Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:55 AM UTC

PDB ID	:	1HCY / pdb_00001hcy
Title	:	CRYSTAL STRUCTURE OF HEXAMERIC HAEMOCYANIN FROM PANULIRUS INTERRUPTUS REFINED AT 3.2 ANGSTROMS RESOLUTION
Authors	:	Volbeda, A.; Hol, W.G.J.
Deposited on	:	1991-05-15
Resolution	:	3.20 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:

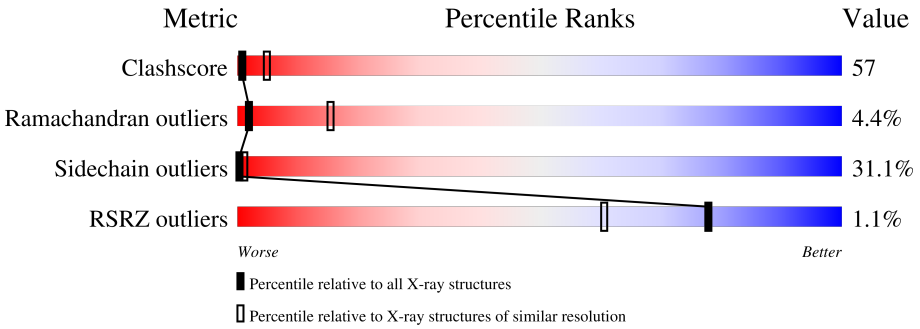
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	657	23% 52% 21%
1	B	657	23% 51% 22%
1	C	657	22% 52% 21%
1	D	657	22% 52% 22%
1	E	657	21% 52% 21%
1	F	657	23% 51% 21%
2	G	2	100%

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Mol	Chain	Length	Quality of chain
2	H	2	100%
2	I	2	100%
2	J	2	100%
2	K	2	100%
2	L	2	100%

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
2	NAG	G	1	X	-	-	-
2	NAG	H	1	X	-	-	-
2	NAG	I	1	X	-	-	-
2	NAG	J	1	X	-	-	-
2	NAG	K	1	X	-	-	-
2	NAG	L	1	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31790 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 ARTHROPODAN HEMOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	B	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	C	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	D	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	E	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	F	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ASP	GLU	conflict	UNP P04254
A	163	PRO	GLN	conflict	UNP P04254
A	458	ASN	LYS	conflict	UNP P04254
A	514	SER	LYS	conflict	UNP P04254
B	32	ASP	GLU	conflict	UNP P04254
B	163	PRO	GLN	conflict	UNP P04254
B	458	ASN	LYS	conflict	UNP P04254
B	514	SER	LYS	conflict	UNP P04254
C	32	ASP	GLU	conflict	UNP P04254
C	163	PRO	GLN	conflict	UNP P04254
C	458	ASN	LYS	conflict	UNP P04254
C	514	SER	LYS	conflict	UNP P04254
D	32	ASP	GLU	conflict	UNP P04254
D	163	PRO	GLN	conflict	UNP P04254
D	458	ASN	LYS	conflict	UNP P04254
D	514	SER	LYS	conflict	UNP P04254
E	32	ASP	GLU	conflict	UNP P04254

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Chain	Residue	Modelled	Actual	Comment	Reference
E	163	PRO	GLN	conflict	UNP P04254
E	458	ASN	LYS	conflict	UNP P04254
E	514	SER	LYS	conflict	UNP P04254
F	32	ASP	GLU	conflict	UNP P04254
F	163	PRO	GLN	conflict	UNP P04254
F	458	ASN	LYS	conflict	UNP P04254
F	514	SER	LYS	conflict	UNP P04254

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	G	2	Total C N O 28 16 2 10	0	0	0
2	H	2	Total C N O 28 16 2 10	0	0	0
2	I	2	Total C N O 28 16 2 10	0	0	0
2	J	2	Total C N O 28 16 2 10	0	0	0
2	K	2	Total C N O 28 16 2 10	0	0	0
2	L	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cu 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	176	Total O 176 176	0	0
4	B	4	Total O 4 4	0	0

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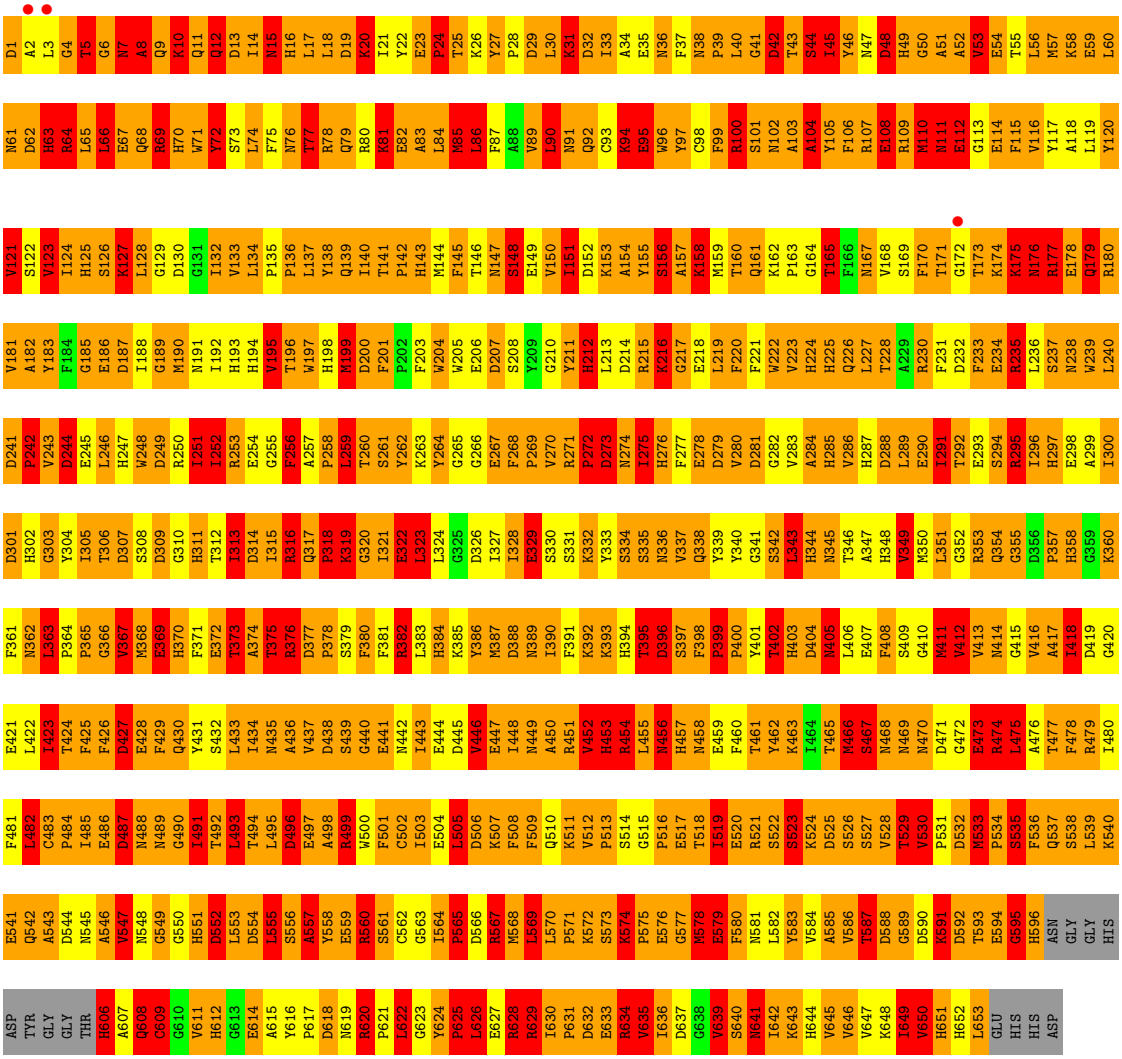
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total O 2 2	0	0
4	E	3	Total O 3 3	0	0
4	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

