CB	2.07	1.26
2:B:54:MET:HB3	2:B:55:ASN:OD1	1.32	1.26
2:D:84:PHE:CD1	2:D:84:PHE:CB	2.16	1.26
2:B:53:VAL:C	2:B:54:MET:CA	2.08	1.26
2:B:84:PHE:CB	2:B:84:PHE:CD1	2.18	1.26
1:C:110:ALA:CA	1:C:110:ALA:C	2.08	1.26
2:D:34:TYR:CE2	2:D:34:TYR:CE1	2.09	1.26
2:D:3:THR:OG1	2:D:3:THR:CB	1.83	1.26
1:C:114:PRO:CB	1:C:114:PRO:CG	2.13	1.25
2:D:48:SER:CB	2:D:48:SER:OG	1.81	1.25
1:A:3:SER:CB	1:A:3:SER:OG	1.83	1.25
2:B:84:PHE:CG	2:B:84:PHE:CE2	1.77	1.25
1:C:45:HIS:NE2	1:C:45:HIS:CD2	1.78	1.25
2:D:2:LEU:HD23	2:D:7:LYS:CG	1.66	1.25
2:B:74:LEU:HD13	2:B:77:LEU:CB	1.65	1.25
1:A:85:ASN:CB	1:A:85:ASN:CG	2.10	1.24
2:B:42:GLN:C	2:B:43:HIS:N	1.93	1.24
1:A:103:HIS:CG	1:A:103:HIS:ND1	1.71	1.24
2:B:145:HIS:O	2:D:1:MET:SD	1.95	1.24
1:A:124:ASN:CB	1:A:124:ASN:C	2.10	1.24
1:C:85:ASN:CA	1:C:85:ASN:O	1.83	1.24
1:A:79:THR:CB	1:A:80:LEU:HD23	1.67	1.24
2:B:95:LEU:CA	2:B:95:LEU:CG	2.14	1.24
2:D:145:HIS:ND1	2:D:145:HIS:CG	2.06	1.24
1:A:18:GLY:O	1:A:19:GLY:N	1.69	1.23
1:A:89:HIS:NE2	1:A:89:HIS:CE1	1.68	1.23
2:D:95:LEU:CG	2:D:95:LEU:CD1	2.14	1.23
2:D:55:ASN:CA	2:D:55:ASN:CB	2.17	1.23
2:B:41:PHE:CD2	2:B:44:PHE:CE1	2.24	1.23
3:D:146:HEM:C1B	3:D:146:HEM:NB	1.85	1.23
2:B:75:LYS:HG3	2:B:76:HIS:CE1	1.72	1.22
2:D:51:GLY:O	2:D:52:ALA:HA	1.34	1.22
1:A:112:HIS:CG	1:A:112:HIS:ND1	1.71	1.22
1:C:29:LEU:CD2	1:C:29:LEU:CG	2.16	1.22
1:C:114:PRO:N	1:C:114:PRO:CG	2.00	1.22
1:A:72:HIS:NE2	1:A:72:HIS:CE1	1.94	1.22
2:B:92:CYS:SG	2:B:92:CYS:CB	2.27	1.22
1:A:49:SER:CB	1:A:52:SER:HB3	1.68	1.22
1:A:77:PRO:C	1:A:77:PRO:CA	2.12	1.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLN:CD	1:A:70:GLN:OE1	1.80	1.22
2:D:90:LEU:CB	2:D:90:LEU:CD1	2.19	1.21
1:A:8:SER:O	1:A:8:SER:CA	1.87	1.21
2:B:7:LYS:NZ	2:B:7:LYS:CE	2.04	1.21
1:C:61:LYS:CE	1:C:61:LYS:NZ	2.03	1.21
1:C:74:ASN:CB	1:C:74:ASN:CG	2.13	1.21
2:D:72:GLN:HE21	2:D:73:GLY:N	1.39	1.21
1:C:98:PHE:C	1:C:99:LYS:N	1.99	1.21
1:A:85:ASN:C	1:A:85:ASN:CB	2.13	1.20
2:D:7:LYS:O	2:D:7:LYS:CA	1.89	1.20
2:B:117:PHE:CD1	2:B:117:PHE:CZ	2.30	1.20
2:B:38:GLN:O	2:B:39:ARG:N	1.72	1.20
2:B:41:PHE:CD2	2:B:44:PHE:CZ	2.30	1.20
2:B:1:MET:CG	2:B:1:MET:SD	2.30	1.19
1:A:131:ASN:N	1:A:131:ASN:CA	2.05	1.19
1:C:56:LYS:CG	1:C:56:LYS:HA	1.72	1.19
1:C:89:HIS:HB2	1:C:139:LYS:NZ	1.53	1.19
2:B:68:ASP:N	2:B:71:THR:HG21	1.57	1.19
1:C:141:ARG:C	1:C:141:ARG:O	1.84	1.19
1:A:119:PRO:CA	1:A:119:PRO:CG	2.20	1.19
2:B:41:PHE:HD2	2:B:44:PHE:CZ	1.60	1.19
2:B:130:GLN:CG	2:B:130:GLN:NE2	2.06	1.19
1:A:94:ASN:CA	1:A:94:ASN:O	1.88	1.19
1:A:108:THR:CA	1:A:108:THR:HB	1.51	1.19
1:C:135:VAL:CG2	1:C:135:VAL:CG1	2.20	1.18
1:A:91:LEU:CD2	1:A:91:LEU:CD1	2.21	1.18
2:D:7:LYS:CA	2:D:7:LYS:CB	2.20	1.18
1:A:79:THR:CA	1:A:79:THR:CG2	2.21	1.18
2:B:93:ASN:CG	2:B:93:ASN:CA	2.16	1.18
1:A:91:LEU:HD23	3:A:142:HEM:C4D	1.79	1.18
1:A:100:LEU:CB	1:A:100:LEU:CD1	2.21	1.18
1:A:31:ARG:CG	2:B:126:GLN:HE21	1.57	1.17
1:A:36:PHE:O	1:A:39:THR:HG22	1.40	1.17
2:B:75:LYS:N	2:B:75:LYS:CA	2.07	1.17
1:C:20:ASN:N	1:C:20:ASN:C	2.02	1.17
2:D:2:LEU:HD23	2:D:7:LYS:HG2	1.22	1.17
2:D:70:PHE:HD1	2:D:71:THR:OG1	1.22	1.17
2:B:3:THR:CG2	2:B:5:GLU:C	2.17	1.17
2:B:95:LEU:CA	2:B:95:LEU:HG	1.73	1.17
2:D:126:GLN:OE1	2:D:126:GLN:CD	1.87	1.17
1:A:105:LEU:CD1	1:A:105:LEU:CD2	2.23	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:THR:HG22	2:B:5:GLU:C	1.68	1.17
2:B:62:HIS:CG	2:B:62:HIS:CB	2.28	1.17
2:B:77:LEU:CB	2:B:77:LEU:C	2.16	1.17
1:A:49:SER:CB	1:A:49:SER:OG	1.93	1.16
1:C:52:SER:HB3	1:C:55:GLN:HE21	1.08	1.16
2:D:2:LEU:CD1	2:D:2:LEU:HB3	1.65	1.16
1:A:60:GLN:CA	1:A:61:LYS:N	2.09	1.16
2:B:15:GLY:C	2:B:15:GLY:O	1.89	1.16
2:B:64:LYS:N	2:B:64:LYS:C	2.03	1.16
1:C:87:HIS:HA	1:C:91:LEU:HD12	1.17	1.16
1:A:74:ASN:C	1:A:74:ASN:O	1.87	1.16
2:D:75:LYS:CD	2:D:75:LYS:CE	2.24	1.16
2:D:10:VAL:C	2:D:10:VAL:HB	1.71	1.16
2:D:81:LYS:CB	2:D:81:LYS:N	2.06	1.16
1:A:99:LYS:CG	1:A:99:LYS:CD	2.24	1.16
2:B:102:PHE:CD1	2:B:102:PHE:CD2	2.10	1.16
1:C:72:HIS:HB2	1:C:74:ASN:HD21	0.99	1.16
2:B:3:THR:CG2	2:B:6:GLU:N	2.09	1.15
1:C:46:PHE:CZ	1:C:46:PHE:CD2	2.18	1.15
2:D:85:ALA:N	2:D:85:ALA:CA	2.08	1.15
2:D:94:LYS:HG3	2:D:95:LEU:HD23	1.29	1.15
2:B:55:ASN:C	2:B:60:LYS:HZ3	1.54	1.15
2:B:133:VAL:O	2:B:133:VAL:CA	1.93	1.15
2:D:6:GLU:HB2	2:D:128:LEU:HD23	1.22	1.15
2:D:10:VAL:CG1	2:D:128:LEU:HD22	1.76	1.15
1:A:42:TYR:O	1:A:42:TYR:CA	1.95	1.15
1:A:132:ASP:CG	1:A:132:ASP:OD2	1.88	1.15
2:B:1:MET:N	2:B:1:MET:CA	2.10	1.15
2:B:71:THR:N	2:B:71:THR:C	2.03	1.15
3:A:142:HEM:C3D	3:A:142:HEM:CMD	2.30	1.14
2:D:59:VAL:CG2	2:D:59:VAL:CG1	2.25	1.14
2:B:71:THR:N	2:B:71:THR:HA	1.55	1.14
2:D:105:LEU:CD1	2:D:105:LEU:HD22	1.72	1.14
2:D:105:LEU:CD1	2:D:105:LEU:HB2	1.65	1.14
2:D:10:VAL:HG11	2:D:128:LEU:HD22	1.29	1.14
2:D:62:HIS:CG	2:D:62:HIS:CE1	2.33	1.14
1:A:109:LEU:C	1:A:109:LEU:CA	2.19	1.14
1:C:69:ALA:C	1:C:69:ALA:CB	2.21	1.14
2:D:75:LYS:O	2:D:75:LYS:C	1.90	1.14
1:A:39:THR:CB	1:A:40:LYS:HZ3	1.61	1.14
1:A:137:THR:CA	1:A:137:THR:OG1	1.95	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ALA:H	1:C:56:LYS:HE2	1.12	1.14
2:D:11:THR:N	2:D:11:THR:CB	2.08	1.14
2:B:68:ASP:CG	2:B:71:THR:CG2	2.20	1.13
2:B:80:LEU:CD2	2:B:80:LEU:CB	2.25	1.13
2:D:14:TRP:NE1	2:D:71:THR:HG23	1.62	1.13
2:B:68:ASP:OD2	2:B:71:THR:HG21	1.48	1.13
1:C:56:LYS:CG	1:C:56:LYS:CB	2.26	1.13
1:A:62:VAL:CG1	1:A:62:VAL:HG21	1.64	1.13
2:B:55:ASN:C	2:B:60:LYS:NZ	2.05	1.12
2:D:11:THR:CA	2:D:11:THR:OG1	1.95	1.12
2:D:53:VAL:HG22	2:D:54:MET:HE2	1.30	1.12
2:D:111:LEU:O	2:D:112:VAL:N	1.82	1.12
1:A:49:SER:HB2	1:A:52:SER:CB	1.80	1.12
1:A:114:PRO:CD	1:A:114:PRO:HB2	1.62	1.12
2:B:1:MET:N	2:B:2:LEU:HD23	1.63	1.12
2:B:68:ASP:HB3	2:B:71:THR:O	1.46	1.12
1:C:138:SER:CB	1:C:138:SER:OG	1.96	1.12
2:D:51:GLY:O	2:D:52:ALA:CA	1.97	1.12
1:A:31:ARG:CG	1:A:31:ARG:NE	2.11	1.12
2:D:1:MET:N	2:D:1:MET:C	2.06	1.12
2:D:103:ARG:CB	2:D:103:ARG:C	2.21	1.12
2:B:1:MET:SD	2:B:1:MET:CE	2.37	1.12
1:A:119:PRO:CG	1:A:119:PRO:CD	2.27	1.11
2:B:56:ASN:O	2:B:56:ASN:CA	1.97	1.11
2:B:80:LEU:CD2	2:B:80:LEU:HB3	1.75	1.11
2:D:39:ARG:NE	2:D:39:ARG:CG	2.10	1.11
2:B:118:GLY:N	2:B:118:GLY:C	2.07	1.11
1:A:108:THR:CB	1:A:108:THR:HA	1.70	1.11
2:D:19:VAL:CG2	2:D:19:VAL:HA	1.81	1.11
2:B:64:LYS:NZ	2:B:64:LYS:HB3	1.66	1.11
2:B:81:LYS:NZ	2:B:142:HIS:CG	2.18	1.11
1:A:30:GLN:NE2	1:A:30:GLN:CD	2.08	1.11
1:A:65:ALA:CB	1:A:65:ALA:C	2.23	1.11
2:B:11:THR:O	2:B:12:GLY:N	1.84	1.11
2:B:95:LEU:H	2:B:95:LEU:HB2	1.07	1.11
1:C:38:THR:C	1:C:38:THR:O	1.92	1.11
2:D:14:TRP:HE1	2:D:71:THR:HG23	1.09	1.11
2:D:34:TYR:CZ	2:D:34:TYR:CD2	2.21	1.11
2:D:7:LYS:NZ	2:D:7:LYS:CE	2.14	1.10
1:A:41:THR:CA	1:A:41:THR:CG2	2.29	1.10
1:A:137:THR:CG2	1:A:137:THR:OG1	1.98	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:THR:CG2	2:B:5:GLU:CB	2.09	1.10
2:B:47:LEU:HD12	2:B:53:VAL:HG23	1.32	1.10
1:C:114:PRO:N	1:C:114:PRO:CB	2.13	1.10
2:D:28:GLY:CA	2:D:54:MET:HE1	1.80	1.10
2:D:53:VAL:HG22	2:D:54:MET:CE	1.81	1.10
2:D:84:PHE:CD1	2:D:84:PHE:HB2	1.79	1.10
1:A:140:TYR:CB	1:A:140:TYR:CD1	2.33	1.10
2:B:4:ALA:CA	2:B:5:GLU:N	2.15	1.10
2:B:113:VAL:CG1	2:B:113:VAL:HA	1.77	1.10
2:D:7:LYS:CB	2:D:7:LYS:C	2.23	1.10
1:A:26:ALA:HA	1:A:29:LEU:CD2	1.81	1.10
2:B:10:VAL:HG11	2:B:128:LEU:HD22	1.31	1.10
1:A:126:ASN:CA	1:A:127:LYS:N	2.15	1.10
1:A:127:LYS:O	1:A:127:LYS:CA	1.99	1.10
1:C:44:PRO:CB	1:C:44:PRO:CD	2.29	1.10
1:C:75:ASP:CB	1:C:75:ASP:N	2.15	1.09
2:D:18:ASP:CB	2:D:18:ASP:N	2.12	1.09
2:D:70:PHE:O	2:D:70:PHE:CA	2.00	1.09
1:C:55:GLN:CB	1:C:55:GLN:CD	2.23	1.09
2:D:93:ASN:CB	2:D:93:ASN:C	2.23	1.09
2:D:100:GLN:CG	2:D:100:GLN:HA	1.83	1.09
2:D:131:LYS:NZ	2:D:131:LYS:CD	2.13	1.09
1:A:74:ASN:O	1:A:75:ASP:HA	1.53	1.09
1:A:91:LEU:HD21	3:A:142:HEM:HAD1	1.29	1.09
1:A:118:THR:CG2	1:A:118:THR:CA	2.30	1.09
1:C:45:HIS:HE1	3:C:142:HEM:HBD1	0.99	1.09
2:B:87:LEU:CD1	2:B:87:LEU:CD2	2.29	1.09
1:C:108:THR:CG2	1:C:108:THR:HB	1.61	1.09
2:D:100:GLN:CG	2:D:100:GLN:CA	2.31	1.09
1:A:137:THR:CB	1:A:137:THR:N	2.15	1.08
2:B:21:VAL:C	2:B:21:VAL:HB	1.75	1.08
1:C:7:LYS:HG2	1:C:73:LEU:HB2	1.34	1.08
2:D:2:LEU:HD22	2:D:4:ALA:HA	1.18	1.08
2:D:68:ASP:CG	2:D:68:ASP:CA	2.27	1.08
2:B:68:ASP:OD2	2:B:71:THR:CG2	1.99	1.08
2:B:69:ALA:CB	2:B:69:ALA:HA	1.63	1.08
2:B:87:LEU:C	2:B:87:LEU:N	2.11	1.08
1:C:4:ALA:CB	1:C:4:ALA:N	2.13	1.08
2:B:43:HIS:C	2:B:43:HIS:N	2.09	1.08
2:D:99:PRO:HD2	2:D:144:TYR:OH	1.51	1.08
1:A:105:LEU:CD1	1:A:105:LEU:CB	2.31	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:CB	1:A:41:THR:C	2.27	1.08
1:A:77:PRO:CA	1:A:77:PRO:N	1.75	1.08
2:D:42:GLN:HA	2:D:42:GLN:HG2	1.29	1.08
1:A:26:ALA:HA	1:A:29:LEU:HD22	1.29	1.07
1:A:114:PRO:HB2	1:A:114:PRO:HD2	1.08	1.07
1:A:100:LEU:CB	1:A:100:LEU:CD2	2.33	1.07
1:A:56:LYS:HE3	1:A:56:LYS:HA	1.33	1.07
2:B:124:ASN:C	2:B:125:VAL:CA	2.27	1.07
2:B:14:TRP:HE1	2:B:68:ASP:CG	1.62	1.07
1:A:10:VAL:O	1:A:13:ALA:HB3	1.55	1.06
1:A:18:GLY:O	1:A:18:GLY:C	0.82	1.06
1:A:20:ASN:CG	1:A:20:ASN:HA	1.72	1.06
2:B:4:ALA:C	2:B:4:ALA:O	0.82	1.06
2:B:38:GLN:C	2:B:38:GLN:O	0.82	1.06
2:B:43:HIS:CD2	3:B:146:HEM:O2A	2.07	1.06
1:C:80:LEU:C	1:C:80:LEU:HA	1.63	1.06
2:D:140:LEU:CD1	2:D:140:LEU:CD2	2.33	1.06
1:A:26:ALA:HB1	1:A:56:LYS:CE	1.86	1.06
1:A:93:VAL:CG2	1:A:93:VAL:HB	1.79	1.06
2:B:3:THR:H	2:B:6:GLU:HB2	1.19	1.06
2:B:101:ASN:O	3:B:146:HEM:HBB1	1.54	1.06
1:C:87:HIS:CG	1:C:87:HIS:ND1	1.69	1.06
2:B:41:PHE:CG	2:B:44:PHE:CE1	2.42	1.06
2:B:54:MET:CA	2:B:54:MET:CG	2.33	1.06
1:C:29:LEU:CD2	1:C:29:LEU:CD1	2.34	1.06
2:B:140:LEU:CD1	2:B:140:LEU:CB	2.32	1.06
1:C:70:GLN:CB	1:C:70:GLN:C	2.28	1.06
1:A:79:THR:HB	1:A:80:LEU:CD2	1.86	1.06
2:B:22:VAL:C	2:B:23:GLY:CA	2.28	1.06
2:B:64:LYS:HB3	2:B:64:LYS:HZ2	0.94	1.05
2:D:57:PRO:N	2:D:57:PRO:HG2	1.62	1.05
1:A:105:LEU:HA	1:A:108:THR:HG22	1.37	1.05
2:D:44:PHE:CA	2:D:44:PHE:CG	2.39	1.05
2:D:70:PHE:O	2:D:70:PHE:C	1.98	1.05
3:D:146:HEM:CBA	3:D:146:HEM:C2A	2.39	1.05
1:A:34:LEU:HD11	2:B:123:PRO:HB2	1.38	1.05
1:A:108:THR:C	1:A:108:THR:O	0.81	1.05
2:B:1:MET:HG3	2:B:77:LEU:O	1.55	1.05
2:B:34:TYR:CE2	2:B:34:TYR:CG	2.43	1.05
2:B:81:LYS:CD	2:B:81:LYS:CG	2.35	1.05
1:A:91:LEU:CD2	3:A:142:HEM:HAD1	1.85	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HD23	3:A:142:HEM:C3D	1.92	1.05
1:A:136:LEU:CD1	1:A:136:LEU:CB	2.34	1.05
2:B:11:THR:O	2:B:11:THR:C	0.80	1.05
2:B:74:LEU:CD1	2:B:77:LEU:HB2	1.86	1.05
1:A:12:ALA:C	1:A:12:ALA:O	0.80	1.04
2:B:63:GLY:HA2	2:B:66:VAL:HG13	1.36	1.04
2:B:75:LYS:CG	2:B:76:HIS:ND1	2.20	1.04
2:B:113:VAL:CG1	2:B:113:VAL:CA	2.34	1.04
1:C:133:SER:CB	1:C:133:SER:HA	1.84	1.04
2:D:2:LEU:CB	2:D:2:LEU:N	2.20	1.04
2:D:68:ASP:CB	2:D:68:ASP:C	2.30	1.04
2:D:73:GLY:C	2:D:73:GLY:N	2.15	1.04
1:A:3:SER:CB	1:A:3:SER:C	2.30	1.04
1:A:57:ALA:CB	1:A:57:ALA:N	2.19	1.04
2:B:69:ALA:CA	2:B:69:ALA:HB1	1.52	1.04
2:B:133:VAL:O	2:B:133:VAL:C	0.80	1.04
1:C:45:HIS:CE1	3:C:142:HEM:HBD1	1.91	1.04
1:C:140:TYR:O	1:C:141:ARG:HD3	1.58	1.04
2:D:65:ARG:CA	2:D:66:VAL:N	2.19	1.04
2:B:118:GLY:C	2:B:119:GLY:CA	2.30	1.04
1:C:17:VAL:C	1:C:18:GLY:CA	2.30	1.04
1:C:24:TYR:CB	1:C:24:TYR:CD2	2.40	1.04
1:C:55:GLN:CD	1:C:55:GLN:HB2	1.83	1.04
1:C:135:VAL:CG2	1:C:135:VAL:HG11	1.85	1.04
2:B:88:SER:OG	2:B:143:LYS:HB3	1.55	1.03
2:B:94:LYS:CD	2:B:94:LYS:CB	2.37	1.03
2:B:103:ARG:NH1	2:B:103:ARG:NE	2.04	1.03
1:C:23:ALA:CB	1:C:23:ALA:C	2.31	1.03
1:C:72:HIS:HB2	1:C:74:ASN:ND2	1.73	1.03
2:D:28:GLY:C	2:D:54:MET:HE1	1.82	1.03
2:D:123:PRO:C	2:D:123:PRO:HA	1.78	1.03
1:A:16:LYS:NZ	1:A:16:LYS:HD3	1.71	1.03
1:A:76:LEU:O	1:A:77:PRO:C	2.01	1.03
1:C:22:PRO:CD	1:C:22:PRO:CA	2.35	1.03
2:D:16:LYS:HD3	2:D:16:LYS:HB2	1.09	1.03
2:D:145:HIS:NE2	2:D:145:HIS:CD2	2.27	1.03
1:C:56:LYS:NZ	1:C:59:GLY:HA3	1.74	1.03
2:D:123:PRO:CD	2:D:123:PRO:N	2.22	1.03
2:B:3:THR:N	2:B:6:GLU:HB2	1.72	1.03
2:B:76:HIS:N	2:B:76:HIS:CB	2.22	1.03
2:B:84:PHE:CD1	2:B:84:PHE:CD2	2.43	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:LEU:C	2:B:110:ALA:CA	2.31	1.03
2:B:139:ALA:O	2:B:143:LYS:HB2	1.57	1.03
2:D:5:GLU:HB3	2:D:9:ALA:HB3	1.41	1.03
2:D:84:PHE:CB	2:D:84:PHE:N	2.21	1.03
2:B:56:ASN:O	2:B:56:ASN:C	0.78	1.02
2:B:69:ALA:CA	2:B:69:ALA:HB2	1.52	1.02
2:B:144:TYR:CG	2:B:144:TYR:CE2	2.46	1.02
1:C:98:PHE:C	1:C:98:PHE:O	0.78	1.02
2:D:19:VAL:CG2	2:D:19:VAL:CA	2.38	1.02
2:B:1:MET:HG2	2:B:77:LEU:HD11	1.04	1.02
2:B:144:TYR:CD2	2:B:144:TYR:CB	2.42	1.02
2:D:103:ARG:C	2:D:103:ARG:HB3	1.84	1.02
1:A:48:LEU:CA	1:A:48:LEU:CG	2.38	1.02
2:B:4:ALA:N	2:B:5:GLU:N	2.08	1.02
2:B:30:LEU:HD23	2:B:105:LEU:HA	1.35	1.02
2:D:107:ASN:N	2:D:107:ASN:CB	2.23	1.02
1:C:70:GLN:CB	1:C:70:GLN:N	2.21	1.02
2:D:34:TYR:CE2	2:D:34:TYR:OH	2.10	1.02
2:D:59:VAL:CB	2:D:59:VAL:C	2.33	1.02
1:A:56:LYS:HE3	1:A:56:LYS:CA	1.83	1.02
1:A:85:ASN:CA	1:A:85:ASN:O	2.08	1.02
2:D:105:LEU:HB2	2:D:105:LEU:HD12	1.37	1.02
3:D:146:HEM:NA	3:D:146:HEM:C4A	1.73	1.02
1:A:42:TYR:C	1:A:42:TYR:O	0.77	1.01
1:A:89:HIS:CD2	1:A:139:LYS:HD2	1.94	1.01
1:C:86:LEU:CD1	1:C:86:LEU:CD2	2.37	1.01
2:B:118:GLY:N	2:B:118:GLY:HA2	1.35	1.01
1:C:84:SER:CB	1:C:84:SER:OG	2.06	1.01
1:C:140:TYR:O	1:C:140:TYR:HD1	1.42	1.01
2:B:1:MET:HG3	2:B:77:LEU:HD13	1.02	1.01
2:B:69:ALA:CA	2:B:69:ALA:HB3	1.52	1.01
2:B:103:ARG:CZ	2:B:103:ARG:NH1	0.86	1.01
1:C:83:LEU:CD2	1:C:83:LEU:CB	2.38	1.01
2:D:130:GLN:CG	2:D:130:GLN:HA	1.86	1.01
2:D:145:HIS:C	2:D:145:HIS:CB	2.34	1.01
1:A:85:ASN:HD21	1:A:90:LYS:HE3	1.25	1.01
2:D:42:GLN:OE1	2:D:42:GLN:CD	2.04	1.01
2:B:80:LEU:HB3	2:B:81:LYS:O	1.60	1.00
2:B:128:LEU:CD2	2:B:128:LEU:HG	1.88	1.00
1:C:133:SER:C	1:C:133:SER:N	2.16	1.00
3:C:142:HEM:C4C	3:C:142:HEM:HHD	1.60	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:GLN:NE2	2:D:73:GLY:N	2.08	1.00
2:D:128:LEU:C	2:D:129:PHE:CA	2.32	1.00
1:A:91:LEU:CD2	3:A:142:HEM:C3D	2.43	1.00
1:C:124:ASN:ND2	1:C:124:ASN:OD1	1.94	1.00
2:D:41:PHE:CE2	2:D:41:PHE:CG	2.48	1.00
2:D:81:LYS:HB3	2:D:81:LYS:H	1.26	1.00
2:D:140:LEU:CD1	2:D:140:LEU:CB	2.38	1.00
1:A:2:LEU:HG	1:A:73:LEU:HD23	1.44	1.00
2:B:109:LEU:CB	2:B:109:LEU:CD1	2.40	1.00
1:A:57:ALA:HA	1:A:60:GLN:CD	1.87	1.00
2:B:19:VAL:HG23	2:B:68:ASP:OD2	1.62	1.00
2:B:70:PHE:C	2:B:71:THR:CA	2.34	1.00
2:B:84:PHE:CB	2:B:84:PHE:CD2	2.45	1.00
1:C:30:GLN:CD	1:C:30:GLN:CB	2.35	1.00
1:C:102:SER:C	1:C:103:HIS:CA	2.34	1.00
1:C:9:ASN:CG	1:C:9:ASN:OD1	0.76	1.00
1:C:10:VAL:CG2	1:C:10:VAL:CG1	2.40	1.00
2:B:65:ARG:NH2	2:B:65:ARG:NH1	2.08	1.00
2:D:2:LEU:HG	2:D:7:LYS:HE3	1.42	1.00
2:B:98:ASN:HB3	2:B:100:GLN:H	1.28	0.99
2:B:98:ASN:OD1	1:C:96:VAL:HG11	1.59	0.99
1:A:108:THR:O	1:A:109:LEU:N	1.95	0.99
2:B:2:LEU:CG	2:B:6:GLU:HB3	1.92	0.99
2:B:80:LEU:CD2	2:B:80:LEU:CD1	2.40	0.99
1:C:135:VAL:HG11	1:C:135:VAL:HG21	1.40	0.99
2:D:140:LEU:CD1	2:D:140:LEU:HB2	1.92	0.99
2:B:118:GLY:N	2:B:118:GLY:HA3	1.35	0.99
2:D:2:LEU:CB	2:D:2:LEU:C	2.34	0.99
1:A:127:LYS:CD	1:A:127:LYS:HZ2	1.68	0.99
2:B:17:VAL:C	2:B:17:VAL:HG12	1.85	0.99
2:B:41:PHE:C	2:B:41:PHE:O	0.74	0.99
2:D:22:VAL:HG12	2:D:67:LEU:HD13	1.45	0.99
2:D:69:ALA:C	2:D:69:ALA:CB	2.35	0.99
1:A:26:ALA:HB1	1:A:56:LYS:NZ	1.78	0.99
2:B:2:LEU:HB3	2:B:131:LYS:NZ	1.76	0.99
2:B:71:THR:CA	2:B:71:THR:N	0.85	0.99
1:A:62:VAL:HG21	1:A:62:VAL:HG11	1.03	0.99
1:C:44:PRO:CG	1:C:44:PRO:CA	2.40	0.99
2:D:101:ASN:O	3:D:146:HEM:HBB1	1.62	0.99
2:B:41:PHE:CB	2:B:44:PHE:CE1	2.45	0.99
2:B:141:ALA:N	2:B:141:ALA:CB	2.24	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:LEU:O	2:D:77:LEU:HD11	1.61	0.99
2:D:93:ASN:C	2:D:93:ASN:HB3	1.85	0.99
1:A:36:PHE:CB	1:A:36:PHE:CD2	2.43	0.99
1:A:94:ASN:O	1:A:94:ASN:C	0.74	0.99
1:A:74:ASN:O	1:A:75:ASP:CA	2.11	0.98
2:B:75:LYS:CG	2:B:75:LYS:CE	2.40	0.98
3:C:142:HEM:CHD	3:C:142:HEM:C4C	0.94	0.98
2:B:142:HIS:O	2:B:144:TYR:N	1.95	0.98
2:D:75:LYS:CB	2:D:75:LYS:C	2.36	0.98
2:D:81:LYS:N	2:D:81:LYS:HB3	1.77	0.98
2:D:108:VAL:O	2:D:109:LEU:N	1.94	0.98
1:A:136:LEU:HD23	1:A:136:LEU:H	1.24	0.98
1:A:126:ASN:C	1:A:126:ASN:CB	2.36	0.98
1:C:61:LYS:CB	1:C:61:LYS:HA	1.93	0.98
2:B:20:ASP:HB2	2:B:64:LYS:HD2	1.46	0.98
2:B:32:VAL:N	2:B:32:VAL:HB	1.79	0.98
1:C:95:PRO:HG3	1:C:141:ARG:CZ	1.92	0.98
2:B:22:VAL:C	2:B:22:VAL:N	2.20	0.98
2:B:77:LEU:HD13	2:B:77:LEU:O	1.64	0.98
2:D:108:VAL:O	2:D:108:VAL:C	0.73	0.98
1:A:8:SER:O	1:A:8:SER:HA	1.62	0.98
2:B:1:MET:H2	2:B:2:LEU:CD2	1.76	0.98
1:A:9:ASN:N	1:A:9:ASN:CB	2.26	0.97
1:A:11:LYS:C	1:A:11:LYS:O	0.73	0.97
1:A:1:VAL:CG1	1:A:1:VAL:CG2	2.42	0.97
1:A:10:VAL:C	1:A:10:VAL:CB	2.37	0.97
1:A:77:PRO:C	1:A:78:GLY:CA	2.37	0.97
1:C:44:PRO:C	1:C:45:HIS:CA	2.37	0.97
2:D:130:GLN:CB	2:D:130:GLN:HG2	1.48	0.97
2:B:140:LEU:C	2:B:141:ALA:CA	2.37	0.97
1:C:61:LYS:CG	1:C:61:LYS:CA	2.43	0.97
1:C:9:ASN:OD1	1:C:9:ASN:ND2	1.97	0.97
1:A:91:LEU:HD21	3:A:142:HEM:CAD	1.95	0.97
2:D:52:ALA:CB	2:D:52:ALA:N	2.28	0.97
2:B:66:VAL:CG1	2:B:66:VAL:CG2	2.41	0.97
1:A:31:ARG:HG2	2:B:126:GLN:HE21	1.27	0.97
2:D:2:LEU:HG	2:D:7:LYS:CE	1.95	0.97
2:D:137:ALA:HB1	2:D:140:LEU:HD13	1.47	0.97
1:A:43:PHE:CA	1:A:44:PRO:N	2.27	0.97
2:B:94:LYS:CG	2:B:94:LYS:CE	2.42	0.97
2:B:109:LEU:CB	2:B:109:LEU:HD22	1.95	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:THR:C	1:C:108:THR:N	2.23	0.97
2:D:72:GLN:NE2	2:D:73:GLY:CA	2.28	0.97
2:B:75:LYS:N	2:B:75:LYS:C	2.23	0.97
2:B:117:PHE:O	2:B:120:GLN:OE1	1.81	0.97
1:C:89:HIS:HB2	1:C:139:LYS:HZ3	1.18	0.97
2:B:36:TRP:CD2	2:B:36:TRP:CZ2	2.36	0.96
1:C:119:PRO:C	1:C:119:PRO:CB	2.36	0.96
2:D:8:ALA:C	2:D:8:ALA:O	2.08	0.96
2:D:130:GLN:CB	2:D:130:GLN:HG3	1.48	0.96
2:B:87:LEU:CD1	2:B:87:LEU:HD21	1.94	0.96
2:D:72:GLN:HE21	2:D:73:GLY:CA	1.77	0.96
2:B:3:THR:HG23	2:B:5:GLU:CA	1.94	0.96
2:B:103:ARG:CD	2:B:103:ARG:HB3	1.95	0.96
1:C:71:GLY:C	1:C:71:GLY:N	2.22	0.96
2:D:25:GLN:HB3	2:D:112:VAL:HG21	1.45	0.96
2:D:42:GLN:CB	2:D:42:GLN:CD	2.37	0.96
1:A:106:LEU:CD2	1:A:106:LEU:CD1	2.42	0.96
2:B:16:LYS:HD3	2:B:117:PHE:HE1	1.28	0.96
1:A:110:ALA:O	1:A:114:PRO:HG3	1.64	0.96
2:B:1:MET:HG2	2:B:77:LEU:HD12	1.45	0.96
2:B:31:LEU:C	2:B:32:VAL:CA	2.38	0.96
1:C:53:ALA:O	1:C:57:ALA:HB3	1.66	0.96
2:B:71:THR:CB	2:B:71:THR:H	1.78	0.96
2:B:77:LEU:CB	2:B:77:LEU:N	2.29	0.96
2:B:124:ASN:C	2:B:125:VAL:HA	1.85	0.96
1:C:76:LEU:CD2	1:C:76:LEU:HG	1.91	0.96
1:C:78:GLY:C	1:C:79:THR:CA	2.37	0.96
2:D:22:VAL:HG12	2:D:67:LEU:CD1	1.95	0.96
2:D:59:VAL:CG2	2:D:59:VAL:HG13	1.94	0.96
2:D:72:GLN:NE2	2:D:73:GLY:H	1.62	0.96
2:D:131:LYS:C	2:D:132:VAL:CA	2.38	0.96
2:D:130:GLN:CG	2:D:130:GLN:HB2	1.45	0.96
2:B:60:LYS:NZ	2:B:60:LYS:CD	2.28	0.95
2:B:76:HIS:ND1	2:B:76:HIS:CG	1.81	0.95
2:B:80:LEU:HD22	2:B:82:GLY:HA2	1.48	0.95
1:A:81:SER:CB	1:A:81:SER:HA	1.93	0.95
2:B:81:LYS:NZ	2:B:142:HIS:ND1	2.15	0.95
2:D:130:GLN:CG	2:D:130:GLN:HB3	1.45	0.95
1:A:2:LEU:CD1	1:A:2:LEU:CD2	2.44	0.95
2:D:94:LYS:CG	2:D:95:LEU:HD23	1.97	0.95
2:D:131:LYS:HZ2	2:D:131:LYS:HD3	1.30	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:TYR:CD2	2:B:34:TYR:HE2	1.65	0.95
1:C:56:LYS:HZ1	1:C:59:GLY:HA3	1.28	0.95
1:C:28:ALA:N	1:C:28:ALA:CB	2.29	0.95
1:A:87:HIS:NE2	1:A:87:HIS:CD2	1.70	0.95
2:B:126:GLN:C	2:B:126:GLN:N	2.24	0.95
1:A:108:THR:HB	1:A:108:THR:HA	1.36	0.95
1:A:124:ASN:CA	1:A:124:ASN:HB2	1.45	0.95
2:D:131:LYS:NZ	2:D:131:LYS:HD3	1.79	0.95
2:B:57:PRO:O	2:B:60:LYS:HB3	1.66	0.95
2:D:2:LEU:HD23	2:D:7:LYS:HB3	1.48	0.95
2:D:2:LEU:CD2	2:D:7:LYS:HG2	1.97	0.95
2:D:144:TYR:CZ	2:D:144:TYR:CD1	2.38	0.95
2:B:128:LEU:CB	2:B:128:LEU:N	2.29	0.94
1:C:48:LEU:HD12	1:C:49:SER:HB2	1.49	0.94
2:D:72:GLN:NE2	2:D:73:GLY:HA2	1.82	0.94
3:D:146:HEM:CMB	3:D:146:HEM:C1B	2.50	0.94
2:B:2:LEU:HB2	2:B:6:GLU:CB	1.96	0.94
2:B:44:PHE:C	2:B:45:GLY:CA	2.40	0.94
2:B:128:LEU:C	2:B:128:LEU:HA	1.90	0.94
2:D:126:GLN:HE22	2:D:130:GLN:HB2	1.29	0.94
2:B:20:ASP:CB	2:B:64:LYS:HD2	1.97	0.94
2:D:34:TYR:N	2:D:34:TYR:C	2.25	0.94
2:D:107:ASN:N	2:D:107:ASN:C	2.24	0.94
2:D:111:LEU:CA	2:D:112:VAL:N	2.29	0.94
2:D:2:LEU:HB3	2:D:2:LEU:HD12	1.47	0.94
1:A:1:VAL:HG12	1:C:141:ARG:O	1.68	0.94
1:A:91:LEU:HD21	1:A:91:LEU:HD11	1.49	0.94
3:A:142:HEM:C1D	3:A:142:HEM:CMD	2.50	0.94
2:B:1:MET:N	2:B:2:LEU:CD2	2.29	0.94
2:B:68:ASP:N	2:B:71:THR:HG22	1.70	0.94
2:B:70:PHE:O	2:B:71:THR:CA	2.16	0.94
1:A:16:LYS:CD	1:A:16:LYS:HZ2	1.55	0.94
1:A:17:VAL:CG2	1:A:17:VAL:CG1	2.44	0.94
1:A:79:THR:HB	1:A:80:LEU:HD23	0.95	0.94
2:B:84:PHE:CD1	2:B:84:PHE:HB2	2.03	0.94
2:D:69:ALA:CA	2:D:70:PHE:N	2.30	0.94
1:A:124:ASN:CA	1:A:124:ASN:HB3	1.45	0.94
2:B:1:MET:CG	2:B:77:LEU:HD11	1.76	0.94
2:B:45:GLY:N	2:B:45:GLY:C	2.26	0.94
2:D:30:LEU:C	2:D:30:LEU:CB	2.41	0.94
2:D:111:LEU:C	2:D:112:VAL:N	0.84	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:142:HEM:NB	3:A:142:HEM:CHC	2.28	0.94
1:A:43:PHE:HA	1:A:44:PRO:N	1.82	0.94
1:C:52:SER:HB3	1:C:55:GLN:NE2	1.82	0.94
2:B:81:LYS:HZ2	2:B:142:HIS:CE1	1.85	0.93
1:C:91:LEU:CB	1:C:91:LEU:N	2.30	0.93
1:A:136:LEU:HD23	1:A:136:LEU:N	1.81	0.93
2:B:107:ASN:ND2	2:B:107:ASN:CB	2.30	0.93
1:C:85:ASN:CB	1:C:85:ASN:C	2.40	0.93
2:D:108:VAL:O	2:D:108:VAL:HA	1.66	0.93
2:B:141:ALA:C	2:B:142:HIS:CA	2.38	0.93
2:D:27:LEU:CD1	2:D:27:LEU:CD2	2.44	0.93
2:D:75:LYS:CG	2:D:75:LYS:CA	2.46	0.93
2:D:142:HIS:CB	2:D:142:HIS:HA	1.94	0.93
2:B:22:VAL:HG12	2:B:67:LEU:HD21	1.49	0.93
2:B:24:ALA:CB	2:B:24:ALA:HA	1.93	0.93
1:C:67:THR:CG2	1:C:67:THR:OG1	2.16	0.93
1:C:68:LYS:CG	1:C:68:LYS:CA	2.45	0.93
1:A:45:HIS:CB	1:A:45:HIS:C	2.41	0.93
2:B:59:VAL:CG1	2:B:59:VAL:CA	2.45	0.93
2:B:109:LEU:CB	2:B:109:LEU:HD23	1.95	0.93
2:D:34:TYR:CE2	2:D:34:TYR:CZ	0.93	0.93
1:A:11:LYS:C	1:A:12:ALA:CA	2.42	0.93
1:A:20:ASN:CG	1:A:20:ASN:CA	2.41	0.93
1:A:52:SER:C	1:A:56:LYS:HG2	1.93	0.93
2:B:46:ASN:CA	2:B:46:ASN:CG	2.41	0.93
3:A:142:HEM:C2D	3:A:142:HEM:C3D	0.93	0.93
2:D:2:LEU:HD23	2:D:7:LYS:CB	1.99	0.93
2:D:100:GLN:CA	2:D:100:GLN:HG3	1.98	0.93
1:C:135:VAL:O	1:C:138:SER:HB2	1.68	0.93
1:A:43:PHE:CB	1:A:43:PHE:CD2	2.52	0.93
1:A:119:PRO:C	1:A:120:ALA:CA	2.41	0.93
1:C:52:SER:C	1:C:53:ALA:CA	2.40	0.93
1:C:91:LEU:CG	1:C:91:LEU:CA	2.47	0.93
1:C:115:THR:CG2	1:C:115:THR:HB	1.97	0.93
2:D:59:VAL:HA	2:D:59:VAL:HG22	1.51	0.93
2:D:75:LYS:CG	2:D:75:LYS:HB3	1.42	0.93
1:A:13:ALA:HB1	1:A:125:LEU:HD21	1.50	0.92
1:A:25:GLY:CA	1:A:26:ALA:N	2.32	0.92
1:A:106:LEU:N	1:A:106:LEU:CB	2.32	0.92
1:A:127:LYS:CA	1:A:128:PHE:N	2.32	0.92
2:B:84:PHE:CG	2:B:84:PHE:CD2	0.92	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PHE:CA	1:C:37:PRO:N	2.30	0.92
2:D:144:TYR:HD1	2:D:145:HIS:H	1.10	0.92
2:B:17:VAL:C	2:B:17:VAL:CG1	2.42	0.92
2:B:75:LYS:HG3	2:B:76:HIS:ND1	1.80	0.92
1:C:85:ASN:CG	1:C:89:HIS:HB3	1.93	0.92
1:C:140:TYR:CB	1:C:140:TYR:CD2	2.51	0.92
2:D:75:LYS:CG	2:D:75:LYS:HB2	1.42	0.92
1:A:62:VAL:CG2	1:A:62:VAL:HG11	1.76	0.92
2:B:1:MET:HE1	2:B:78:ASP:OD2	1.65	0.92
2:B:16:LYS:HD3	2:B:117:PHE:CE1	2.02	0.92
2:B:84:PHE:CG	2:B:84:PHE:HD2	1.70	0.92
2:B:31:LEU:CD1	2:B:31:LEU:HG	1.94	0.92
1:C:60:GLN:CG	1:C:60:GLN:CA	2.47	0.92
1:A:36:PHE:O	1:A:39:THR:CG2	2.17	0.92
2:B:103:ARG:CG	2:B:103:ARG:NE	2.31	0.92
2:B:60:LYS:HD2	2:B:60:LYS:HZ2	1.33	0.92
2:B:62:HIS:CG	2:B:62:HIS:CA	2.53	0.92
2:B:95:LEU:HD11	3:B:146:HEM:C3A	2.05	0.92
1:C:92:ARG:CD	1:C:92:ARG:CB	2.47	0.92
2:B:68:ASP:HA	2:B:71:THR:HG23	1.07	0.92
2:D:11:THR:C	2:D:11:THR:HA	1.91	0.92
2:D:67:LEU:CB	2:D:67:LEU:HA	2.00	0.92
2:D:102:PHE:N	2:D:102:PHE:C	2.27	0.92
1:A:57:ALA:HA	1:A:60:GLN:NE2	1.84	0.92
2:D:2:LEU:CD2	2:D:4:ALA:HA	2.00	0.92
2:B:106:GLY:HA3	2:B:133:VAL:HG22	1.51	0.91
1:C:45:HIS:HE1	3:C:142:HEM:CBD	1.82	0.91
1:A:127:LYS:C	1:A:128:PHE:N	0.82	0.91
2:B:34:TYR:CE2	2:B:34:TYR:CD2	0.91	0.91
2:B:117:PHE:CG	2:B:117:PHE:CE1	2.41	0.91
1:A:85:ASN:ND2	1:A:90:LYS:HE3	1.84	0.91
2:B:13:PHE:CA	2:B:13:PHE:O	2.18	0.91
2:B:32:VAL:N	2:B:32:VAL:CB	2.32	0.91
2:D:67:LEU:CA	2:D:67:LEU:CG	2.48	0.91
2:B:103:ARG:CB	2:B:103:ARG:CD	2.49	0.91
2:B:113:VAL:HG12	2:B:117:PHE:CD2	2.04	0.91
1:C:80:LEU:HD23	1:C:135:VAL:CG2	2.00	0.91
2:B:75:LYS:CG	2:B:76:HIS:CE1	2.53	0.91
1:C:126:ASN:ND2	1:C:126:ASN:OD1	2.03	0.91
1:C:113:LEU:HD23	1:C:113:LEU:H	1.36	0.91
2:B:128:LEU:CA	2:B:128:LEU:O	2.17	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:LEU:CD2	2:D:3:THR:O	2.15	0.91
2:D:127:ALA:CB	2:D:127:ALA:C	2.44	0.91
1:A:47:ASP:OD2	1:A:49:SER:HA	1.70	0.91
1:A:80:LEU:CB	1:A:80:LEU:HG	2.00	0.91
2:B:10:VAL:HG13	2:B:128:LEU:HD21	0.91	0.91
2:B:67:LEU:C	2:B:71:THR:HG22	1.96	0.91
1:C:3:SER:C	1:C:3:SER:N	2.29	0.91
2:D:51:GLY:C	2:D:52:ALA:CA	2.42	0.91
2:D:100:GLN:CB	2:D:100:GLN:HA	1.99	0.91
1:A:42:TYR:C	1:A:43:PHE:CA	2.44	0.91
3:B:146:HEM:C3D	3:B:146:HEM:CBD	2.54	0.91
2:B:71:THR:CB	2:B:71:THR:N	2.33	0.90
2:B:74:LEU:HD13	2:B:77:LEU:HB2	0.91	0.90
1:C:44:PRO:CD	1:C:44:PRO:CA	2.49	0.90
1:C:76:LEU:CD1	1:C:76:LEU:HG	2.01	0.90
1:A:141:ARG:HB3	1:C:1:VAL:HG23	1.50	0.90
2:B:74:LEU:HD22	2:B:77:LEU:HD23	1.53	0.90
1:C:54:GLN:CG	1:C:54:GLN:CA	2.50	0.90
2:B:116:ASN:CB	2:B:116:ASN:HA	2.00	0.90
2:B:145:HIS:CB	2:B:145:HIS:N	2.34	0.90
2:B:25:GLN:OE1	2:B:112:VAL:CG1	2.19	0.90
2:B:33:VAL:HG12	2:B:34:TYR:CE1	2.06	0.90
2:D:75:LYS:CD	2:D:75:LYS:CB	2.49	0.90
2:B:86:GLN:CG	2:B:86:GLN:CA	2.50	0.90
1:C:87:HIS:ND1	1:C:87:HIS:CB	2.33	0.90
2:D:17:VAL:C	2:D:17:VAL:N	2.28	0.90
2:D:57:PRO:CA	2:D:57:PRO:CG	2.37	0.90
2:D:68:ASP:C	2:D:68:ASP:N	2.26	0.90
2:B:41:PHE:CD2	2:B:44:PHE:HE1	1.85	0.90
2:B:116:ASN:CA	2:B:116:ASN:CG	2.45	0.90
1:C:93:VAL:HG13	3:C:142:HEM:HAC	1.54	0.90
1:C:52:SER:CB	1:C:55:GLN:HE21	1.84	0.90
2:D:107:ASN:HB2	2:D:107:ASN:H	1.35	0.90
2:B:20:ASP:HB3	2:B:64:LYS:CE	2.02	0.90
1:C:133:SER:C	1:C:134:THR:CA	2.45	0.90
1:C:17:VAL:C	1:C:17:VAL:N	2.30	0.89
1:C:39:THR:CA	1:C:39:THR:HB	2.01	0.89
1:C:89:HIS:HB2	1:C:139:LYS:HZ2	1.36	0.89
3:A:142:HEM:CBA	3:A:142:HEM:C2A	2.54	0.89
1:C:89:HIS:HE1	1:C:90:LYS:HG2	1.36	0.89
2:D:53:VAL:CG2	2:D:54:MET:HE2	2.02	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:PRO:CA	2:D:57:PRO:CD	2.46	0.89
1:A:124:ASN:CB	1:A:124:ASN:CA	0.90	0.89
2:B:36:TRP:CE2	2:B:36:TRP:CZ2	0.90	0.89
1:C:36:PHE:CB	1:C:36:PHE:C	2.46	0.89
2:D:100:GLN:O	2:D:101:ASN:HA	1.72	0.89
2:B:69:ALA:CB	2:B:69:ALA:CA	0.89	0.89
1:C:115:THR:C	1:C:115:THR:N	2.29	0.89
1:A:39:THR:HG23	1:A:40:LYS:NZ	1.88	0.89
1:A:132:ASP:OD2	1:A:132:ASP:CB	2.20	0.89
1:C:45:HIS:CE1	3:C:142:HEM:CGD	2.56	0.89
2:D:2:LEU:HB3	2:D:2:LEU:HD13	1.52	0.89
1:A:135:VAL:CG2	1:A:135:VAL:CG1	2.51	0.89
2:D:2:LEU:HD22	2:D:4:ALA:CA	2.03	0.89
2:D:14:TRP:CA	2:D:14:TRP:O	2.19	0.89
2:D:75:LYS:CB	2:D:75:LYS:HG3	1.37	0.89
2:B:23:GLY:C	2:B:24:ALA:CA	2.46	0.89
2:B:36:TRP:CE2	2:B:36:TRP:HZ2	1.65	0.89
2:B:144:TYR:O	2:D:1:MET:HE1	1.73	0.89
2:D:2:LEU:HG	2:D:7:LYS:CD	2.02	0.89
2:D:71:THR:CG2	2:D:71:THR:CA	2.51	0.89
2:B:17:VAL:C	2:B:17:VAL:CB	2.44	0.89
2:B:54:MET:CB	2:B:55:ASN:OD1	2.20	0.89
1:C:61:LYS:CD	1:C:61:LYS:CB	2.45	0.89
2:D:7:LYS:O	2:D:7:LYS:C	0.70	0.89
1:A:3:SER:O	1:A:4:ALA:CA	2.20	0.88
2:B:16:LYS:N	2:B:16:LYS:CB	2.36	0.88
2:B:19:VAL:CB	2:B:19:VAL:C	2.46	0.88
2:B:130:GLN:NE2	2:B:130:GLN:CD	0.78	0.88
1:C:113:LEU:CD2	1:C:113:LEU:H	1.86	0.88
2:D:7:LYS:O	2:D:8:ALA:N	0.75	0.88
2:B:22:VAL:CG2	2:B:22:VAL:HA	2.01	0.88
2:D:109:LEU:C	2:D:109:LEU:N	2.30	0.88
1:A:69:ALA:N	1:A:69:ALA:C	2.31	0.88
1:A:115:THR:OG1	1:A:115:THR:CA	2.20	0.88
1:A:136:LEU:C	1:A:136:LEU:CB	2.47	0.88
2:B:2:LEU:HB2	2:B:3:THR:H	1.37	0.88
2:B:3:THR:CB	2:B:5:GLU:HB3	2.03	0.88
2:B:117:PHE:CD1	2:B:117:PHE:CE1	0.88	0.88
2:D:25:GLN:HE22	2:D:115:ARG:HH22	1.22	0.88
2:D:119:GLY:N	2:D:119:GLY:C	2.31	0.88
2:D:130:GLN:CD	2:D:130:GLN:CB	2.46	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:142:HEM:C2D	3:A:142:HEM:HAD2	2.07	0.88
2:B:41:PHE:CG	2:B:44:PHE:HE1	1.88	0.88
1:C:89:HIS:CE1	1:C:90:LYS:HG2	2.08	0.88
1:C:56:LYS:NZ	1:C:59:GLY:CA	2.36	0.88
1:C:97:ASN:CA	1:C:98:PHE:N	2.36	0.88
1:A:2:LEU:CB	1:A:2:LEU:HA	2.00	0.88
2:B:40:PHE:HB3	3:B:146:HEM:CMA	2.03	0.88
2:B:87:LEU:HD21	2:B:87:LEU:HD11	1.56	0.88
2:B:118:GLY:CA	2:B:118:GLY:N	0.73	0.88
1:C:95:PRO:HG3	1:C:141:ARG:NH1	1.89	0.88
2:D:100:GLN:HA	2:D:100:GLN:HG3	1.52	0.88
2:D:131:LYS:CG	2:D:131:LYS:CA	2.52	0.88
2:B:2:LEU:CD1	2:B:6:GLU:HB3	2.04	0.88
1:C:110:ALA:C	1:C:110:ALA:N	2.32	0.88
2:B:11:THR:CA	2:B:11:THR:O	2.21	0.87
1:C:131:ASN:CB	1:C:131:ASN:C	2.47	0.87
1:A:49:SER:HB2	1:A:52:SER:HB3	0.89	0.87
2:B:38:GLN:NE2	2:B:47:LEU:O	2.07	0.87
1:A:85:ASN:C	1:A:85:ASN:HD22	1.81	0.87
2:B:14:TRP:NE1	2:B:68:ASP:CG	2.32	0.87
2:B:131:LYS:CD	2:B:131:LYS:NZ	2.37	0.87
1:C:68:LYS:NZ	1:C:68:LYS:CD	2.37	0.87
1:C:140:TYR:O	1:C:140:TYR:CD1	2.28	0.87
2:D:55:ASN:O	2:D:60:LYS:HD3	1.74	0.87
1:A:16:LYS:HZ2	1:A:16:LYS:HD2	1.37	0.87
1:A:85:ASN:HD22	1:A:86:LEU:N	1.72	0.87
1:C:93:VAL:HG13	3:C:142:HEM:CAC	2.05	0.87
1:A:25:GLY:O	1:A:29:LEU:HD22	1.75	0.87
1:A:67:THR:CA	1:A:68:LYS:N	2.35	0.87
2:B:10:VAL:HG13	2:B:128:LEU:CD2	1.72	0.87
1:C:84:SER:C	1:C:84:SER:HB2	1.98	0.87
2:B:75:LYS:CG	2:B:75:LYS:HE3	2.05	0.87
2:D:28:GLY:HA3	2:D:54:MET:HE1	1.55	0.87
2:D:68:ASP:CG	2:D:68:ASP:HA	1.98	0.87
1:A:108:THR:CA	1:A:108:THR:O	2.22	0.86
1:A:11:LYS:O	1:A:11:LYS:CA	2.22	0.86
2:B:79:ASP:O	2:B:80:LEU:N	2.06	0.86
1:C:29:LEU:CA	1:C:29:LEU:HB3	2.06	0.86
2:D:14:TRP:HE1	2:D:71:THR:CG2	1.87	0.86
2:D:107:ASN:N	2:D:107:ASN:HB2	1.88	0.86
2:B:2:LEU:HD12	2:B:6:GLU:HB3	1.55	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ASP:CB	2:B:71:THR:O	2.22	0.86
1:C:104:SER:C	1:C:104:SER:CB	2.48	0.86
1:A:124:ASN:CB	1:A:124:ASN:HA	1.35	0.86
2:D:22:VAL:CG1	2:D:22:VAL:CG2	2.53	0.86
1:A:3:SER:C	1:A:4:ALA:CA	2.49	0.86
1:C:14:TRP:HB2	1:C:70:GLN:HE22	1.40	0.86
2:D:34:TYR:CZ	2:D:34:TYR:HE2	1.59	0.86
2:D:34:TYR:HB3	2:D:36:TRP:CZ2	2.10	0.86
2:D:53:VAL:CG2	2:D:54:MET:CE	2.53	0.86
1:A:33:PHE:HB3	1:A:40:LYS:HG3	1.57	0.86
1:A:114:PRO:CD	1:A:114:PRO:CA	2.54	0.86
2:B:144:TYR:O	2:D:1:MET:SD	2.33	0.86
1:C:55:GLN:CB	1:C:55:GLN:HA	2.04	0.86
2:D:45:GLY:C	2:D:46:ASN:CA	2.48	0.86
2:D:126:GLN:NE2	2:D:130:GLN:HB2	1.91	0.86
2:B:87:LEU:CA	2:B:87:LEU:O	2.23	0.86
1:C:89:HIS:N	1:C:139:LYS:HG3	1.91	0.86
2:D:75:LYS:CB	2:D:75:LYS:HG2	1.37	0.86
1:A:126:ASN:ND2	1:A:126:ASN:OD1	2.08	0.86
2:B:57:PRO:CD	2:B:57:PRO:HB3	2.02	0.86
2:B:144:TYR:O	2:D:1:MET:CE	2.23	0.86
2:D:20:ASP:C	2:D:21:VAL:CA	2.44	0.86
1:A:46:PHE:HB2	1:A:48:LEU:HD23	1.55	0.86
1:C:48:LEU:CD1	1:C:49:SER:HB2	2.05	0.86
1:C:137:THR:O	1:C:138:SER:N	2.07	0.86
2:D:110:ALA:C	2:D:110:ALA:CB	2.48	0.86
1:A:22:PRO:CB	1:A:22:PRO:CD	2.54	0.85
3:A:142:HEM:CAA	3:A:142:HEM:CGA	2.54	0.85
1:C:100:LEU:N	1:C:100:LEU:C	2.34	0.85
2:D:34:TYR:N	2:D:34:TYR:CB	2.37	0.85
2:B:94:LYS:C	2:B:94:LYS:CB	2.49	0.85
2:D:14:TRP:C	2:D:14:TRP:N	2.32	0.85
1:A:16:LYS:HD3	1:A:16:LYS:HZ3	1.38	0.85
2:B:133:VAL:CG2	2:B:133:VAL:CG1	2.53	0.85
1:A:9:ASN:N	1:A:9:ASN:HB2	1.89	0.85
2:B:3:THR:HG23	2:B:5:GLU:CG	2.06	0.85
2:B:19:VAL:CG2	2:B:68:ASP:H	1.90	0.85
1:C:14:TRP:C	1:C:15:GLY:CA	2.49	0.85
2:D:1:MET:HG3	2:D:131:LYS:HZ1	1.42	0.85
2:D:75:LYS:HB3	2:D:76:HIS:H	1.42	0.85
1:A:39:THR:CA	1:A:40:LYS:HZ3	1.89	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:GLN:OE1	2:B:112:VAL:HG12	1.74	0.85
2:D:11:THR:HA	2:D:14:TRP:H	1.40	0.85
2:D:67:LEU:HD23	2:D:71:THR:HG21	1.59	0.85
2:D:90:LEU:CD1	2:D:90:LEU:HB3	2.04	0.85
1:A:96:VAL:HG11	2:D:100:GLN:HG2	1.58	0.85
1:A:104:SER:CB	1:A:104:SER:C	2.49	0.85
2:B:128:LEU:HA	2:B:128:LEU:O	1.76	0.85
2:D:31:LEU:CA	2:D:31:LEU:CG	2.54	0.85
1:A:89:HIS:HD2	1:A:139:LYS:HD2	1.38	0.85
2:D:121:PHE:CB	2:D:121:PHE:C	2.49	0.85
3:A:142:HEM:CBD	3:A:142:HEM:HAD2	2.07	0.85
2:B:14:TRP:NE1	2:B:68:ASP:OD1	2.10	0.85
2:B:70:PHE:CZ	2:B:70:PHE:CD1	2.59	0.85
2:D:78:ASP:CA	2:D:79:ASP:N	2.38	0.85
1:C:80:LEU:CD1	1:C:80:LEU:CB	2.55	0.84
1:C:3:SER:C	1:C:3:SER:CB	2.51	0.84
1:C:30:GLN:CG	1:C:30:GLN:OE1	2.24	0.84
1:C:97:ASN:C	1:C:97:ASN:CB	2.50	0.84
2:D:95:LEU:HD23	2:D:95:LEU:N	1.91	0.84
1:A:16:LYS:H	1:A:17:VAL:N	1.75	0.84
1:A:105:LEU:CD1	1:A:105:LEU:HD22	2.05	0.84
2:B:80:LEU:HD23	2:B:81:LYS:O	1.77	0.84
2:D:14:TRP:CA	2:D:15:GLY:N	2.38	0.84
2:D:73:GLY:CA	2:D:73:GLY:O	2.24	0.84
2:D:144:TYR:CD1	2:D:145:HIS:N	2.45	0.84
1:A:83:LEU:C	1:A:84:SER:CA	2.49	0.84
1:C:121:VAL:C	1:C:122:HIS:CA	2.50	0.84
1:A:35:SER:CB	1:A:35:SER:HA	2.05	0.84
2:B:3:THR:C	2:B:4:ALA:CA	2.50	0.84
2:B:20:ASP:O	2:B:21:VAL:CG2	2.25	0.84
1:C:89:HIS:ND1	1:C:89:HIS:C	2.34	0.84
2:D:75:LYS:HB3	2:D:76:HIS:N	1.93	0.84
2:D:76:HIS:CG	2:D:76:HIS:H	1.96	0.84
1:A:31:ARG:HD3	2:B:126:GLN:HG3	1.59	0.84
2:B:106:GLY:CA	2:B:133:VAL:HG22	2.07	0.84
1:A:1:VAL:CG1	1:A:1:VAL:CA	2.56	0.84
1:A:46:PHE:CB	1:A:48:LEU:HD23	2.07	0.84
1:A:128:PHE:CD1	1:A:128:PHE:CZ	2.58	0.84
2:B:75:LYS:HG3	2:B:76:HIS:HE1	1.40	0.84
2:B:95:LEU:N	2:B:95:LEU:HB2	1.74	0.84
1:C:72:HIS:CB	1:C:74:ASN:HD21	1.89	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:HH21	2:B:126:GLN:CB	1.88	0.84
1:C:43:PHE:HB3	1:C:46:PHE:HD1	1.43	0.84
2:D:2:LEU:CB	2:D:2:LEU:HD13	2.01	0.84
1:A:104:SER:CB	1:A:104:SER:OG	2.26	0.84
2:B:2:LEU:HD12	2:B:6:GLU:CB	2.06	0.84
2:B:34:TYR:CE2	2:B:34:TYR:HD2	1.54	0.84
2:B:56:ASN:O	2:B:57:PRO:N	2.09	0.84
2:B:74:LEU:HD13	2:B:77:LEU:CG	2.06	0.84
1:C:54:GLN:CB	1:C:54:GLN:C	2.49	0.84
1:C:86:LEU:CB	1:C:86:LEU:C	2.50	0.84
3:C:142:HEM:CHD	3:C:142:HEM:NC	2.41	0.83
2:D:16:LYS:CD	2:D:16:LYS:HB3	2.07	0.83
2:B:2:LEU:HD12	2:B:6:GLU:CG	2.08	0.83
1:C:29:LEU:CD2	1:C:29:LEU:HD13	2.06	0.83
1:C:85:ASN:C	1:C:85:ASN:N	2.33	0.83
1:C:92:ARG:CG	1:C:92:ARG:NE	2.41	0.83
2:D:130:GLN:CG	2:D:130:GLN:CB	0.84	0.83
1:A:86:LEU:C	1:A:87:HIS:HA	2.02	0.83
2:B:101:ASN:C	3:B:146:HEM:HBB1	2.04	0.83
2:B:117:PHE:CD1	2:B:117:PHE:HE1	1.54	0.83
1:C:7:LYS:HG2	1:C:73:LEU:CB	2.08	0.83
1:C:87:HIS:CA	1:C:91:LEU:HD12	2.04	0.83
2:D:2:LEU:CB	2:D:2:LEU:HD12	2.01	0.83
2:D:67:LEU:CD2	2:D:71:THR:HG21	2.09	0.83
2:D:105:LEU:CB	2:D:105:LEU:HD13	2.06	0.83
1:A:76:LEU:C	1:A:77:PRO:CA	2.51	0.83
1:A:88:ALA:O	1:A:92:ARG:HA	1.77	0.83
2:B:25:GLN:CD	2:B:112:VAL:HG11	2.04	0.83
2:B:74:LEU:HD22	2:B:77:LEU:CD2	2.09	0.83
1:C:69:ALA:C	1:C:69:ALA:N	2.36	0.83
2:D:25:GLN:CG	2:D:25:GLN:OE1	2.27	0.83
2:D:95:LEU:HD12	2:D:97:VAL:CG2	2.08	0.83
1:A:3:SER:HB3	1:A:6:ASN:HD22	1.42	0.83
2:B:4:ALA:CA	2:B:4:ALA:O	2.27	0.83
2:B:60:LYS:NZ	2:B:60:LYS:HD2	1.91	0.83
2:B:103:ARG:CZ	2:B:103:ARG:HH11	1.49	0.83
2:D:44:PHE:CD2	2:D:58:LYS:HB3	2.13	0.83
2:D:99:PRO:CD	2:D:144:TYR:OH	2.27	0.83
1:A:33:PHE:HD1	1:A:40:LYS:HE3	1.42	0.83
2:B:67:LEU:C	2:B:71:THR:CG2	2.50	0.83
2:B:103:ARG:CZ	2:B:103:ARG:HH12	1.49	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:HIS:CD2	1:C:46:PHE:CE1	2.67	0.83
1:C:103:HIS:O	1:C:107:VAL:HG12	1.78	0.83
1:A:55:GLN:CA	1:A:55:GLN:CG	2.54	0.83
1:A:18:GLY:O	1:A:18:GLY:CA	2.26	0.82
2:B:68:ASP:CA	2:B:71:THR:HG23	1.68	0.82
2:B:88:SER:CB	2:B:143:LYS:HB3	2.08	0.82
2:B:113:VAL:HG12	2:B:117:PHE:HD2	1.43	0.82
1:C:122:HIS:ND1	1:C:122:HIS:HB2	1.91	0.82
2:B:3:THR:HB	2:B:6:GLU:HB2	1.61	0.82
2:D:26:ALA:C	2:D:26:ALA:CB	2.53	0.82
1:A:127:LYS:HZ2	1:A:127:LYS:HD2	1.43	0.82
2:B:15:GLY:C	2:B:16:LYS:CA	2.51	0.82
1:C:45:HIS:CB	1:C:45:HIS:C	2.51	0.82
1:C:122:HIS:ND1	1:C:122:HIS:CB	2.36	0.82
1:A:86:LEU:CD2	1:A:86:LEU:CB	2.58	0.82
2:D:62:HIS:CE1	2:D:62:HIS:CD2	2.67	0.82
1:A:48:LEU:CB	1:A:48:LEU:HA	2.08	0.82
2:B:2:LEU:CB	2:B:6:GLU:HB3	2.08	0.82
2:B:3:THR:HG21	2:B:5:GLU:CD	2.04	0.82
1:A:31:ARG:NE	1:A:31:ARG:HG2	1.94	0.82
2:B:52:ALA:N	2:B:52:ALA:CB	2.43	0.82
2:B:53:VAL:O	2:B:59:VAL:HG21	1.80	0.82
2:B:65:ARG:N	2:B:65:ARG:C	2.34	0.82
2:B:95:LEU:N	2:B:95:LEU:C	2.37	0.82
1:C:48:LEU:HA	1:C:55:GLN:OE1	1.80	0.82
1:C:111:SER:O	1:C:114:PRO:HG3	1.80	0.82
2:D:75:LYS:CG	2:D:75:LYS:CB	0.82	0.82
1:A:43:PHE:C	1:A:44:PRO:CA	2.52	0.82
1:A:112:HIS:ND1	1:A:112:HIS:CB	2.40	0.82
1:C:45:HIS:CD2	1:C:46:PHE:CD1	2.68	0.82
1:C:88:ALA:CB	1:C:139:LYS:HB2	2.09	0.82
1:A:7:LYS:CA	1:A:8:SER:N	2.40	0.82
1:C:29:LEU:CA	1:C:29:LEU:HB2	2.06	0.82
1:A:53:ALA:CA	1:A:56:LYS:HG2	2.10	0.82
2:B:31:LEU:CD1	2:B:31:LEU:CD2	2.58	0.82
1:C:27:GLN:C	1:C:28:ALA:CA	2.52	0.82
2:D:141:ALA:C	2:D:142:HIS:CA	2.53	0.82
2:B:70:PHE:CZ	2:B:70:PHE:CG	2.67	0.81
1:C:88:ALA:HB1	1:C:139:LYS:HB2	1.61	0.81
1:C:90:LYS:C	1:C:91:LEU:CA	2.52	0.81
2:D:49:SER:O	2:D:53:VAL:CG1	2.27	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:OG1	1:A:137:THR:HA	1.79	0.81
1:A:137:THR:OG1	1:A:137:THR:HG23	1.80	0.81
1:C:83:LEU:HD11	3:C:142:HEM:HMA1	1.62	0.81
1:C:130:ALA:N	1:C:130:ALA:CB	2.43	0.81
2:D:31:LEU:C	2:D:31:LEU:N	2.38	0.81
2:B:4:ALA:CA	2:B:5:GLU:H	1.89	0.81
1:C:101:LEU:O	1:C:105:LEU:HB3	1.78	0.81
1:C:129:LEU:CB	1:C:129:LEU:CD2	2.57	0.81
2:D:12:GLY:N	2:D:12:GLY:C	2.38	0.81
2:D:103:ARG:CD	2:D:103:ARG:CB	2.58	0.81
1:A:20:ASN:O	1:A:23:ALA:HB3	1.80	0.81
1:A:50:HIS:CG	1:A:50:HIS:CA	2.62	0.81
2:B:34:TYR:N	2:B:34:TYR:C	2.38	0.81
1:C:69:ALA:C	1:C:69:ALA:HB3	2.03	0.81
1:C:135:VAL:O	1:C:138:SER:CB	2.29	0.81
2:D:61:ALA:CB	2:D:61:ALA:C	2.52	0.81
2:D:78:ASP:C	2:D:78:ASP:N	2.37	0.81
2:B:3:THR:HG22	2:B:6:GLU:CA	2.11	0.81
2:B:128:LEU:CD1	2:B:128:LEU:CB	2.58	0.81
1:C:138:SER:CB	1:C:138:SER:N	2.44	0.81
2:D:137:ALA:HB1	2:D:140:LEU:CD1	2.09	0.81
1:A:29:LEU:CD2	1:A:29:LEU:CD1	2.58	0.81
2:B:1:MET:H2	2:B:2:LEU:HD23	1.30	0.81
2:B:130:GLN:CD	2:B:130:GLN:HE22	1.43	0.81
1:C:22:PRO:CB	1:C:22:PRO:HD2	2.11	0.81
2:B:19:VAL:CA	2:B:19:VAL:CG2	2.59	0.81
2:B:59:VAL:O	2:B:59:VAL:CA	2.28	0.81
2:B:130:GLN:CD	2:B:130:GLN:HE21	1.42	0.81
1:C:41:THR:CG2	1:C:41:THR:HB	2.10	0.81
2:D:76:HIS:CB	2:D:76:HIS:N	2.44	0.81
1:A:57:ALA:CB	1:A:57:ALA:H	1.92	0.81
3:B:146:HEM:C3D	3:B:146:HEM:CHA	2.64	0.81
1:C:43:PHE:CB	1:C:43:PHE:N	2.44	0.81
2:D:11:THR:N	2:D:11:THR:CG2	2.42	0.81
2:D:67:LEU:CA	2:D:67:LEU:O	2.29	0.81
1:A:2:LEU:CB	1:A:2:LEU:HG	2.08	0.81
1:A:85:ASN:CA	1:A:85:ASN:CG	2.53	0.81
2:B:32:VAL:N	2:B:32:VAL:C	2.37	0.81
2:B:32:VAL:CB	2:B:32:VAL:CG2	2.59	0.81
1:C:39:THR:CB	1:C:39:THR:N	2.40	0.81
1:A:89:HIS:HD2	1:A:139:LYS:HG2	1.46	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ARG:NH1	3:B:146:HEM:CGD	2.44	0.80
2:B:98:ASN:HB3	2:B:100:GLN:N	1.95	0.80
2:B:106:GLY:CA	2:B:133:VAL:CG2	2.59	0.80
1:A:52:SER:C	1:A:54:GLN:N	2.39	0.80
2:B:39:ARG:NH1	2:B:40:PHE:CE1	2.48	0.80
1:A:109:LEU:HD12	1:A:117:PHE:HE1	1.46	0.80
3:A:142:HEM:CBD	3:A:142:HEM:HAD1	2.07	0.80
2:B:1:MET:CE	2:B:78:ASP:OD2	2.29	0.80
2:B:2:LEU:HB2	2:B:6:GLU:HB3	1.64	0.80
2:B:65:ARG:HD3	3:B:146:HEM:HBD1	1.64	0.80
1:C:14:TRP:HB2	1:C:70:GLN:NE2	1.96	0.80
1:C:79:THR:CA	1:C:79:THR:OG1	2.28	0.80
1:A:110:ALA:HB1	2:B:115:ARG:HB2	1.63	0.80
2:B:2:LEU:HB3	2:B:131:LYS:HZ1	1.46	0.80
1:C:84:SER:OG	1:C:136:LEU:HD22	1.82	0.80
2:B:64:LYS:HZ2	2:B:64:LYS:CB	1.87	0.80
1:C:93:VAL:HG11	3:C:142:HEM:C3C	2.16	0.80
2:D:112:VAL:CG1	2:D:112:VAL:CA	2.59	0.80
2:B:41:PHE:HB3	2:B:44:PHE:CE1	2.16	0.80
1:C:22:PRO:CD	1:C:22:PRO:HB2	2.10	0.80
2:D:50:ALA:O	2:D:53:VAL:HG13	1.82	0.80
1:A:81:SER:C	1:A:82:ASN:CA	2.49	0.80
2:B:77:LEU:HD13	2:B:77:LEU:C	2.07	0.80
1:C:99:LYS:CG	1:C:99:LYS:CE	2.59	0.80
2:D:115:ARG:CB	2:D:115:ARG:N	2.44	0.80
2:B:117:PHE:CE1	2:B:117:PHE:HD1	1.56	0.80
2:B:136:VAL:C	2:B:136:VAL:CB	2.51	0.80
2:D:99:PRO:HD2	2:D:144:TYR:CZ	2.17	0.80
1:A:31:ARG:CG	1:A:31:ARG:HE	1.95	0.80
1:C:45:HIS:NE2	1:C:46:PHE:CE1	2.50	0.80
1:C:49:SER:HA	1:C:55:GLN:OE1	1.82	0.80
1:C:108:THR:CB	1:C:108:THR:C	2.54	0.80
1:C:133:SER:CA	1:C:134:THR:N	2.43	0.80
2:D:17:VAL:C	2:D:17:VAL:CB	2.55	0.80
1:A:26:ALA:HB2	1:A:59:GLY:HA3	1.63	0.79
1:A:58:HIS:CB	1:A:58:HIS:HA	2.10	0.79
1:C:56:LYS:CG	1:C:56:LYS:CA	2.56	0.79
1:C:110:ALA:O	1:C:114:PRO:HB3	1.82	0.79
1:C:138:SER:CB	1:C:138:SER:C	2.54	0.79
1:C:22:PRO:O	1:C:56:LYS:CE	2.30	0.79
2:D:16:LYS:HD3	2:D:16:LYS:HB3	1.57	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:ASN:C	3:D:146:HEM:HBB1	2.06	0.79
1:A:63:ALA:CB	1:A:63:ALA:C	2.53	0.79
1:A:119:PRO:CG	1:A:119:PRO:N	2.46	0.79
1:C:104:SER:C	1:C:104:SER:N	2.39	0.79
1:A:39:THR:OG1	1:A:40:LYS:NZ	2.16	0.79
1:A:122:HIS:CA	1:A:123:ALA:N	2.42	0.79
2:B:2:LEU:HB2	2:B:6:GLU:OE2	1.83	0.79
1:C:24:TYR:CG	1:C:24:TYR:HA	2.17	0.79
1:C:70:GLN:OE1	1:C:70:GLN:O	2.00	0.79
2:D:47:LEU:CA	2:D:47:LEU:HB3	2.09	0.79
2:D:124:ASN:CB	2:D:124:ASN:C	2.56	0.79
2:B:2:LEU:HB2	2:B:3:THR:N	1.96	0.79
2:B:122:THR:OG1	2:B:125:VAL:N	2.15	0.79
1:C:84:SER:OG	1:C:136:LEU:HD13	1.82	0.79
2:D:131:LYS:CB	2:D:131:LYS:CD	2.56	0.79
1:C:116:ASN:CA	1:C:116:ASN:O	2.31	0.79
1:C:117:PHE:CA	1:C:117:PHE:O	2.30	0.79
2:D:121:PHE:CA	2:D:121:PHE:CG	2.60	0.79
2:D:124:ASN:CG	2:D:124:ASN:CA	2.55	0.79
2:D:31:LEU:HD11	2:D:41:PHE:CE1	2.17	0.79
1:A:8:SER:O	1:A:9:ASN:N	2.16	0.79
1:A:91:LEU:CD2	1:A:91:LEU:HD11	2.07	0.79
2:D:14:TRP:CD1	2:D:14:TRP:CB	2.64	0.79
1:A:2:LEU:HD13	1:A:3:SER:N	1.98	0.79
1:A:124:ASN:HB3	1:A:124:ASN:HA	1.17	0.79
1:A:3:SER:CB	1:A:6:ASN:HD22	1.96	0.78
1:A:88:ALA:C	1:A:88:ALA:N	2.41	0.78
2:B:91:HIS:HA	2:B:95:LEU:HD23	1.65	0.78
2:D:47:LEU:CB	2:D:47:LEU:HA	2.10	0.78
2:D:86:GLN:CA	2:D:86:GLN:O	2.29	0.78
2:D:94:LYS:HG3	2:D:95:LEU:CD2	2.10	0.78
1:A:34:LEU:CA	1:A:34:LEU:CG	2.61	0.78
2:B:1:MET:HG3	2:B:77:LEU:CD1	1.81	0.78
2:B:88:SER:OG	2:B:143:LYS:CB	2.31	0.78
1:C:70:GLN:C	1:C:70:GLN:HB3	2.08	0.78
1:C:83:LEU:CG	1:C:83:LEU:CA	2.61	0.78
1:A:91:LEU:HD21	3:A:142:HEM:C3D	2.15	0.78
2:B:5:GLU:O	2:B:8:ALA:HB3	1.83	0.78
2:B:65:ARG:NH2	2:B:65:ARG:HH12	1.81	0.78
1:C:29:LEU:CB	1:C:29:LEU:HA	2.07	0.78
2:B:54:MET:CA	2:B:54:MET:HG3	2.14	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ALA:H	1:C:56:LYS:CE	1.92	0.78
2:B:1:MET:N	2:B:77:LEU:HD11	1.99	0.78
2:B:95:LEU:HG	2:B:95:LEU:HA	1.65	0.78
1:C:59:GLY:C	1:C:59:GLY:N	2.41	0.78
2:D:79:ASP:C	2:D:81:LYS:HD2	2.09	0.78
1:A:2:LEU:HD13	1:A:3:SER:H	1.46	0.78
1:A:31:ARG:CD	1:A:31:ARG:HG3	2.12	0.78
2:B:7:LYS:CA	2:B:8:ALA:N	2.46	0.78
1:C:137:THR:N	1:C:137:THR:C	2.42	0.78
2:B:62:HIS:CG	2:B:62:HIS:HA	2.18	0.78
1:C:3:SER:CA	1:C:4:ALA:N	2.42	0.78
1:C:84:SER:C	1:C:84:SER:HB3	2.08	0.78
1:A:103:HIS:CA	1:A:103:HIS:CG	2.64	0.78
2:D:6:GLU:CB	2:D:128:LEU:HD23	2.09	0.78
2:B:34:TYR:N	2:B:35:PRO:CD	2.47	0.78
2:B:98:ASN:OD1	2:B:98:ASN:CB	2.32	0.78
2:B:117:PHE:CD1	2:B:117:PHE:CE2	2.72	0.78
1:C:67:THR:CG2	1:C:67:THR:CA	2.62	0.78
1:A:31:ARG:CD	1:A:31:ARG:HG2	2.12	0.77
1:A:31:ARG:CB	2:B:126:GLN:HE21	1.93	0.77
1:A:39:THR:CB	1:A:40:LYS:NZ	2.45	0.77
2:B:3:THR:H	2:B:6:GLU:CB	1.97	0.77
1:C:45:HIS:CE1	1:C:46:PHE:HE1	2.03	0.77
2:D:4:ALA:CA	2:D:5:GLU:N	2.44	0.77
1:A:31:ARG:CG	2:B:126:GLN:NE2	2.42	0.77
1:A:42:TYR:C	1:A:43:PHE:HA	2.08	0.77
1:C:56:LYS:HZ1	1:C:59:GLY:CA	1.95	0.77
2:D:3:THR:N	2:D:3:THR:C	2.42	0.77
1:A:52:SER:C	1:A:54:GLN:H	1.92	0.77
2:B:20:ASP:HB3	2:B:64:LYS:CD	2.15	0.77
1:C:21:ALA:O	1:C:22:PRO:CA	2.30	0.77
1:C:68:LYS:CB	1:C:68:LYS:CD	2.63	0.77
2:D:124:ASN:C	2:D:124:ASN:N	2.41	0.77
2:B:62:HIS:CD2	2:B:66:VAL:CB	2.67	0.77
2:B:74:LEU:CB	2:B:74:LEU:CD2	2.63	0.77
2:B:80:LEU:HB2	2:B:82:GLY:HA3	1.66	0.77
2:B:98:ASN:HB3	2:B:101:ASN:H	1.50	0.77
1:C:91:LEU:CB	1:C:91:LEU:CD1	2.63	0.77
1:A:33:PHE:CD1	1:A:40:LYS:HE3	2.19	0.77
1:A:91:LEU:CD2	3:A:142:HEM:CAD	2.60	0.77
2:D:2:LEU:CD2	2:D:7:LYS:CG	2.57	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:ARG:CA	2:D:65:ARG:O	2.31	0.77