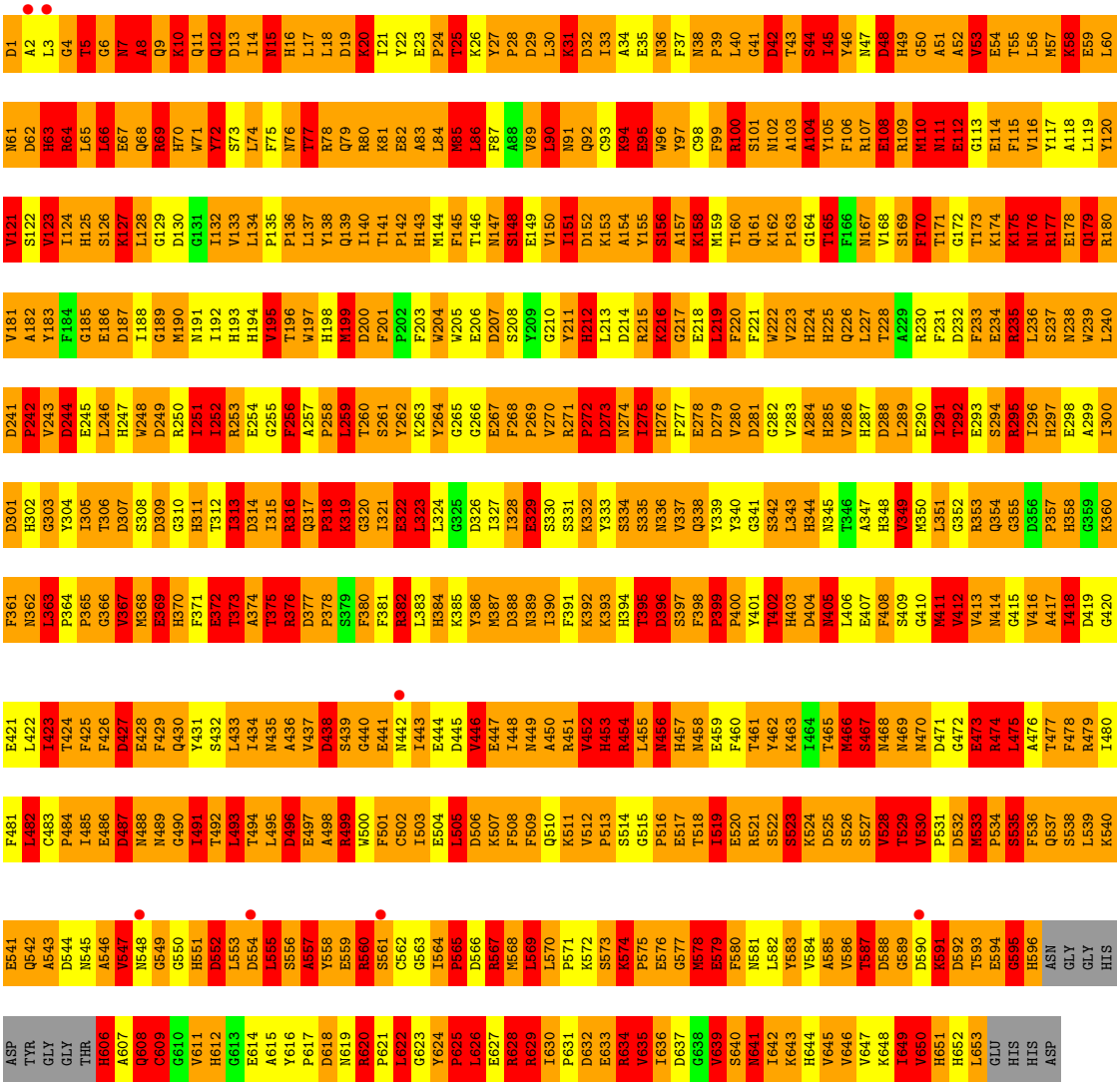
• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain A:



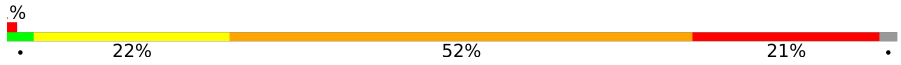
• Molecule 1: ARTHROPODAN HEMOCYANIN

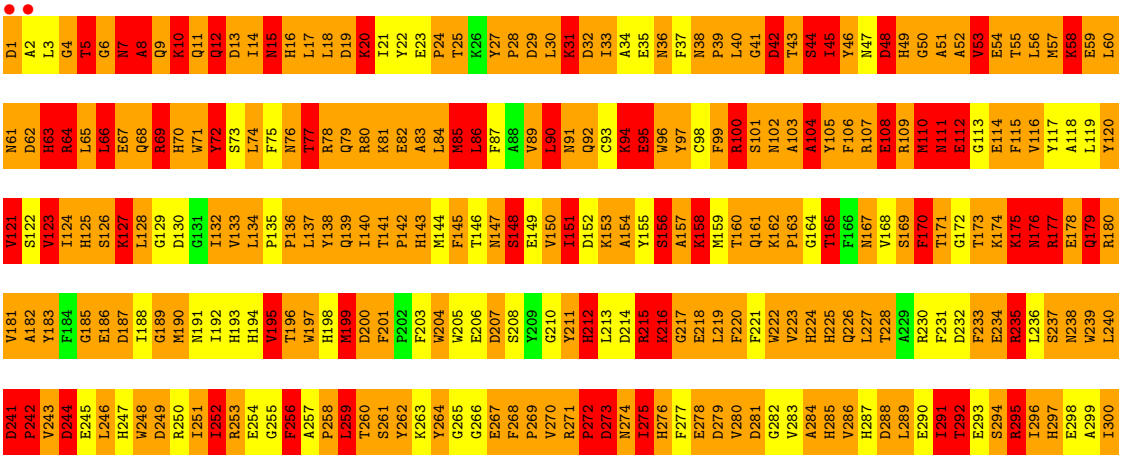
Chain B:

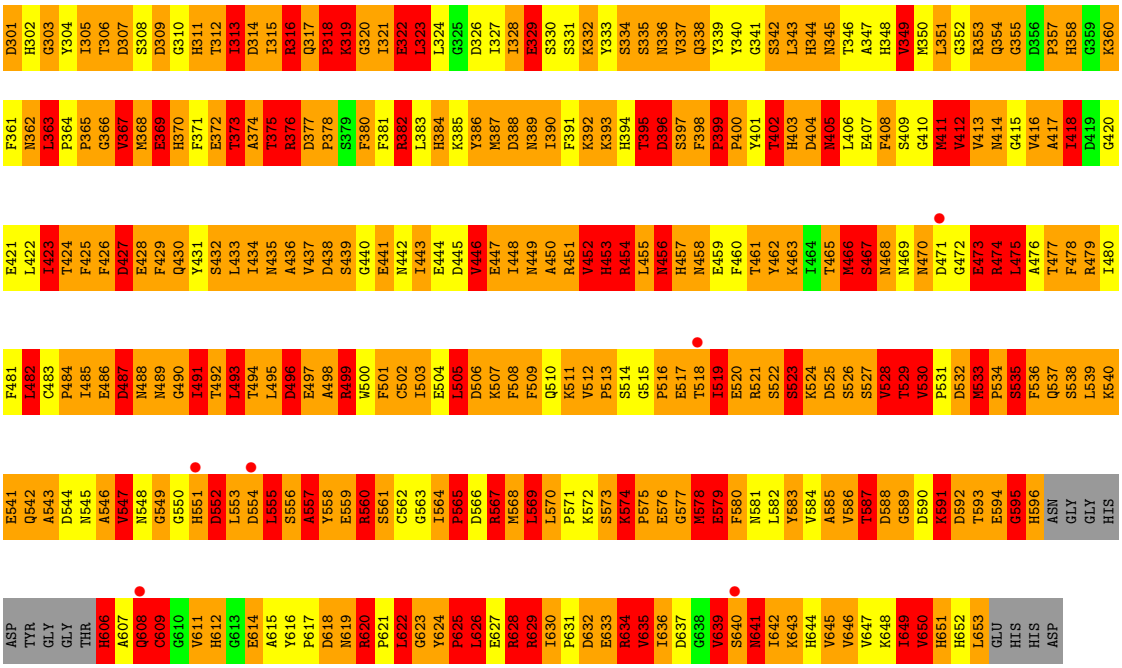


• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain C:

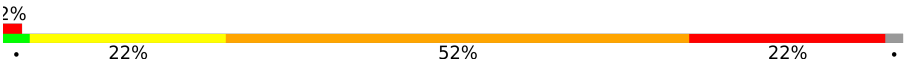


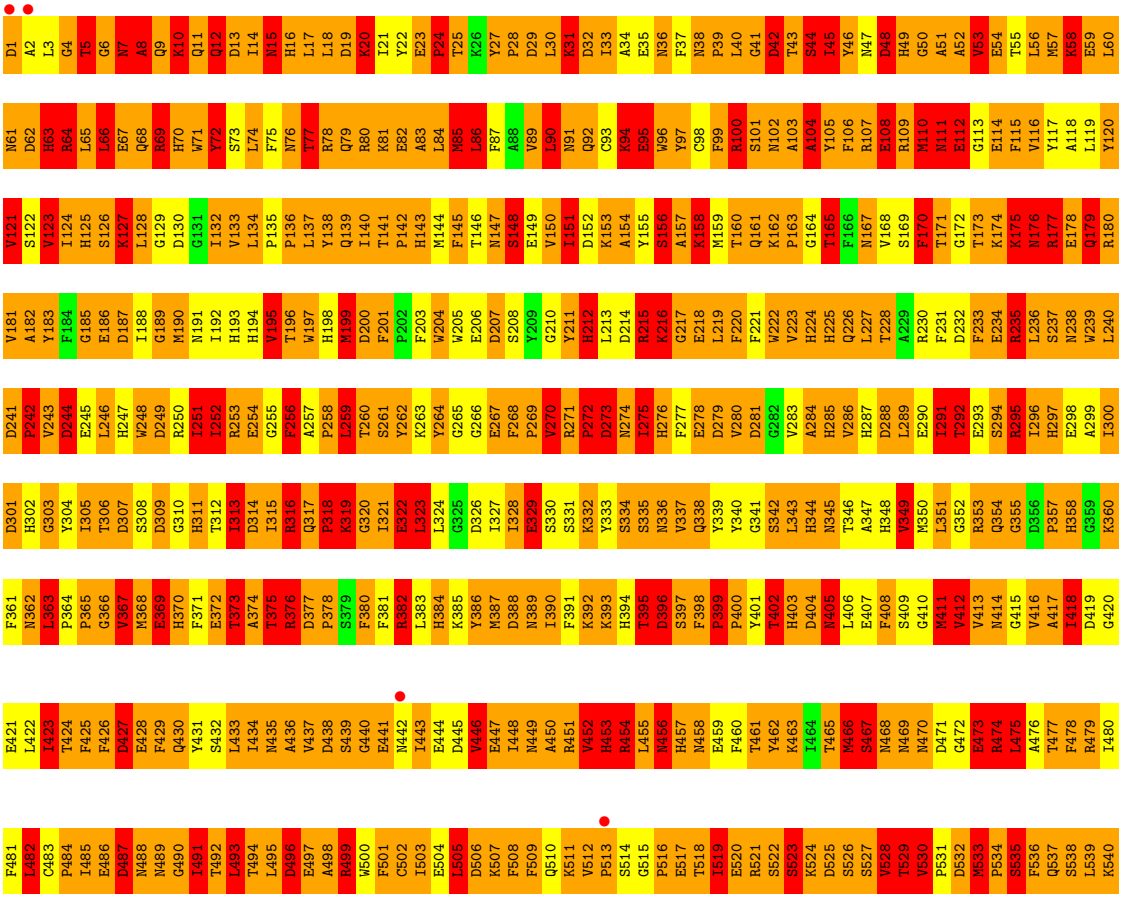


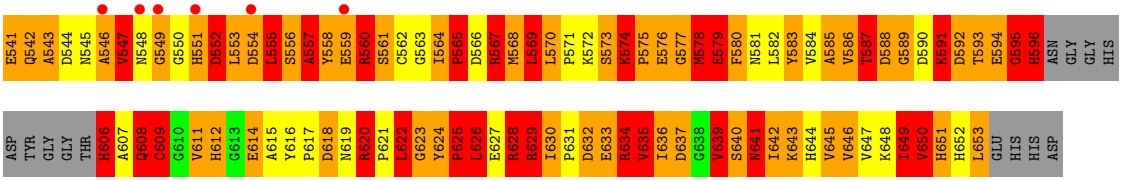


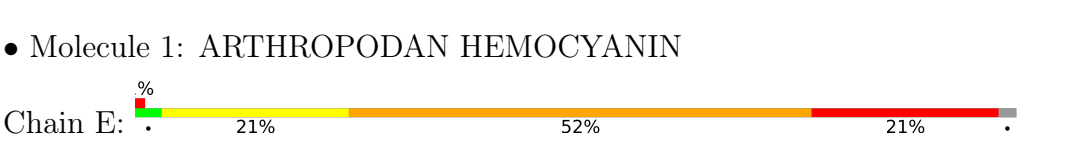
• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain D:



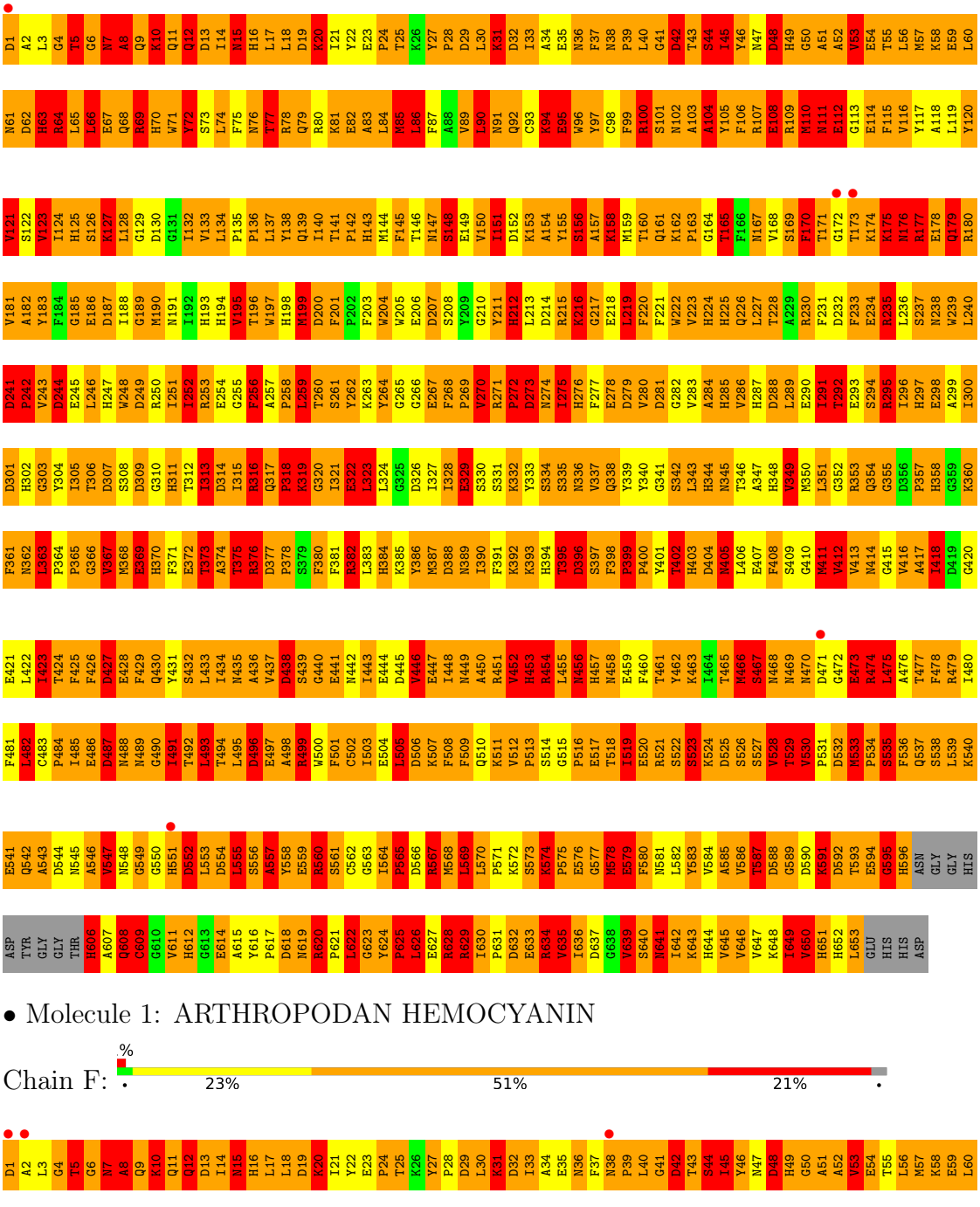






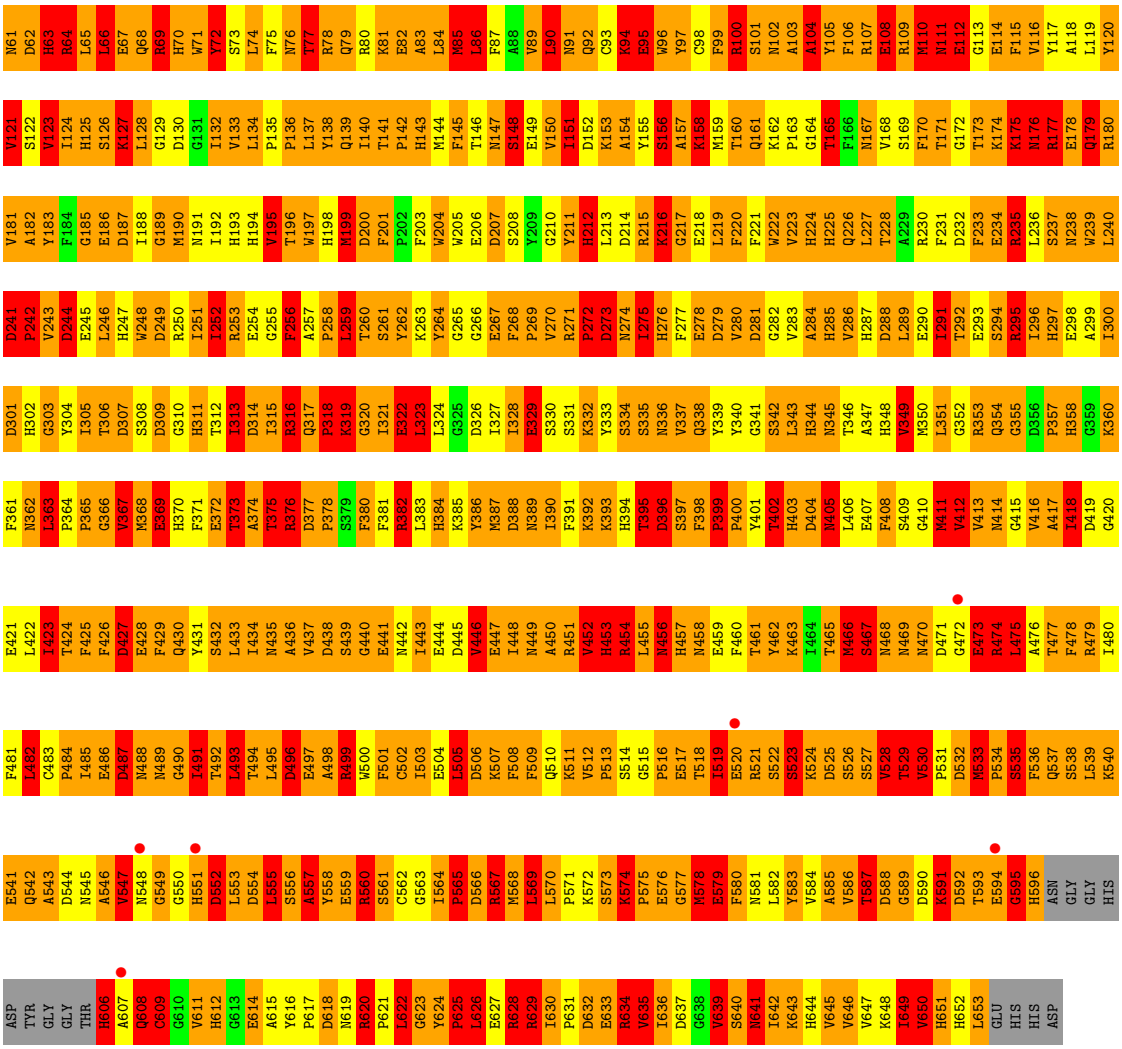
• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain E:



• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain F:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

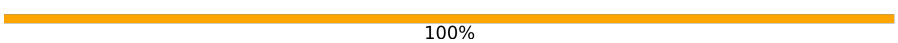
Chain G:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.80Å 193.10Å 122.20Å 90.00° 118.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 8.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.20) 71.9 (8.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	CORELS, PROLSQ	Depositor
R, R_{free}	0.221 , (Not available) 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 38.3	EDS
L-test for twinning[1]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.095 for -h-l,k,h 0.095 for l,k,-h-l 0.105 for h,-k,-h-l 0.097 for -h-l,-k,l 0.104 for l,-k,h	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	31790	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	2.16	163/5385 (3.0%)	4.71	1837/7301 (25.2%)
1	B	2.16	164/5385 (3.0%)	4.71	1833/7301 (25.1%)
1	C	2.16	163/5385 (3.0%)	4.71	1832/7301 (25.1%)
1	D	2.16	162/5385 (3.0%)	4.71	1834/7301 (25.1%)
1	E	2.16	163/5385 (3.0%)	4.71	1831/7301 (25.1%)
1	F	2.16	162/5385 (3.0%)	4.71	1836/7301 (25.1%)
All	All	2.16	977/32310 (3.0%)	4.71	11003/43806 (25.1%)

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	0	7
1	B	0	7
1	C	0	7
1	D	0	7
1	E	0	7
1	F	0	7
All	All	0	42