2:B:76:HIS:O	2:B:78:ASP:HB3	1.84	0.77
2:B:1:MET:O	2:B:2:LEU:HD23	1.84	0.77
1:C:68:LYS:HD3	1:C:79:THR:HG22	1.66	0.77
2:D:34:TYR:O	2:D:37:THR:HB	1.85	0.77
1:A:46:PHE:CD1	1:A:55:GLN:NE2	2.52	0.77
1:A:57:ALA:O	1:A:60:GLN:HB3	1.85	0.77
2:B:49:SER:HB3	2:B:52:ALA:CB	2.15	0.77
2:B:108:VAL:CG2	2:B:108:VAL:CA	2.62	0.77
1:A:48:LEU:CD2	1:A:48:LEU:CD1	2.62	0.77
1:A:85:ASN:C	1:A:85:ASN:ND2	2.41	0.77
2:B:84:PHE:CG	2:B:84:PHE:CA	2.67	0.77
3:B:146:HEM:HMA2	3:B:146:HEM:HHB	1.67	0.77
1:A:86:LEU:C	1:A:87:HIS:CA	2.58	0.77
2:B:62:HIS:N	2:B:62:HIS:C	2.43	0.77
2:B:64:LYS:N	2:B:64:LYS:CB	2.43	0.77
2:B:136:VAL:C	2:B:136:VAL:N	2.42	0.77
1:C:17:VAL:CG1	1:C:17:VAL:CG2	2.62	0.77
2:B:123:PRO:HB3	2:B:126:GLN:NE2	2.00	0.76
1:C:45:HIS:CB	1:C:45:HIS:N	2.48	0.76
2:B:76:HIS:N	2:B:76:HIS:ND1	2.33	0.76
1:A:16:LYS:CD	1:A:16:LYS:HZ3	1.86	0.76
2:B:2:LEU:HD12	2:B:6:GLU:HG2	1.66	0.76
2:B:20:ASP:CB	2:B:64:LYS:CD	2.63	0.76
2:B:69:ALA:CB	2:B:70:PHE:N	2.49	0.76
1:C:22:PRO:HD2	1:C:22:PRO:HB2	1.67	0.76
1:C:26:ALA:N	1:C:56:LYS:HE2	1.96	0.76
1:C:108:THR:C	1:C:108:THR:HB	2.09	0.76
1:A:35:SER:CB	1:A:35:SER:C	2.56	0.76
2:B:33:VAL:O	2:B:35:PRO:HD2	1.85	0.76
2:B:76:HIS:C	2:B:78:ASP:HB3	2.10	0.76
1:A:41:THR:CB	1:A:41:THR:N	2.38	0.76
2:B:20:ASP:O	2:B:21:VAL:HG23	1.85	0.76
1:A:1:VAL:CG1	1:C:141:ARG:O	2.33	0.76
2:B:9:ALA:C	2:B:10:VAL:CA	2.57	0.76
2:B:25:GLN:CG	2:B:112:VAL:HG11	2.16	0.76
2:B:47:LEU:HD12	2:B:53:VAL:CG2	2.13	0.76
2:B:130:GLN:NE2	2:B:130:GLN:OE1	2.17	0.76
1:A:94:ASN:OD1	1:A:96:VAL:HG22	1.86	0.76
1:C:3:SER:CA	1:C:3:SER:OG	2.34	0.76
1:A:70:GLN:C	1:A:73:LEU:HD12	2.11	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:C	1:A:85:ASN:HB3	2.11	0.76
1:C:21:ALA:C	1:C:22:PRO:CA	2.59	0.76
1:C:87:HIS:HB3	1:C:93:VAL:HG21	1.68	0.76
2:D:2:LEU:HD22	2:D:3:THR:C	2.11	0.76
1:A:3:SER:O	1:A:4:ALA:HA	1.84	0.76
1:C:45:HIS:CE1	1:C:46:PHE:CE1	2.73	0.76
1:C:134:THR:CA	1:C:134:THR:CG2	2.63	0.76
1:A:93:VAL:CG1	1:A:93:VAL:CA	2.64	0.76
1:A:119:PRO:CB	1:A:119:PRO:C	2.57	0.76
1:A:12:ALA:O	1:A:13:ALA:N	2.19	0.75
1:A:39:THR:CG2	1:A:40:LYS:NZ	2.47	0.75
1:C:24:TYR:CG	1:C:24:TYR:CA	2.68	0.75
1:C:53:ALA:N	1:C:53:ALA:HA	1.95	0.75
2:D:49:SER:O	2:D:53:VAL:HG12	1.85	0.75
2:D:76:HIS:CG	2:D:76:HIS:CA	2.69	0.75
2:D:100:GLN:HA	2:D:100:GLN:OE1	1.86	0.75
2:D:120:GLN:CG	2:D:120:GLN:CA	2.62	0.75
1:A:50:HIS:CB	1:A:50:HIS:ND1	2.48	0.75
2:B:5:GLU:CB	2:B:5:GLU:N	2.49	0.75
2:B:26:ALA:CA	2:B:27:LEU:N	2.46	0.75
1:C:74:ASN:N	1:C:74:ASN:C	2.44	0.75
1:C:93:VAL:CG1	3:C:142:HEM:CAC	2.64	0.75
1:C:113:LEU:C	1:C:114:PRO:CA	2.59	0.75
2:D:100:GLN:C	2:D:101:ASN:CA	2.25	0.75
1:A:76:LEU:HB2	1:A:77:PRO:CD	2.16	0.75
1:A:136:LEU:CD1	1:A:136:LEU:CD2	2.57	0.75
2:D:2:LEU:HD23	2:D:7:LYS:CD	2.16	0.75
2:D:43:HIS:CB	2:D:43:HIS:N	2.49	0.75
2:B:134:ALA:O	2:B:138:ASN:HB2	1.85	0.75
1:C:43:PHE:C	1:C:44:PRO:CA	2.58	0.75
1:C:81:SER:CB	1:C:81:SER:N	2.46	0.75
2:D:59:VAL:HG13	2:D:59:VAL:HG21	1.68	0.75
2:D:95:LEU:HD12	2:D:97:VAL:HG21	1.67	0.75
2:D:103:ARG:CG	2:D:103:ARG:NE	2.48	0.75
2:B:81:LYS:NZ	2:B:142:HIS:CE1	2.55	0.75
2:B:103:ARG:HB3	2:B:103:ARG:HD2	1.69	0.75
1:C:88:ALA:HB1	1:C:139:LYS:CB	2.16	0.75
1:C:134:THR:N	1:C:134:THR:C	2.43	0.75
1:A:56:LYS:HE3	1:A:56:LYS:N	2.00	0.75
1:A:29:LEU:CB	1:A:29:LEU:HA	2.12	0.75
2:B:6:GLU:CD	2:B:131:LYS:HZ1	1.95	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ALA:O	1:C:57:ALA:CB	2.35	0.75
2:D:81:LYS:CD	2:D:81:LYS:NZ	2.50	0.75
1:A:55:GLN:NE2	1:A:55:GLN:OE1	2.18	0.75
2:B:75:LYS:C	2:B:76:HIS:CA	2.60	0.75
1:C:42:TYR:CD1	3:C:142:HEM:HBC1	2.22	0.75
1:C:139:LYS:CB	1:C:139:LYS:CD	2.65	0.75
1:A:45:HIS:CA	1:A:45:HIS:CG	2.68	0.74
1:A:126:ASN:C	1:A:126:ASN:N	2.43	0.74
2:B:3:THR:O	2:B:4:ALA:CA	2.35	0.74
2:B:43:HIS:CE1	3:B:146:HEM:O2A	2.40	0.74
2:B:83:ALA:CB	2:B:83:ALA:N	2.50	0.74
1:C:3:SER:CB	1:C:4:ALA:N	2.50	0.74
2:D:55:ASN:O	2:D:60:LYS:CD	2.35	0.74
1:A:73:LEU:CD2	1:A:73:LEU:CD1	2.65	0.74
2:B:10:VAL:HG11	2:B:128:LEU:HD23	1.58	0.74
1:C:17:VAL:HG13	1:C:24:TYR:CD2	2.22	0.74
2:D:93:ASN:CA	2:D:93:ASN:O	2.35	0.74
2:B:41:PHE:HB2	2:B:44:PHE:CD1	2.22	0.74
1:C:129:LEU:CB	1:C:129:LEU:HG	2.13	0.74
2:D:53:VAL:HG22	2:D:54:MET:HE3	1.68	0.74
2:B:37:THR:N	2:B:37:THR:CB	2.49	0.74
1:C:46:PHE:CD2	1:C:54:GLN:HB3	2.22	0.74
2:D:1:MET:HG3	2:D:131:LYS:NZ	2.01	0.74
2:B:16:LYS:CE	2:B:16:LYS:CG	2.65	0.74
2:B:74:LEU:CD1	2:B:77:LEU:CG	2.65	0.74
2:B:80:LEU:HD22	2:B:82:GLY:CA	2.17	0.74
1:C:113:LEU:CD2	1:C:113:LEU:N	2.51	0.74
2:D:140:LEU:CD1	2:D:140:LEU:HD22	2.16	0.74
1:A:2:LEU:CA	1:A:2:LEU:CG	2.66	0.74
1:A:41:THR:CG2	1:A:41:THR:HA	2.16	0.74
2:B:140:LEU:O	2:B:141:ALA:CA	2.36	0.74
2:D:10:VAL:HG11	2:D:128:LEU:CD1	2.17	0.74
1:A:3:SER:CB	1:A:3:SER:N	2.51	0.74
1:A:39:THR:HG23	1:A:40:LYS:HE2	1.69	0.74
1:A:46:PHE:HB2	1:A:48:LEU:CD2	2.18	0.74
3:A:142:HEM:CHA	3:A:142:HEM:ND	2.50	0.74
2:B:2:LEU:CB	2:B:2:LEU:C	2.61	0.74
2:B:123:PRO:HA	2:B:126:GLN:NE2	2.01	0.74
1:A:6:ASN:O	1:A:10:VAL:HG23	1.88	0.73
2:B:128:LEU:CA	2:B:128:LEU:CG	2.66	0.73
1:C:35:SER:HB3	2:D:127:ALA:HA	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:CD	1:C:61:LYS:HA	2.17	0.73
2:D:47:LEU:CA	2:D:47:LEU:HB2	2.09	0.73
1:A:73:LEU:CD2	1:A:73:LEU:CB	2.66	0.73
2:D:36:TRP:C	2:D:36:TRP:CB	2.60	0.73
2:D:78:ASP:CA	2:D:78:ASP:CG	2.52	0.73
1:A:127:LYS:C	1:A:128:PHE:C	2.56	0.73
1:A:135:VAL:CA	1:A:136:LEU:N	2.49	0.73
2:B:41:PHE:CA	2:B:41:PHE:O	2.36	0.73
1:C:67:THR:CG2	1:C:67:THR:HA	2.19	0.73
1:C:100:LEU:CB	1:C:100:LEU:CD2	2.65	0.73
2:D:4:ALA:C	2:D:4:ALA:CB	2.61	0.73
2:D:36:TRP:C	2:D:36:TRP:N	2.46	0.73
2:D:105:LEU:HD22	2:D:105:LEU:HD11	1.70	0.73
2:B:54:MET:N	2:B:54:MET:CB	2.51	0.73
1:C:39:THR:CB	1:C:39:THR:C	2.62	0.73
1:C:89:HIS:CB	1:C:139:LYS:NZ	2.45	0.73
2:D:10:VAL:HG11	2:D:128:LEU:HD13	1.69	0.73
1:A:124:ASN:CG	1:A:124:ASN:CA	2.61	0.73
2:B:2:LEU:CA	2:B:2:LEU:CG	2.67	0.73
2:B:41:PHE:HD2	2:B:44:PHE:HZ	1.30	0.73
1:C:45:HIS:CE1	3:C:142:HEM:CBD	2.64	0.73
2:D:67:LEU:C	2:D:68:ASP:C	2.55	0.73
2:D:71:THR:CG2	2:D:71:THR:C	2.61	0.73
1:A:106:LEU:N	1:A:106:LEU:HB2	2.03	0.73
2:B:103:ARG:CG	2:B:103:ARG:HB3	2.15	0.73
2:D:31:LEU:CB	2:D:31:LEU:HA	2.12	0.73
2:D:59:VAL:CG1	2:D:59:VAL:HG21	2.17	0.73
2:D:84:PHE:HB2	2:D:84:PHE:HD1	1.49	0.73
2:B:53:VAL:O	2:B:59:VAL:CG2	2.37	0.73
2:B:136:VAL:CA	2:B:136:VAL:O	2.37	0.73
1:C:131:ASN:CA	1:C:131:ASN:CG	2.62	0.73
2:D:19:VAL:O	2:D:21:VAL:N	2.22	0.73
1:A:31:ARG:HG2	2:B:126:GLN:NE2	2.02	0.73
1:A:93:VAL:CG1	1:A:93:VAL:HA	2.18	0.73
2:B:62:HIS:HE1	3:B:146:HEM:CHA	2.02	0.73
2:B:102:PHE:CE2	2:B:141:ALA:HB2	2.24	0.73
1:C:95:PRO:HG3	1:C:141:ARG:HH12	1.52	0.73
1:C:103:HIS:CB	1:C:103:HIS:ND1	2.52	0.73
2:D:56:ASN:O	2:D:56:ASN:CA	2.36	0.73
2:B:98:ASN:CB	2:B:100:GLN:H	2.01	0.72
2:D:103:ARG:O	2:D:107:ASN:HB2	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:PHE:CD1	2:B:102:PHE:CB	2.54	0.72
1:C:80:LEU:HD23	1:C:135:VAL:HG22	1.70	0.72
2:D:76:HIS:CG	2:D:76:HIS:N	2.57	0.72
1:A:41:THR:CG2	1:A:41:THR:OG1	2.28	0.72
2:B:6:GLU:N	2:B:6:GLU:C	2.45	0.72
2:B:10:VAL:CG1	2:B:10:VAL:CA	2.67	0.72
2:B:22:VAL:CG2	2:B:22:VAL:CG1	2.67	0.72
2:B:22:VAL:N	2:B:23:GLY:N	2.37	0.72
2:B:47:LEU:HD12	2:B:53:VAL:HA	1.71	0.72
1:C:116:ASN:C	1:C:116:ASN:CB	2.53	0.72
1:C:137:THR:O	1:C:138:SER:CA	2.37	0.72
2:D:79:ASP:CB	2:D:79:ASP:C	2.63	0.72
2:D:103:ARG:HB3	2:D:103:ARG:O	1.89	0.72
2:B:103:ARG:CG	2:B:103:ARG:HB2	2.15	0.72
1:C:108:THR:HB	1:C:108:THR:HG22	1.68	0.72
2:D:6:GLU:CA	2:D:6:GLU:CG	2.64	0.72
2:D:126:GLN:OE1	2:D:126:GLN:NE2	2.22	0.72
1:A:79:THR:CB	1:A:79:THR:C	2.62	0.72
1:A:89:HIS:CD2	1:A:139:LYS:HG2	2.25	0.72
2:B:39:ARG:CB	2:B:39:ARG:CD	2.67	0.72
2:B:46:ASN:C	2:B:47:LEU:HD13	2.14	0.72
1:C:131:ASN:CB	1:C:131:ASN:N	2.48	0.72
2:D:27:LEU:HD11	2:D:62:HIS:HB3	1.70	0.72
1:A:31:ARG:HD3	2:B:126:GLN:CG	2.18	0.72
2:B:106:GLY:HA2	2:B:133:VAL:CG2	2.18	0.72
2:B:140:LEU:O	2:B:141:ALA:HA	1.89	0.72
3:B:146:HEM:HHA	3:B:146:HEM:HAD2	1.71	0.72
2:D:144:TYR:OH	2:D:144:TYR:CE2	2.43	0.72
2:D:46:ASN:N	2:D:46:ASN:CB	2.52	0.72
2:D:50:ALA:C	2:D:50:ALA:N	2.46	0.72
2:D:25:GLN:NE2	2:D:115:ARG:HH22	1.88	0.72
2:D:34:TYR:HA	2:D:36:TRP:CZ3	2.25	0.72
1:A:126:ASN:C	1:A:126:ASN:HB3	2.14	0.72
1:A:126:ASN:N	1:A:127:LYS:N	2.38	0.72
2:B:55:ASN:CA	2:B:56:ASN:N	2.52	0.72
1:A:12:ALA:CA	1:A:13:ALA:N	2.52	0.72
1:A:32:MET:N	1:A:32:MET:CB	2.45	0.72
2:B:25:GLN:N	2:B:25:GLN:C	2.48	0.72
2:B:33:VAL:C	2:B:35:PRO:CD	2.63	0.72
2:B:130:GLN:CG	2:B:130:GLN:HE21	1.89	0.72
1:C:32:MET:CB	1:C:32:MET:N	2.53	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLY:O	1:C:72:HIS:HB3	1.90	0.72
2:B:41:PHE:CB	2:B:44:PHE:CD1	2.73	0.71
2:B:80:LEU:CD2	2:B:80:LEU:HD13	2.20	0.71
2:B:81:LYS:NZ	2:B:142:HIS:CD2	2.58	0.71
1:C:14:TRP:CB	1:C:70:GLN:HE22	2.03	0.71
2:D:90:LEU:CB	2:D:90:LEU:HD13	2.20	0.71
2:B:22:VAL:O	2:B:23:GLY:CA	2.38	0.71
2:B:33:VAL:C	2:B:35:PRO:HD2	2.14	0.71
1:C:56:LYS:HZ2	1:C:59:GLY:N	1.88	0.71
2:D:79:ASP:CG	2:D:81:LYS:HE2	2.14	0.71
1:A:105:LEU:N	1:A:105:LEU:CB	2.52	0.71
2:B:8:ALA:CB	2:B:8:ALA:N	2.50	0.71
2:B:75:LYS:HG2	2:B:76:HIS:ND1	2.05	0.71
2:B:98:ASN:CB	2:B:101:ASN:H	2.03	0.71
1:C:17:VAL:CA	1:C:18:GLY:N	2.46	0.71
1:C:23:ALA:CB	1:C:23:ALA:N	2.53	0.71
2:D:84:PHE:CE1	2:D:136:VAL:HG13	2.26	0.71
1:A:22:PRO:CG	1:A:22:PRO:CA	2.68	0.71
1:A:80:LEU:O	1:A:84:SER:N	2.23	0.71
2:D:19:VAL:CG2	2:D:19:VAL:CG1	2.68	0.71
2:D:50:ALA:CA	2:D:50:ALA:O	2.39	0.71
2:D:145:HIS:CG	2:D:145:HIS:CE1	2.77	0.71
1:C:36:PHE:HA	1:C:37:PRO:CD	2.21	0.71
2:D:6:GLU:HB2	2:D:128:LEU:CD2	2.12	0.71
2:D:90:LEU:CB	2:D:90:LEU:HD12	2.20	0.71
1:A:11:LYS:CA	1:A:12:ALA:N	2.53	0.71
1:A:127:LYS:O	1:A:127:LYS:HA	1.91	0.71
2:B:68:ASP:CG	2:B:68:ASP:CA	2.60	0.71
2:D:67:LEU:O	2:D:71:THR:CB	2.38	0.71
2:D:68:ASP:C	2:D:68:ASP:HB3	2.16	0.71
2:D:77:LEU:CB	2:D:77:LEU:CD1	2.69	0.71
2:D:123:PRO:CA	2:D:124:ASN:N	2.53	0.71
2:B:64:LYS:NZ	2:B:64:LYS:CB	2.49	0.71
2:B:101:ASN:CA	2:B:101:ASN:O	2.38	0.71
2:B:140:LEU:CD1	2:B:140:LEU:HB3	2.20	0.71
2:D:87:LEU:HD12	2:D:90:LEU:HD12	1.71	0.71
1:A:109:LEU:HD12	1:A:117:PHE:CE1	2.24	0.71
2:B:2:LEU:HB2	2:B:6:GLU:CG	2.20	0.71
2:B:38:GLN:O	2:B:39:ARG:CA	2.39	0.71
2:B:84:PHE:HB2	2:B:84:PHE:HD1	1.55	0.71
2:B:93:ASN:O	2:B:96:HIS:CE1	2.44	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ARG:NH2	2:B:103:ARG:NE	2.36	0.71
2:D:86:GLN:CA	2:D:86:GLN:CG	2.58	0.71
2:D:131:LYS:CB	2:D:131:LYS:C	2.63	0.71
2:B:105:LEU:C	2:B:105:LEU:N	2.48	0.71
2:B:117:PHE:CD1	2:B:117:PHE:CD2	2.65	0.71
2:D:41:PHE:O	2:D:42:GLN:N	2.18	0.71
1:A:87:HIS:CB	1:A:87:HIS:CD2	2.71	0.70
2:B:133:VAL:O	2:B:133:VAL:HA	1.91	0.70
2:B:144:TYR:CD2	2:B:144:TYR:HB3	2.26	0.70
1:A:29:LEU:CB	1:A:29:LEU:HG	2.17	0.70
1:A:40:LYS:CG	1:A:40:LYS:CA	2.65	0.70
1:A:57:ALA:HA	1:A:60:GLN:CG	2.21	0.70
1:A:118:THR:CG2	1:A:118:THR:OG1	2.39	0.70
2:D:70:PHE:HB3	2:D:71:THR:HB	1.73	0.70
2:B:10:VAL:CG1	2:B:128:LEU:HD22	1.98	0.70
1:A:124:ASN:C	1:A:124:ASN:HB2	1.99	0.70
1:C:86:LEU:CD1	1:C:86:LEU:CB	2.69	0.70
2:D:31:LEU:CG	2:D:31:LEU:HA	2.22	0.70
1:A:76:LEU:O	1:A:77:PRO:O	2.10	0.70
1:A:105:LEU:HA	1:A:108:THR:CG2	2.18	0.70
1:A:106:LEU:N	1:A:106:LEU:C	2.47	0.70
1:A:135:VAL:C	1:A:135:VAL:CB	2.64	0.70
2:B:94:LYS:N	2:B:95:LEU:H	1.89	0.70
1:C:56:LYS:NZ	1:C:59:GLY:N	2.39	0.70
2:D:25:GLN:HB3	2:D:112:VAL:CG2	2.21	0.70
2:D:48:SER:O	2:D:49:SER:HB3	1.91	0.70
2:D:124:ASN:CG	2:D:124:ASN:HA	2.14	0.70
1:A:13:ALA:CB	1:A:125:LEU:HD21	2.22	0.70
1:A:48:LEU:CA	1:A:48:LEU:HG	2.21	0.70
2:B:11:THR:CA	2:B:11:THR:OG1	2.40	0.70
2:B:11:THR:CB	2:B:11:THR:N	2.54	0.70
2:B:44:PHE:O	2:B:45:GLY:CA	2.38	0.70
2:B:76:HIS:ND1	2:B:76:HIS:CB	2.54	0.70
2:B:80:LEU:CB	2:B:82:GLY:HA3	2.22	0.70
2:B:94:LYS:N	2:B:95:LEU:N	2.40	0.70
1:C:98:PHE:CA	1:C:99:LYS:N	2.54	0.70
2:D:60:LYS:CD	2:D:60:LYS:NZ	2.55	0.70
2:D:70:PHE:CD2	2:D:136:VAL:HG11	2.27	0.70
2:B:47:LEU:CD1	2:B:53:VAL:HG23	2.16	0.70
2:B:121:PHE:CE2	2:B:126:GLN:HA	2.27	0.70
1:C:9:ASN:HB3	1:C:124:ASN:HB2	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:VAL:HG22	1:C:24:TYR:CE2	2.27	0.70
3:C:142:HEM:CAB	3:C:142:HEM:C4B	2.61	0.70
2:D:2:LEU:CG	2:D:7:LYS:HD3	2.22	0.70
2:D:109:LEU:CD2	2:D:109:LEU:CD1	2.69	0.70
2:B:74:LEU:CD1	2:B:77:LEU:CB	2.57	0.70
1:C:45:HIS:NE2	1:C:46:PHE:HE1	1.89	0.70
1:A:14:TRP:HD1	1:A:70:GLN:HE21	1.39	0.69
1:A:33:PHE:HB3	1:A:40:LYS:CG	2.22	0.69
2:B:1:MET:C	2:B:2:LEU:HD23	2.17	0.69
2:D:99:PRO:O	2:D:102:PHE:HB2	1.90	0.69
2:D:131:LYS:CB	2:D:131:LYS:N	2.54	0.69
2:B:25:GLN:OE1	2:B:112:VAL:HG11	1.90	0.69
1:C:119:PRO:C	1:C:119:PRO:HB2	2.16	0.69
2:D:14:TRP:C	2:D:14:TRP:CB	2.63	0.69
2:B:3:THR:CB	2:B:6:GLU:HB2	2.22	0.69
2:B:95:LEU:HD11	3:B:146:HEM:CMA	2.22	0.69
1:C:44:PRO:CG	1:C:44:PRO:N	2.45	0.69
2:D:10:VAL:HG13	2:D:128:LEU:HD22	1.73	0.69
2:D:31:LEU:CA	2:D:31:LEU:O	2.40	0.69
2:D:71:THR:C	2:D:71:THR:HG22	2.17	0.69
2:B:55:ASN:OD1	2:B:55:ASN:N	2.25	0.69
1:A:94:ASN:CA	1:A:94:ASN:CG	2.64	0.69
1:A:96:VAL:C	1:A:97:ASN:CA	2.62	0.69
1:C:118:THR:OG1	1:C:118:THR:CG2	2.40	0.69
2:D:2:LEU:HD13	2:D:3:THR:N	2.06	0.69
2:D:23:GLY:N	2:D:67:LEU:HD12	2.07	0.69
2:D:75:LYS:HG3	2:D:76:HIS:CD2	2.28	0.69
2:D:109:LEU:CA	2:D:109:LEU:O	2.37	0.69
1:A:22:PRO:CD	1:A:22:PRO:CA	2.69	0.69
1:A:89:HIS:HD2	1:A:139:LYS:CD	2.04	0.69
1:A:89:HIS:C	1:A:89:HIS:ND1	2.51	0.69
1:C:79:THR:CB	1:C:79:THR:C	2.65	0.69
1:C:80:LEU:CD1	1:C:80:LEU:CD2	2.69	0.69
2:D:131:LYS:CA	2:D:131:LYS:HG3	2.22	0.69
2:D:143:LYS:CB	2:D:143:LYS:C	2.60	0.69
2:B:22:VAL:HG12	2:B:67:LEU:CD2	2.20	0.69
1:C:14:TRP:CB	1:C:70:GLN:NE2	2.55	0.69
1:C:104:SER:CA	1:C:105:LEU:N	2.56	0.69
2:D:27:LEU:CD1	2:D:62:HIS:HB3	2.22	0.69
2:D:87:LEU:CB	2:D:87:LEU:N	2.48	0.69
1:A:3:SER:O	1:A:4:ALA:C	2.35	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ALA:O	1:A:60:GLN:CG	2.41	0.69
1:A:98:PHE:CE1	1:A:136:LEU:HD12	2.28	0.69
1:A:132:ASP:OD1	1:A:136:LEU:HD11	1.93	0.69
2:B:20:ASP:OD1	2:B:20:ASP:CB	2.41	0.69
2:B:21:VAL:CA	2:B:21:VAL:CG2	2.70	0.69
2:B:27:LEU:CD2	2:B:66:VAL:HG11	2.23	0.69
2:B:40:PHE:HB3	3:B:146:HEM:HMA2	1.74	0.69
2:B:46:ASN:CB	2:B:46:ASN:OD1	2.40	0.69
2:B:102:PHE:HE2	2:B:141:ALA:HB2	1.58	0.69
1:C:36:PHE:HA	1:C:37:PRO:HD3	1.74	0.69
1:C:46:PHE:CB	1:C:46:PHE:CD1	2.74	0.69
1:C:89:HIS:O	1:C:90:LYS:CA	2.41	0.69
1:C:130:ALA:O	1:C:130:ALA:CA	2.35	0.69
2:D:59:VAL:CA	2:D:59:VAL:O	2.40	0.69
2:D:67:LEU:HA	2:D:67:LEU:CG	2.15	0.69
2:D:84:PHE:CB	2:D:84:PHE:H	2.06	0.69
2:D:86:GLN:C	2:D:86:GLN:HA	2.12	0.69
1:A:94:ASN:N	1:A:94:ASN:C	2.49	0.69
1:A:106:LEU:CD2	1:A:106:LEU:CB	2.71	0.69
1:C:95:PRO:O	1:C:98:PHE:HB2	1.93	0.69
1:A:83:LEU:O	1:A:84:SER:CA	2.40	0.69
1:A:124:ASN:CB	1:A:124:ASN:OD1	2.41	0.69
2:B:2:LEU:CB	2:B:3:THR:N	2.56	0.69
3:B:146:HEM:C4A	3:B:146:HEM:CMA	2.76	0.69
2:D:59:VAL:C	2:D:59:VAL:N	2.51	0.69
2:B:86:GLN:CG	2:B:86:GLN:NE2	2.55	0.68
2:B:143:LYS:CD	2:B:143:LYS:NZ	2.56	0.68
1:C:30:GLN:CD	1:C:30:GLN:HB2	2.17	0.68
2:D:61:ALA:CB	2:D:62:HIS:N	2.55	0.68
2:D:79:ASP:CA	2:D:81:LYS:HD2	2.22	0.68
1:A:39:THR:HG23	1:A:40:LYS:HZ1	1.56	0.68
2:B:2:LEU:CB	2:B:6:GLU:OE2	2.42	0.68
2:B:33:VAL:HG12	2:B:34:TYR:CZ	2.27	0.68
2:B:97:VAL:CB	2:B:97:VAL:C	2.66	0.68
2:D:61:ALA:CB	2:D:61:ALA:N	2.50	0.68
2:D:79:ASP:O	2:D:81:LYS:HD3	1.94	0.68
2:D:91:HIS:HA	2:D:95:LEU:HG	1.75	0.68
2:D:95:LEU:HD11	3:D:146:HEM:CHB	2.24	0.68
2:B:23:GLY:N	2:B:23:GLY:C	2.48	0.68
2:B:38:GLN:O	2:B:39:ARG:HA	1.91	0.68
1:C:136:LEU:CB	1:C:136:LEU:HA	2.14	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:HIS:HA	2:D:142:HIS:CG	2.28	0.68
2:D:143:LYS:CB	2:D:143:LYS:N	2.56	0.68
2:B:43:HIS:C	2:B:43:HIS:CB	2.65	0.68
2:B:43:HIS:ND1	2:B:43:HIS:HA	2.07	0.68
1:C:12:ALA:O	1:C:12:ALA:CA	2.42	0.68
1:C:72:HIS:CD2	1:C:72:HIS:CB	2.72	0.68
1:C:84:SER:OG	1:C:136:LEU:CD2	2.42	0.68
1:C:54:GLN:CA	1:C:54:GLN:O	2.42	0.68
1:C:87:HIS:HB3	1:C:93:VAL:CG2	2.23	0.68
2:D:79:ASP:O	2:D:79:ASP:OD1	2.11	0.68
2:D:104:LEU:CG	2:D:104:LEU:CA	2.71	0.68
1:A:43:PHE:CD2	1:A:43:PHE:HB3	2.27	0.68
1:A:127:LYS:NZ	1:A:127:LYS:HD3	2.03	0.68
2:B:69:ALA:C	2:B:69:ALA:HB1	1.87	0.68
2:D:2:LEU:CG	2:D:7:LYS:CD	2.72	0.68
2:D:10:VAL:HG21	2:D:128:LEU:HB2	1.75	0.68
2:D:14:TRP:CD1	2:D:74:LEU:HD23	2.29	0.68
2:D:14:TRP:CE2	2:D:71:THR:HG23	2.28	0.68
2:B:53:VAL:C	2:B:54:MET:HA	2.17	0.68
2:B:103:ARG:CG	2:B:103:ARG:HE	2.06	0.68
2:D:110:ALA:O	2:D:114:ALA:N	2.27	0.68
2:B:26:ALA:CA	2:B:26:ALA:O	2.40	0.68
2:B:75:LYS:O	2:B:76:HIS:O	2.11	0.68
1:C:84:SER:CA	1:C:84:SER:OG	2.42	0.68
1:C:110:ALA:C	1:C:110:ALA:CB	2.66	0.68
2:D:102:PHE:N	2:D:102:PHE:CB	2.53	0.68
1:A:47:ASP:C	1:A:49:SER:H	2.01	0.68
1:A:82:ASN:N	1:A:82:ASN:CB	2.54	0.68
3:A:142:HEM:HMD1	3:A:142:HEM:HHD	1.75	0.68
2:B:19:VAL:HG13	2:B:64:LYS:HE2	1.75	0.68
2:B:57:PRO:CB	2:B:57:PRO:HD3	2.21	0.68
2:B:71:THR:CA	2:B:71:THR:H	1.33	0.68
1:C:68:LYS:CG	1:C:68:LYS:HA	2.22	0.68
2:D:103:ARG:NH2	2:D:130:GLN:O	2.24	0.68
1:A:14:TRP:CD1	1:A:70:GLN:HE21	2.13	0.67
2:D:124:ASN:CA	2:D:124:ASN:O	2.43	0.67
2:B:24:ALA:C	2:B:25:GLN:CA	2.66	0.67
2:B:41:PHE:HB2	2:B:44:PHE:CE1	2.30	0.67
2:B:54:MET:HG3	2:B:54:MET:HA	1.76	0.67
2:D:81:LYS:CB	2:D:81:LYS:CD	2.69	0.67
2:B:55:ASN:C	2:B:60:LYS:HZ1	1.96	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:146:HEM:CMA	3:B:146:HEM:HHB	2.23	0.67
1:C:16:LYS:N	1:C:16:LYS:CB	2.56	0.67
2:D:86:GLN:CB	2:D:86:GLN:HA	2.15	0.67
2:D:92:CYS:CA	2:D:92:CYS:SG	2.81	0.67
2:D:94:LYS:HD2	2:D:95:LEU:CD2	2.24	0.67
1:A:72:HIS:O	1:A:72:HIS:ND1	2.25	0.67
1:A:86:LEU:CD2	1:A:86:LEU:CD1	2.70	0.67
2:B:31:LEU:HB3	2:B:53:VAL:HG21	1.75	0.67
2:B:34:TYR:CE2	2:B:34:TYR:OH	2.42	0.67
1:C:22:PRO:O	1:C:56:LYS:HE2	1.94	0.67
1:C:86:LEU:HD12	1:C:91:LEU:HD11	1.76	0.67
2:D:2:LEU:C	2:D:2:LEU:HD13	2.18	0.67
1:A:127:LYS:O	1:A:130:ALA:HB3	1.95	0.67
2:B:53:VAL:O	2:B:54:MET:CA	2.42	0.67
2:B:64:LYS:CG	2:B:64:LYS:CE	2.73	0.67
1:C:11:LYS:N	1:C:11:LYS:HG2	2.09	0.67
1:C:31:ARG:O	1:C:34:LEU:HB2	1.95	0.67
2:D:76:HIS:CB	2:D:76:HIS:CD2	2.78	0.67
2:B:5:GLU:N	2:B:5:GLU:C	2.51	0.67
2:B:25:GLN:N	2:B:25:GLN:HA	1.99	0.67
2:B:59:VAL:O	2:B:62:HIS:HB3	1.94	0.67
2:B:59:VAL:HG23	2:B:60:LYS:N	2.07	0.67
2:B:131:LYS:O	2:B:134:ALA:HB3	1.95	0.67
2:D:11:THR:HB	2:D:129:PHE:CZ	2.29	0.67
2:B:70:PHE:HD1	2:B:71:THR:HB	1.60	0.67
2:D:26:ALA:C	2:D:26:ALA:N	2.51	0.67
2:D:50:ALA:O	2:D:54:MET:HG2	1.94	0.67
2:D:75:LYS:HB3	2:D:76:HIS:CD2	2.29	0.67
2:D:142:HIS:CA	2:D:142:HIS:CG	2.64	0.67
1:A:76:LEU:H	1:A:76:LEU:CD2	2.06	0.67
1:A:100:LEU:CD2	1:A:100:LEU:HB3	2.23	0.67
2:D:66:VAL:O	2:D:69:ALA:HB3	1.94	0.67
2:D:128:LEU:N	2:D:128:LEU:CB	2.58	0.67
1:A:127:LYS:CD	1:A:127:LYS:CB	2.73	0.67
1:C:76:LEU:CD1	1:C:76:LEU:CB	2.73	0.67
1:A:87:HIS:CG	1:A:87:HIS:CA	2.77	0.67
1:A:89:HIS:HD2	1:A:139:LYS:CG	2.07	0.67
1:A:105:LEU:CA	1:A:108:THR:HG22	2.21	0.67
1:A:114:PRO:HG2	2:B:115:ARG:HA	1.76	0.67
2:B:94:LYS:C	2:B:94:LYS:N	2.53	0.67
2:B:97:VAL:CA	2:B:97:VAL:CG1	2.70	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LEU:HD11	3:C:142:HEM:CHA	2.25	0.67
1:A:110:ALA:O	1:A:114:PRO:CG	2.40	0.66
1:A:116:ASN:N	1:A:116:ASN:C	2.53	0.66
2:B:49:SER:HB3	2:B:52:ALA:HB2	1.76	0.66
2:B:68:ASP:HA	2:B:71:THR:HG22	0.67	0.66
2:B:80:LEU:CD2	2:B:81:LYS:O	2.43	0.66
1:C:68:LYS:HA	1:C:68:LYS:HG2	1.77	0.66
2:D:39:ARG:CG	2:D:39:ARG:HE	2.06	0.66
2:D:49:SER:O	2:D:53:VAL:HG13	1.95	0.66
2:D:59:VAL:HA	2:D:59:VAL:HG23	1.73	0.66
2:B:40:PHE:C	2:B:40:PHE:N	2.53	0.66
2:B:140:LEU:CD2	2:B:140:LEU:CB	2.68	0.66
1:C:113:LEU:O	1:C:114:PRO:CA	2.43	0.66
2:D:13:PHE:O	2:D:14:TRP:O	2.14	0.66
2:D:130:GLN:CG	2:D:130:GLN:NE2	2.54	0.66
1:A:42:TYR:O	1:A:43:PHE:HA	1.95	0.66
2:B:72:GLN:N	2:B:72:GLN:C	2.54	0.66
2:D:56:ASN:O	2:D:57:PRO:C	2.38	0.66
2:D:88:SER:O	2:D:143:LYS:HE2	1.95	0.66
2:B:94:LYS:CD	2:B:94:LYS:HB3	2.23	0.66
2:D:95:LEU:N	2:D:95:LEU:CD2	2.58	0.66
1:A:43:PHE:HA	1:A:44:PRO:CD	2.25	0.66
2:B:34:TYR:N	2:B:35:PRO:HD2	2.10	0.66
2:B:128:LEU:C	2:B:128:LEU:N	2.45	0.66
1:C:101:LEU:CB	1:C:101:LEU:N	2.58	0.66
2:D:20:ASP:OD1	2:D:64:LYS:HB2	1.96	0.66
2:D:94:LYS:CD	2:D:95:LEU:HD23	2.25	0.66
2:D:110:ALA:N	2:D:110:ALA:HA	2.02	0.66
1:A:9:ASN:OD1	1:A:9:ASN:CB	2.42	0.66
1:A:104:SER:C	1:A:105:LEU:CA	2.66	0.66
1:A:136:LEU:H	1:A:136:LEU:CD2	1.94	0.66
2:B:3:THR:C	2:B:5:GLU:H	2.01	0.66
1:A:42:TYR:O	1:A:44:PRO:HD2	1.96	0.66
2:B:125:VAL:CG1	2:B:125:VAL:CG2	2.72	0.66
1:C:132:ASP:O	1:C:136:LEU:HD23	1.95	0.66
2:D:27:LEU:CD1	2:D:27:LEU:CB	2.69	0.66
2:D:145:HIS:CD2	2:D:145:HIS:CE1	2.84	0.66
1:C:83:LEU:CD2	1:C:83:LEU:CD1	2.70	0.66
2:D:14:TRP:CZ2	2:D:71:THR:HG23	2.31	0.66
2:D:19:VAL:HG12	2:D:64:LYS:HD2	1.78	0.66
2:D:138:ASN:N	2:D:138:ASN:C	2.48	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:GLY:HA2	2:B:66:VAL:CG1	2.21	0.66
2:B:93:ASN:CG	2:B:93:ASN:HA	2.17	0.66
1:C:64:ASN:CB	1:C:64:ASN:N	2.55	0.66
2:D:88:SER:CB	2:D:88:SER:C	2.59	0.66
2:D:124:ASN:CB	2:D:124:ASN:OD1	2.44	0.66
1:A:44:PRO:N	1:A:45:HIS:CD2	2.63	0.66
2:B:13:PHE:HE1	2:B:120:GLN:HB2	1.61	0.66
3:B:146:HEM:CMA	3:B:146:HEM:CHB	2.74	0.66
1:C:61:LYS:CG	1:C:61:LYS:HA	2.18	0.66
1:C:118:THR:CB	1:C:118:THR:HG1	2.07	0.66
2:D:95:LEU:CB	2:D:95:LEU:CD2	2.74	0.66
2:D:101:ASN:O	2:D:104:LEU:HB2	1.96	0.66
1:A:34:LEU:CD1	2:B:123:PRO:HB2	2.19	0.65
1:A:45:HIS:ND1	1:A:46:PHE:CD2	2.64	0.65
2:B:109:LEU:CD1	2:B:109:LEU:HB3	2.26	0.65
1:C:44:PRO:O	1:C:45:HIS:C	2.40	0.65
1:C:140:TYR:CG	1:C:140:TYR:CA	2.77	0.65
2:D:117:PHE:O	2:D:120:GLN:HB2	1.96	0.65
1:A:16:LYS:CA	1:A:17:VAL:N	2.56	0.65
1:A:43:PHE:CZ	3:A:142:HEM:HMD1	2.31	0.65
2:B:2:LEU:CD2	2:B:2:LEU:CD1	2.72	0.65
2:D:32:VAL:HG11	2:D:50:ALA:HA	1.77	0.65
1:A:34:LEU:CB	1:A:34:LEU:C	2.70	0.65
2:B:30:LEU:HD23	2:B:105:LEU:CA	2.18	0.65
1:C:26:ALA:HB2	1:C:56:LYS:HD2	1.76	0.65
1:C:66:LEU:CD2	1:C:66:LEU:CB	2.63	0.65
2:D:83:ALA:C	2:D:83:ALA:N	2.51	0.65
2:D:103:ARG:CD	2:D:103:ARG:HB2	2.26	0.65
1:A:91:LEU:CD2	3:A:142:HEM:C4D	2.66	0.65
1:C:3:SER:HB2	1:C:4:ALA:N	2.11	0.65
1:C:133:SER:CA	1:C:133:SER:O	2.41	0.65
2:D:63:GLY:O	2:D:66:VAL:HB	1.95	0.65
1:A:31:ARG:HH21	2:B:126:GLN:HB2	1.60	0.65
1:A:80:LEU:CG	1:A:80:LEU:CA	2.74	0.65
2:B:57:PRO:CD	2:B:57:PRO:HA	2.20	0.65
2:B:78:ASP:OD2	2:B:78:ASP:HA	1.95	0.65
2:B:94:LYS:CA	2:B:95:LEU:N	2.59	0.65
2:D:34:TYR:HB3	2:D:36:TRP:CH2	2.31	0.65
2:D:70:PHE:O	2:D:73:GLY:HA3	1.96	0.65
2:D:93:ASN:CA	2:D:94:LYS:N	2.55	0.65
1:A:3:SER:HB3	1:A:6:ASN:ND2	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASN:CB	1:A:20:ASN:OD1	2.45	0.65
2:B:75:LYS:N	2:B:75:LYS:O	2.29	0.65
2:B:126:GLN:CD	2:B:126:GLN:CB	2.69	0.65
1:C:43:PHE:HB3	1:C:46:PHE:CD1	2.28	0.65
2:D:105:LEU:HB2	3:D:146:HEM:HBB2	1.76	0.65
1:C:36:PHE:HA	1:C:37:PRO:N	2.10	0.65
1:C:89:HIS:CB	1:C:139:LYS:HZ3	2.01	0.65
1:A:39:THR:HG23	1:A:40:LYS:CE	2.26	0.65
1:A:133:SER:O	1:A:137:THR:HB	1.97	0.65
2:B:68:ASP:CB	2:B:71:THR:CG2	2.36	0.65
1:C:66:LEU:CD2	1:C:66:LEU:HG	2.13	0.65
1:A:80:LEU:CD2	1:A:80:LEU:HG	2.16	0.65
1:A:124:ASN:O	1:A:127:LYS:HB3	1.97	0.65
2:B:5:GLU:C	2:B:8:ALA:HB3	2.22	0.65
2:B:113:VAL:HA	2:B:113:VAL:HG12	1.75	0.65
1:C:87:HIS:HA	1:C:91:LEU:CD1	2.11	0.65
2:D:14:TRP:HA	2:D:14:TRP:HE3	1.61	0.65
1:A:88:ALA:O	1:A:92:ARG:CA	2.45	0.65
1:A:100:LEU:CB	1:A:100:LEU:HD13	2.22	0.65
2:B:3:THR:CG2	2:B:5:GLU:CD	2.70	0.65
2:B:94:LYS:CB	2:B:94:LYS:HD2	2.25	0.65
1:C:32:MET:CG	1:C:39:THR:HG21	2.27	0.65
1:C:80:LEU:O	1:C:81:SER:N	2.25	0.65
2:D:84:PHE:CB	2:D:84:PHE:C	2.70	0.65
2:D:87:LEU:HD12	2:D:90:LEU:CD1	2.27	0.65
2:D:94:LYS:C	2:D:94:LYS:HD3	2.22	0.65
1:A:31:ARG:CB	2:B:126:GLN:NE2	2.59	0.64
1:A:39:THR:CG2	1:A:40:LYS:HZ3	2.06	0.64
2:B:87:LEU:C	2:B:87:LEU:CB	2.70	0.64
2:D:2:LEU:HB3	2:D:2:LEU:N	2.12	0.64
2:D:71:THR:HG22	2:D:71:THR:O	1.97	0.64
1:A:35:SER:HB3	2:B:127:ALA:HA	1.78	0.64
2:B:144:TYR:O	2:B:145:HIS:O	2.14	0.64
2:D:19:VAL:HA	2:D:19:VAL:HG22	1.75	0.64
1:A:93:VAL:C	1:A:94:ASN:CA	2.66	0.64
2:B:75:LYS:HG3	2:B:75:LYS:HE3	1.77	0.64
2:D:142:HIS:CB	2:D:142:HIS:C	2.66	0.64
1:A:58:HIS:CA	1:A:58:HIS:CG	2.74	0.64
1:A:105:LEU:C	1:A:106:LEU:CA	2.70	0.64
2:B:55:ASN:C	2:B:55:ASN:HA	2.17	0.64
1:C:109:LEU:O	1:C:113:LEU:HD22	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:CB	1:A:100:LEU:HD12	2.22	0.64
2:B:3:THR:HG23	2:B:5:GLU:HB3	0.65	0.64
2:B:5:GLU:N	2:B:6:GLU:N	2.45	0.64
2:B:79:ASP:HA	2:B:80:LEU:HG	1.78	0.64
2:B:81:LYS:HZ2	2:B:142:HIS:CD2	2.16	0.64
1:C:49:SER:HA	1:C:55:GLN:HE22	1.61	0.64
1:C:86:LEU:CD2	3:C:142:HEM:CBA	2.76	0.64
2:D:109:LEU:CD2	2:D:109:LEU:CB	2.74	0.64
1:A:16:LYS:O	1:A:17:VAL:N	2.29	0.64
1:A:118:THR:CG2	1:A:118:THR:HA	2.25	0.64
2:B:2:LEU:HG	2:B:6:GLU:HB3	1.78	0.64
1:C:32:MET:HG2	1:C:39:THR:HG21	1.80	0.64
2:D:16:LYS:CD	2:D:16:LYS:HB2	1.88	0.64
1:A:85:ASN:C	1:A:85:ASN:CG	2.65	0.64
2:B:26:ALA:C	2:B:26:ALA:N	2.55	0.64
2:B:38:GLN:CA	2:B:38:GLN:O	2.44	0.64
1:C:95:PRO:CG	1:C:141:ARG:HH12	2.09	0.64
1:C:105:LEU:CD1	1:C:105:LEU:HG	2.18	0.64
2:B:24:ALA:CB	2:B:60:LYS:HA	2.27	0.64
1:C:94:ASN:N	1:C:94:ASN:ND2	2.46	0.64
2:D:115:ARG:CA	2:D:115:ARG:CG	2.75	0.64
2:B:70:PHE:CD1	2:B:71:THR:HB	2.32	0.64
2:B:74:LEU:CD2	2:B:77:LEU:HG	2.28	0.64
2:B:124:ASN:O	2:B:125:VAL:HA	1.98	0.64
1:C:9:ASN:CG	1:C:9:ASN:CA	2.70	0.64
1:C:93:VAL:CA	1:C:93:VAL:CG1	2.75	0.64
2:D:31:LEU:HA	2:D:37:THR:HG22	1.80	0.64
1:A:43:PHE:CE2	3:A:142:HEM:CMD	2.81	0.64
1:A:111:SER:HA	2:B:114:ALA:O	1.98	0.64
2:B:88:SER:HB2	2:B:143:LYS:HB3	1.79	0.64
1:C:72:HIS:CB	1:C:74:ASN:ND2	2.54	0.64
2:D:7:LYS:O	2:D:8:ALA:C	2.40	0.64
2:D:32:VAL:HG13	2:D:53:VAL:HG21	1.80	0.64
1:A:37:PRO:HA	1:A:40:LYS:HD3	1.80	0.63
1:C:53:ALA:CB	1:C:53:ALA:C	2.71	0.63
1:A:26:ALA:HB1	1:A:56:LYS:HE3	1.78	0.63
1:A:72:HIS:CE1	1:A:79:THR:HG21	2.33	0.63
2:B:98:ASN:C	2:B:100:GLN:H	1.99	0.63
1:C:89:HIS:HB2	1:C:139:LYS:CD	2.28	0.63
1:C:137:THR:N	1:C:137:THR:CB	2.54	0.63
2:D:74:LEU:CD1	2:D:132:VAL:HG21	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NE	1:A:31:ARG:HG3	2.11	0.63
2:B:77:LEU:N	2:B:78:ASP:HB3	2.13	0.63
2:B:80:LEU:HB3	2:B:82:GLY:CA	2.28	0.63
2:B:118:GLY:CA	2:B:118:GLY:H	1.29	0.63
2:D:38:GLN:CG	2:D:38:GLN:OE1	2.42	0.63
2:B:43:HIS:ND1	2:B:43:HIS:CD2	2.66	0.63
1:C:43:PHE:CB	1:C:43:PHE:C	2.69	0.63
1:C:86:LEU:CD2	3:C:142:HEM:HBA2	2.28	0.63
2:D:19:VAL:CG2	2:D:19:VAL:N	2.62	0.63
2:D:64:LYS:NZ	2:D:68:ASP:OD1	2.28	0.63
2:D:94:LYS:CD	2:D:95:LEU:N	2.61	0.63
2:B:21:VAL:HG12	2:B:25:GLN:NE2	2.14	0.63
2:B:41:PHE:CA	2:B:42:GLN:N	2.62	0.63
1:C:15:GLY:C	1:C:16:LYS:CA	2.69	0.63
2:D:31:LEU:HD11	2:D:41:PHE:CD1	2.34	0.63
2:D:95:LEU:CG	2:D:95:LEU:N	2.62	0.63
2:D:122:THR:H	2:D:125:VAL:HG12	1.63	0.63
1:A:57:ALA:O	1:A:60:GLN:CB	2.47	0.63
1:A:105:LEU:N	1:A:105:LEU:HB2	2.12	0.63
2:B:57:PRO:CA	2:B:57:PRO:HD3	2.17	0.63
1:C:89:HIS:CD2	1:C:139:LYS:HZ3	2.16	0.63
2:D:94:LYS:CD	2:D:94:LYS:C	2.72	0.63
2:B:91:HIS:C	2:B:144:TYR:OH	2.42	0.63
1:C:39:THR:O	1:C:42:TYR:HB2	1.98	0.63
1:C:75:ASP:CB	1:C:75:ASP:C	2.72	0.63
1:C:76:LEU:HB3	1:C:80:LEU:HD22	1.80	0.63
2:D:75:LYS:CD	2:D:75:LYS:HG3	2.14	0.63
1:A:37:PRO:O	1:A:40:LYS:HD2	1.99	0.63
1:A:84:SER:O	1:A:88:ALA:HB2	1.99	0.63
1:A:122:HIS:C	1:A:122:HIS:CB	2.66	0.63
1:C:52:SER:C	1:C:53:ALA:HA	2.20	0.63
1:C:129:LEU:C	1:C:130:ALA:CA	2.67	0.63
2:B:82:GLY:O	2:B:85:ALA:HB2	1.99	0.63
2:D:86:GLN:CA	2:D:87:LEU:N	2.58	0.63
2:D:87:LEU:CB	2:D:87:LEU:C	2.72	0.63
1:A:79:THR:CA	1:A:79:THR:HG22	2.26	0.62
1:A:82:ASN:N	1:A:82:ASN:HB2	2.13	0.62
2:B:41:PHE:C	2:B:42:GLN:CA	2.68	0.62
2:B:81:LYS:HZ3	2:B:142:HIS:CG	2.16	0.62
1:C:40:LYS:HD3	1:C:48:LEU:HD11	1.80	0.62
1:C:115:THR:CG2	1:C:115:THR:OG1	2.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:VAL:HG13	2:D:109:LEU:HD21	1.81	0.62
2:D:74:LEU:O	2:D:75:LYS:O	2.17	0.62
2:D:84:PHE:HD2	2:D:87:LEU:HD23	1.63	0.62
2:B:81:LYS:HD2	2:B:142:HIS:HB3	1.81	0.62
2:B:91:HIS:O	2:B:96:HIS:HA	1.99	0.62
1:C:6:ASN:CA	1:C:7:LYS:N	2.54	0.62
1:C:68:LYS:NZ	1:C:68:LYS:HD3	2.12	0.62
1:C:130:ALA:O	1:C:134:THR:OG1	2.13	0.62
2:D:25:GLN:CD	2:D:25:GLN:CB	2.72	0.62
2:D:96:HIS:CA	2:D:97:VAL:N	2.57	0.62
2:B:40:PHE:N	2:B:40:PHE:CD1	2.67	0.62
1:C:11:LYS:N	1:C:11:LYS:CB	2.60	0.62
2:D:75:LYS:O	2:D:77:LEU:HD11	1.99	0.62
1:A:76:LEU:O	1:A:77:PRO:CA	2.47	0.62
1:A:88:ALA:HB3	1:A:89:HIS:HB2	1.80	0.62
2:B:40:PHE:HB3	3:B:146:HEM:HMA3	1.81	0.62
2:B:143:LYS:CG	2:B:143:LYS:HA	2.28	0.62
1:C:42:TYR:CG	3:C:142:HEM:HBC1	2.34	0.62
1:C:103:HIS:CG	1:C:103:HIS:CA	2.82	0.62
1:A:10:VAL:C	1:A:10:VAL:HB	2.23	0.62
1:C:61:LYS:CG	1:C:61:LYS:HD3	2.16	0.62
1:C:89:HIS:CB	1:C:139:LYS:HG3	2.30	0.62
2:D:6:GLU:O	2:D:6:GLU:HG3	1.99	0.62
2:D:61:ALA:HB3	2:D:62:HIS:H	1.65	0.62
2:D:84:PHE:HB2	2:D:84:PHE:H	1.63	0.62
1:A:27:GLN:O	1:A:30:GLN:HB3	2.00	0.62
2:B:74:LEU:CD1	2:B:74:LEU:CD2	2.74	0.62
2:B:80:LEU:CB	2:B:81:LYS:O	2.43	0.62
2:B:98:ASN:HB3	2:B:101:ASN:N	2.15	0.62
2:B:125:VAL:O	2:B:125:VAL:HG12	2.00	0.62
1:C:25:GLY:N	1:C:25:GLY:C	2.53	0.62
1:C:115:THR:N	1:C:116:ASN:N	2.48	0.62
2:D:26:ALA:CA	2:D:26:ALA:O	2.45	0.62
2:D:78:ASP:N	2:D:79:ASP:N	2.47	0.62
1:A:27:GLN:OE1	1:A:112:HIS:HE1	1.83	0.62
1:A:42:TYR:O	1:A:43:PHE:N	2.28	0.62
2:B:1:MET:H1	2:B:77:LEU:HD11	1.64	0.62
1:C:129:LEU:O	1:C:130:ALA:C	2.43	0.62
2:D:27:LEU:HD12	2:D:63:GLY:N	2.15	0.62
1:A:136:LEU:C	1:A:136:LEU:HB2	2.25	0.62
2:B:70:PHE:HE2	2:B:133:VAL:HG23	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:O	1:A:31:ARG:CA	2.32	0.62
1:A:88:ALA:HB3	1:A:89:HIS:CB	2.30	0.62
2:D:7:LYS:N	2:D:10:VAL:HG22	2.15	0.62
2:B:4:ALA:C	2:B:8:ALA:HB2	2.24	0.62
2:B:80:LEU:HB3	2:B:81:LYS:C	2.25	0.62
2:B:103:ARG:NH2	2:B:103:ARG:NH1	2.44	0.62
2:B:138:ASN:ND2	2:B:138:ASN:CB	2.56	0.62
2:B:144:TYR:CE2	2:B:144:TYR:CD1	2.87	0.62
1:C:46:PHE:CE2	1:C:54:GLN:HG2	2.34	0.62
1:C:90:LYS:N	1:C:90:LYS:C	2.58	0.62
2:D:130:GLN:CA	2:D:130:GLN:HE21	2.13	0.62
1:A:43:PHE:CA	1:A:43:PHE:CG	2.76	0.61
1:A:46:PHE:HB3	1:A:48:LEU:HD23	1.82	0.61
2:D:19:VAL:CG1	2:D:64:LYS:HD2	2.29	0.61
1:A:2:LEU:CB	1:A:2:LEU:CD1	2.78	0.61
2:B:1:MET:N	2:B:1:MET:C	2.58	0.61
2:B:18:ASP:CG	2:B:18:ASP:CA	2.71	0.61
1:C:89:HIS:CD2	1:C:139:LYS:NZ	2.68	0.61
2:D:50:ALA:C	2:D:53:VAL:HG13	2.24	0.61
2:D:94:LYS:HD2	2:D:95:LEU:HD22	1.81	0.61
1:A:27:GLN:OE1	1:A:112:HIS:CE1	2.53	0.61
1:A:132:ASP:O	1:A:135:VAL:HG23	2.00	0.61
1:C:46:PHE:CD2	1:C:54:GLN:CB	2.83	0.61
2:D:52:ALA:HA	2:D:55:ASN:H	1.63	0.61
2:D:6:GLU:O	2:D:6:GLU:CG	2.48	0.61
2:D:33:VAL:O	2:D:33:VAL:HG22	1.98	0.61
2:D:128:LEU:N	2:D:128:LEU:C	2.58	0.61
2:D:130:GLN:CG	2:D:130:GLN:OE1	2.48	0.61
1:A:10:VAL:C	1:A:10:VAL:N	2.59	0.61
1:C:84:SER:HA	1:C:136:LEU:HD13	1.83	0.61
1:C:95:PRO:HG3	1:C:141:ARG:NH2	2.15	0.61
2:D:39:ARG:NE	2:D:39:ARG:HG2	2.09	0.61
1:A:43:PHE:CB	1:A:43:PHE:N	2.61	0.61
1:A:76:LEU:H	1:A:76:LEU:HD23	1.64	0.61
1:A:105:LEU:CD2	1:A:105:LEU:HD11	2.25	0.61
2:B:64:LYS:N	2:B:65:ARG:N	2.48	0.61
2:D:28:GLY:O	2:D:54:MET:HE1	2.00	0.61
2:D:75:LYS:CD	2:D:75:LYS:HG2	2.14	0.61
1:A:42:TYR:C	1:A:44:PRO:HD2	2.25	0.61
2:B:43:HIS:CE1	3:B:146:HEM:CGA	2.83	0.61
2:B:97:VAL:HG12	2:B:101:ASN:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ASN:HB3	1:C:124:ASN:CB	2.31	0.61
1:C:87:HIS:O	1:C:91:LEU:HB2	2.00	0.61
1:C:90:LYS:N	1:C:90:LYS:CB	2.62	0.61
3:D:146:HEM:C4C	3:D:146:HEM:CAC	2.74	0.61
1:A:31:ARG:CD	2:B:126:GLN:HE21	2.14	0.61
1:A:52:SER:OG	1:A:52:SER:CA	2.48	0.61
1:A:106:LEU:HD23	1:A:126:ASN:HD22	1.66	0.61
2:B:39:ARG:CZ	2:B:40:PHE:CZ	2.82	0.61
2:B:80:LEU:HB3	2:B:80:LEU:HD23	1.78	0.61
1:C:60:GLN:NE2	1:C:64:ASN:HD21	1.98	0.61
1:C:99:LYS:CD	1:C:99:LYS:CB	2.59	0.61
1:A:43:PHE:HB2	1:A:48:LEU:HD22	1.83	0.61
1:A:86:LEU:O	1:A:91:LEU:HB2	2.00	0.61
1:A:124:ASN:CB	1:A:124:ASN:H	2.06	0.61
2:B:140:LEU:CD1	2:B:140:LEU:CD2	2.79	0.61
2:D:79:ASP:OD1	2:D:81:LYS:CD	2.49	0.61
2:D:84:PHE:HB2	2:D:84:PHE:N	2.14	0.61
1:A:42:TYR:HB3	3:A:142:HEM:CMD	2.31	0.61
2:B:70:PHE:HD1	2:B:71:THR:CB	2.13	0.61
1:C:109:LEU:O	1:C:113:LEU:CD2	2.49	0.61
2:D:2:LEU:CG	2:D:7:LYS:CE	2.75	0.61
2:D:56:ASN:C	2:D:56:ASN:HD22	2.09	0.61
2:B:2:LEU:CB	2:B:131:LYS:HZ1	2.14	0.60
2:B:27:LEU:HD21	2:B:66:VAL:HG11	1.80	0.60
1:C:86:LEU:HD21	3:C:142:HEM:CBA	2.31	0.60
1:A:9:ASN:N	1:A:9:ASN:C	2.54	0.60
1:A:16:LYS:CE	1:A:16:LYS:CG	2.74	0.60
1:A:89:HIS:CD2	1:A:139:LYS:CD	2.77	0.60
2:B:65:ARG:HH12	2:B:65:ARG:HH22	1.49	0.60
2:B:121:PHE:CZ	2:B:126:GLN:HA	2.36	0.60
2:D:141:ALA:N	2:D:142:HIS:N	2.49	0.60
1:A:75:ASP:O	1:A:79:THR:N	2.35	0.60
1:A:14:TRP:O	1:A:17:VAL:HG23	2.01	0.60
1:A:50:HIS:CG	1:A:50:HIS:HA	2.35	0.60
2:B:46:ASN:CB	2:B:46:ASN:C	2.72	0.60
1:C:44:PRO:O	1:C:45:HIS:CA	2.49	0.60
1:C:113:LEU:HD23	1:C:113:LEU:N	2.10	0.60
1:C:114:PRO:CA	1:C:114:PRO:CG	2.78	0.60
1:C:129:LEU:O	1:C:130:ALA:CA	2.50	0.60
2:D:72:GLN:HE22	2:D:73:GLY:HA2	1.61	0.60
2:B:104:LEU:O	2:B:107:ASN:HB2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:CG	1:C:61:LYS:HD2	2.15	0.60
2:D:41:PHE:HB2	2:D:44:PHE:CE1	2.36	0.60
2:D:110:ALA:HB1	2:D:126:GLN:OE1	2.00	0.60
2:B:134:ALA:C	2:B:138:ASN:HD22	2.09	0.60
2:D:5:GLU:CB	2:D:9:ALA:HB3	2.25	0.60
2:D:79:ASP:OD1	2:D:81:LYS:HD3	2.02	0.60
1:A:118:THR:CG2	1:A:118:THR:N	2.65	0.60
2:B:80:LEU:CD1	2:B:80:LEU:HD21	2.32	0.60
2:B:82:GLY:O	2:B:85:ALA:CB	2.50	0.60
2:D:2:LEU:CD2	2:D:7:LYS:CD	2.78	0.60
2:D:59:VAL:C	2:D:59:VAL:HB	2.23	0.60
1:A:36:PHE:CG	1:A:36:PHE:CA	2.81	0.60
1:A:61:LYS:CB	1:A:61:LYS:C	2.74	0.60
1:A:76:LEU:HB2	1:A:77:PRO:HD3	1.82	0.60
1:A:94:ASN:OD1	1:A:96:VAL:CG2	2.49	0.60
1:C:73:LEU:C	1:C:74:ASN:CA	2.71	0.60
1:C:89:HIS:CB	1:C:139:LYS:CG	2.80	0.60
1:C:121:VAL:C	1:C:122:HIS:C	2.68	0.60
2:D:14:TRP:CE3	2:D:14:TRP:HA	2.34	0.60
2:D:25:GLN:CD	2:D:115:ARG:NH2	2.59	0.60
2:D:137:ALA:CB	2:D:140:LEU:CD1	2.80	0.60
1:A:1:VAL:CB	1:A:1:VAL:C	2.70	0.60
1:A:62:VAL:CG1	1:A:62:VAL:HG22	2.23	0.60
1:A:79:THR:CG2	1:A:79:THR:HA	2.24	0.60
2:B:62:HIS:CD2	2:B:62:HIS:O	2.55	0.60
2:B:123:PRO:CB	2:B:126:GLN:NE2	2.64	0.60
1:C:131:ASN:CB	1:C:131:ASN:OD1	2.49	0.60
2:D:116:ASN:CA	2:D:117:PHE:N	2.60	0.60
1:A:2:LEU:HB3	1:A:7:LYS:HD3	1.82	0.60
2:B:95:LEU:HD11	3:B:146:HEM:C2A	2.37	0.60
1:C:26:ALA:CB	1:C:56:LYS:HD2	2.31	0.60
1:C:36:PHE:O	1:C:39:THR:HG22	2.01	0.60
2:D:11:THR:CA	2:D:11:THR:HG1	2.14	0.60
2:D:14:TRP:CB	2:D:15:GLY:N	2.65	0.60
2:D:123:PRO:CD	2:D:123:PRO:HG3	2.17	0.60
1:A:31:ARG:HH21	2:B:126:GLN:HB3	1.66	0.59
1:A:55:GLN:HB3	1:A:56:LYS:HZ3	1.67	0.59
1:A:106:LEU:CD2	1:A:106:LEU:HD11	2.32	0.59
2:B:34:TYR:CE2	2:B:34:TYR:CD1	2.89	0.59
2:B:137:ALA:N	2:B:137:ALA:CB	2.54	0.59
1:C:139:LYS:CB	1:C:139:LYS:HD3	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:ASN:ND2	2:D:57:PRO:HD2	2.17	0.59
2:B:80:LEU:C	2:B:81:LYS:C	2.69	0.59
2:B:105:LEU:CB	3:B:146:HEM:HBB2	2.32	0.59
3:B:146:HEM:HMA2	3:B:146:HEM:CHB	2.30	0.59
1:C:27:GLN:OE1	1:C:31:ARG:NH1	2.36	0.59
1:C:56:LYS:CE	1:C:59:GLY:HA3	2.32	0.59
2:D:87:LEU:CA	2:D:87:LEU:CG	2.71	0.59
2:B:22:VAL:O	2:B:23:GLY:HA2	2.03	0.59
1:C:48:LEU:HA	1:C:55:GLN:CD	2.27	0.59
1:A:29:LEU:HD23	1:A:29:LEU:O	2.02	0.59
2:B:38:GLN:C	2:B:38:GLN:N	2.59	0.59
1:C:70:GLN:O	1:C:73:LEU:HD11	2.02	0.59
2:D:10:VAL:CA	2:D:11:THR:N	2.64	0.59
2:D:129:PHE:N	2:D:129:PHE:CB	2.64	0.59
2:B:2:LEU:HB2	2:B:6:GLU:HB2	1.83	0.59
2:B:7:LYS:HE3	2:B:74:LEU:HD11	1.84	0.59
2:B:16:LYS:N	2:B:16:LYS:HB3	2.18	0.59
2:B:19:VAL:CG2	2:B:68:ASP:OD2	2.46	0.59
2:B:126:GLN:CA	2:B:127:ALA:N	2.60	0.59
1:C:15:GLY:N	1:C:15:GLY:C	2.58	0.59
2:D:56:ASN:C	2:D:57:PRO:HG2	2.25	0.59
2:D:59:VAL:HB	2:D:60:LYS:N	2.18	0.59
1:A:26:ALA:CB	1:A:59:GLY:HA3	2.31	0.59
1:A:36:PHE:HB3	1:A:100:LEU:HD13	1.84	0.59
1:A:70:GLN:O	1:A:73:LEU:HD12	2.03	0.59
3:A:142:HEM:HMD1	3:A:142:HEM:CHD	2.32	0.59
2:B:68:ASP:H	2:B:71:THR:HG21	1.61	0.59
2:B:78:ASP:OD2	2:B:79:ASP:HB2	2.02	0.59
1:C:87:HIS:O	1:C:93:VAL:HG23	2.01	0.59
2:D:28:GLY:HA3	2:D:54:MET:CE	2.30	0.59
2:D:103:ARG:NH2	2:D:130:GLN:NE2	2.50	0.59
2:B:58:LYS:CB	2:B:58:LYS:CD	2.77	0.59
2:D:115:ARG:HH21	2:D:115:ARG:HG2	1.68	0.59
2:B:41:PHE:HB3	2:B:43:HIS:HB3	1.82	0.59
1:C:47:ASP:CB	1:C:47:ASP:OD1	2.47	0.59
3:C:142:HEM:CAB	3:C:142:HEM:C2B	2.73	0.59
2:D:10:VAL:CG1	2:D:128:LEU:CD2	2.69	0.59
2:D:123:PRO:CD	2:D:123:PRO:HG2	2.17	0.59
2:D:126:GLN:NE2	2:D:130:GLN:CB	2.64	0.59
1:A:7:LYS:C	1:A:7:LYS:N	2.60	0.59
1:A:72:HIS:HB2	1:A:74:ASN:HD21	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:N	1:A:116:ASN:CB	2.64	0.59
1:A:136:LEU:CA	1:A:137:THR:N	2.66	0.59
2:B:52:ALA:N	2:B:52:ALA:C	2.60	0.59
1:C:86:LEU:HD22	3:C:142:HEM:HBA2	1.84	0.59
1:C:113:LEU:CD2	1:C:113:LEU:CD1	2.79	0.59
2:D:52:ALA:CB	2:D:52:ALA:C	2.70	0.59
1:A:85:ASN:HA	1:A:139:LYS:HE3	1.85	0.58
2:D:70:PHE:CA	2:D:71:THR:HB	2.32	0.58
1:A:91:LEU:HD23	3:A:142:HEM:C2D	2.37	0.58
2:B:22:VAL:CG1	2:B:67:LEU:HD21	2.30	0.58
2:B:36:TRP:C	2:B:37:THR:CA	2.75	0.58
2:B:42:GLN:O	2:B:43:HIS:N	2.35	0.58
1:A:31:ARG:HE	1:A:31:ARG:HG3	1.66	0.58
1:A:36:PHE:CZ	2:B:130:GLN:HG3	2.37	0.58
2:B:55:ASN:HA	2:B:60:LYS:NZ	2.18	0.58
2:B:109:LEU:O	2:B:110:ALA:CA	2.50	0.58
2:B:130:GLN:CB	2:B:130:GLN:N	2.65	0.58
1:C:46:PHE:CG	1:C:46:PHE:CA	2.86	0.58
1:C:76:LEU:CD2	1:C:76:LEU:CB	2.78	0.58
2:D:2:LEU:CD2	2:D:7:LYS:HB3	2.28	0.58
2:D:4:ALA:CA	2:D:5:GLU:CA	2.77	0.58
2:D:83:ALA:C	2:D:83:ALA:CB	2.76	0.58
2:D:143:LYS:CE	2:D:143:LYS:CG	2.72	0.58
1:A:57:ALA:CA	1:A:60:GLN:NE2	2.61	0.58
2:B:75:LYS:CB	2:B:76:HIS:ND1	2.66	0.58
2:D:17:VAL:C	2:D:17:VAL:CG2	2.76	0.58
1:A:52:SER:O	1:A:54:GLN:N	2.36	0.58
2:B:113:VAL:CG1	2:B:113:VAL:CG2	2.82	0.58
1:C:32:MET:CA	1:C:32:MET:HB3	2.16	0.58
1:A:79:THR:CA	1:A:79:THR:OG1	2.38	0.58
2:B:101:ASN:HB3	3:B:146:HEM:HAB	1.85	0.58
2:B:125:VAL:CG1	2:B:125:VAL:O	2.52	0.58
2:D:67:LEU:HA	2:D:67:LEU:HD23	1.84	0.58
2:D:79:ASP:C	2:D:81:LYS:CD	2.76	0.58
2:D:79:ASP:OD1	2:D:81:LYS:HE2	2.02	0.58
2:B:18:ASP:O	2:B:20:ASP:OD2	2.22	0.58
2:B:39:ARG:HH12	2:B:40:PHE:HZ	0.62	0.58
2:B:97:VAL:CG1	3:B:146:HEM:HMB2	2.34	0.58
1:C:96:VAL:CG2	1:C:96:VAL:CG1	2.79	0.58
2:D:90:LEU:HD13	2:D:91:HIS:HD1	1.68	0.58
2:D:115:ARG:CA	2:D:115:ARG:HG3	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:CG	1:A:100:LEU:HA	2.31	0.58
2:D:84:PHE:CG	2:D:84:PHE:CA	2.85	0.58
1:A:29:LEU:HB2	1:A:32:MET:HE2	1.86	0.58
2:B:2:LEU:HB2	2:B:6:GLU:CD	2.28	0.58
2:B:3:THR:N	2:B:6:GLU:CB	2.58	0.58
1:C:116:ASN:CA	1:C:117:PHE:N	2.45	0.58
2:D:31:LEU:HA	2:D:31:LEU:HG	1.84	0.58
2:D:46:ASN:OD1	2:D:52:ALA:HB3	2.04	0.58
1:A:72:HIS:HD1	1:A:72:HIS:C	2.12	0.58
2:B:84:PHE:HE2	3:B:146:HEM:CBC	2.16	0.58
2:B:123:PRO:HB3	2:B:126:GLN:HE22	1.68	0.58
1:A:118:THR:O	1:A:122:HIS:N	2.28	0.57
2:B:77:LEU:CD1	2:B:77:LEU:C	2.78	0.57
1:C:17:VAL:HG12	1:C:21:ALA:HB2	1.86	0.57
1:C:86:LEU:HD21	3:C:142:HEM:HBA1	1.85	0.57
2:D:12:GLY:O	2:D:13:PHE:C	2.47	0.57
2:D:30:LEU:HG	2:D:37:THR:HG21	1.84	0.57
2:B:7:LYS:HE3	2:B:74:LEU:CD1	2.34	0.57
2:B:49:SER:HB3	2:B:52:ALA:HB3	1.86	0.57
2:B:105:LEU:HB3	3:B:146:HEM:HBB2	1.86	0.57
1:C:20:ASN:O	1:C:21:ALA:N	2.30	0.57
2:D:77:LEU:H	2:D:77:LEU:HD12	1.68	0.57
1:A:79:THR:CA	1:A:79:THR:HG23	2.26	0.57
3:A:142:HEM:C1D	3:A:142:HEM:HMD1	2.36	0.57
2:B:20:ASP:O	2:B:21:VAL:HG22	2.03	0.57
2:B:60:LYS:NZ	2:B:60:LYS:HB2	2.20	0.57
2:B:81:LYS:CE	2:B:142:HIS:ND1	2.67	0.57
1:C:58:HIS:C	1:C:59:GLY:C	2.72	0.57
1:C:89:HIS:CB	1:C:139:LYS:HZ2	2.13	0.57
2:D:20:ASP:CG	2:D:64:LYS:HB2	2.29	0.57
1:A:80:LEU:CD2	1:A:80:LEU:CD1	2.79	0.57
1:A:112:HIS:ND1	1:A:112:HIS:HB2	2.16	0.57
2:B:13:PHE:CE1	2:B:120:GLN:HB2	2.40	0.57
1:A:32:MET:CA	1:A:33:PHE:N	2.65	0.57
1:A:53:ALA:CA	1:A:56:LYS:CG	2.82	0.57
1:A:100:LEU:CD1	1:A:100:LEU:HB2	2.27	0.57
2:B:145:HIS:CB	2:B:145:HIS:C	2.72	0.57
1:C:91:LEU:N	1:C:91:LEU:C	2.57	0.57
1:C:118:THR:OG1	1:C:121:VAL:HG23	2.05	0.57
2:D:67:LEU:O	2:D:71:THR:HB	2.04	0.57
2:D:79:ASP:OD1	2:D:81:LYS:CE	2.53	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:LEU:CD1	3:D:146:HEM:CHB	2.82	0.57
1:A:1:VAL:C	1:A:1:VAL:N	2.63	0.57
2:B:20:ASP:HA	2:B:64:LYS:HG2	1.87	0.57
2:B:106:GLY:CA	2:B:133:VAL:HG21	2.35	0.57
1:C:43:PHE:CE2	1:C:58:HIS:NE2	2.73	0.57
1:C:49:SER:CB	1:C:49:SER:HG	2.09	0.57
2:D:41:PHE:CB	2:D:44:PHE:CE1	2.88	0.57
1:A:33:PHE:HD1	1:A:40:LYS:CE	2.14	0.57
1:A:42:TYR:HB2	1:A:43:PHE:CE1	2.40	0.57
1:A:43:PHE:CD2	1:A:43:PHE:CD1	2.50	0.57
1:A:46:PHE:HB3	1:A:55:GLN:HE22	1.69	0.57
2:B:92:CYS:HB2	2:B:144:TYR:CZ	2.40	0.57
2:B:131:LYS:NZ	2:B:131:LYS:HD2	2.16	0.57
1:C:100:LEU:CB	1:C:100:LEU:CD1	2.80	0.57
1:A:100:LEU:HA	1:A:100:LEU:HD23	1.87	0.57
2:B:6:GLU:OE1	2:B:131:LYS:CE	2.52	0.57
2:B:16:LYS:O	2:B:117:PHE:HZ	1.86	0.57
2:B:98:ASN:C	2:B:100:GLN:N	2.63	0.57
1:C:70:GLN:HG2	1:C:128:PHE:CZ	2.39	0.57
1:C:117:PHE:HE2	2:D:111:LEU:HD11	1.69	0.57
1:A:41:THR:C	1:A:41:THR:HB	2.27	0.56
1:A:43:PHE:CD2	1:A:46:PHE:CE1	2.93	0.56
1:C:80:LEU:O	1:C:84:SER:HB2	2.05	0.56
2:D:144:TYR:HD1	2:D:145:HIS:N	1.86	0.56
1:A:73:LEU:HA	1:A:76:LEU:HD21	1.87	0.56
2:B:19:VAL:HG21	2:B:68:ASP:H	1.66	0.56
1:C:54:GLN:O	1:C:57:ALA:HB3	2.05	0.56
1:A:29:LEU:CB	1:A:29:LEU:N	2.68	0.56
2:B:39:ARG:HD3	1:C:92:ARG:HB2	1.86	0.56
2:B:136:VAL:C	2:B:136:VAL:CG1	2.79	0.56
1:C:66:LEU:CD2	1:C:66:LEU:CD1	2.78	0.56
1:C:80:LEU:HD23	1:C:135:VAL:HG21	1.85	0.56
1:C:92:ARG:CD	1:C:92:ARG:HB2	2.35	0.56
1:C:93:VAL:CG1	3:C:142:HEM:C3C	2.88	0.56
2:D:1:MET:CG	2:D:131:LYS:NZ	2.67	0.56
2:D:54:MET:O	2:D:60:LYS:HD2	2.05	0.56
1:A:70:GLN:CD	1:A:70:GLN:HG2	2.19	0.56
2:B:94:LYS:H	2:B:95:LEU:HB2	1.70	0.56
1:C:17:VAL:HG22	1:C:24:TYR:HE2	1.67	0.56
1:C:83:LEU:CB	1:C:83:LEU:C	2.70	0.56
1:C:141:ARG:CD	1:C:141:ARG:CB	2.81	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:GLN:NE2	2:D:115:ARG:NH2	2.53	0.56
2:D:65:ARG:HA	2:D:68:ASP:HB2	1.86	0.56
1:A:14:TRP:CD1	1:A:67:THR:HG23	2.40	0.56
1:A:31:ARG:NH2	2:B:126:GLN:HB2	2.21	0.56
1:A:105:LEU:N	1:A:106:LEU:N	2.52	0.56
1:A:132:ASP:O	1:A:136:LEU:HG	2.05	0.56
2:B:57:PRO:HB3	2:B:57:PRO:HD3	1.86	0.56
1:C:11:LYS:HD2	1:C:70:GLN:HE22	1.69	0.56
2:D:44:PHE:CB	2:D:44:PHE:C	2.79	0.56
2:D:56:ASN:O	2:D:59:VAL:N	2.39	0.56
2:B:14:TRP:O	2:B:17:VAL:HG23	2.05	0.56
2:B:24:ALA:O	2:B:28:GLY:HA3	2.05	0.56
1:C:93:VAL:O	1:C:140:TYR:OH	2.24	0.56
2:D:72:GLN:HE21	2:D:72:GLN:C	2.11	0.56
2:D:124:ASN:O	2:D:128:LEU:HD12	2.04	0.56
1:A:35:SER:CA	1:A:35:SER:OG	2.52	0.56
2:B:1:MET:H3	2:B:2:LEU:CD2	2.18	0.56
2:B:25:GLN:HG3	2:B:112:VAL:HG11	1.87	0.56
2:B:33:VAL:C	2:B:35:PRO:HD3	2.30	0.56
1:C:43:PHE:HE2	1:C:58:HIS:NE2	2.03	0.56
1:C:133:SER:C	1:C:134:THR:C	2.72	0.56
1:A:55:GLN:HB3	1:A:56:LYS:NZ	2.21	0.56
1:A:65:ALA:CB	1:A:65:ALA:N	2.59	0.56
2:B:21:VAL:CA	2:B:21:VAL:CG1	2.65	0.56
2:B:43:HIS:CA	2:B:43:HIS:O	2.48	0.56
2:D:1:MET:C	2:D:1:MET:H3	2.10	0.56
2:B:1:MET:H3	2:B:2:LEU:HD23	1.68	0.56
2:B:2:LEU:CB	2:B:131:LYS:NZ	2.62	0.56
2:B:70:PHE:HD1	2:B:71:THR:H	1.54	0.56
2:B:97:VAL:HG11	3:B:146:HEM:CMB	2.36	0.56
2:B:134:ALA:O	2:B:138:ASN:ND2	2.37	0.56
2:D:10:VAL:HG23	2:D:11:THR:HG22	1.87	0.56
2:D:61:ALA:CB	2:D:62:HIS:H	2.17	0.56
2:D:79:ASP:O	2:D:81:LYS:CD	2.54	0.56
1:A:26:ALA:CB	1:A:56:LYS:CE	2.72	0.56
1:A:63:ALA:CB	1:A:63:ALA:HA	2.16	0.56
2:B:101:ASN:C	3:B:146:HEM:CBB	2.79	0.56
2:B:125:VAL:C	2:B:126:GLN:C	2.74	0.56
1:A:26:ALA:O	1:A:30:GLN:HB3	2.06	0.55
1:A:32:MET:N	1:A:32:MET:HB3	2.21	0.55
1:A:43:PHE:CB	1:A:43:PHE:C	2.74	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ALA:O	2:B:28:GLY:CA	2.53	0.55
1:C:44:PRO:CB	1:C:44:PRO:N	2.59	0.55
1:C:88:ALA:HB3	1:C:139:LYS:HB2	1.87	0.55
2:D:75:LYS:C	2:D:75:LYS:HB3	2.21	0.55
1:A:2:LEU:CD1	1:A:2:LEU:HD22	2.32	0.55
3:A:142:HEM:HMA2	3:A:142:HEM:HHB	1.87	0.55
2:B:6:GLU:O	2:B:9:ALA:HB3	2.05	0.55
2:B:65:ARG:HD3	3:B:146:HEM:CBD	2.35	0.55
1:C:32:MET:CE	1:C:101:LEU:HG	2.36	0.55
1:C:69:ALA:CA	1:C:70:GLN:N	2.54	0.55
1:C:88:ALA:HB2	1:C:136:LEU:O	2.07	0.55
1:C:101:LEU:HD12	3:C:142:HEM:HHC	1.88	0.55
2:D:67:LEU:HA	2:D:67:LEU:CD2	2.36	0.55
2:D:88:SER:CB	2:D:88:SER:N	2.65	0.55
2:B:24:ALA:HB2	2:B:60:LYS:HA	1.89	0.55
2:B:80:LEU:CB	2:B:82:GLY:CA	2.84	0.55
2:B:102:PHE:CD1	2:B:140:LEU:HD12	2.42	0.55
2:D:138:ASN:N	2:D:138:ASN:CB	2.64	0.55
3:D:146:HEM:CAA	3:D:146:HEM:CHA	2.83	0.55
1:A:31:ARG:NH2	2:B:126:GLN:CB	2.65	0.55
1:A:32:MET:SD	1:A:101:LEU:HB2	2.46	0.55
2:B:92:CYS:HB2	2:B:144:TYR:CE2	2.41	0.55
1:C:93:VAL:CG1	3:C:142:HEM:HAC	2.30	0.55
2:D:51:GLY:O	2:D:54:MET:HB2	2.06	0.55
1:A:74:ASN:HD22	1:A:74:ASN:N	2.04	0.55
1:A:131:ASN:N	1:A:131:ASN:C	2.63	0.55
2:B:21:VAL:HB	2:B:22:VAL:N	2.20	0.55
2:B:97:VAL:HG21	3:B:146:HEM:C1B	2.41	0.55
1:A:70:GLN:CD	1:A:70:GLN:HG3	2.19	0.55
1:A:139:LYS:CD	1:A:139:LYS:NZ	2.70	0.55
2:B:4:ALA:O	2:B:8:ALA:HB2	2.06	0.55
1:A:72:HIS:HE1	1:A:79:THR:OG1	1.89	0.55
1:A:140:TYR:CD1	1:A:140:TYR:HB2	2.40	0.55
2:B:97:VAL:CG1	3:B:146:HEM:CMB	2.85	0.55
2:B:106:GLY:CA	2:B:107:ASN:N	2.63	0.55
2:B:130:GLN:CB	2:B:130:GLN:CD	2.79	0.55
1:C:117:PHE:CD2	1:C:117:PHE:O	2.59	0.55
1:C:140:TYR:C	1:C:141:ARG:HD3	2.31	0.55
2:D:47:LEU:HD12	2:D:53:VAL:HA	1.87	0.55
1:A:105:LEU:N	1:A:105:LEU:C	2.51	0.55
2:B:70:PHE:HA	2:B:84:PHE:HZ	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:VAL:HG12	2:B:117:PHE:CE2	2.42	0.55
1:C:60:GLN:CA	1:C:60:GLN:HG2	2.35	0.55
2:D:110:ALA:N	2:D:110:ALA:C	2.65	0.55
2:B:3:THR:CG2	2:B:5:GLU:CG	2.78	0.55
1:C:7:LYS:O	1:C:11:LYS:HB2	2.06	0.55
1:C:15:GLY:N	1:C:16:LYS:N	2.53	0.55
1:C:23:ALA:HA	1:C:56:LYS:HD3	1.89	0.55
1:C:99:LYS:C	1:C:100:LEU:CA	2.71	0.55
2:B:13:PHE:HE1	2:B:120:GLN:CB	2.20	0.55
2:B:47:LEU:CD1	2:B:53:VAL:HA	2.37	0.55
2:B:125:VAL:CG1	2:B:125:VAL:CA	2.81	0.55
1:C:32:MET:CA	1:C:32:MET:HB2	2.16	0.55
2:D:111:LEU:C	2:D:112:VAL:HA	2.22	0.55
2:D:145:HIS:C	2:D:145:HIS:HB2	2.30	0.55
1:A:43:PHE:HA	1:A:44:PRO:HD2	1.89	0.54
2:B:24:ALA:HB1	2:B:60:LYS:HA	1.89	0.54
2:B:54:MET:O	2:B:59:VAL:CG2	2.56	0.54
2:B:85:ALA:O	2:B:88:SER:HB2	2.06	0.54
2:B:109:LEU:CD2	2:B:109:LEU:CA	2.80	0.54
2:B:122:THR:HG1	2:B:125:VAL:H	1.53	0.54
1:C:17:VAL:O	1:C:18:GLY:CA	2.54	0.54
1:C:83:LEU:HB3	1:C:84:SER:OG	2.07	0.54
1:C:84:SER:HA	1:C:87:HIS:HD1	1.72	0.54
2:D:65:ARG:N	2:D:66:VAL:N	2.55	0.54
2:D:90:LEU:HB3	2:D:90:LEU:HD12	1.85	0.54
1:A:17:VAL:CG2	1:A:17:VAL:CA	2.78	0.54
1:A:43:PHE:HA	1:A:45:HIS:NE2	2.22	0.54
1:A:48:LEU:CD2	1:A:48:LEU:HG	2.22	0.54
1:C:83:LEU:CD1	3:C:142:HEM:HMA1	2.35	0.54
2:D:10:VAL:HG23	2:D:11:THR:CG2	2.35	0.54
2:D:56:ASN:C	2:D:56:ASN:ND2	2.64	0.54
1:A:26:ALA:HB1	1:A:56:LYS:HZ1	1.67	0.54
2:B:74:LEU:C	2:B:75:LYS:C	2.68	0.54
1:C:32:MET:CB	1:C:32:MET:C	2.77	0.54
2:D:112:VAL:CG1	2:D:112:VAL:HA	2.37	0.54
1:A:26:ALA:O	1:A:30:GLN:CB	2.55	0.54
1:A:41:THR:CA	1:A:41:THR:HG23	2.35	0.54
1:A:93:VAL:HG21	3:A:142:HEM:C3C	2.42	0.54
1:A:119:PRO:HD3	2:B:29:ARG:NH1	2.23	0.54
2:B:63:GLY:CA	2:B:66:VAL:HG13	2.24	0.54
1:C:18:GLY:N	1:C:18:GLY:C	2.57	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASN:OD1	1:C:89:HIS:HB3	2.08	0.54
2:D:33:VAL:C	2:D:34:TYR:CA	2.76	0.54
2:D:70:PHE:CE2	2:D:136:VAL:HG11	2.42	0.54
2:D:104:LEU:CB	2:D:104:LEU:CD1	2.85	0.54
1:A:26:ALA:CA	1:A:29:LEU:HD22	2.21	0.54
1:C:36:PHE:C	1:C:37:PRO:CD	2.76	0.54
2:D:70:PHE:CD1	2:D:71:THR:OG1	2.13	0.54
3:D:146:HEM:CAA	3:D:146:HEM:CGA	2.85	0.54
2:B:128:LEU:CB	2:B:128:LEU:HA	2.21	0.54
2:B:143:LYS:CG	2:B:143:LYS:CA	2.83	0.54
1:C:39:THR:HB	1:C:39:THR:N	2.17	0.54
2:D:95:LEU:HD11	3:D:146:HEM:C4A	2.43	0.54
1:A:1:VAL:CG1	1:A:1:VAL:HG22	2.35	0.54
1:A:19:GLY:O	1:A:22:PRO:HG2	2.08	0.54
1:A:26:ALA:CB	1:A:56:LYS:HE3	2.37	0.54
1:A:42:TYR:O	1:A:43:PHE:CA	2.55	0.54
1:A:62:VAL:HG23	3:A:142:HEM:C1B	2.42	0.54
2:B:27:LEU:HD23	2:B:66:VAL:CG1	2.38	0.54
2:B:95:LEU:CB	2:B:95:LEU:C	2.75	0.54
1:C:86:LEU:O	1:C:91:LEU:N	2.26	0.54
2:D:14:TRP:HB3	2:D:15:GLY:N	2.22	0.54
2:B:30:LEU:CD2	2:B:105:LEU:HB2	2.37	0.54
1:C:99:LYS:CD	1:C:99:LYS:HB3	2.37	0.54
2:D:16:LYS:CB	2:D:16:LYS:O	2.55	0.54
1:A:21:ALA:O	1:A:22:PRO:C	2.50	0.54
2:B:19:VAL:HA	2:B:67:LEU:HD23	1.90	0.54
2:B:75:LYS:CD	2:B:75:LYS:CB	2.83	0.54
1:C:42:TYR:CG	3:C:142:HEM:CBC	2.90	0.54
1:C:86:LEU:CD2	3:C:142:HEM:HBA1	2.37	0.54
2:D:14:TRP:O	2:D:17:VAL:HG13	2.07	0.54
2:D:32:VAL:CG1	2:D:53:VAL:HG21	2.38	0.54
1:A:96:VAL:HG11	2:D:100:GLN:CG	2.36	0.54
1:C:64:ASN:CA	1:C:64:ASN:CG	2.70	0.54
1:C:89:HIS:C	1:C:90:LYS:CA	2.78	0.54
2:D:115:ARG:NH2	2:D:115:ARG:HG2	2.16	0.54
2:D:129:PHE:N	2:D:129:PHE:CG	2.75	0.54
1:A:67:THR:C	1:A:67:THR:CB	2.76	0.53
1:A:72:HIS:CE1	1:A:79:THR:OG1	2.61	0.53
1:A:85:ASN:CG	1:A:90:LYS:HE3	2.32	0.53
1:A:109:LEU:CA	1:A:110:ALA:N	2.67	0.53
2:B:39:ARG:CG	2:B:39:ARG:CA	2.82	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:SER:CA	2:B:49:SER:O	2.57	0.53
2:B:54:MET:C	2:B:55:ASN:OD1	2.51	0.53
2:B:114:ALA:O	2:B:118:GLY:HA2	2.07	0.53
1:C:91:LEU:CD1	1:C:91:LEU:CD2	2.76	0.53
1:C:128:PHE:O	1:C:131:ASN:HB2	2.09	0.53
2:D:101:ASN:HB2	3:D:146:HEM:HAB	1.90	0.53
1:A:132:ASP:OD2	1:A:132:ASP:HB2	2.07	0.53
2:B:94:LYS:HB3	2:B:94:LYS:HD2	1.85	0.53
1:C:99:LYS:CG	1:C:99:LYS:HE3	2.37	0.53
2:D:30:LEU:CA	2:D:31:LEU:N	2.64	0.53
1:A:40:LYS:CE	1:A:40:LYS:N	2.71	0.53
1:A:44:PRO:CA	1:A:45:HIS:HD2	2.21	0.53
1:A:110:ALA:HB2	1:A:117:PHE:CE2	2.44	0.53
2:B:70:PHE:CE2	2:B:133:VAL:HG23	2.44	0.53
1:C:126:ASN:C	1:C:126:ASN:CB	2.73	0.53
2:D:34:TYR:N	2:D:34:TYR:CG	2.77	0.53
2:D:67:LEU:CA	2:D:67:LEU:CD2	2.87	0.53
2:D:127:ALA:C	2:D:128:LEU:CA	2.66	0.53
2:D:130:GLN:CD	2:D:130:GLN:HA	2.31	0.53
1:A:37:PRO:HA	1:A:40:LYS:CD	2.38	0.53
2:B:34:TYR:HB3	2:B:36:TRP:CZ2	2.44	0.53
2:B:125:VAL:CA	2:B:125:VAL:O	2.46	0.53
1:C:71:GLY:CA	1:C:72:HIS:N	2.65	0.53
1:C:83:LEU:HD11	3:C:142:HEM:CMA	2.36	0.53
1:A:127:LYS:CB	1:A:128:PHE:N	2.71	0.53
2:B:10:VAL:HG12	2:B:129:PHE:CE2	2.43	0.53
1:C:108:THR:CA	1:C:108:THR:O	2.54	0.53
1:A:37:PRO:C	1:A:40:LYS:HD2	2.34	0.53
2:B:80:LEU:HB3	2:B:80:LEU:HD22	1.82	0.53
2:B:133:VAL:CG2	2:B:133:VAL:HG11	2.36	0.53
1:A:21:ALA:HB3	1:A:22:PRO:CD	2.38	0.53
1:A:100:LEU:CD2	1:A:100:LEU:HA	2.38	0.53
1:A:113:LEU:O	1:A:117:PHE:HB2	2.08	0.53
2:B:43:HIS:HA	2:B:43:HIS:HD1	1.72	0.53
2:B:74:LEU:C	2:B:75:LYS:CA	2.69	0.53
2:B:86:GLN:CG	2:B:86:GLN:HA	2.38	0.53
2:B:128:LEU:CB	2:B:128:LEU:H	2.16	0.53
1:C:60:GLN:NE2	1:C:64:ASN:ND2	2.57	0.53
1:C:70:GLN:N	1:C:70:GLN:HB2	2.19	0.53
1:C:76:LEU:O	1:C:80:LEU:N	2.34	0.53
2:D:7:LYS:O	2:D:7:LYS:CB	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:HIS:ND1	2:D:76:HIS:O	2.41	0.53
2:D:77:LEU:HD12	2:D:77:LEU:N	2.24	0.53
2:D:85:ALA:N	2:D:85:ALA:CB	2.72	0.53
2:B:30:LEU:HG	2:B:105:LEU:HD23	1.90	0.53
2:B:70:PHE:CD1	2:B:71:THR:N	2.77	0.53
1:A:73:LEU:HD21	1:A:128:PHE:HD2	1.73	0.53
2:B:13:PHE:C	2:B:13:PHE:N	2.65	0.53
2:B:86:GLN:CB	2:B:86:GLN:CD	2.75	0.53
1:C:19:GLY:C	1:C:19:GLY:N	2.55	0.53
1:C:23:ALA:C	1:C:23:ALA:HB1	2.29	0.53
1:C:43:PHE:HE2	1:C:58:HIS:CE1	2.27	0.53
1:C:107:VAL:HG23	2:D:114:ALA:HB3	1.91	0.53
2:D:55:ASN:CB	2:D:55:ASN:C	2.81	0.53
2:D:90:LEU:HB3	2:D:90:LEU:HD13	1.86	0.53
1:A:63:ALA:HA	1:A:66:LEU:HB2	1.89	0.53
1:A:74:ASN:CB	1:A:74:ASN:ND2	2.72	0.53
1:A:97:ASN:N	1:A:97:ASN:C	2.61	0.53
1:A:138:SER:CB	1:A:138:SER:HG	2.10	0.53
1:A:140:TYR:CG	1:A:140:TYR:CA	2.79	0.53
2:B:41:PHE:HB3	2:B:44:PHE:CD1	2.41	0.53
2:B:97:VAL:HG11	3:B:146:HEM:C2B	2.44	0.53
3:B:146:HEM:CMB	3:B:146:HEM:C3B	2.61	0.53
1:C:29:LEU:CB	1:C:29:LEU:CD2	2.79	0.53
2:B:34:TYR:N	2:B:34:TYR:CB	2.64	0.52
2:B:61:ALA:C	2:B:62:HIS:CA	2.76	0.52
2:B:95:LEU:HD11	3:B:146:HEM:HMA1	1.91	0.52
2:D:5:GLU:CD	2:D:5:GLU:CB	2.75	0.52
2:D:99:PRO:O	2:D:100:GLN:C	2.52	0.52
1:A:127:LYS:CE	1:A:127:LYS:CG	2.84	0.52
2:B:41:PHE:CD2	2:B:44:PHE:HZ	2.05	0.52
2:B:53:VAL:O	2:B:54:MET:HA	2.09	0.52
2:B:80:LEU:O	2:B:81:LYS:N	2.41	0.52
2:B:140:LEU:CD1	2:B:140:LEU:HB2	2.37	0.52
2:D:28:GLY:C	2:D:54:MET:CE	2.71	0.52
2:D:81:LYS:HD3	2:D:82:GLY:H	1.75	0.52
1:A:34:LEU:CB	1:A:34:LEU:HA	2.24	0.52
2:B:74:LEU:CD1	2:B:77:LEU:HG	2.38	0.52
1:C:65:ALA:O	1:C:68:LYS:HB2	2.10	0.52
2:D:77:LEU:CG	2:D:77:LEU:CA	2.79	0.52
1:A:122:HIS:C	1:A:122:HIS:N	2.57	0.52
2:B:7:LYS:C	2:B:7:LYS:CB	2.81	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:PHE:HD1	2:B:71:THR:N	2.07	0.52
2:B:124:ASN:O	2:B:125:VAL:CA	2.56	0.52
1:C:43:PHE:CB	1:C:43:PHE:CD1	2.85	0.52
1:C:45:HIS:N	1:C:45:HIS:CG	2.77	0.52
1:C:117:PHE:C	1:C:117:PHE:N	2.62	0.52
2:D:37:THR:O	2:D:40:PHE:HD1	1.93	0.52
2:D:94:LYS:CG	2:D:95:LEU:N	2.69	0.52
2:D:140:LEU:HB2	2:D:140:LEU:HD13	1.88	0.52
1:A:14:TRP:HD1	1:A:70:GLN:NE2	2.08	0.52
1:A:60:GLN:C	1:A:60:GLN:N	2.66	0.52
1:C:3:SER:HB2	1:C:5:ALA:H	1.73	0.52
1:C:89:HIS:ND1	1:C:89:HIS:O	2.42	0.52
2:D:79:ASP:CB	2:D:79:ASP:O	2.58	0.52
1:A:33:PHE:HB3	1:A:40:LYS:HE3	1.90	0.52
1:A:116:ASN:CA	1:A:116:ASN:H	2.05	0.52
2:B:59:VAL:CG2	2:B:60:LYS:N	2.72	0.52
1:C:111:SER:O	1:C:114:PRO:CG	2.57	0.52
1:A:2:LEU:O	1:A:7:LYS:HE2	2.09	0.52
1:A:80:LEU:CG	1:A:80:LEU:N	2.72	0.52
2:B:31:LEU:CD1	2:B:31:LEU:HD21	2.39	0.52
2:B:62:HIS:HE1	3:B:146:HEM:C1A	2.27	0.52
1:C:57:ALA:O	1:C:60:GLN:CB	2.58	0.52
1:C:86:LEU:HA	1:C:90:LYS:HB2	1.91	0.52
1:C:110:ALA:HB1	2:D:115:ARG:HB2	1.92	0.52
1:C:137:THR:O	1:C:139:LYS:N	2.42	0.52
2:D:59:VAL:HB	2:D:60:LYS:H	1.75	0.52
2:D:67:LEU:CA	2:D:67:LEU:HD23	2.39	0.52
2:D:79:ASP:CB	2:D:79:ASP:N	2.61	0.52
1:A:42:TYR:O	1:A:45:HIS:NE2	2.42	0.52
3:A:142:HEM:CMD	3:A:142:HEM:CHD	2.87	0.52
2:D:11:THR:CA	2:D:14:TRP:H	2.17	0.52
2:D:84:PHE:C	2:D:85:ALA:CA	2.81	0.52
2:D:99:PRO:O	2:D:102:PHE:N	2.38	0.52
1:A:83:LEU:O	1:A:84:SER:HA	2.10	0.52
1:A:100:LEU:CB	1:A:100:LEU:HD23	2.36	0.52
2:B:52:ALA:C	2:B:54:MET:N	2.61	0.52
2:B:87:LEU:O	2:B:88:SER:C	2.53	0.52
1:C:28:ALA:N	1:C:29:LEU:N	2.58	0.52
1:C:104:SER:C	1:C:104:SER:HB3	2.34	0.52
1:C:116:ASN:C	1:C:116:ASN:HA	2.17	0.52
2:D:37:THR:O	2:D:41:PHE:CE1	2.63	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:CD1	1:A:136:LEU:HB2	2.36	0.51
2:B:59:VAL:CG1	2:B:59:VAL:HA	2.39	0.51
2:D:103:ARG:HB2	2:D:103:ARG:HD3	1.92	0.51
1:A:32:MET:N	1:A:33:PHE:N	2.58	0.51
2:B:6:GLU:OE1	2:B:131:LYS:NZ	2.43	0.51
2:B:56:ASN:O	2:B:58:LYS:N	2.44	0.51
2:B:110:ALA:C	2:B:111:LEU:CA	2.74	0.51
1:C:29:LEU:CD2	1:C:29:LEU:HB2	2.41	0.51
1:C:95:PRO:HA	1:C:98:PHE:HD2	1.74	0.51
1:C:96:VAL:CG2	1:C:96:VAL:CA	2.87	0.51
2:B:6:GLU:OE1	2:B:131:LYS:HE2	2.10	0.51
3:B:146:HEM:CHA	3:B:146:HEM:HAD2	2.37	0.51
1:C:55:GLN:O	1:C:56:LYS:O	2.28	0.51
1:C:111:SER:C	1:C:111:SER:HA	2.18	0.51
2:D:101:ASN:N	2:D:102:PHE:H	2.05	0.51
2:D:141:ALA:CA	2:D:142:HIS:N	2.74	0.51
2:B:62:HIS:N	2:B:62:HIS:CB	2.64	0.51
2:B:86:GLN:CG	2:B:86:GLN:C	2.83	0.51
1:C:1:VAL:C	1:C:1:VAL:N	2.68	0.51
1:C:9:ASN:CB	1:C:9:ASN:OD1	2.50	0.51
2:D:3:THR:O	2:D:5:GLU:HA	2.10	0.51
2:D:86:GLN:CB	2:D:86:GLN:N	2.67	0.51
2:D:91:HIS:HD2	2:D:102:PHE:CE1	2.28	0.51
1:A:11:LYS:C	1:A:12:ALA:HA	2.34	0.51
1:A:32:MET:CE	1:A:32:MET:CG	2.87	0.51
1:A:70:GLN:C	1:A:73:LEU:CD1	2.81	0.51
1:A:72:HIS:HE1	1:A:79:THR:CB	2.23	0.51
1:A:87:HIS:HE1	3:A:142:HEM:C4A	2.27	0.51
1:A:115:THR:CB	1:A:115:THR:HG1	2.10	0.51
2:B:2:LEU:HD13	2:B:131:LYS:NZ	2.25	0.51
2:B:55:ASN:O	2:B:57:PRO:N	2.43	0.51
2:B:104:LEU:N	2:B:104:LEU:C	2.54	0.51
2:B:123:PRO:HA	2:B:126:GLN:CD	2.35	0.51
1:C:57:ALA:O	1:C:60:GLN:HB3	2.10	0.51
2:D:55:ASN:CG	2:D:55:ASN:CA	2.77	0.51
2:B:49:SER:C	2:B:49:SER:N	2.58	0.51
1:C:72:HIS:HE1	1:C:79:THR:OG1	1.92	0.51
1:C:138:SER:CA	1:C:138:SER:OG	2.59	0.51
3:C:142:HEM:HHD	3:C:142:HEM:CAC	2.40	0.51
2:D:141:ALA:C	2:D:142:HIS:HA	2.34	0.51
1:A:25:GLY:C	1:A:29:LEU:HD22	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:HB3	1:A:40:LYS:CD	2.41	0.51
1:A:97:ASN:HD22	1:A:100:LEU:HD11	1.76	0.51
2:B:7:LYS:HD2	2:B:77:LEU:HD12	1.91	0.51
2:B:58:LYS:C	2:B:59:VAL:CA	2.65	0.51
2:B:123:PRO:CB	2:B:126:GLN:HE22	2.22	0.51
1:C:111:SER:CA	1:C:112:HIS:N	2.74	0.51
1:A:10:VAL:C	1:A:10:VAL:CG1	2.84	0.51
1:A:131:ASN:N	1:A:131:ASN:HB2	2.26	0.51
2:B:30:LEU:HA	2:B:108:VAL:HG21	1.93	0.51
2:B:97:VAL:HG11	3:B:146:HEM:HMB2	1.93	0.51
2:B:117:PHE:O	2:B:118:GLY:CA	2.46	0.51
2:B:141:ALA:C	2:B:142:HIS:C	2.78	0.51
1:C:84:SER:OG	1:C:136:LEU:CD1	2.58	0.51
2:D:76:HIS:H	2:D:76:HIS:CD2	2.28	0.51
2:D:91:HIS:O	2:D:95:LEU:HG	2.10	0.51
1:A:14:TRP:HB3	1:A:70:GLN:NE2	2.26	0.51
3:A:142:HEM:CMA	3:A:142:HEM:HHB	2.41	0.51
2:B:14:TRP:HZ2	2:B:67:LEU:HG	1.76	0.51
2:B:84:PHE:CE2	3:B:146:HEM:CBC	2.94	0.51
1:C:55:GLN:O	1:C:56:LYS:NZ	2.44	0.51
1:A:100:LEU:HD12	1:A:100:LEU:HB2	1.88	0.51
2:B:19:VAL:C	2:B:19:VAL:CG1	2.83	0.51
2:B:106:GLY:C	2:B:133:VAL:HG21	2.36	0.51
1:C:10:VAL:CG2	1:C:10:VAL:HG11	2.36	0.51
1:C:89:HIS:HB2	1:C:139:LYS:CG	2.41	0.51
2:D:75:LYS:CB	2:D:76:HIS:N	2.59	0.51
1:A:89:HIS:ND1	1:A:90:LYS:N	2.58	0.50
1:C:45:HIS:CG	1:C:46:PHE:CE1	2.99	0.50
2:D:17:VAL:C	2:D:17:VAL:HG23	2.35	0.50
2:D:44:PHE:CB	2:D:44:PHE:H	2.24	0.50
1:A:1:VAL:HG22	1:A:1:VAL:HG13	1.90	0.50
1:A:4:ALA:O	1:A:8:SER:HB2	2.10	0.50
1:A:64:ASN:C	1:A:64:ASN:CB	2.77	0.50
2:B:6:GLU:CA	2:B:6:GLU:CG	2.72	0.50
2:B:36:TRP:CG	1:C:94:ASN:HA	2.46	0.50
2:B:41:PHE:HA	2:B:42:GLN:N	2.26	0.50
2:B:77:LEU:C	2:B:77:LEU:HB3	2.27	0.50
2:B:136:VAL:C	2:B:136:VAL:HG12	2.36	0.50
1:C:102:SER:C	1:C:103:HIS:C	2.79	0.50
2:D:25:GLN:HE22	2:D:116:ASN:CG	2.18	0.50
2:D:120:GLN:CG	2:D:120:GLN:HA	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ASN:OD1	2:B:98:ASN:HB2	2.09	0.50
1:C:68:LYS:HD3	1:C:79:THR:CG2	2.38	0.50
1:C:102:SER:C	1:C:103:HIS:HA	2.32	0.50
3:C:142:HEM:CHD	3:C:142:HEM:CAC	2.89	0.50
2:D:138:ASN:O	2:D:139:ALA:C	2.54	0.50
1:A:44:PRO:N	1:A:45:HIS:HD2	2.08	0.50
1:A:68:LYS:C	1:A:69:ALA:CA	2.59	0.50
1:A:72:HIS:CE1	1:A:79:THR:CB	2.94	0.50
2:B:36:TRP:HA	1:C:92:ARG:HB3	1.92	0.50
2:D:130:GLN:CA	2:D:130:GLN:NE2	2.75	0.50
1:A:56:LYS:NZ	1:A:56:LYS:CD	2.63	0.50
1:A:85:ASN:CB	1:A:85:ASN:ND2	2.74	0.50
1:C:56:LYS:HA	1:C:56:LYS:CD	2.41	0.50
1:C:61:LYS:HA	1:C:61:LYS:HD2	1.90	0.50
1:C:114:PRO:CA	1:C:114:PRO:CD	2.87	0.50
2:D:69:ALA:C	2:D:69:ALA:HB1	2.34	0.50
1:A:5:ALA:O	1:A:8:SER:C	2.54	0.50
1:A:12:ALA:CB	1:A:12:ALA:C	2.84	0.50
1:A:53:ALA:N	1:A:56:LYS:HG2	2.26	0.50
1:A:99:LYS:CD	1:A:99:LYS:CB	2.90	0.50
1:A:135:VAL:C	1:A:135:VAL:HB	2.35	0.50
2:B:17:VAL:CA	2:B:18:ASP:N	2.62	0.50
1:C:14:TRP:CG	1:C:70:GLN:NE2	2.79	0.50
1:C:58:HIS:O	1:C:59:GLY:C	2.55	0.50
1:C:74:ASN:H	1:C:75:ASP:N	2.10	0.50
1:C:89:HIS:CA	1:C:139:LYS:HG3	2.42	0.50
1:C:110:ALA:CA	1:C:110:ALA:O	2.58	0.50
2:D:93:ASN:HB3	2:D:93:ASN:O	2.09	0.50
2:D:141:ALA:O	2:D:143:LYS:CA	2.60	0.50
1:A:41:THR:CA	1:A:41:THR:HG22	2.35	0.50
2:B:80:LEU:CA	2:B:81:LYS:O	2.59	0.50
1:A:47:ASP:C	1:A:49:SER:N	2.56	0.50
1:A:67:THR:HG22	1:A:70:GLN:NE2	2.27	0.50
2:B:46:ASN:CG	2:B:46:ASN:HA	2.32	0.50
2:B:54:MET:HB3	2:B:55:ASN:CG	2.35	0.50
1:C:39:THR:CB	1:C:39:THR:H	2.22	0.50
1:C:94:ASN:ND2	1:C:97:ASN:OD1	2.45	0.50
2:D:56:ASN:C	2:D:57:PRO:CD	2.74	0.50
2:D:81:LYS:CE	2:D:81:LYS:CG	2.90	0.50
1:A:42:TYR:CA	1:A:43:PHE:N	2.65	0.50
1:A:49:SER:HB3	1:A:52:SER:HB3	1.83	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:VAL:O	1:A:121:VAL:HG23	2.12	0.50
2:B:1:MET:O	2:B:2:LEU:CD2	2.58	0.50
2:B:31:LEU:O	2:B:32:VAL:CA	2.59	0.50
2:B:49:SER:C	2:B:49:SER:CB	2.78	0.50
1:C:107:VAL:HG23	2:D:114:ALA:CB	2.42	0.50
2:D:30:LEU:C	2:D:31:LEU:C	2.80	0.50
2:D:106:GLY:HA3	2:D:133:VAL:CG1	2.42	0.50
1:A:4:ALA:N	1:A:4:ALA:CB	2.71	0.49
1:A:72:HIS:ND1	1:A:72:HIS:C	2.65	0.49
2:B:3:THR:C	2:B:5:GLU:N	2.65	0.49
2:B:3:THR:HB	2:B:6:GLU:CB	2.39	0.49
2:B:46:ASN:CB	2:B:46:ASN:O	2.60	0.49
2:B:115:ARG:CB	2:B:115:ARG:C	2.81	0.49
3:B:146:HEM:CAD	3:B:146:HEM:CHA	2.90	0.49
1:C:60:GLN:O	1:C:64:ASN:N	2.45	0.49
2:D:75:LYS:HB2	2:D:75:LYS:HG2	1.32	0.49
2:D:95:LEU:CD1	2:D:97:VAL:CG2	2.87	0.49
1:A:88:ALA:CB	1:A:89:HIS:HB2	2.42	0.49
1:A:126:ASN:HB3	1:A:127:LYS:N	2.26	0.49
2:B:62:HIS:CG	2:B:62:HIS:C	2.90	0.49
2:D:110:ALA:C	2:D:110:ALA:HB3	2.34	0.49
1:A:100:LEU:HB3	1:A:100:LEU:HD22	1.91	0.49
1:A:107:VAL:HG23	2:B:111:LEU:HD22	1.93	0.49
2:B:55:ASN:O	2:B:57:PRO:CD	2.61	0.49
2:B:94:LYS:CE	2:B:94:LYS:HG3	2.39	0.49
1:C:83:LEU:C	1:C:83:LEU:HG	2.37	0.49
1:C:123:ALA:HB3	1:C:124:ASN:HD22	1.77	0.49
2:D:42:GLN:CA	2:D:42:GLN:HG2	2.01	0.49
2:D:70:PHE:HB3	2:D:71:THR:CB	2.40	0.49
1:A:57:ALA:CA	1:A:60:GLN:CG	2.90	0.49
1:A:85:ASN:C	1:A:85:ASN:N	2.68	0.49
1:A:109:LEU:C	1:A:109:LEU:HB3	2.37	0.49
2:B:23:GLY:N	2:B:24:ALA:N	2.60	0.49
2:B:65:ARG:O	2:B:67:LEU:N	2.44	0.49
2:B:66:VAL:CG1	2:B:66:VAL:CA	2.76	0.49
2:D:25:GLN:HE22	2:D:115:ARG:NH2	2.00	0.49
2:D:28:GLY:O	2:D:54:MET:CE	2.60	0.49
2:D:54:MET:CG	2:D:54:MET:CE	2.90	0.49
2:D:70:PHE:CB	2:D:71:THR:HB	2.42	0.49
2:D:83:ALA:CA	2:D:84:PHE:N	2.70	0.49
1:A:44:PRO:CD	1:A:45:HIS:CD2	2.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:SER:O	1:C:107:VAL:HG13	2.13	0.49
2:D:71:THR:CG2	2:D:71:THR:OG1	2.61	0.49
1:A:27:GLN:HE22	1:A:31:ARG:HH11	1.60	0.49
2:B:81:LYS:CD	2:B:142:HIS:HB3	2.42	0.49
1:C:16:LYS:C	1:C:17:VAL:C	2.80	0.49
1:C:30:GLN:NE2	1:C:30:GLN:HB2	2.27	0.49
2:D:50:ALA:O	2:D:53:VAL:CG1	2.59	0.49
2:D:139:ALA:O	2:D:142:HIS:N	2.45	0.49
1:A:2:LEU:CG	1:A:2:LEU:HA	2.43	0.49
1:A:53:ALA:O	1:A:53:ALA:HA	2.12	0.49
1:A:56:LYS:CE	1:A:56:LYS:N	2.72	0.49
1:A:77:PRO:C	1:A:78:GLY:C	2.80	0.49
1:C:21:ALA:O	1:C:22:PRO:HA	2.09	0.49
1:C:29:LEU:CD1	1:C:59:GLY:HA2	2.42	0.49
1:C:85:ASN:HA	1:C:88:ALA:HB3	1.95	0.49
2:D:29:ARG:HG3	2:D:112:VAL:HG11	1.94	0.49
2:D:69:ALA:CB	2:D:70:PHE:N	2.70	0.49
1:A:43:PHE:HB3	1:A:46:PHE:CD1	2.47	0.49
1:A:43:PHE:HD2	1:A:46:PHE:CE1	2.30	0.49
1:A:103:HIS:CB	1:A:103:HIS:ND1	2.59	0.49
2:B:62:HIS:O	2:B:66:VAL:HG12	2.13	0.49
2:D:58:LYS:O	2:D:61:ALA:HB3	2.12	0.49
1:A:94:ASN:N	1:A:94:ASN:O	2.45	0.49
2:B:124:ASN:O	2:B:127:ALA:HB3	2.12	0.49
1:C:6:ASN:C	1:C:7:LYS:CA	2.82	0.49
1:C:16:LYS:CD	1:C:16:LYS:CB	2.89	0.49
1:C:45:HIS:ND1	3:C:142:HEM:CGD	2.75	0.49
1:C:113:LEU:O	1:C:117:PHE:N	2.46	0.49
2:D:53:VAL:CG2	2:D:54:MET:HE3	2.34	0.49
2:D:130:GLN:HA	2:D:130:GLN:NE2	2.28	0.49
2:B:74:LEU:O	2:B:75:LYS:HG2	2.13	0.49
2:B:115:ARG:CA	2:B:115:ARG:CG	2.90	0.49
1:C:45:HIS:CE1	1:C:46:PHE:CZ	3.00	0.49
1:C:65:ALA:HB1	1:C:83:LEU:CD2	2.43	0.49
2:D:10:VAL:HG11	2:D:128:LEU:HD11	1.95	0.49
2:D:14:TRP:CZ2	2:D:71:THR:CG2	2.96	0.49
2:D:93:ASN:C	2:D:93:ASN:N	2.55	0.49
1:A:16:LYS:HB2	1:A:113:LEU:HD21	1.95	0.48
1:A:32:MET:C	1:A:32:MET:N	2.64	0.48
1:A:70:GLN:NE2	1:A:70:GLN:OE1	2.46	0.48
1:A:91:LEU:N	1:A:91:LEU:C	2.66	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLY:O	2:B:24:ALA:CA	2.58	0.48
2:B:44:PHE:HD2	2:B:58:LYS:HG2	1.77	0.48
2:B:67:LEU:C	2:B:71:THR:HG21	2.24	0.48
2:B:144:TYR:HB3	2:B:145:HIS:NE2	2.23	0.48
1:C:140:TYR:CE1	1:C:141:ARG:NH2	2.81	0.48
1:A:32:MET:N	1:A:33:PHE:H	2.10	0.48
2:B:19:VAL:CG1	2:B:20:ASP:N	2.75	0.48
2:B:66:VAL:CG2	2:B:66:VAL:HG11	2.39	0.48
1:C:76:LEU:HB3	1:C:80:LEU:CD2	2.43	0.48
2:D:95:LEU:HD13	3:D:146:HEM:HMA2	1.94	0.48
2:D:131:LYS:C	2:D:132:VAL:HA	2.33	0.48
2:D:141:ALA:O	2:D:143:LYS:C	2.56	0.48
1:A:17:VAL:CG2	1:A:17:VAL:HG11	2.40	0.48
1:C:17:VAL:CG1	1:C:24:TYR:CD2	2.95	0.48
1:C:83:LEU:HB3	1:C:84:SER:HG	1.77	0.48
1:C:130:ALA:C	1:C:130:ALA:N	2.59	0.48
2:D:43:HIS:CE1	3:D:146:HEM:CGA	2.96	0.48
2:D:121:PHE:O	2:D:122:THR:O	2.32	0.48
2:B:27:LEU:CD2	2:B:66:VAL:CG1	2.92	0.48
2:B:43:HIS:N	2:B:44:PHE:N	2.61	0.48
2:B:44:PHE:CD2	2:B:58:LYS:HG2	2.49	0.48
1:C:17:VAL:HG13	1:C:24:TYR:CE2	2.48	0.48
1:A:16:LYS:N	1:A:17:VAL:N	2.53	0.48
1:A:91:LEU:CD2	3:A:142:HEM:C2D	2.95	0.48
1:A:106:LEU:HB3	2:B:111:LEU:HD11	1.94	0.48
2:B:2:LEU:CB	2:B:6:GLU:CD	2.86	0.48
2:B:11:THR:CB	2:B:11:THR:HG1	2.12	0.48
2:B:26:ALA:C	2:B:26:ALA:CB	2.66	0.48
2:B:26:ALA:HB2	2:B:112:VAL:CG2	2.43	0.48
2:B:84:PHE:O	2:B:85:ALA:C	2.57	0.48
2:B:97:VAL:HG11	3:B:146:HEM:HAB	1.95	0.48
1:C:109:LEU:O	1:C:112:HIS:N	2.44	0.48
2:D:59:VAL:CA	2:D:59:VAL:HG23	2.29	0.48
1:A:84:SER:OG	1:A:136:LEU:HA	2.13	0.48
2:B:92:CYS:CB	2:B:144:TYR:CZ	2.96	0.48
2:B:92:CYS:N	2:B:144:TYR:OH	2.45	0.48
1:C:7:LYS:HE2	1:C:7:LYS:HB2	1.95	0.48
1:C:11:LYS:HD3	1:C:70:GLN:OE1	2.14	0.48
1:C:12:ALA:O	1:C:16:LYS:HB2	2.14	0.48
1:C:84:SER:C	1:C:84:SER:N	2.66	0.48
1:C:99:LYS:HE3	1:C:99:LYS:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:HIS:ND1	2:D:62:HIS:CB	2.67	0.48
2:D:75:LYS:O	2:D:77:LEU:CD1	2.60	0.48
2:D:95:LEU:CB	2:D:95:LEU:CD1	2.91	0.48
2:D:104:LEU:CG	2:D:104:LEU:HA	2.43	0.48
2:D:127:ALA:C	2:D:127:ALA:HB3	2.34	0.48
2:B:107:ASN:ND2	2:B:107:ASN:HB2	2.23	0.48
1:C:22:PRO:O	1:C:56:LYS:HE3	2.11	0.48
1:C:130:ALA:O	1:C:131:ASN:N	2.36	0.48
2:D:11:THR:OG1	2:D:11:THR:CG2	2.56	0.48
2:D:57:PRO:O	2:D:58:LYS:C	2.54	0.48
2:D:94:LYS:CD	2:D:95:LEU:CD2	2.87	0.48
2:D:119:GLY:N	2:D:120:GLN:N	2.62	0.48
1:A:43:PHE:O	1:A:48:LEU:HD21	2.14	0.48
1:A:72:HIS:CE1	1:A:79:THR:CG2	2.96	0.48
1:A:98:PHE:HE2	1:A:137:THR:HG1	1.58	0.48
1:A:114:PRO:HB3	2:B:115:ARG:HG2	1.96	0.48
2:B:62:HIS:CD2	2:B:62:HIS:C	2.92	0.48
2:B:74:LEU:HD12	2:B:75:LYS:O	2.14	0.48
2:B:92:CYS:O	2:B:96:HIS:ND1	2.33	0.48
1:C:45:HIS:N	1:C:45:HIS:CD2	2.82	0.48
1:C:46:PHE:CE2	1:C:54:GLN:HB3	2.49	0.48
2:D:14:TRP:CE3	2:D:14:TRP:CA	2.93	0.48
2:D:55:ASN:O	2:D:55:ASN:ND2	2.45	0.48
1:A:57:ALA:H	1:A:57:ALA:HB3	1.74	0.48
1:A:84:SER:N	1:A:84:SER:HA	2.12	0.48
1:A:86:LEU:CA	1:A:87:HIS:N	2.62	0.48
1:C:36:PHE:CB	1:C:36:PHE:N	2.69	0.48
2:D:74:LEU:HD12	2:D:132:VAL:HG21	1.95	0.48
1:A:19:GLY:CA	1:A:20:ASN:N	2.68	0.48
2:B:50:ALA:O	2:B:51:GLY:C	2.56	0.48
2:D:43:HIS:CA	2:D:43:HIS:HB2	2.23	0.48
2:D:72:GLN:C	2:D:73:GLY:C	2.82	0.48
2:D:92:CYS:CA	2:D:92:CYS:O	2.42	0.48
1:A:40:LYS:CB	1:A:40:LYS:CD	2.88	0.47
1:C:45:HIS:CE1	3:C:142:HEM:O2D	2.67	0.47
1:C:47:ASP:O	1:C:52:SER:OG	2.31	0.47
2:D:36:TRP:N	2:D:37:THR:N	2.62	0.47
2:D:96:HIS:C	2:D:96:HIS:N	2.72	0.47
2:D:101:ASN:N	2:D:102:PHE:N	2.62	0.47
2:D:104:LEU:HA	2:D:104:LEU:CD2	2.43	0.47
2:D:106:GLY:HA3	2:D:133:VAL:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:CE2	3:A:142:HEM:HMD1	2.48	0.47
1:A:69:ALA:N	1:A:70:GLN:N	2.62	0.47
2:B:66:VAL:CG1	2:B:66:VAL:HG21	2.39	0.47
1:C:135:VAL:O	1:C:136:LEU:N	2.44	0.47
2:D:84:PHE:O	2:D:88:SER:N	2.44	0.47
1:A:21:ALA:HB1	1:A:63:ALA:HB1	1.95	0.47
1:A:39:THR:C	1:A:40:LYS:HZ3	2.20	0.47
2:B:1:MET:N	2:B:2:LEU:HD21	2.23	0.47
2:B:33:VAL:H	2:B:35:PRO:HD3	1.79	0.47
1:C:85:ASN:OD1	1:C:89:HIS:CB	2.62	0.47
1:A:79:THR:HA	1:A:79:THR:HG23	1.93	0.47
2:B:93:ASN:O	2:B:96:HIS:HE1	1.93	0.47
2:B:130:GLN:HE21	2:B:130:GLN:HG2	1.75	0.47
1:C:137:THR:CA	1:C:137:THR:O	2.59	0.47
2:D:19:VAL:O	2:D:20:ASP:C	2.54	0.47
2:D:27:LEU:HD12	2:D:63:GLY:CA	2.45	0.47
2:D:61:ALA:O	2:D:64:LYS:HB3	2.14	0.47
2:B:91:HIS:HA	2:B:95:LEU:CD2	2.41	0.47
2:D:31:LEU:CB	2:D:31:LEU:N	2.66	0.47
2:D:141:ALA:C	2:D:141:ALA:N	2.66	0.47
2:B:46:ASN:HA	2:B:46:ASN:ND2	2.30	0.47
2:B:54:MET:O	2:B:59:VAL:HG23	2.15	0.47
2:B:118:GLY:HA2	2:B:118:GLY:H	1.26	0.47
1:C:19:GLY:CA	1:C:20:ASN:N	2.56	0.47
1:C:113:LEU:O	1:C:116:ASN:HB3	2.15	0.47
2:D:6:GLU:CB	2:D:6:GLU:N	2.66	0.47
1:A:32:MET:CE	1:A:32:MET:HG2	2.44	0.47
1:A:46:PHE:HA	1:A:54:GLN:OE1	2.14	0.47
1:A:141:ARG:OXT	1:C:1:VAL:O	2.32	0.47
2:B:31:LEU:HB3	2:B:53:VAL:CG2	2.44	0.47
2:B:73:GLY:C	2:B:74:LEU:O	2.58	0.47
2:B:95:LEU:CG	2:B:95:LEU:HA	2.24	0.47
1:C:46:PHE:CE2	1:C:54:GLN:CG	2.98	0.47
1:C:80:LEU:O	1:C:81:SER:CA	2.62	0.47
1:C:110:ALA:O	1:C:114:PRO:CB	2.59	0.47
1:C:141:ARG:O	1:C:141:ARG:N	2.48	0.47
2:D:7:LYS:NZ	2:D:78:ASP:OD2	2.44	0.47
2:D:30:LEU:CG	2:D:37:THR:HG21	2.44	0.47
2:D:47:LEU:CB	2:D:47:LEU:N	2.68	0.47
2:D:67:LEU:O	2:D:68:ASP:C	2.57	0.47
2:D:70:PHE:N	2:D:71:THR:HB	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:105:LEU:CD2	2:D:105:LEU:HD11	2.29	0.47
1:A:42:TYR:HB2	1:A:43:PHE:CD1	2.50	0.47
2:B:77:LEU:N	2:B:78:ASP:CB	2.78	0.47
2:D:19:VAL:CG2	2:D:19:VAL:HG13	2.44	0.47
1:A:60:GLN:N	1:A:61:LYS:N	2.62	0.47
2:B:7:LYS:NZ	2:B:7:LYS:CD	2.78	0.47
2:B:32:VAL:HG11	2:B:50:ALA:CB	2.45	0.47
2:B:59:VAL:O	2:B:62:HIS:CB	2.60	0.47
2:B:87:LEU:O	2:B:89:GLY:N	2.48	0.47
1:C:22:PRO:N	1:C:22:PRO:C	2.61	0.47
1:C:86:LEU:CD1	1:C:86:LEU:HD22	2.39	0.47
2:D:84:PHE:HD2	2:D:87:LEU:CD2	2.28	0.47
1:A:86:LEU:CD1	1:A:91:LEU:HD22	2.45	0.47
2:B:14:TRP:CZ2	2:B:67:LEU:HG	2.49	0.47
2:B:86:GLN:C	2:B:87:LEU:C	2.82	0.47
2:B:106:GLY:HA3	2:B:133:VAL:CG2	2.28	0.47
2:B:133:VAL:O	2:B:134:ALA:CA	2.60	0.47
1:C:11:LYS:HD2	1:C:70:GLN:NE2	2.30	0.47
1:C:29:LEU:HD13	1:C:29:LEU:HD22	1.91	0.47
2:D:90:LEU:HD13	2:D:91:HIS:ND1	2.30	0.47
2:D:101:ASN:O	2:D:104:LEU:CB	2.63	0.47
1:A:26:ALA:CB	1:A:56:LYS:NZ	2.66	0.46
2:B:8:ALA:CB	2:B:8:ALA:H	2.29	0.46
2:B:21:VAL:HG12	2:B:25:GLN:HE21	1.79	0.46
2:B:78:ASP:O	2:B:80:LEU:O	2.31	0.46
2:B:92:CYS:N	2:B:144:TYR:CZ	2.83	0.46
1:C:26:ALA:N	1:C:56:LYS:CE	2.67	0.46
1:A:85:ASN:O	1:A:87:HIS:N	2.48	0.46
2:B:16:LYS:CD	2:B:117:PHE:CE1	2.85	0.46
2:B:70:PHE:CZ	2:B:109:LEU:HD11	2.49	0.46
1:C:10:VAL:HG11	1:C:128:PHE:CG	2.50	0.46
2:D:81:LYS:O	2:D:85:ALA:HB2	2.15	0.46
2:D:105:LEU:CD1	2:D:105:LEU:HB3	2.25	0.46
1:A:114:PRO:CG	2:B:115:ARG:HG3	2.46	0.46
2:D:94:LYS:CG	2:D:95:LEU:CD2	2.82	0.46
1:A:41:THR:CB	1:A:41:THR:H	2.23	0.46
1:A:42:TYR:C	1:A:44:PRO:CD	2.88	0.46
2:B:94:LYS:H	2:B:95:LEU:H	1.59	0.46
1:C:75:ASP:CA	1:C:76:LEU:N	2.74	0.46
2:D:16:LYS:CB	2:D:16:LYS:C	2.77	0.46
2:D:27:LEU:HD12	2:D:62:HIS:C	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TRP:C	1:A:17:VAL:HG23	2.40	0.46
1:A:33:PHE:CB	1:A:40:LYS:HE3	2.45	0.46
2:B:16:LYS:O	2:B:117:PHE:CZ	2.68	0.46
3:B:146:HEM:C3D	3:B:146:HEM:HBD2	2.48	0.46
1:A:77:PRO:CA	1:A:77:PRO:O	2.60	0.46
1:A:94:ASN:HD21	1:A:96:VAL:HG22	1.81	0.46
1:A:126:ASN:CB	1:A:127:LYS:N	2.66	0.46
1:A:139:LYS:O	1:A:140:TYR:C	2.58	0.46
2:B:74:LEU:HD22	2:B:77:LEU:HG	1.94	0.46
1:C:83:LEU:CB	1:C:83:LEU:N	2.67	0.46
1:A:141:ARG:C	1:A:141:ARG:HA	2.22	0.46
2:B:98:ASN:HA	2:B:99:PRO:HD2	1.44	0.46
2:B:102:PHE:CD1	2:B:140:LEU:CD1	2.99	0.46
2:B:141:ALA:O	2:B:144:TYR:HB2	2.16	0.46
2:B:21:VAL:C	2:B:21:VAL:CG1	2.70	0.46
1:C:10:VAL:HG11	1:C:128:PHE:CD1	2.50	0.46
1:C:11:LYS:O	1:C:12:ALA:C	2.55	0.46
1:A:14:TRP:CE3	1:A:14:TRP:HA	2.51	0.46
1:A:27:GLN:O	1:A:31:ARG:HB2	2.16	0.46
2:B:3:THR:CA	2:B:6:GLU:HB2	2.45	0.46
2:B:67:LEU:O	2:B:69:ALA:HB3	2.14	0.46
1:C:130:ALA:O	1:C:130:ALA:HA	2.14	0.46
1:A:3:SER:HB2	1:A:6:ASN:HD22	1.75	0.46
1:A:104:SER:CB	1:A:104:SER:HA	2.21	0.46
2:B:39:ARG:NE	1:C:92:ARG:O	2.49	0.46
2:B:109:LEU:C	2:B:110:ALA:HA	2.33	0.46
1:C:54:GLN:CA	1:C:54:GLN:HG3	2.43	0.46
2:D:19:VAL:HG12	2:D:64:LYS:HA	1.97	0.46
1:A:11:LYS:O	1:A:12:ALA:CA	2.63	0.45
2:B:27:LEU:HD23	2:B:66:VAL:HG11	1.94	0.45
2:B:68:ASP:C	2:B:71:THR:HG22	2.33	0.45
1:C:106:LEU:HD23	2:D:111:LEU:HD21	1.97	0.45
1:A:36:PHE:CZ	2:B:130:GLN:CG	2.99	0.45
1:A:64:ASN:C	1:A:64:ASN:N	2.66	0.45
1:A:73:LEU:C	1:A:74:ASN:HD22	2.24	0.45
1:A:76:LEU:C	1:A:77:PRO:C	2.84	0.45
2:B:66:VAL:CG2	2:B:66:VAL:O	2.64	0.45
1:C:85:ASN:O	1:C:85:ASN:OD1	2.34	0.45
1:C:130:ALA:C	1:C:133:SER:HB2	2.42	0.45
2:D:94:LYS:HD3	2:D:95:LEU:N	2.26	0.45
2:D:97:VAL:O	2:D:144:TYR:OH	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:GLN:O	2:D:127:ALA:O	2.34	0.45
2:D:132:VAL:N	2:D:133:VAL:N	2.64	0.45
3:D:146:HEM:HMA2	3:D:146:HEM:HHB	1.79	0.45
1:C:93:VAL:HG11	3:C:142:HEM:C2C	2.51	0.45
2:D:145:HIS:O	2:D:145:HIS:OXT	2.28	0.45
1:A:49:SER:CB	1:A:52:SER:CB	2.61	0.45
1:A:79:THR:CB	1:A:80:LEU:CD2	2.63	0.45
2:B:24:ALA:N	2:B:25:GLN:N	2.64	0.45
1:C:84:SER:CA	1:C:136:LEU:HD13	2.46	0.45
1:A:98:PHE:CZ	1:A:136:LEU:HB2	2.52	0.45
2:B:46:ASN:CA	2:B:46:ASN:ND2	2.77	0.45
2:B:126:GLN:CD	2:B:126:GLN:HB3	2.42	0.45
1:C:56:LYS:NZ	1:C:56:LYS:O	2.48	0.45
2:D:69:ALA:CA	2:D:69:ALA:O	2.49	0.45
2:D:75:LYS:HB3	2:D:75:LYS:HG3	1.34	0.45
1:A:127:LYS:HB3	1:A:128:PHE:N	2.32	0.45
2:B:16:LYS:CE	2:B:16:LYS:HG3	2.47	0.45
1:C:22:PRO:C	1:C:56:LYS:HD3	2.42	0.45
1:C:26:ALA:HA	1:C:56:LYS:NZ	2.31	0.45
2:D:22:VAL:CG1	2:D:22:VAL:CA	2.71	0.45
2:D:112:VAL:CG1	2:D:112:VAL:CG2	2.75	0.45
1:A:95:PRO:HB3	1:A:137:THR:CG2	2.46	0.45
2:B:29:ARG:HB3	2:B:108:VAL:CG1	2.46	0.45
2:B:62:HIS:C	2:B:66:VAL:HG12	2.41	0.45
1:C:17:VAL:CG1	1:C:24:TYR:HD2	2.30	0.45
2:D:2:LEU:CD2	2:D:4:ALA:CA	2.78	0.45
2:D:14:TRP:O	2:D:14:TRP:N	2.43	0.45
1:A:106:LEU:CD2	1:A:126:ASN:HD22	2.30	0.45
2:B:74:LEU:O	2:B:76:HIS:HB2	2.17	0.45
2:B:104:LEU:O	2:B:108:VAL:N	2.50	0.45
2:D:100:GLN:C	2:D:102:PHE:H	2.25	0.45
2:D:122:THR:N	2:D:125:VAL:HG12	2.29	0.45
2:D:122:THR:OG1	2:D:125:VAL:N	2.47	0.45
1:A:16:LYS:HD2	1:A:116:ASN:HB3	1.99	0.45
2:B:11:THR:O	2:B:12:GLY:CA	2.64	0.45
2:B:47:LEU:HB3	2:B:53:VAL:HG23	1.99	0.45
1:C:74:ASN:N	1:C:75:ASP:N	2.65	0.45
2:D:94:LYS:HD3	2:D:95:LEU:CA	2.47	0.45
1:A:33:PHE:CG	1:A:48:LEU:HD13	2.52	0.45
1:A:116:ASN:N	1:A:117:PHE:N	2.64	0.45
2:B:94:LYS:NZ	2:B:94:LYS:HE2	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:LEU:HD22	2:B:109:LEU:CA	2.46	0.45
2:D:4:ALA:CA	2:D:5:GLU:HA	2.45	0.45
2:D:36:TRP:O	2:D:37:THR:C	2.59	0.45
2:D:74:LEU:HD13	2:D:132:VAL:HG21	1.97	0.45
2:D:110:ALA:CB	2:D:126:GLN:OE1	2.65	0.45
2:D:140:LEU:CD2	2:D:140:LEU:HD11	2.38	0.45
1:A:105:LEU:C	1:A:108:THR:HG22	2.41	0.44
1:C:38:THR:CG2	1:C:38:THR:OG1	2.63	0.44
1:C:61:LYS:CD	1:C:61:LYS:CA	2.92	0.44
2:D:6:GLU:CB	2:D:6:GLU:HA	2.22	0.44
2:D:94:LYS:HD3	2:D:95:LEU:HA	1.99	0.44
2:B:43:HIS:CA	2:B:43:HIS:ND1	2.76	0.44
2:B:84:PHE:CD2	2:B:84:PHE:CA	3.00	0.44
2:B:122:THR:O	2:B:126:GLN:HB3	2.18	0.44
1:C:27:GLN:OE1	1:C:112:HIS:HE1	2.00	0.44
2:D:10:VAL:C	2:D:11:THR:HG22	2.43	0.44
2:D:14:TRP:CD1	2:D:74:LEU:CD2	2.98	0.44
2:D:131:LYS:HG3	2:D:131:LYS:HA	1.96	0.44
1:A:85:ASN:CA	1:A:139:LYS:HE3	2.47	0.44
2:B:12:GLY:O	2:B:13:PHE:C	2.60	0.44
2:B:104:LEU:N	2:B:104:LEU:CB	2.76	0.44
2:B:128:LEU:C	2:B:128:LEU:HD22	2.42	0.44
1:C:20:ASN:O	1:C:22:PRO:N	2.51	0.44
2:D:33:VAL:O	2:D:33:VAL:CG2	2.62	0.44
2:B:33:VAL:HG12	2:B:34:TYR:CD1	2.51	0.44
1:C:52:SER:CB	1:C:55:GLN:NE2	2.61	0.44
1:A:132:ASP:O	1:A:136:LEU:CD2	2.65	0.44
1:C:39:THR:HB	1:C:39:THR:H	1.80	0.44
1:C:45:HIS:CA	1:C:45:HIS:CG	2.83	0.44
1:C:73:LEU:O	1:C:74:ASN:CA	2.65	0.44
1:C:87:HIS:ND1	1:C:87:HIS:HB2	2.27	0.44
1:C:89:HIS:ND1	1:C:90:LYS:HG2	2.27	0.44
3:D:146:HEM:CHA	3:D:146:HEM:HAA2	2.46	0.44
1:A:122:HIS:NE2	2:B:29:ARG:HG2	2.33	0.44
1:A:128:PHE:O	1:A:131:ASN:N	2.50	0.44
3:A:142:HEM:CMD	3:A:142:HEM:HHD	2.43	0.44
2:B:71:THR:HG23	2:B:71:THR:O	2.17	0.44
1:C:32:MET:HG3	1:C:39:THR:HG21	1.98	0.44
1:C:46:PHE:HB3	1:C:47:ASP:O	2.18	0.44
2:D:130:GLN:HE21	2:D:130:GLN:C	2.26	0.44
2:D:137:ALA:HA	2:D:140:LEU:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:CG2	1:A:80:LEU:HD23	2.39	0.44
2:B:55:ASN:C	2:B:56:ASN:CA	2.82	0.44
2:D:28:GLY:CA	2:D:54:MET:CE	2.73	0.44
2:D:137:ALA:CB	2:D:140:LEU:HD12	2.48	0.44
1:A:95:PRO:C	1:A:97:ASN:N	2.75	0.44
2:B:62:HIS:CE1	3:B:146:HEM:C1A	3.06	0.44
2:B:97:VAL:CG2	2:B:97:VAL:CG1	2.90	0.44
1:C:15:GLY:N	1:C:16:LYS:H	2.16	0.44
2:D:32:VAL:CG1	2:D:50:ALA:HA	2.44	0.44
1:A:7:LYS:C	1:A:7:LYS:CB	2.85	0.44
2:B:11:THR:CG2	2:B:11:THR:OG1	2.65	0.44
2:B:20:ASP:HB3	2:B:64:LYS:HE2	1.94	0.44
2:B:70:PHE:HA	2:B:84:PHE:CZ	2.52	0.44
1:C:69:ALA:N	1:C:70:GLN:N	2.64	0.44
2:D:10:VAL:CG2	2:D:11:THR:HG22	2.48	0.44
2:D:31:LEU:CD1	2:D:41:PHE:CE1	2.96	0.44
2:D:56:ASN:HD22	2:D:57:PRO:HG2	1.83	0.44
1:A:35:SER:HB3	2:B:126:GLN:OE1	2.17	0.43
1:A:45:HIS:CB	1:A:45:HIS:O	2.66	0.43
2:B:64:LYS:CE	2:B:64:LYS:HA	2.49	0.43
1:C:42:TYR:HB3	1:C:43:PHE:CD1	2.53	0.43
2:D:14:TRP:HZ2	2:D:71:THR:CG2	2.30	0.43
2:D:79:ASP:HA	2:D:81:LYS:HD2	1.99	0.43
2:D:92:CYS:C	2:D:92:CYS:SG	3.00	0.43
1:A:57:ALA:C	1:A:61:LYS:HD3	2.42	0.43
1:A:87:HIS:CD2	3:A:142:HEM:NC	2.86	0.43
2:B:26:ALA:HB2	2:B:112:VAL:HG21	2.01	0.43
1:C:45:HIS:ND1	3:C:142:HEM:O2D	2.51	0.43
1:C:80:LEU:CD1	1:C:80:LEU:HB2	2.46	0.43
1:C:102:SER:O	1:C:103:HIS:C	2.61	0.43
2:D:55:ASN:O	2:D:60:LYS:HD2	2.15	0.43
1:A:45:HIS:ND1	1:A:46:PHE:CE2	2.81	0.43
2:B:3:THR:CG2	2:B:5:GLU:CA	2.63	0.43
2:B:39:ARG:HD3	1:C:92:ARG:O	2.18	0.43
2:B:81:LYS:NZ	2:B:142:HIS:NE2	2.65	0.43
2:B:128:LEU:CD2	2:B:128:LEU:C	2.91	0.43
1:C:44:PRO:CB	1:C:44:PRO:HD3	2.40	0.43
1:C:60:GLN:CG	1:C:60:GLN:HA	2.43	0.43
1:C:81:SER:O	1:C:82:ASN:C	2.57	0.43
1:C:105:LEU:CD1	1:C:105:LEU:CD2	2.90	0.43
1:C:110:ALA:C	1:C:111:SER:C	2.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:SER:C	1:C:140:TYR:N	2.73	0.43
2:D:122:THR:HA	2:D:123:PRO:CD	2.47	0.43
1:A:1:VAL:CG2	1:A:1:VAL:HG13	2.36	0.43
1:A:73:LEU:HD21	1:A:128:PHE:CD2	2.52	0.43
1:A:137:THR:CG2	1:A:137:THR:HG1	2.23	0.43
3:C:142:HEM:HBB2	3:C:142:HEM:CMB	2.48	0.43
2:D:55:ASN:ND2	2:D:57:PRO:CD	2.81	0.43
2:D:75:LYS:CD	2:D:75:LYS:NZ	2.81	0.43
2:D:100:GLN:C	2:D:100:GLN:HG3	2.43	0.43
1:A:79:THR:C	1:A:80:LEU:CD2	2.91	0.43
2:B:32:VAL:CG1	2:B:32:VAL:O	2.64	0.43
2:B:66:VAL:HG11	2:B:66:VAL:HG21	1.99	0.43
2:B:109:LEU:CB	2:B:109:LEU:HD13	2.40	0.43
1:C:17:VAL:CG2	1:C:17:VAL:HA	2.44	0.43
1:C:36:PHE:CZ	2:D:130:GLN:OE1	2.72	0.43
2:D:18:ASP:O	2:D:19:VAL:O	2.31	0.43
2:B:53:VAL:CG1	2:B:54:MET:N	2.82	0.43
1:C:49:SER:CA	1:C:55:GLN:HE22	2.29	0.43
1:C:122:HIS:HD2	2:D:29:ARG:HD3	1.83	0.43
2:D:30:LEU:O	2:D:37:THR:CG2	2.66	0.43
1:A:105:LEU:O	1:A:108:THR:HG22	2.19	0.43
2:B:1:MET:SD	2:B:1:MET:CB	3.01	0.43
2:B:2:LEU:CD1	2:B:6:GLU:CG	2.90	0.43
2:B:84:PHE:CZ	3:B:146:HEM:HBC1	2.54	0.43
2:B:92:CYS:CA	2:B:144:TYR:CZ	3.02	0.43
1:C:32:MET:HE1	1:C:101:LEU:HG	2.00	0.43
1:C:74:ASN:O	1:C:75:ASP:N	2.28	0.43
1:C:94:ASN:N	1:C:94:ASN:HD22	2.16	0.43
1:C:94:ASN:ND2	1:C:94:ASN:O	2.40	0.43
1:C:140:TYR:CG	1:C:140:TYR:N	2.85	0.43
1:A:135:VAL:CG2	1:A:135:VAL:HG13	2.45	0.43
2:B:28:GLY:O	2:B:31:LEU:HB2	2.18	0.43
2:B:41:PHE:C	2:B:41:PHE:CB	2.85	0.43
1:C:10:VAL:CG1	1:C:128:PHE:CD1	3.02	0.43
1:C:39:THR:CA	1:C:39:THR:OG1	2.54	0.43
1:C:46:PHE:HA	1:C:54:GLN:OE1	2.19	0.43
1:C:70:GLN:CA	1:C:72:HIS:H	2.31	0.43
2:D:95:LEU:CD1	3:D:146:HEM:C4A	3.02	0.43
2:D:124:ASN:HA	2:D:124:ASN:ND2	2.34	0.43
2:D:130:GLN:CA	2:D:130:GLN:CD	2.91	0.43
1:A:14:TRP:CD1	1:A:70:GLN:NE2	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:VAL:C	2:B:22:VAL:C	2.87	0.43
2:B:133:VAL:O	2:B:134:ALA:C	2.61	0.43
2:D:25:GLN:NE2	2:D:116:ASN:OD1	2.52	0.43
1:A:70:GLN:HA	1:A:73:LEU:HD11	2.01	0.43
2:B:3:THR:O	2:B:4:ALA:HA	2.17	0.43
2:B:7:LYS:CA	2:B:8:ALA:H	2.27	0.43
2:B:49:SER:O	2:B:49:SER:N	2.52	0.43
2:B:101:ASN:HD22	2:B:101:ASN:HA	1.67	0.43
2:B:106:GLY:HA2	2:B:133:VAL:HG21	1.95	0.43
3:D:146:HEM:CHA	3:D:146:HEM:NA	2.70	0.43
1:A:2:LEU:CG	1:A:73:LEU:HD23	2.32	0.42
2:B:5:GLU:CB	2:B:5:GLU:H	2.28	0.42
2:B:84:PHE:CD2	2:B:84:PHE:HA	2.54	0.42
2:D:77:LEU:CG	2:D:77:LEU:N	2.81	0.42
2:D:109:LEU:HD13	2:D:113:VAL:CG2	2.49	0.42
1:A:2:LEU:CD2	1:A:2:LEU:HD11	2.44	0.42
2:B:1:MET:HE3	2:B:78:ASP:OD2	2.17	0.42
2:B:97:VAL:HG13	3:B:146:HEM:CMB	2.49	0.42
1:C:46:PHE:HD2	1:C:54:GLN:CG	2.32	0.42
1:C:83:LEU:CA	1:C:83:LEU:HG	2.47	0.42
1:C:97:ASN:C	1:C:97:ASN:HB3	2.40	0.42
2:D:11:THR:C	2:D:11:THR:N	2.75	0.42
1:A:26:ALA:O	1:A:30:GLN:HB2	2.20	0.42
2:B:34:TYR:N	2:B:35:PRO:HD3	2.29	0.42
2:B:43:HIS:CD2	2:B:43:HIS:CE1	3.04	0.42
1:C:44:PRO:N	1:C:44:PRO:C	2.72	0.42
1:C:60:GLN:HG2	1:C:60:GLN:HA	2.00	0.42
2:D:19:VAL:N	2:D:19:VAL:HG23	2.33	0.42
2:D:50:ALA:C	2:D:50:ALA:CB	2.78	0.42
2:D:134:ALA:O	2:D:135:GLY:C	2.56	0.42
1:A:6:ASN:HD21	1:A:127:LYS:NZ	2.17	0.42
2:B:2:LEU:HB3	2:B:131:LYS:HZ3	1.75	0.42
2:B:26:ALA:N	2:B:27:LEU:N	2.67	0.42
2:B:62:HIS:CE1	3:B:146:HEM:C4D	3.08	0.42
1:C:117:PHE:O	1:C:117:PHE:HD2	2.00	0.42
2:D:100:GLN:C	2:D:102:PHE:N	2.76	0.42
1:A:53:ALA:HA	1:A:56:LYS:CG	2.49	0.42
1:A:86:LEU:HD21	3:A:142:HEM:HBA2	2.01	0.42
2:B:30:LEU:HD21	2:B:105:LEU:HB2	2.00	0.42
2:B:43:HIS:C	2:B:43:HIS:CG	2.97	0.42
2:B:55:ASN:C	2:B:56:ASN:C	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LEU:O	2:B:75:LYS:C	2.62	0.42
2:B:109:LEU:HD23	2:B:109:LEU:HA	2.01	0.42
1:C:68:LYS:CB	1:C:68:LYS:HD3	2.49	0.42
1:C:70:GLN:CB	1:C:71:GLY:N	2.78	0.42
1:C:86:LEU:CD2	1:C:86:LEU:HD11	2.40	0.42
1:C:131:ASN:CB	1:C:131:ASN:H	2.28	0.42
2:D:65:ARG:NH1	2:D:65:ARG:NH2	2.57	0.42
2:D:70:PHE:O	2:D:84:PHE:CZ	2.72	0.42
1:A:100:LEU:CB	1:A:100:LEU:HD22	2.36	0.42
2:B:105:LEU:HB2	3:B:146:HEM:HBB2	2.00	0.42
1:C:32:MET:HG2	1:C:39:THR:CG2	2.49	0.42
1:C:140:TYR:CB	1:C:140:TYR:CD1	2.63	0.42
2:D:67:LEU:C	2:D:67:LEU:N	2.73	0.42
2:D:81:LYS:HD3	2:D:82:GLY:N	2.34	0.42
3:D:146:HEM:CGD	3:D:146:HEM:CAD	2.90	0.42
1:A:10:VAL:CA	1:A:11:LYS:N	2.54	0.42
2:B:1:MET:CB	2:B:77:LEU:HD11	2.45	0.42
2:B:22:VAL:CG2	2:B:113:VAL:HG13	2.50	0.42
2:B:64:LYS:CE	2:B:64:LYS:CB	2.97	0.42
2:B:74:LEU:HD21	2:B:77:LEU:HG	2.02	0.42
2:B:91:HIS:HE1	3:B:146:HEM:ND	2.18	0.42
1:C:6:ASN:CG	1:C:124:ASN:HB3	2.45	0.42
1:C:33:PHE:O	1:C:37:PRO:HG3	2.19	0.42
1:C:72:HIS:C	1:C:74:ASN:ND2	2.78	0.42
2:D:95:LEU:HD13	3:D:146:HEM:CMA	2.50	0.42
2:D:105:LEU:O	2:D:106:GLY:C	2.60	0.42
2:D:126:GLN:O	2:D:127:ALA:C	2.51	0.42
1:A:31:ARG:HH21	2:B:126:GLN:CG	2.33	0.42
1:A:95:PRO:HB3	1:A:137:THR:HG23	2.01	0.42
2:B:1:MET:CA	2:B:2:LEU:HD23	2.50	0.42
2:B:62:HIS:HE1	3:B:146:HEM:C4D	2.38	0.42
2:B:106:GLY:O	2:B:133:VAL:HG21	2.20	0.42
1:C:28:ALA:C	1:C:104:SER:HB3	2.45	0.42
1:C:49:SER:HA	1:C:55:GLN:NE2	2.31	0.42
1:C:54:GLN:C	1:C:54:GLN:N	2.63	0.42
1:C:56:LYS:CB	1:C:56:LYS:CD	2.98	0.42
2:D:140:LEU:C	2:D:142:HIS:N	2.77	0.42
2:B:98:ASN:HB2	2:B:101:ASN:H	1.81	0.42
1:C:10:VAL:CG1	1:C:10:VAL:HG22	2.40	0.42
1:C:17:VAL:HG13	1:C:24:TYR:HD2	1.77	0.42
2:D:30:LEU:C	2:D:30:LEU:HB3	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:LEU:O	2:D:90:LEU:HD22	2.19	0.42
2:D:100:GLN:CB	2:D:100:GLN:N	2.73	0.42
1:C:14:TRP:CG	1:C:70:GLN:HE21	2.38	0.42
1:C:43:PHE:CB	1:C:43:PHE:O	2.67	0.42
1:C:61:LYS:HA	1:C:61:LYS:HD3	2.00	0.42
1:C:72:HIS:C	1:C:72:HIS:ND1	2.78	0.42
1:C:130:ALA:CA	1:C:133:SER:HB2	2.50	0.42
2:D:141:ALA:O	2:D:144:TYR:HB2	2.20	0.42
1:A:43:PHE:HB2	1:A:48:LEU:CD2	2.50	0.41
1:A:93:VAL:HB	1:A:93:VAL:HG23	1.90	0.41
2:B:13:PHE:C	2:B:13:PHE:CB	2.86	0.41
2:B:70:PHE:O	2:B:73:GLY:N	2.52	0.41
2:B:77:LEU:C	2:B:77:LEU:CG	2.89	0.41
2:B:109:LEU:O	2:B:110:ALA:HA	2.19	0.41
3:A:142:HEM:CMA	3:A:142:HEM:CHB	2.98	0.41
2:B:53:VAL:HG13	2:B:54:MET:N	2.35	0.41
2:B:105:LEU:C	2:B:105:LEU:CB	2.81	0.41
2:B:133:VAL:HG21	2:B:133:VAL:HG11	2.02	0.41
2:B:138:ASN:O	2:B:139:ALA:C	2.63	0.41
1:C:29:LEU:CD1	1:C:59:GLY:CA	2.98	0.41
2:D:2:LEU:CB	2:D:7:LYS:HD3	2.50	0.41
2:D:43:HIS:CE1	3:D:146:HEM:CBA	3.03	0.41
2:D:98:ASN:O	2:D:100:GLN:N	2.52	0.41
1:A:31:ARG:HG2	2:B:123:PRO:HB3	2.01	0.41
1:A:135:VAL:CA	1:A:135:VAL:CG2	2.90	0.41
2:B:109:LEU:HD23	2:B:109:LEU:CA	2.48	0.41
1:C:47:ASP:CB	1:C:47:ASP:OD2	2.48	0.41
2:D:37:THR:O	2:D:40:PHE:CD1	2.73	0.41
2:D:75:LYS:NZ	2:D:76:HIS:HD2	2.18	0.41
1:A:74:ASN:O	1:A:74:ASN:CA	2.57	0.41
1:A:119:PRO:HG3	2:B:54:MET:SD	2.61	0.41
2:B:80:LEU:HB3	2:B:82:GLY:N	2.34	0.41
2:B:115:ARG:HH21	2:B:115:ARG:HD2	1.36	0.41
1:C:36:PHE:CE1	2:D:103:ARG:NH1	2.89	0.41
1:C:44:PRO:O	1:C:46:PHE:N	2.54	0.41
1:C:68:LYS:CD	1:C:68:LYS:HZ2	2.30	0.41
1:C:72:HIS:C	1:C:74:ASN:HD22	2.29	0.41
1:C:95:PRO:HD3	1:C:141:ARG:HH22	1.85	0.41
2:D:43:HIS:N	2:D:43:HIS:HB2	2.31	0.41
2:D:105:LEU:HD13	2:D:105:LEU:HB3	1.97	0.41
2:D:131:LYS:C	2:D:132:VAL:C	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:O	1:A:136:LEU:HD21	2.21	0.41
2:B:6:GLU:CB	2:B:6:GLU:HA	2.23	0.41
2:B:126:GLN:N	2:B:127:ALA:N	2.65	0.41
2:D:102:PHE:HB3	2:D:137:ALA:CB	2.51	0.41
1:A:46:PHE:HD1	1:A:55:GLN:OE1	2.04	0.41
1:A:48:LEU:HG	1:A:48:LEU:N	2.35	0.41
2:B:10:VAL:CG1	2:B:10:VAL:CG2	2.88	0.41
2:B:55:ASN:C	2:B:57:PRO:N	2.79	0.41
1:C:97:ASN:N	1:C:98:PHE:N	2.67	0.41
2:D:6:GLU:CA	2:D:6:GLU:O	2.57	0.41
2:D:41:PHE:HB3	2:D:44:PHE:CE1	2.56	0.41
2:D:131:LYS:O	2:D:132:VAL:CA	2.63	0.41
1:A:14:TRP:HD1	1:A:67:THR:HG23	1.84	0.41
1:A:60:GLN:HE21	1:A:61:LYS:CD	2.33	0.41
1:A:62:VAL:CG2	3:A:142:HEM:C1B	3.03	0.41
2:D:65:ARG:C	2:D:65:ARG:CB	2.81	0.41
1:A:42:TYR:N	1:A:43:PHE:N	2.69	0.41
1:A:43:PHE:CE2	3:A:142:HEM:C2D	3.09	0.41
1:A:50:HIS:HA	1:A:50:HIS:CD2	2.56	0.41
2:B:74:LEU:O	2:B:75:LYS:CA	2.69	0.41
2:B:84:PHE:CG	2:B:84:PHE:HA	2.52	0.41
1:C:42:TYR:CB	1:C:43:PHE:CD1	3.03	0.41
1:C:54:GLN:CG	1:C:54:GLN:HA	2.43	0.41
1:C:89:HIS:CE1	1:C:90:LYS:CG	2.94	0.41
2:D:2:LEU:C	2:D:3:THR:CA	2.70	0.41
1:A:45:HIS:CE1	1:A:46:PHE:CE2	3.09	0.41
2:B:40:PHE:HE2	2:B:95:LEU:O	2.03	0.41
2:B:70:PHE:CD1	2:B:71:THR:CB	2.94	0.41
2:B:113:VAL:CG2	2:B:113:VAL:HB	2.30	0.41
2:B:128:LEU:CD1	2:B:128:LEU:HB3	2.46	0.41
1:C:7:LYS:CB	1:C:7:LYS:HG2	2.21	0.41
1:C:18:GLY:N	1:C:18:GLY:O	2.54	0.41
1:C:73:LEU:C	1:C:74:ASN:HD22	2.28	0.41
1:C:95:PRO:CG	1:C:141:ARG:NH1	2.68	0.41
1:C:129:LEU:CD2	1:C:129:LEU:HB3	2.49	0.41
1:C:134:THR:N	1:C:134:THR:CB	2.81	0.41
3:C:142:HEM:HBB2	3:C:142:HEM:HMB1	2.03	0.41
2:D:38:GLN:CD	2:D:38:GLN:CB	2.83	0.41
1:A:48:LEU:O	1:A:50:HIS:N	2.53	0.41
2:B:19:VAL:HG13	2:B:20:ASP:N	2.36	0.41
2:B:34:TYR:HB3	2:B:36:TRP:CH2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:PRO:HD3	2:B:57:PRO:HA	1.96	0.41
2:D:11:THR:N	2:D:11:THR:HG22	2.30	0.41
2:D:41:PHE:O	2:D:42:GLN:HA	2.21	0.41
1:A:31:ARG:NH2	2:B:126:GLN:HB3	2.34	0.40
2:B:25:GLN:O	2:B:29:ARG:N	2.54	0.40
2:B:141:ALA:HA	2:B:144:TYR:CD1	2.56	0.40
1:C:13:ALA:HB2	1:C:121:VAL:HG11	2.02	0.40
1:C:48:LEU:HD12	1:C:48:LEU:C	2.46	0.40
1:C:116:ASN:O	1:C:116:ASN:HA	2.17	0.40
2:D:43:HIS:CA	2:D:43:HIS:HB3	2.23	0.40
2:D:102:PHE:N	2:D:103:ARG:N	2.61	0.40
2:D:126:GLN:CD	2:D:126:GLN:C	2.80	0.40
1:A:94:ASN:HD22	2:D:36:TRP:NE1	2.19	0.40
2:B:30:LEU:HD23	2:B:105:LEU:CB	2.50	0.40
2:B:105:LEU:HB2	3:B:146:HEM:CBB	2.51	0.40
1:C:17:VAL:O	1:C:18:GLY:HA3	2.20	0.40
1:C:32:MET:N	1:C:32:MET:HB3	2.30	0.40
1:C:46:PHE:CD2	1:C:54:GLN:CG	3.04	0.40
2:D:75:LYS:C	2:D:76:HIS:CA	2.79	0.40
1:A:39:THR:CG2	1:A:40:LYS:HZ1	2.23	0.40
2:B:36:TRP:HE1	2:B:101:ASN:HD21	1.69	0.40
1:C:84:SER:HB3	1:C:136:LEU:HA	2.02	0.40
1:C:134:THR:O	1:C:135:VAL:C	2.64	0.40
2:D:64:LYS:CG	2:D:64:LYS:CE	2.83	0.40
2:B:6:GLU:CD	2:B:131:LYS:NZ	2.74	0.40
2:B:38:GLN:C	2:B:38:GLN:CB	2.86	0.40
2:B:44:PHE:HD2	2:B:58:LYS:CG	2.34	0.40
2:B:76:HIS:N	2:B:76:HIS:HB2	2.27	0.40
1:C:48:LEU:HD13	1:C:49:SER:HB2	1.96	0.40
2:D:53:VAL:CG2	2:D:53:VAL:C	2.94	0.40
1:A:53:ALA:O	1:A:53:ALA:CA	2.54	0.40
2:B:34:TYR:HB3	2:B:36:TRP:CE2	2.56	0.40
2:B:52:ALA:O	2:B:53:VAL:C	2.64	0.40
2:B:138:ASN:ND2	2:B:138:ASN:HB2	2.33	0.40
1:C:2:LEU:HD12	1:C:7:LYS:HG3	2.02	0.40
1:C:35:SER:CB	2:D:127:ALA:HA	2.47	0.40
1:C:56:LYS:O	1:C:57:ALA:C	2.65	0.40
1:C:85:ASN:C	1:C:85:ASN:HB3	2.41	0.40
1:C:131:ASN:CA	1:C:131:ASN:ND2	2.84	0.40
2:D:91:HIS:HD2	2:D:102:PHE:HE1	1.68	0.40
2:D:95:LEU:CD1	2:D:97:VAL:HG21	2.43	0.40