All (977) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	273	ASP	N-CA	11.35	1.60	1.46
1	C	273	ASP	N-CA	11.34	1.60	1.46
1	A	273	ASP	N-CA	11.33	1.60	1.46
1	D	273	ASP	N-CA	11.33	1.60	1.46
1	B	273	ASP	N-CA	11.33	1.60	1.46
1	F	273	ASP	N-CA	11.28	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	215	ARG	N-CA	10.26	1.58	1.46
1	E	215	ARG	N-CA	10.23	1.58	1.46
1	F	217	GLY	N-CA	10.23	1.60	1.45
1	B	215	ARG	N-CA	10.23	1.58	1.46
1	D	217	GLY	N-CA	10.23	1.60	1.45
1	F	215	ARG	N-CA	10.22	1.58	1.46
1	A	215	ARG	N-CA	10.22	1.58	1.46
1	C	217	GLY	N-CA	10.22	1.60	1.45
1	B	217	GLY	N-CA	10.21	1.60	1.45
1	A	217	GLY	N-CA	10.20	1.60	1.45
1	C	215	ARG	N-CA	10.20	1.58	1.46
1	E	217	GLY	N-CA	10.14	1.60	1.45
1	E	390	ILE	C-O	-9.02	1.14	1.23
1	A	390	ILE	C-O	-9.00	1.14	1.23
1	F	390	ILE	C-O	-8.99	1.14	1.23
1	C	390	ILE	C-O	-8.99	1.14	1.23
1	B	390	ILE	C-O	-8.97	1.14	1.23
1	D	390	ILE	C-O	-8.97	1.14	1.23
1	B	410	GLY	N-CA	8.69	1.57	1.45
1	F	410	GLY	N-CA	8.69	1.57	1.45
1	A	410	GLY	N-CA	8.67	1.57	1.45
1	E	410	GLY	N-CA	8.67	1.57	1.45
1	C	410	GLY	N-CA	8.66	1.57	1.45
1	D	410	GLY	N-CA	8.63	1.57	1.45
1	C	367	VAL	C-N	-8.32	1.21	1.33
1	F	367	VAL	C-N	-8.28	1.21	1.33
1	A	367	VAL	C-N	-8.28	1.21	1.33
1	D	367	VAL	C-N	-8.28	1.21	1.33
1	E	367	VAL	C-N	-8.26	1.21	1.33
1	B	367	VAL	C-N	-8.25	1.21	1.33
1	B	494	THR	CA-CB	8.17	1.64	1.53
1	E	494	THR	CA-CB	8.17	1.64	1.53
1	B	487	ASP	N-CA	-8.14	1.36	1.46
1	D	494	THR	CA-CB	8.13	1.64	1.53
1	D	487	ASP	N-CA	-8.12	1.36	1.46
1	A	494	THR	CA-CB	8.12	1.64	1.53
1	F	487	ASP	N-CA	-8.11	1.36	1.46
1	C	494	THR	CA-CB	8.11	1.64	1.53
1	D	551	HIS	CA-CB	8.10	1.66	1.53
1	E	487	ASP	N-CA	-8.09	1.36	1.46
1	C	551	HIS	CA-CB	8.09	1.66	1.53
1	F	494	THR	CA-CB	8.09	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	487	ASP	N-CA	-8.08	1.36	1.46
1	C	487	ASP	N-CA	-8.08	1.36	1.46
1	B	70	HIS	C-O	8.07	1.33	1.23
1	D	70	HIS	C-O	8.07	1.33	1.23
1	A	70	HIS	C-O	8.04	1.33	1.23
1	A	551	HIS	CA-CB	8.04	1.66	1.53
1	B	551	HIS	CA-CB	8.04	1.66	1.53
1	F	70	HIS	C-O	8.03	1.33	1.23
1	E	70	HIS	C-O	8.03	1.33	1.23
1	F	551	HIS	CA-CB	8.03	1.66	1.53
1	E	551	HIS	CA-CB	8.02	1.66	1.53
1	C	70	HIS	C-O	8.01	1.33	1.23
1	B	70	HIS	N-CA	7.96	1.55	1.46
1	E	70	HIS	N-CA	7.95	1.55	1.46
1	F	70	HIS	N-CA	7.95	1.55	1.46
1	A	70	HIS	N-CA	7.94	1.55	1.46
1	C	70	HIS	N-CA	7.92	1.55	1.46
1	D	70	HIS	N-CA	7.92	1.55	1.46
1	E	494	THR	N-CA	-7.90	1.37	1.46
1	C	132	ILE	CA-CB	7.88	1.63	1.54
1	E	132	ILE	CA-CB	7.88	1.63	1.54
1	B	132	ILE	CA-CB	7.88	1.63	1.54
1	D	132	ILE	CA-CB	7.88	1.63	1.54
1	C	494	THR	N-CA	-7.88	1.37	1.46
1	D	494	THR	N-CA	-7.88	1.37	1.46
1	A	494	THR	N-CA	-7.86	1.37	1.46
1	B	494	THR	N-CA	-7.86	1.37	1.46
1	F	494	THR	N-CA	-7.86	1.37	1.46
1	A	132	ILE	CA-CB	7.85	1.63	1.54
1	F	92	GLN	CA-CB	-7.83	1.41	1.53
1	F	132	ILE	CA-CB	7.82	1.63	1.54
1	C	92	GLN	CA-CB	-7.80	1.41	1.53
1	A	92	GLN	CA-CB	-7.79	1.41	1.53
1	B	92	GLN	CA-CB	-7.78	1.41	1.53
1	B	216	LYS	C-O	7.78	1.33	1.24
1	E	92	GLN	CA-CB	-7.76	1.41	1.53
1	D	92	GLN	CA-CB	-7.76	1.41	1.53
1	A	216	LYS	C-O	7.74	1.33	1.24
1	F	216	LYS	C-O	7.74	1.33	1.24
1	E	216	LYS	C-O	7.73	1.33	1.24
1	C	216	LYS	C-O	7.71	1.33	1.24
1	D	216	LYS	C-O	7.65	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	496	ASP	CA-CB	-7.57	1.40	1.53
1	E	496	ASP	CA-CB	-7.56	1.40	1.53