All (80) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:O	2:D:49:SER:CB[4_555]	0.51	1.69
1:A:75:ASP:C	2:D:55:ASN:CG[4_555]	0.81	1.39
1:A:74:ASN:CG	2:D:54:MET:CA[4_555]	0.92	1.28
1:A:2:LEU:O	2:D:49:SER:CA[4_555]	1.05	1.15
1:A:7:LYS:NZ	2:D:51:GLY:N[4_555]	1.06	1.14
1:A:1:VAL:N	2:D:48:SER:O[4_555]	1.09	1.11
1:A:74:ASN:CG	2:D:54:MET:C[4_555]	1.10	1.10
1:A:2:LEU:C	2:D:49:SER:CB[4_555]	1.13	1.07
1:A:75:ASP:N	2:D:55:ASN:CB[4_555]	1.13	1.07
1:A:75:ASP:CG	2:D:55:ASN:O[4_555]	1.14	1.06
1:A:75:ASP:CA	2:D:55:ASN:CB[4_555]	1.19	1.01
1:A:75:ASP:C	2:D:55:ASN:OD1[4_555]	1.22	0.98
1:A:75:ASP:CB	2:D:55:ASN:O[4_555]	1.27	0.93
1:A:74:ASN:OD1	2:D:54:MET:CA[4_555]	1.28	0.92
1:A:75:ASP:N	2:D:55:ASN:CA[4_555]	1.29	0.91
1:A:75:ASP:O	2:D:55:ASN:OD1[4_555]	1.31	0.89
1:A:75:ASP:CB	2:D:55:ASN:C[4_555]	1.36	0.84
1:A:7:LYS:NZ	2:D:51:GLY:CA[4_555]	1.38	0.82
1:A:75:ASP:CA	2:D:55:ASN:CG[4_555]	1.42	0.78
1:A:73:LEU:O	2:D:51:GLY:O[4_555]	1.44	0.76
1:A:74:ASN:C	2:D:55:ASN:N[4_555]	1.45	0.75
1:A:74:ASN:C	2:D:55:ASN:CA[4_555]	1.49	0.71
1:A:75:ASP:OD1	2:D:60:LYS:CD[4_555]	1.50	0.70
1:A:75:ASP:CB	2:D:55:ASN:ND2[4_555]	1.50	0.70
1:A:75:ASP:C	2:D:55:ASN:CB[4_555]	1.52	0.68
1:A:75:ASP:OD2	2:D:57:PRO:CA[4_555]	1.56	0.64
1:A:90:LYS:NZ	1:C:82:ASN:ND2[4_545]	1.57	0.63
1:A:74:ASN:CA	2:D:52:ALA:CA[4_555]	1.59	0.61
1:A:74:ASN:CG	2:D:54:MET:CB[4_555]	1.59	0.61
1:A:75:ASP:OD2	2:D:57:PRO:N[4_555]	1.63	0.57
1:A:74:ASN:OD1	2:D:54:MET:CB[4_555]	1.64	0.56
1:A:74:ASN:CB	2:D:54:MET:N[4_555]	1.65	0.55
1:A:74:ASN:CA	2:D:55:ASN:N[4_555]	1.66	0.54
1:A:74:ASN:N	2:D:51:GLY:O[4_555]	1.67	0.53
1:A:75:ASP:OD1	2:D:55:ASN:O[4_555]	1.69	0.51
1:A:7:LYS:NZ	2:D:50:ALA:C[4_555]	1.70	0.50
1:A:90:LYS:CD	1:C:82:ASN:ND2[4_545]	1.71	0.49
1:A:76:LEU:N	2:D:55:ASN:OD1[4_555]	1.73	0.47
1:A:74:ASN:CB	2:D:51:GLY:O[4_555]	1.74	0.46
1:A:74:ASN:CB	2:D:55:ASN:N[4_555]	1.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:N	2:D:55:ASN:CB[4_555]	1.74	0.46
1:A:74:ASN:CB	2:D:54:MET:C[4_555]	1.76	0.44
1:A:76:LEU:N	2:D:55:ASN:CG[4_555]	1.78	0.42
1:A:73:LEU:C	2:D:51:GLY:O[4_555]	1.80	0.40
1:A:74:ASN:O	2:D:56:ASN:N[4_555]	1.80	0.40
1:A:7:LYS:NZ	2:D:51:GLY:C[4_555]	1.81	0.39
1:A:75:ASP:N	2:D:55:ASN:N[4_555]	1.82	0.38
1:A:2:LEU:O	2:D:49:SER:OG[4_555]	1.84	0.36
1:A:73:LEU:O	2:D:51:GLY:C[4_555]	1.84	0.36
1:A:75:ASP:OD2	2:D:57:PRO:CD[4_555]	1.85	0.35
1:A:74:ASN:O	2:D:52:ALA:O[4_555]	1.87	0.33
1:A:75:ASP:CA	2:D:55:ASN:C[4_555]	1.88	0.32
1:A:74:ASN:CA	2:D:51:GLY:O[4_555]	1.89	0.31
1:A:90:LYS:CE	1:C:82:ASN:ND2[4_545]	1.89	0.31
1:A:74:ASN:OD1	2:D:54:MET:C[4_555]	1.90	0.30
1:A:75:ASP:CB	2:D:55:ASN:CA[4_555]	1.90	0.30
1:A:7:LYS:CE	2:D:51:GLY:CA[4_555]	1.91	0.29
1:A:76:LEU:CA	2:D:55:ASN:OD1[4_555]	1.91	0.29
1:A:2:LEU:CA	2:D:49:SER:OG[4_555]	1.92	0.28
1:A:75:ASP:CA	2:D:55:ASN:CA[4_555]	1.92	0.28
1:A:75:ASP:O	2:D:55:ASN:CG[4_555]	1.94	0.26
1:A:7:LYS:CE	2:D:51:GLY:N[4_555]	1.95	0.25
1:A:75:ASP:O	2:D:55:ASN:ND2[4_555]	1.95	0.25
1:A:74:ASN:CB	2:D:54:MET:CA[4_555]	1.98	0.22
1:A:75:ASP:OD1	2:D:60:LYS:CG[4_555]	2.00	0.20
1:A:74:ASN:C	2:D:55:ASN:CB[4_555]	2.01	0.19
1:A:75:ASP:CA	2:D:55:ASN:ND2[4_555]	2.01	0.19
1:A:75:ASP:C	2:D:55:ASN:ND2[4_555]	2.02	0.18
1:A:1:VAL:CA	2:D:48:SER:O[4_555]	2.04	0.16
1:A:76:LEU:C	2:D:55:ASN:OD1[4_555]	2.04	0.16
1:A:2:LEU:C	2:D:49:SER:OG[4_555]	2.06	0.14
1:A:74:ASN:CA	2:D:52:ALA:C[4_555]	2.06	0.14
1:A:75:ASP:N	2:D:55:ASN:CG[4_555]	2.07	0.13
1:A:75:ASP:CB	2:D:56:ASN:N[4_555]	2.07	0.13
1:A:74:ASN:CG	2:D:54:MET:N[4_555]	2.09	0.11
1:A:75:ASP:CG	2:D:57:PRO:CD[4_555]	2.09	0.11
1:A:2:LEU:CB	2:D:49:SER:OG[4_555]	2.11	0.09
1:A:74:ASN:O	2:D:55:ASN:C[4_555]	2.13	0.07
1:A:1:VAL:N	2:D:48:SER:C[4_555]	2.17	0.03
1:A:75:ASP:CB	2:D:55:ASN:CG[4_555]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/141 (99%)	74 (53%)	34 (24%)	31 (22%)	0	0
1	C	139/141 (99%)	78 (56%)	28 (20%)	33 (24%)	0	0
2	B	143/145 (99%)	75 (52%)	28 (20%)	40 (28%)	0	0
2	D	143/145 (99%)	78 (54%)	26 (18%)	39 (27%)	0	0
All	All	564/572 (99%)	305 (54%)	116 (21%)	143 (25%)	0	0

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	6	ASN
1	A	13	ALA
1	A	15	GLY
1	A	17	VAL
1	A	30	GLN
1	A	31	ARG
1	A	40	LYS
1	A	47	ASP
1	A	53	ALA
1	A	72	HIS
1	A	74	ASN
1	A	89	HIS
1	A	109	LEU
1	A	110	ALA
2	B	7	LYS
2	B	19	VAL
2	B	20	ASP
2	B	21	VAL
2	B	33	VAL
2	B	46	ASN
2	B	56	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	57	PRO
2	B	66	VAL
2	B	68	ASP
2	B	72	GLN
2	B	74	LEU
2	B	76	HIS
2	B	85	ALA
2	B	86	GLN
2	B	93	ASN
2	B	96	HIS
2	B	122	THR
2	B	137	ALA
1	C	3	SER
1	C	21	ALA
1	C	45	HIS
1	C	48	LEU
1	C	63	ALA
1	C	64	ASN
1	C	75	ASP
1	C	83	LEU
1	C	84	SER
1	C	86	LEU
1	C	102	SER
1	C	110	ALA
1	C	138	SER
2	D	2	LEU
2	D	6	GLU
2	D	7	LYS
2	D	14	TRP
2	D	20	ASP
2	D	43	HIS
2	D	46	ASN
2	D	49	SER
2	D	59	VAL
2	D	72	GLN
2	D	73	GLY
2	D	75	LYS
2	D	78	ASP
2	D	124	ASN
2	D	144	TYR
1	A	14	TRP
1	A	25	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	29	LEU
1	A	49	SER
1	A	86	LEU
1	A	88	ALA
1	A	99	LYS
1	A	132	ASP
1	A	140	TYR
2	B	15	GLY
2	B	28	GLY
2	B	43	HIS
2	B	52	ALA
2	B	69	ALA
2	B	81	LYS
2	B	89	GLY
2	B	95	LEU
2	B	118	GLY
1	C	7	LYS
1	C	10	VAL
1	C	44	PRO
1	C	61	LYS
1	C	130	ALA
2	D	8	ALA
2	D	9	ALA
2	D	12	GLY
2	D	16	LYS
2	D	44	PHE
2	D	58	LYS
2	D	60	LYS
2	D	61	ALA
2	D	64	LYS
2	D	71	THR
2	D	82	GLY
2	D	110	ALA
2	D	116	ASN
2	D	134	ALA
2	D	143	LYS
1	A	66	LEU
1	A	82	ASN
1	A	136	LEU
1	A	139	LYS
2	B	60	LYS
2	B	67	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	75	LYS
2	B	112	VAL
2	B	143	LYS
1	C	24	TYR
1	C	31	ARG
1	C	68	LYS
1	C	124	ASN
1	C	139	LYS
2	D	92	CYS
2	D	128	LEU
2	D	139	ALA
1	A	37	PRO
2	B	2	LEU
2	B	31	LEU
2	B	83	ALA
2	B	127	ALA
1	C	57	ALA
1	C	109	LEU
2	D	3	THR
2	D	99	PRO
2	D	122	THR
1	A	50	HIS
1	A	128	PHE
1	C	9	ASN
1	C	17	VAL
1	C	37	PRO
1	C	74	ASN
1	C	118	THR
1	C	133	SER
2	D	62	HIS
1	C	56	LYS
2	D	86	GLN
2	D	19	VAL
1	C	96	VAL
2	B	17	VAL
2	B	82	GLY
2	B	132	VAL