1	A	496	ASP	CA-CB	-7.54	1.40	1.53
1	F	496	ASP	CA-CB	-7.53	1.40	1.53
1	D	496	ASP	CA-CB	-7.51	1.40	1.53
1	C	496	ASP	CA-CB	-7.49	1.40	1.53
1	B	384	HIS	CD2-NE2	7.47	1.46	1.37
1	E	384	HIS	CD2-NE2	7.46	1.46	1.37
1	A	384	HIS	CD2-NE2	7.45	1.46	1.37
1	D	384	HIS	CD2-NE2	7.45	1.46	1.37
1	F	384	HIS	CD2-NE2	7.43	1.46	1.37
1	C	384	HIS	CD2-NE2	7.42	1.46	1.37
1	A	358	HIS	N-CA	7.27	1.55	1.46
1	E	358	HIS	N-CA	7.27	1.55	1.46
1	F	358	HIS	N-CA	7.26	1.55	1.46
1	C	454	ARG	N-CA	7.26	1.54	1.45
1	D	358	HIS	N-CA	7.26	1.55	1.46
1	A	454	ARG	N-CA	7.25	1.54	1.45
1	B	454	ARG	N-CA	7.25	1.54	1.45
1	C	358	HIS	N-CA	7.25	1.55	1.46
1	E	454	ARG	N-CA	7.24	1.54	1.45
1	B	358	HIS	N-CA	7.23	1.55	1.46
1	D	454	ARG	N-CA	7.23	1.54	1.45
1	B	214	ASP	C-O	7.20	1.33	1.24
1	A	214	ASP	C-O	7.20	1.33	1.24
1	D	214	ASP	C-O	7.19	1.33	1.24
1	F	454	ARG	N-CA	7.19	1.54	1.45
1	F	214	ASP	C-O	7.19	1.33	1.24
1	C	214	ASP	C-O	7.17	1.33	1.24
1	D	366	GLY	N-CA	7.14	1.51	1.44
1	E	214	ASP	C-O	7.13	1.32	1.24
1	F	366	GLY	N-CA	7.12	1.51	1.44
1	F	636	ILE	N-CA	7.09	1.54	1.46
1	A	636	ILE	N-CA	7.08	1.54	1.46
1	B	636	ILE	N-CA	7.08	1.54	1.46
1	B	143	HIS	CG-CD2	-7.08	1.28	1.35
1	F	214	ASP	N-CA	-7.07	1.37	1.46
1	F	480	ILE	CA-CB	7.07	1.63	1.54
1	C	366	GLY	N-CA	7.07	1.51	1.44
1	D	214	ASP	N-CA	-7.07	1.37	1.46
1	E	143	HIS	CG-CD2	-7.05	1.28	1.35
1	A	366	GLY	N-CA	7.05	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	366	GLY	N-CA	7.05	1.51	1.44
1	E	636	ILE	N-CA	7.05	1.54	1.46
1	E	85	MET	N-CA	7.05	1.55	1.46
1	A	143	HIS	CG-CD2	-7.04	1.28	1.35
1	F	85	MET	N-CA	7.04	1.55	1.46
1	B	480	ILE	CA-CB	7.04	1.63	1.54
1	C	636	ILE	N-CA	7.04	1.54	1.46
1	A	85	MET	N-CA	7.03	1.55	1.46
1	C	143	HIS	CG-CD2	-7.03	1.28	1.35
1	C	214	ASP	N-CA	-7.03	1.37	1.46
1	D	85	MET	N-CA	7.03	1.55	1.46
1	B	366	GLY	N-CA	7.03	1.51	1.44
1	A	214	ASP	N-CA	-7.03	1.37	1.46
1	B	85	MET	N-CA	7.03	1.55	1.46
1	B	214	ASP	N-CA	-7.02	1.37	1.46
1	D	636	ILE	N-CA	7.02	1.54	1.46
1	C	85	MET	N-CA	7.02	1.55	1.46
1	F	430	GLN	N-CA	7.02	1.54	1.46
1	F	143	HIS	CG-CD2	-7.02	1.28	1.35
1	A	430	GLN	N-CA	7.02	1.54	1.46
1	A	480	ILE	CA-CB	7.01	1.63	1.54
1	E	430	GLN	N-CA	7.01	1.54	1.46
1	D	143	HIS	CG-CD2	-6.99	1.28	1.35
1	C	430	GLN	N-CA	6.99	1.54	1.46
1	C	480	ILE	CA-CB	6.98	1.63	1.54
1	D	430	GLN	N-CA	6.98	1.54	1.46
1	B	430	GLN	N-CA	6.98	1.54	1.46
1	D	480	ILE	CA-CB	6.97	1.63	1.54
1	E	214	ASP	N-CA	-6.96	1.37	1.46
1	E	480	ILE	CA-CB	6.95	1.63	1.54
1	B	644	HIS	N-CA	6.86	1.54	1.46
1	A	644	HIS	N-CA	6.85	1.54	1.46
1	E	644	HIS	N-CA	6.84	1.54	1.46
1	C	644	HIS	N-CA	6.83	1.54	1.46
1	D	644	HIS	N-CA	6.83	1.54	1.46
1	F	644	HIS	N-CA	6.79	1.54	1.46
1	A	427	ASP	N-CA	-6.76	1.37	1.46
1	D	427	ASP	N-CA	-6.76	1.37	1.46
1	F	427	ASP	N-CA	-6.76	1.37	1.46
1	E	427	ASP	N-CA	-6.75	1.37	1.46
1	C	347	ALA	CA-CB	-6.72	1.42	1.53
1	C	427	ASP	N-CA	-6.72	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	427	ASP	N-CA	-6.71	1.37	1.46
1	F	125	HIS	CA-CB	6.70	1.64	1.53
1	C	393	LYS	C-N	-6.70	1.24	1.33
1	B	215	ARG	NE-CZ	6.70	1.40	1.33
1	C	125	HIS	CA-CB	6.69	1.64	1.53
1	D	393	LYS	C-N	-6.69	1.24	1.33
1	A	393	LYS	C-N	-6.69	1.24	1.33
1	F	393	LYS	C-N	-6.68	1.24	1.33
1	B	125	HIS	CA-CB	6.68	1.64	1.53
1	E	347	ALA	CA-CB	-6.68	1.42	1.53
1	A	125	HIS	CA-CB	6.68	1.64	1.53
1	A	347	ALA	CA-CB	-6.67	1.42	1.53