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	115/115 (100%)	54 (47%)	61 (53%)	0 0
1	C	115/115 (100%)	63 (55%)	52 (45%)	0 0
2	B	56/113 (50%)	30 (54%)	26 (46%)	0 0
2	D	113/113 (100%)	50 (44%)	63 (56%)	0 0
All	All	399/456 (88%)	197 (49%)	202 (51%)	0 0

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	16	LYS
1	A	17	VAL
1	A	20	ASN
1	A	22	PRO
1	A	24	TYR
1	A	27	GLN
1	A	29	LEU
1	A	30	GLN
1	A	32	MET
1	A	33	PHE
1	A	34	LEU
1	A	37	PRO
1	A	38	THR
1	A	39	THR
1	A	40	LYS
1	A	41	THR
1	A	43	PHE
1	A	45	HIS
1	A	50	HIS
1	A	52	SER
1	A	55	GLN
1	A	56	LYS
1	A	60	GLN
1	A	61	LYS
1	A	62	VAL
1	A	68	LYS
1	A	70	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	LEU
1	A	74	ASN
1	A	76	LEU
1	A	79	THR
1	A	80	LEU
1	A	82	ASN
1	A	84	SER
1	A	85	ASN
1	A	90	LYS
1	A	92	ARG
1	A	93	VAL
1	A	99	LYS
1	A	100	LEU
1	A	104	SER
1	A	105	LEU
1	A	106	LEU
1	A	107	VAL
1	A	108	THR
1	A	109	LEU
1	A	111	SER
1	A	113	LEU
1	A	114	PRO
1	A	118	THR
1	A	121	VAL
1	A	122	HIS
1	A	124	ASN
1	A	133	SER
1	A	135	VAL
1	A	136	LEU
1	A	137	THR
1	A	138	SER
1	A	139	LYS
1	A	141	ARG
2	B	2	LEU
2	B	3	THR
2	B	5	GLU
2	B	7	LYS
2	B	16	LYS
2	B	19	VAL
2	B	95	LEU
2	B	97	VAL
2	B	98	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	99	PRO
2	B	104	LEU
2	B	105	LEU
2	B	109	LEU
2	B	111	LEU
2	B	112	VAL
2	B	113	VAL
2	B	116	ASN
2	B	120	GLN
2	B	121	PHE
2	B	122	THR
2	B	126	GLN
2	B	128	LEU
2	B	129	PHE
2	B	130	GLN
2	B	132	VAL
2	B	138	ASN
1	C	1	VAL
1	C	2	LEU
1	C	3	SER
1	C	6	ASN
1	C	7	LYS
1	C	10	VAL
1	C	11	LYS
1	C	14	TRP
1	C	16	LYS
1	C	20	ASN
1	C	22	PRO
1	C	35	SER
1	C	36	PHE
1	C	39	THR
1	C	45	HIS
1	C	47	ASP
1	C	48	LEU
1	C	52	SER
1	C	55	GLN
1	C	56	LYS
1	C	60	GLN
1	C	61	LYS
1	C	66	LEU
1	C	68	LYS
1	C	72	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	73	LEU
1	C	74	ASN
1	C	76	LEU
1	C	79	THR
1	C	81	SER
1	C	86	LEU
1	C	89	HIS
1	C	90	LYS
1	C	92	ARG
1	C	94	ASN
1	C	99	LYS
1	C	100	LEU
1	C	101	LEU
1	C	104	SER
1	C	106	LEU
1	C	107	VAL
1	C	113	LEU
1	C	115	THR
1	C	116	ASN
1	C	117	PHE
1	C	124	ASN
1	C	129	LEU
1	C	131	ASN
1	C	132	ASP
1	C	135	VAL
1	C	139	LYS
1	C	140	TYR
2	D	1	MET
2	D	2	LEU
2	D	3	THR
2	D	7	LYS
2	D	10	VAL
2	D	11	THR
2	D	14	TRP
2	D	17	VAL
2	D	19	VAL
2	D	20	ASP
2	D	21	VAL
2	D	27	LEU
2	D	31	LEU
2	D	32	VAL
2	D	33	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	37	THR
2	D	39	ARG
2	D	41	PHE
2	D	43	HIS
2	D	47	LEU
2	D	48	SER
2	D	53	VAL
2	D	56	ASN
2	D	58	LYS
2	D	60	LYS
2	D	65	ARG
2	D	66	VAL
2	D	68	ASP
2	D	71	THR
2	D	72	GLN
2	D	75	LYS
2	D	78	ASP
2	D	80	LEU
2	D	81	LYS
2	D	87	LEU
2	D	90	LEU
2	D	94	LYS
2	D	95	LEU
2	D	96	HIS
2	D	98	ASN
2	D	101	ASN
2	D	103	ARG
2	D	104	LEU
2	D	108	VAL
2	D	109	LEU
2	D	111	LEU
2	D	112	VAL
2	D	113	VAL
2	D	115	ARG
2	D	116	ASN
2	D	121	PHE
2	D	124	ASN
2	D	125	VAL
2	D	126	GLN
2	D	128	LEU
2	D	131	LYS
2	D	132	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	133	VAL
2	D	138	ASN
2	D	140	LEU
2	D	142	HIS
2	D	143	LYS
2	D	145	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	60	GLN
1	A	70	GLN
1	A	74	ASN
1	A	85	ASN
1	A	97	ASN
1	A	112	HIS
1	A	126	ASN
2	B	101	ASN
2	B	120	GLN
2	B	126	GLN
2	B	145	HIS
1	C	30	GLN
1	C	45	HIS
1	C	55	GLN
1	C	60	GLN
1	C	64	ASN
1	C	70	GLN
1	C	72	HIS
1	C	74	ASN
1	C	89	HIS
2	D	25	GLN
2	D	43	HIS
2	D	55	ASN
2	D	56	ASN
2	D	72	GLN
2	D	76	HIS
2	D	130	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	A	142	1	50,50,50	10.75	43 (86%)	67,82,82	9.98	59 (88%)
3	HEM	B	146	2	50,50,50	9.11	43 (86%)	67,82,82	8.11	49 (73%)
3	HEM	C	142	1	50,50,50	9.37	42 (84%)	67,82,82	6.08	46 (68%)
3	HEM	D	146	-	50,50,50	11.42	41 (82%)	67,82,82	7.42	54 (80%)

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	A	142	1	-	5/14/54/54	-
3	HEM	B	146	2	-	4/14/54/54	-
3	HEM	C	142	1	-	7/14/54/54	-
3	HEM	D	146	-	-	7/14/54/54	-

All (169) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	146	HEM	C4D-C3D	30.43	1.96	1.45
3	A	142	HEM	CBD-CGD	26.54	2.12	1.50
3	D	146	HEM	C1B-NB	26.42	1.85	1.40
3	D	146	HEM	CBD-CGD	25.73	2.10	1.50
3	A	142	HEM	CHA-C4D	25.59	1.89	1.38
3	D	146	HEM	CHA-C1A	24.70	1.94	1.39
3	D	146	HEM	CMD-C2D	-23.08	1.03	1.50
3	C	142	HEM	CHD-C4C	-22.51	0.94	1.38
3	A	142	HEM	C4A-NA	-22.31	0.97	1.39
3	D	146	HEM	C3C-C4C	21.58	1.83	1.46
3	B	146	HEM	CMA-C3A	21.58	1.95	1.50
3	A	142	HEM	C1B-C2B	-21.56	1.00	1.44
3	D	146	HEM	CBA-CGA	20.65	1.98	1.50
3	C	142	HEM	CMA-C3A	-20.33	1.09	1.50
3	A	142	HEM	C3D-C2D	-20.10	0.93	1.36
3	C	142	HEM	C4D-C3D	-18.88	1.13	1.45
3	D	146	HEM	CAD-C3D	-18.57	1.03	1.51
3	A	142	HEM	CHC-C4B	-17.88	0.98	1.39
3	D	146	HEM	C4A-NA	17.87	1.73	1.39
3	C	142	HEM	O1D-CGD	17.85	1.80	1.22
3	D	146	HEM	CMC-C2C	-16.95	1.16	1.50
3	A	142	HEM	C1D-C2D	16.49	1.78	1.44
3	B	146	HEM	CMB-C2B	16.32	1.84	1.50
3	B	146	HEM	C4A-NA	15.12	1.68	1.39
3	A	142	HEM	C3B-C4B	15.08	1.74	1.44
3	B	146	HEM	C3B-C2B	-14.63	1.07	1.37
3	A	142	HEM	C4B-NB	14.59	1.67	1.38
3	B	146	HEM	C1A-C2A	14.54	1.73	1.44
3	D	146	HEM	CMB-C2B	14.45	1.80	1.50
3	A	142	HEM	CHC-C1C	14.40	1.66	1.38
3	D	146	HEM	CHA-C4D	-14.39	1.09	1.38
3	C	142	HEM	C1C-NC	-14.06	1.13	1.39
3	D	146	HEM	C4D-ND	14.02	1.64	1.40
3	C	142	HEM	C4C-NC	13.84	1.65	1.39
3	C	142	HEM	CMD-C2D	-13.72	1.22	1.50
3	A	142	HEM	CHB-C1B	13.53	1.65	1.38
3	A	142	HEM	C1B-NB	13.53	1.63	1.40
3	B	146	HEM	C1C-C2C	13.35	1.71	1.45
3	D	146	HEM	C4D-C3D	13.30	1.67	1.45
3	C	142	HEM	CBD-CGD	-13.13	1.20	1.50
3	C	142	HEM	C1C-C2C	13.10	1.71	1.45
3	B	146	HEM	C4A-C3A	12.93	1.73	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	C3B-C4B	-12.87	1.20	1.44
3	A	142	HEM	C3B-C2B	12.68	1.62	1.37
3	C	142	HEM	CHB-C4A	12.43	1.67	1.39
3	A	142	HEM	CMA-C3A	12.26	1.75	1.50
3	C	142	HEM	CAB-C3B	12.24	1.80	1.47
3	D	146	HEM	C4A-C3A	-12.16	1.14	1.43
3	D	146	HEM	C1A-C2A	-11.61	1.21	1.44
3	A	142	HEM	CHB-C4A	11.38	1.64	1.39
3	C	142	HEM	CHA-C1A	11.18	1.64	1.39
3	B	146	HEM	C1D-C2D	10.98	1.66	1.44
3	A	142	HEM	O1A-CGA	10.88	1.57	1.22
3	D	146	HEM	C1D-ND	10.83	1.60	1.38
3	C	142	HEM	C3D-C2D	10.49	1.59	1.36
3	B	146	HEM	C3D-C2D	10.47	1.59	1.36
3	B	146	HEM	C3B-C4B	10.36	1.65	1.44
3	B	146	HEM	CAD-C3D	10.21	1.77	1.51
3	B	146	HEM	C1B-C2B	10.17	1.65	1.44
3	D	146	HEM	CHD-C4C	10.08	1.58	1.38
3	A	142	HEM	CAD-C3D	-10.05	1.25	1.51
3	D	146	HEM	CHC-C1C	-9.99	1.18	1.38
3	C	142	HEM	C3C-C2C	9.85	1.57	1.37
3	D	146	HEM	C3B-C4B	-9.49	1.26	1.44
3	C	142	HEM	CMC-C2C	9.34	1.69	1.50
3	A	142	HEM	O1D-CGD	9.10	1.51	1.22
3	D	146	HEM	C3D-C2D	8.96	1.56	1.36
3	C	142	HEM	C4B-NB	8.88	1.56	1.38
3	B	146	HEM	C1C-NC	-8.84	1.23	1.39
3	B	146	HEM	CHC-C4B	8.76	1.59	1.39
3	C	142	HEM	CHC-C1C	8.62	1.55	1.38
3	D	146	HEM	CMA-C3A	-8.42	1.33	1.50
3	C	142	HEM	C1A-NA	8.24	1.55	1.39
3	B	146	HEM	CHB-C4A	-8.22	1.21	1.39
3	A	142	HEM	C4D-ND	-8.13	1.26	1.40
3	A	142	HEM	C3C-C2C	8.08	1.53	1.37
3	A	142	HEM	C4D-C3D	7.90	1.58	1.45
3	A	142	HEM	C2A-C3A	7.86	1.59	1.38
3	B	146	HEM	C3C-C2C	-7.71	1.21	1.37
3	D	146	HEM	C4B-NB	7.69	1.53	1.38
3	C	142	HEM	C1B-NB	7.61	1.53	1.40
3	C	142	HEM	C2A-C3A	7.58	1.58	1.38
3	C	142	HEM	FE-ND	7.52	2.18	1.94
3	C	142	HEM	C4A-C3A	-7.50	1.25	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	146	HEM	C1B-NB	7.47	1.53	1.40
3	A	142	HEM	CBC-CAC	-7.45	0.94	1.30
3	C	142	HEM	O2D-CGD	7.32	1.55	1.30
3	C	142	HEM	CAA-C2A	7.30	1.70	1.51
3	B	146	HEM	CHA-C1A	-7.27	1.23	1.39
3	D	146	HEM	CBA-CAA	7.25	1.77	1.51
3	C	142	HEM	C1A-C2A	-7.25	1.30	1.44
3	B	146	HEM	O1A-CGA	7.17	1.45	1.22
3	B	146	HEM	CHC-C1C	-7.15	1.24	1.38
3	D	146	HEM	C1B-C2B	-7.09	1.30	1.44
3	A	142	HEM	CMC-C2C	7.03	1.65	1.50
3	A	142	HEM	CMB-C2B	7.01	1.65	1.50
3	B	146	HEM	O2D-CGD	6.99	1.53	1.30
3	C	142	HEM	CHA-C4D	6.94	1.52	1.38
3	D	146	HEM	C3C-C2C	6.78	1.50	1.37
3	A	142	HEM	CBA-CAA	6.74	1.75	1.51
3	B	146	HEM	C4B-NB	-6.74	1.25	1.38
3	D	146	HEM	CBC-CAC	-6.74	0.98	1.30
3	A	142	HEM	CBD-CAD	6.58	1.74	1.51
3	C	142	HEM	C4D-ND	6.47	1.51	1.40
3	C	142	HEM	CBB-CAB	-6.10	1.01	1.30
3	D	146	HEM	CHB-C4A	6.07	1.53	1.39
3	C	142	HEM	CHC-C4B	-5.90	1.25	1.39
3	D	146	HEM	CAA-C2A	-5.73	1.36	1.51
3	D	146	HEM	CHD-C1D	-5.72	1.26	1.39
3	D	146	HEM	C1D-C2D	-5.67	1.33	1.44
3	C	142	HEM	CAD-C3D	5.65	1.65	1.51
3	B	146	HEM	O1D-CGD	5.51	1.40	1.22
3	A	142	HEM	C1A-C2A	5.49	1.55	1.44
3	B	146	HEM	FE-NC	5.47	2.13	1.95
3	B	146	HEM	CBB-CAB	5.25	1.55	1.30
3	B	146	HEM	O2A-CGA	-5.16	1.13	1.30
3	D	146	HEM	C4C-NC	-5.04	1.30	1.39
3	C	142	HEM	FE-NA	5.04	2.11	1.95
3	B	146	HEM	CBD-CAD	-5.03	1.34	1.51
3	B	146	HEM	C2A-C3A	-5.00	1.25	1.38
3	C	142	HEM	CHD-C1D	4.98	1.50	1.39
3	D	146	HEM	C3B-C2B	4.89	1.47	1.37
3	B	146	HEM	CHA-C4D	4.81	1.48	1.38
3	C	142	HEM	CHB-C1B	-4.75	1.29	1.38
3	D	146	HEM	O2A-CGA	4.72	1.46	1.30
3	B	146	HEM	C4D-ND	-4.55	1.32	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	C4C-NC	4.54	1.48	1.39
3	A	142	HEM	CAA-C2A	4.48	1.62	1.51
3	A	142	HEM	CAC-C3C	-4.47	1.35	1.47
3	B	146	HEM	CMD-C2D	4.36	1.59	1.50
3	D	146	HEM	CAB-C3B	-4.36	1.35	1.47
3	B	146	HEM	CBD-CGD	-4.15	1.41	1.50
3	C	142	HEM	O1A-CGA	4.11	1.35	1.22
3	A	142	HEM	C1C-NC	3.89	1.46	1.39
3	A	142	HEM	O2D-CGD	-3.82	1.18	1.30
3	B	146	HEM	C1D-ND	3.65	1.46	1.38
3	C	142	HEM	CAC-C3C	3.65	1.57	1.47
3	B	146	HEM	CHD-C4C	3.62	1.45	1.38
3	C	142	HEM	CBD-CAD	3.62	1.64	1.51
3	B	146	HEM	FE-NA	3.59	2.07	1.95
3	A	142	HEM	CMD-C2D	-3.58	1.43	1.50
3	C	142	HEM	FE-NC	-3.58	1.83	1.95
3	B	146	HEM	CBA-CGA	3.42	1.58	1.50
3	B	146	HEM	CAA-C2A	3.40	1.60	1.51
3	C	142	HEM	C4A-NA	3.39	1.46	1.39
3	A	142	HEM	C1A-NA	-3.35	1.33	1.39
3	D	146	HEM	CHB-C1B	3.28	1.45	1.38
3	D	146	HEM	C1C-C2C	3.23	1.51	1.45
3	A	142	HEM	C4A-C3A	3.18	1.50	1.43
3	C	142	HEM	O2A-CGA	3.13	1.41	1.30
3	A	142	HEM	CHD-C4C	3.13	1.44	1.38
3	B	146	HEM	C1A-NA	-3.00	1.34	1.39
3	A	142	HEM	CAB-C3B	-2.99	1.39	1.47
3	C	142	HEM	C1D-ND	-2.91	1.33	1.38
3	A	142	HEM	CHA-C1A	2.85	1.45	1.39
3	B	146	HEM	C3C-C4C	-2.67	1.41	1.46
3	B	146	HEM	CAC-C3C	-2.65	1.40	1.47
3	A	142	HEM	C1C-C2C	-2.61	1.40	1.45
3	A	142	HEM	FE-ND	-2.53	1.87	1.94
3	D	146	HEM	CHC-C4B	-2.48	1.33	1.39
3	B	146	HEM	CAB-C3B	2.48	1.54	1.47
3	D	146	HEM	FE-NB	2.34	2.02	1.94
3	A	142	HEM	O2A-CGA	2.33	1.38	1.30
3	D	146	HEM	FE-NA	2.29	2.02	1.95
3	D	146	HEM	CBB-CAB	2.25	1.41	1.30
3	D	146	HEM	FE-ND	-2.18	1.88	1.94
3	C	142	HEM	C1D-C2D	-2.17	1.40	1.44
3	B	146	HEM	CHB-C1B	-2.14	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	FE-NB	-2.08	1.88	1.94

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	142	HEM	C2B-C1B-NB	27.85	141.86	109.84
3	B	146	HEM	CHA-C4D-ND	27.54	158.43	124.37
3	A	142	HEM	C3D-C4D-ND	25.35	137.98	110.17
3	A	142	HEM	C4D-ND-C1D	-22.73	78.29	105.21
3	D	146	HEM	C3B-C2B-C1B	22.51	123.31	106.41
3	A	142	HEM	CHB-C1B-NB	-22.29	96.79	124.37
3	D	146	HEM	CHD-C1D-ND	-21.41	101.39	124.42
3	A	142	HEM	C4C-C3C-C2C	-19.38	90.01	106.81
3	C	142	HEM	C3C-C2C-C1C	-18.90	89.16	107.05
3	B	146	HEM	CMA-C3A-C4A	-18.55	97.18	125.42
3	A	142	HEM	CBD-CAD-C3D	18.10	162.59	112.53
3	B	146	HEM	C3B-C2B-C1B	17.93	119.88	106.41
3	A	142	HEM	CHC-C1C-NC	-17.12	105.81	124.45
3	B	146	HEM	CMC-C2C-C1C	-17.06	94.68	124.73
3	A	142	HEM	CHA-C4D-ND	-17.05	103.27	124.37
3	D	146	HEM	CHC-C4B-NB	-16.40	106.78	124.42
3	B	146	HEM	C1A-CHA-C4D	-16.27	88.00	126.25
3	D	146	HEM	C4A-C3A-C2A	15.92	125.06	106.82
3	A	142	HEM	CMB-C2B-C1B	15.45	149.18	125.03
3	C	142	HEM	C4B-C3B-C2B	15.19	121.24	107.28
3	A	142	HEM	CMD-C2D-C1D	-14.89	101.77	125.03
3	A	142	HEM	CHD-C4C-NC	-14.48	108.69	124.45
3	B	146	HEM	CHA-C4D-C3D	-14.00	99.41	125.23
3	A	142	HEM	C1B-NB-C4B	-13.96	88.68	105.21
3	B	146	HEM	CHB-C4A-NA	12.91	147.28	123.86
3	A	142	HEM	C3A-C4A-NA	12.83	130.70	110.14
3	D	146	HEM	C3B-C4B-NB	12.52	118.46	109.47
3	B	146	HEM	CMC-C2C-C3C	12.32	158.24	128.43
3	D	146	HEM	CAA-C2A-C3A	12.20	154.43	127.07
3	A	142	HEM	C1A-C2A-C3A	-11.99	88.31	106.87
3	D	146	HEM	C2B-C1B-NB	-11.76	96.32	109.84
3	D	146	HEM	CMB-C2B-C1B	-11.75	106.67	125.03
3	D	146	HEM	C2D-C1D-ND	11.74	123.48	109.90
3	B	146	HEM	C3A-C4A-NA	-11.65	91.47	110.14
3	C	142	HEM	C4C-C3C-C2C	11.59	116.86	106.81
3	D	146	HEM	CMA-C3A-C4A	-11.42	108.03	125.42
3	D	146	HEM	C4D-ND-C1D	-11.10	92.06	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	146	HEM	C4A-C3A-C2A	11.05	119.47	106.82
3	B	146	HEM	C4D-ND-C1D	11.02	118.26	105.21
3	B	146	HEM	C3B-C4B-NB	10.87	117.27	109.47
3	B	146	HEM	CHC-C1C-NC	10.76	136.17	124.45
3	C	142	HEM	O2A-CGA-O1A	-10.68	95.86	123.33
3	D	146	HEM	C2A-C1A-NA	10.64	121.96	110.15
3	C	142	HEM	CHD-C4C-NC	10.58	135.97	124.45
3	A	142	HEM	C2A-C1A-NA	10.57	121.88	110.15
3	B	146	HEM	CHD-C4C-NC	-10.31	113.23	124.45
3	C	142	HEM	C4A-CHB-C1B	-10.23	102.20	126.25
3	C	142	HEM	CHC-C1C-NC	-10.10	113.45	124.45
3	A	142	HEM	CMD-C2D-C3D	10.09	153.45	126.15
3	B	146	HEM	O2D-CGD-O1D	-10.08	97.41	123.33
3	A	142	HEM	C4C-NC-C1C	-10.06	89.41	105.82
3	D	146	HEM	CAA-C2A-C1A	-9.94	105.52	124.94
3	B	146	HEM	CHA-C1A-NA	9.83	141.68	123.86
3	A	142	HEM	CAB-C3B-C2B	9.72	160.03	128.43
3	A	142	HEM	CAA-C2A-C3A	9.67	148.76	127.07
3	B	146	HEM	C2B-C1B-NB	-9.64	98.76	109.84
3	C	142	HEM	O2D-CGD-O1D	-9.50	98.91	123.33
3	A	142	HEM	C1C-CHC-C4B	9.48	146.16	126.02
3	D	146	HEM	C4C-C3C-C2C	-9.39	98.67	106.81
3	C	142	HEM	CAD-CBD-CGD	9.13	137.88	113.67
3	C	142	HEM	O1A-CGA-CBA	8.86	151.20	123.09
3	A	142	HEM	CHB-C4A-C3A	-8.83	101.79	127.43
3	C	142	HEM	CMC-C2C-C1C	8.79	140.20	124.73
3	D	146	HEM	CHA-C1A-NA	-8.73	108.03	123.86
3	D	146	HEM	C1B-NB-C4B	-8.40	95.26	105.21
3	C	142	HEM	CBD-CAD-C3D	8.32	135.55	112.53
3	B	146	HEM	CMA-C3A-C2A	8.17	142.96	125.62
3	C	142	HEM	C2C-C1C-NC	8.07	124.57	109.64
3	D	146	HEM	C3A-C4A-NA	-7.98	97.35	110.14
3	A	142	HEM	CHA-C1A-C2A	-7.90	108.01	125.30
3	A	142	HEM	CHC-C4B-NB	-7.88	115.95	124.42
3	A	142	HEM	O2A-CGA-CBA	-7.87	89.12	114.00
3	B	146	HEM	CAD-C3D-C2D	7.84	142.54	127.87
3	A	142	HEM	CMB-C2B-C3B	-7.83	109.48	128.43
3	A	142	HEM	CAC-C3C-C4C	7.78	143.39	124.82
3	C	142	HEM	CAD-C3D-C4D	7.77	138.24	124.70
3	C	142	HEM	CAD-C3D-C2D	-7.70	113.45	127.87
3	B	146	HEM	C4B-C3B-C2B	-7.66	100.24	107.28
3	C	142	HEM	CHC-C4B-NB	-7.64	116.20	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	146	HEM	C3D-C4D-ND	-7.59	101.85	110.17
3	D	146	HEM	C1C-CHC-C4B	7.59	142.14	126.02
3	B	146	HEM	O2A-CGA-CBA	-7.46	90.42	114.00
3	A	142	HEM	C3B-C2B-C1B	-7.43	100.83	106.41
3	C	142	HEM	O1D-CGD-CBD	7.34	146.38	123.09
3	A	142	HEM	C3B-C4B-NB	-7.15	104.33	109.47
3	C	142	HEM	CHC-C4B-C3B	7.12	139.28	125.07
3	A	142	HEM	C4A-C3A-C2A	-7.06	98.73	106.82
3	C	142	HEM	C3B-C4B-NB	-6.90	104.51	109.47
3	B	146	HEM	CMB-C2B-C1B	-6.82	114.37	125.03
3	A	142	HEM	CBC-CAC-C3C	6.76	161.29	127.53
3	B	146	HEM	CAD-C3D-C4D	-6.74	112.96	124.70
3	A	142	HEM	C2D-C1D-ND	6.64	117.58	109.90
3	C	142	HEM	CHB-C1B-NB	6.61	132.55	124.37
3	A	142	HEM	CHD-C1D-ND	-6.58	117.34	124.42
3	B	146	HEM	C4A-CHB-C1B	-6.55	110.84	126.25
3	B	146	HEM	CHA-C1A-C2A	-6.54	110.98	125.30
3	A	142	HEM	CHC-C4B-C3B	6.54	138.13	125.07
3	C	142	HEM	C2D-C1D-ND	-6.49	102.40	109.90
3	A	142	HEM	CBB-CAB-C3B	-6.43	95.41	127.53
3	D	146	HEM	C4A-NA-C1A	-6.39	95.40	105.82
3	B	146	HEM	O2D-CGD-CBD	6.37	134.11	114.00
3	B	146	HEM	C1D-C2D-C3D	-6.36	100.29	106.98
3	D	146	HEM	CMD-C2D-C1D	-6.36	115.10	125.03
3	D	146	HEM	CHD-C1D-C2D	6.32	135.01	125.03
3	B	146	HEM	C4A-NA-C1A	6.12	115.80	105.82
3	C	142	HEM	CAA-C2A-C1A	6.05	136.75	124.94
3	C	142	HEM	CHD-C1D-ND	6.02	130.90	124.42
3	C	142	HEM	CHB-C4A-C3A	-6.02	109.96	127.43
3	A	142	HEM	CAB-C3B-C4B	-6.02	97.81	124.39
3	D	146	HEM	O1D-CGD-CBD	-6.01	104.02	123.09
3	D	146	HEM	CAC-C3C-C2C	5.99	147.91	128.43
3	A	142	HEM	CHA-C4D-C3D	-5.98	114.19	125.23
3	C	142	HEM	CHB-C4A-NA	5.92	134.60	123.86
3	D	146	HEM	C4C-CHD-C1D	5.81	138.37	126.02
3	B	146	HEM	CHD-C4C-C3C	5.61	134.66	125.21
3	A	142	HEM	C4B-C3B-C2B	-5.57	102.16	107.28
3	D	146	HEM	CHC-C1C-NC	-5.56	118.40	124.45
3	D	146	HEM	CAA-CBA-CGA	-5.55	98.95	113.67
3	C	142	HEM	CAA-CBA-CGA	-5.51	99.04	113.67
3	A	142	HEM	CBA-CAA-C2A	-5.44	97.49	112.53
3	C	142	HEM	CAA-C2A-C3A	-5.36	115.05	127.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	146	HEM	O2D-CGD-CBD	5.23	130.52	114.00
3	D	146	HEM	C4D-C3D-C2D	-5.18	99.35	106.89
3	B	146	HEM	CHC-C4B-NB	-5.09	118.94	124.42
3	A	142	HEM	C3C-C2C-C1C	5.07	111.85	107.05
3	D	146	HEM	CBA-CAA-C2A	-5.01	98.67	112.53
3	A	142	HEM	O1A-CGA-CBA	5.00	138.94	123.09
3	A	142	HEM	CHC-C1C-C2C	4.97	135.83	125.49
3	D	146	HEM	CBC-CAC-C3C	-4.95	102.81	127.53
3	A	142	HEM	CAA-CBA-CGA	-4.86	100.77	113.67
3	C	142	HEM	C1C-CHC-C4B	4.85	136.33	126.02
3	A	142	HEM	O2D-CGD-O1D	4.85	135.80	123.33
3	B	146	HEM	C4C-C3C-C2C	4.84	111.01	106.81
3	C	142	HEM	C4D-C3D-C2D	-4.80	99.90	106.89
3	B	146	HEM	O1A-CGA-CBA	4.79	138.30	123.09
3	D	146	HEM	CAC-C3C-C4C	-4.78	113.41	124.82
3	A	142	HEM	C2C-C1C-NC	4.72	118.36	109.64
3	B	146	HEM	CMD-C2D-C1D	4.59	132.20	125.03
3	D	146	HEM	C1A-C2A-C3A	-4.49	99.92	106.87
3	D	146	HEM	C2C-C1C-NC	4.43	117.83	109.64
3	D	146	HEM	CBD-CAD-C3D	4.41	124.73	112.53
3	B	146	HEM	CHB-C1B-NB	4.40	129.81	124.37
3	D	146	HEM	CAD-C3D-C2D	4.36	136.04	127.87
3	C	142	HEM	CMD-C2D-C1D	-4.36	118.22	125.03
3	C	142	HEM	CHA-C4D-ND	-4.35	118.98	124.37
3	B	146	HEM	C3C-C2C-C1C	-4.21	103.06	107.05
3	B	146	HEM	C4C-NC-C1C	4.19	112.65	105.82
3	B	146	HEM	C4C-CHD-C1D	4.07	134.68	126.02
3	A	142	HEM	CAD-C3D-C2D	4.00	135.35	127.87
3	C	142	HEM	CHB-C1B-C2B	-3.98	115.63	126.95
3	D	146	HEM	CHB-C1B-C2B	3.94	138.14	126.95
3	B	146	HEM	C2C-C1C-NC	-3.88	102.45	109.64
3	A	142	HEM	C4D-C3D-C2D	-3.80	101.36	106.89
3	D	146	HEM	C4B-C3B-C2B	-3.76	103.82	107.28
3	C	142	HEM	C1B-NB-C4B	-3.64	100.89	105.21
3	A	142	HEM	CMC-C2C-C3C	-3.61	119.69	128.43
3	C	142	HEM	CAB-C3B-C2B	-3.61	116.69	128.43
3	D	146	HEM	O2A-CGA-O1A	3.58	132.53	123.33
3	A	142	HEM	C4A-NA-C1A	-3.57	100.00	105.82
3	C	142	HEM	C3B-C2B-C1B	-3.49	103.79	106.41
3	C	142	HEM	C3D-C4D-ND	3.41	113.91	110.17
3	C	142	HEM	C2B-C1B-NB	-3.36	105.97	109.84
3	B	146	HEM	C2D-C1D-ND	3.35	113.78	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	142	HEM	C1D-C2D-C3D	-3.31	103.50	106.98
3	C	142	HEM	C1A-CHA-C4D	-3.29	118.52	126.25
3	D	146	HEM	CHB-C4A-C3A	3.28	136.95	127.43
3	A	142	HEM	CHA-C1A-NA	3.23	129.71	123.86
3	D	146	HEM	C1D-C2D-C3D	3.19	110.34	106.98
3	D	146	HEM	CHD-C4C-NC	3.05	127.78	124.45
3	B	146	HEM	O2A-CGA-O1A	3.03	131.12	123.33
3	B	146	HEM	C4D-C3D-C2D	-3.02	102.50	106.89
3	A	142	HEM	O1D-CGD-CBD	-3.01	113.53	123.09
3	D	146	HEM	C3D-C4D-ND	2.99	113.45	110.17
3	A	142	HEM	CHB-C1B-C2B	-2.91	118.67	126.95
3	A	142	HEM	CMA-C3A-C4A	2.89	129.82	125.42
3	A	142	HEM	C4C-CHD-C1D	2.85	132.08	126.02
3	D	146	HEM	CAD-CBD-CGD	-2.85	106.12	113.67
3	A	142	HEM	CHD-C4C-C3C	-2.80	120.48	125.21
3	D	146	HEM	CHB-C1B-NB	-2.74	120.97	124.37
3	A	142	HEM	CMA-C3A-C2A	2.74	131.44	125.62
3	C	142	HEM	CAC-C3C-C2C	-2.73	119.57	128.43
3	D	146	HEM	CMD-C2D-C3D	2.66	133.33	126.15
3	D	146	HEM	CBB-CAB-C3B	2.65	140.78	127.53
3	C	142	HEM	C3A-C4A-NA	2.65	114.38	110.14
3	D	146	HEM	CHC-C4B-C3B	2.65	130.35	125.07
3	D	146	HEM	C3C-C2C-C1C	-2.62	104.56	107.05
3	B	146	HEM	C2A-C1A-NA	-2.54	107.33	110.15
3	B	146	HEM	CBC-CAC-C3C	2.48	139.91	127.53
3	C	142	HEM	C4A-NA-C1A	-2.39	101.93	105.82
3	D	146	HEM	CHA-C4D-ND	-2.37	121.44	124.37
3	B	146	HEM	CHB-C4A-C3A	-2.32	120.68	127.43
3	B	146	HEM	CHC-C1C-C2C	-2.32	120.66	125.49
3	C	142	HEM	CHC-C1C-C2C	-2.23	120.85	125.49
3	A	142	HEM	O2A-CGA-O1A	2.21	129.02	123.33
3	C	142	HEM	C4D-ND-C1D	2.19	107.80	105.21
3	B	146	HEM	CHD-C1D-ND	-2.17	122.08	124.42
3	D	146	HEM	CHD-C4C-C3C	-2.16	121.57	125.21
3	D	146	HEM	CHA-C1A-C2A	2.15	130.01	125.30
3	C	142	HEM	CBA-CAA-C2A	-2.15	106.59	112.53
3	C	142	HEM	O2A-CGA-CBA	-2.13	107.28	114.00
3	B	146	HEM	CAD-CBD-CGD	-2.12	108.04	113.67
3	C	142	HEM	CBB-CAB-C3B	2.12	138.11	127.53
3	A	142	HEM	CMC-C2C-C1C	2.11	128.44	124.73
3	D	146	HEM	O2A-CGA-CBA	-2.03	107.60	114.00
3	D	146	HEM	C1A-CHA-C4D	2.01	130.98	126.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	146	HEM	CAA-C2A-C3A	2.01	131.57	127.07
3	A	142	HEM	CHB-C4A-NA	2.01	127.50	123.86
3	D	146	HEM	CHA-C4D-C3D	-2.00	121.53	125.23

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	142	HEM	C3A-C2A-CAA-CBA
3	B	146	HEM	C2D-C3D-CAD-CBD
3	D	146	HEM	C3A-C2A-CAA-CBA
3	D	146	HEM	C2C-C3C-CAC-CBC
3	D	146	HEM	C4C-C3C-CAC-CBC
3	B	146	HEM	C4D-C3D-CAD-CBD
3	C	142	HEM	C4D-C3D-CAD-CBD
3	D	146	HEM	C1A-C2A-CAA-CBA
3	D	146	HEM	C3D-CAD-CBD-CGD
3	A	142	HEM	C2A-CAA-CBA-CGA
3	A	142	HEM	C1A-C2A-CAA-CBA
3	D	146	HEM	CAD-CBD-CGD-O2D
3	D	146	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAA-CBA-CGA-O1A
3	C	142	HEM	CAA-CBA-CGA-O2A
3	B	146	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	C4C-C3C-CAC-CBC
3	A	142	HEM	CAD-CBD-CGD-O2D
3	B	146	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	C2C-C3C-CAC-CBC

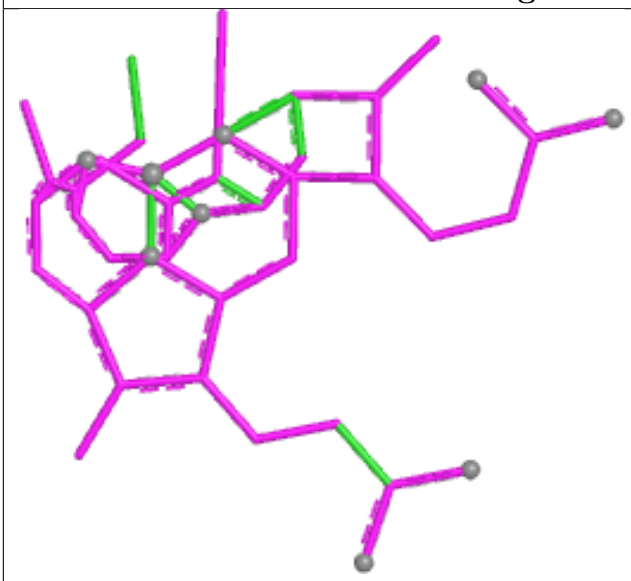
There are no ring outliers.

4 monomers are involved in 176 short contacts:

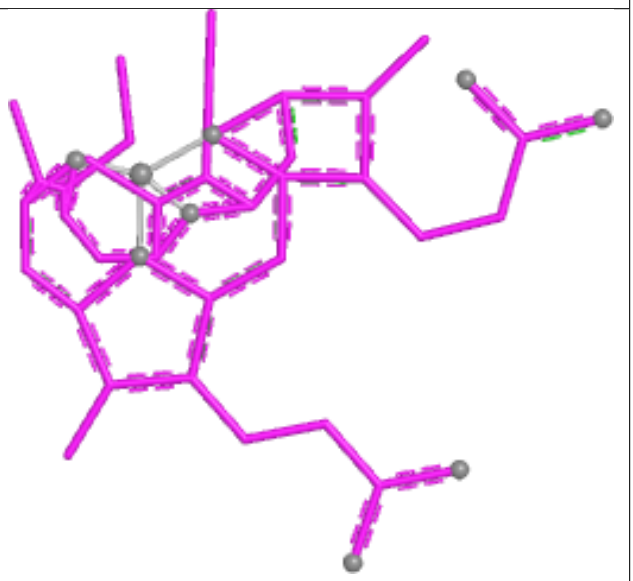
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	142	HEM	49	0
3	B	146	HEM	56	0
3	C	142	HEM	42	0
3	D	146	HEM	29	0

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.

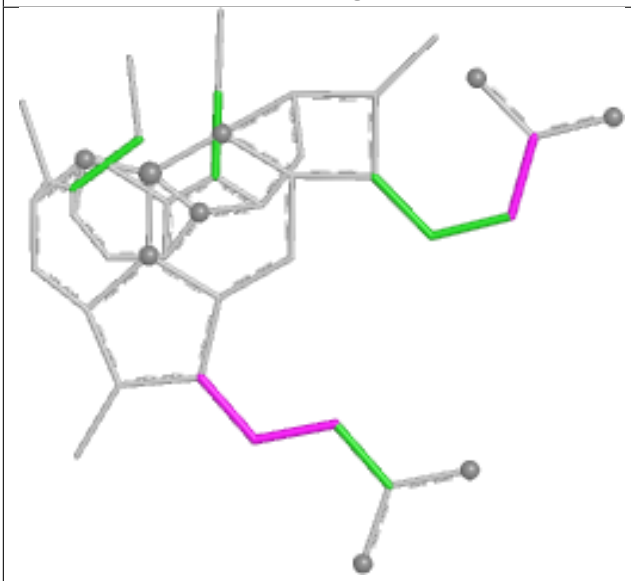
Ligand HEM A 142



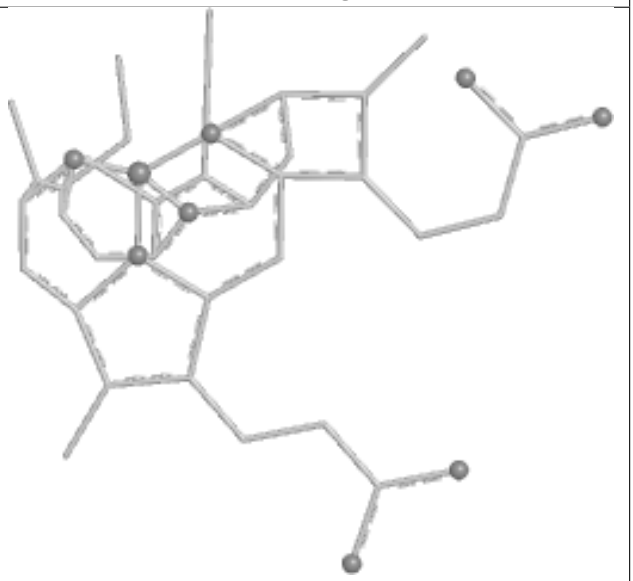
Bond lengths



Bond angles

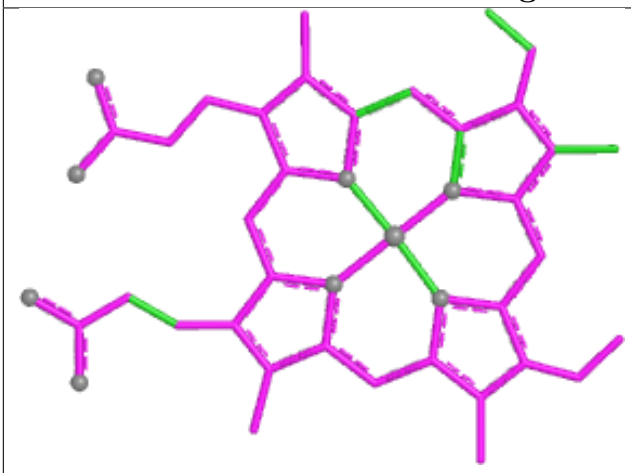


Torsions

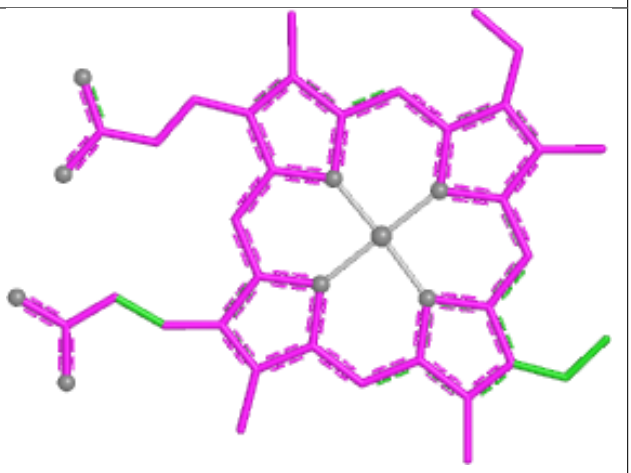


Rings

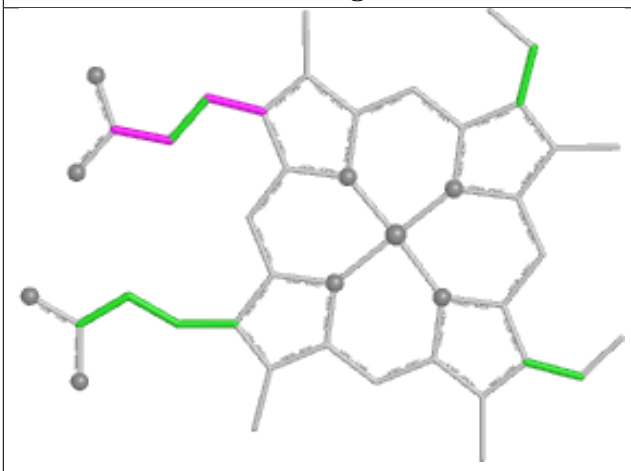
Ligand HEM B 146



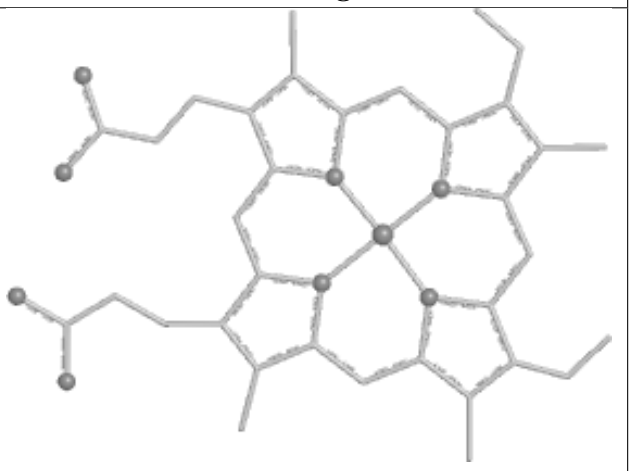
Bond lengths



Bond angles

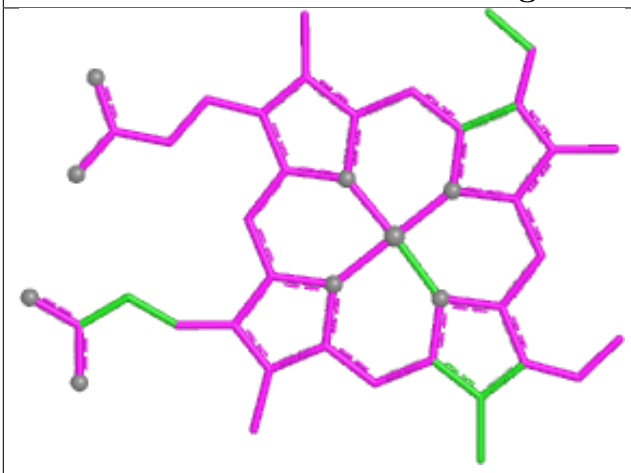


Torsions

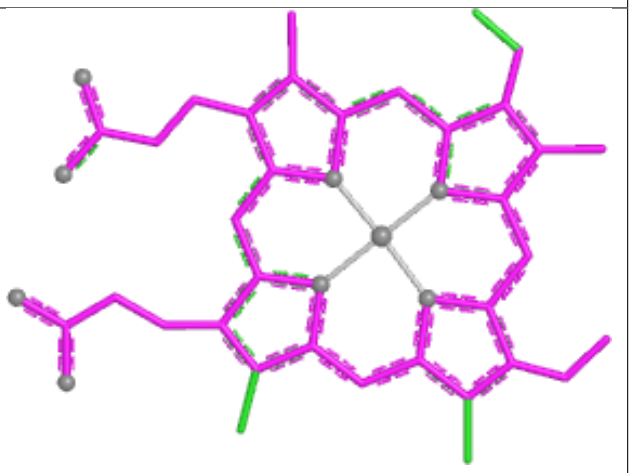


Rings

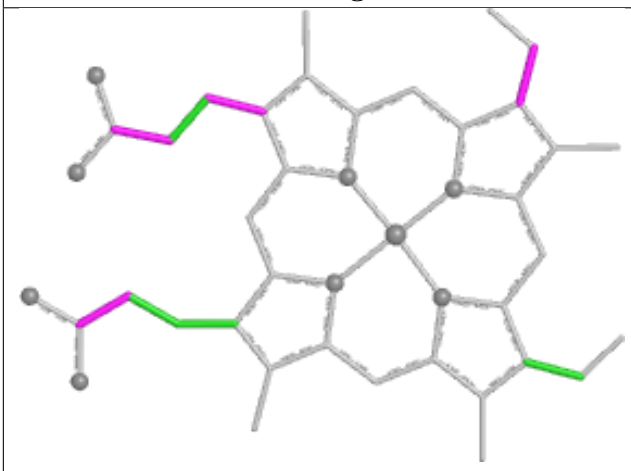
Ligand HEM C 142



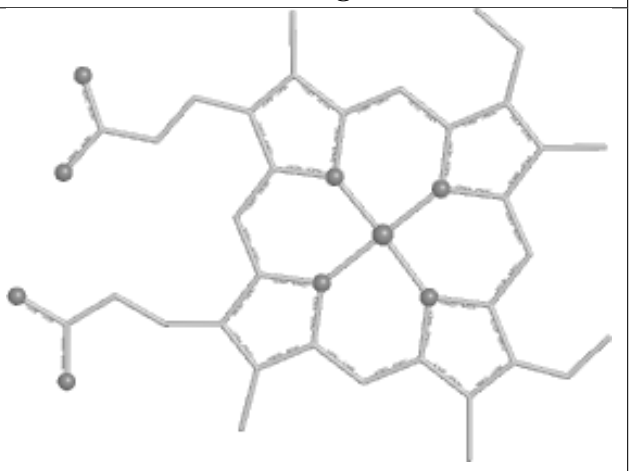
Bond lengths



Bond angles

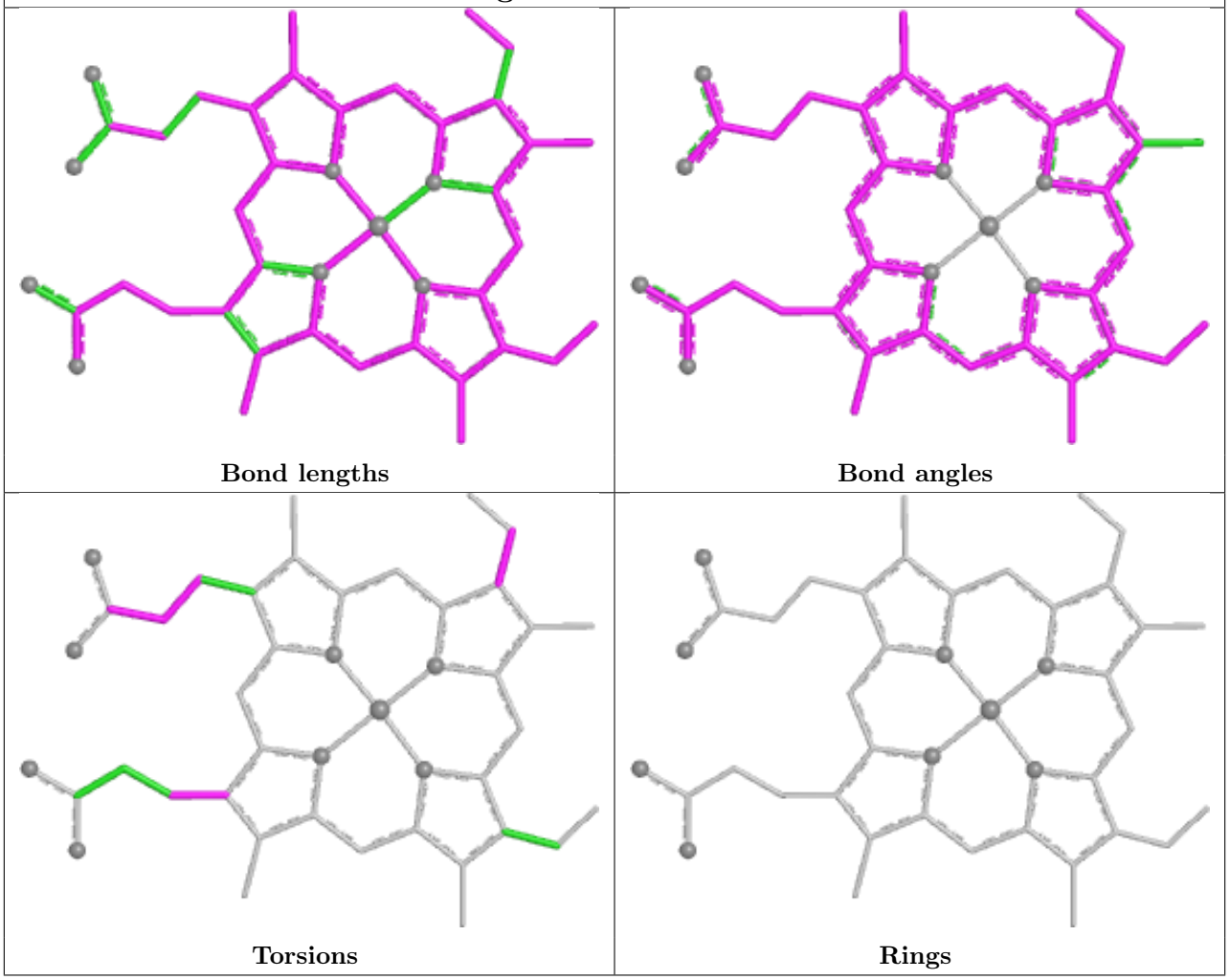


Torsions



Rings

Ligand HEM D 146



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.