1	F	215	ARG	NE-CZ	6.67	1.40	1.33
1	D	125	HIS	CA-CB	6.67	1.64	1.53
1	F	347	ALA	CA-CB	-6.67	1.42	1.53
1	B	393	LYS	C-N	-6.67	1.24	1.33
1	B	347	ALA	CA-CB	-6.66	1.42	1.53
1	E	125	HIS	CA-CB	6.66	1.63	1.53
1	E	393	LYS	C-N	-6.66	1.24	1.33
1	A	215	ARG	NE-CZ	6.65	1.40	1.33
1	D	347	ALA	CA-CB	-6.65	1.42	1.53
1	D	215	ARG	NE-CZ	6.64	1.40	1.33
1	F	573	SER	N-CA	-6.64	1.38	1.47
1	B	573	SER	N-CA	-6.64	1.38	1.47
1	D	573	SER	N-CA	-6.63	1.38	1.47
1	E	215	ARG	NE-CZ	6.63	1.40	1.33
1	A	573	SER	N-CA	-6.62	1.38	1.47
1	E	573	SER	N-CA	-6.60	1.38	1.47
1	E	263	LYS	N-CA	6.59	1.54	1.46
1	C	215	ARG	NE-CZ	6.58	1.40	1.33
1	D	310	GLY	N-CA	6.58	1.54	1.44
1	E	310	GLY	N-CA	6.57	1.54	1.44
1	C	573	SER	N-CA	-6.56	1.38	1.47
1	A	263	LYS	N-CA	6.56	1.54	1.46
1	B	263	LYS	N-CA	6.56	1.54	1.46
1	B	492	THR	CA-CB	6.55	1.64	1.53
1	F	263	LYS	N-CA	6.55	1.54	1.46
1	B	494	THR	CA-C	-6.55	1.44	1.53
1	C	310	GLY	N-CA	6.55	1.54	1.44
1	F	310	GLY	N-CA	6.55	1.54	1.44
1	D	492	THR	CA-CB	6.54	1.64	1.53
1	F	494	THR	CA-C	-6.54	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	THR	CA-C	-6.54	1.44	1.53
1	B	310	GLY	N-CA	6.54	1.54	1.44
1	C	494	THR	CA-C	-6.54	1.44	1.53
1	E	494	THR	CA-C	-6.54	1.44	1.53
1	D	494	THR	CA-C	-6.54	1.44	1.53
1	A	310	GLY	N-CA	6.53	1.54	1.44
1	C	263	LYS	N-CA	6.52	1.54	1.46
1	E	492	THR	CA-CB	6.52	1.64	1.53
1	A	492	THR	CA-CB	6.52	1.64	1.53
1	C	492	THR	CA-CB	6.52	1.64	1.53
1	D	263	LYS	N-CA	6.52	1.54	1.46
1	D	279	ASP	N-CA	6.50	1.54	1.46
1	D	52	ALA	C-N	-6.49	1.25	1.33
1	B	205	TRP	C-N	-6.49	1.24	1.33
1	F	175	LYS	C-N	-6.49	1.24	1.33
1	F	492	THR	CA-CB	6.48	1.64	1.53
1	B	279	ASP	N-CA	6.47	1.54	1.46
1	C	279	ASP	N-CA	6.46	1.54	1.46
1	A	279	ASP	N-CA	6.45	1.54	1.46
1	C	175	LYS	C-N	-6.45	1.24	1.33
1	A	175	LYS	C-N	-6.45	1.24	1.33
1	B	175	LYS	C-N	-6.44	1.24	1.33
1	C	205	TRP	C-N	-6.44	1.24	1.33
1	E	175	LYS	C-N	-6.43	1.24	1.33
1	F	205	TRP	C-N	-6.43	1.24	1.33
1	A	205	TRP	C-N	-6.43	1.24	1.33
1	E	205	TRP	C-N	-6.43	1.24	1.33
1	D	175	LYS	C-N	-6.43	1.24	1.33
1	E	279	ASP	N-CA	6.42	1.54	1.46
1	A	52	ALA	C-N	-6.42	1.26	1.33
1	F	52	ALA	C-N	-6.42	1.26	1.33
1	D	205	TRP	C-N	-6.41	1.24	1.33
1	C	52	ALA	C-N	-6.40	1.26	1.33
1	E	52	ALA	C-N	-6.40	1.26	1.33
1	F	279	ASP	N-CA	6.39	1.54	1.46
1	B	52	ALA	C-N	-6.36	1.26	1.33
1	C	219	LEU	N-CA	6.35	1.53	1.46
1	C	332	LYS	C-N	-6.35	1.24	1.33
1	A	332	LYS	C-N	-6.35	1.24	1.33
1	F	332	LYS	C-N	-6.34	1.24	1.33
1	E	332	LYS	C-N	-6.33	1.24	1.33
1	F	219	LEU	N-CA	6.33	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	219	LEU	N-CA	6.33	1.53	1.46
1	B	332	LYS	C-N	-6.32	1.24	1.33
1	A	219	LEU	N-CA	6.32	1.53	1.46
1	E	219	LEU	N-CA	6.31	1.53	1.46
1	D	332	LYS	C-N	-6.30	1.24	1.33
1	D	333	TYR	C-O	6.30	1.32	1.24
1	B	96	TRP	C-O	6.29	1.31	1.24
1	B	219	LEU	N-CA	6.29	1.53	1.46
1	E	96	TRP	C-O	6.29	1.31	1.24
1	E	333	TYR	C-O	6.29	1.32	1.24
1	C	333	TYR	C-O	6.27	1.32	1.24
1	A	333	TYR	C-O	6.27	1.32	1.24
1	B	266	GLY	N-CA	6.27	1.53	1.45
1	F	333	TYR	C-O	6.27	1.32	1.24
1	C	351	LEU	C-O	6.26	1.32	1.24
1	B	351	LEU	C-O	6.26	1.32	1.24
1	D	351	LEU	C-O	6.26	1.32	1.24
1	E	266	GLY	N-CA	6.26	1.53	1.45
1	F	259	LEU	C-N	-6.25	1.24	1.33
1	D	96	TRP	C-O	6.25	1.31	1.24
1	E	351	LEU	C-O	6.25	1.32	1.24
1	C	266	GLY	N-CA	6.25	1.53	1.45
1	A	96	TRP	C-O	6.24	1.31	1.24
1	A	266	GLY	N-CA	6.24	1.53	1.45
1	C	191	ASN	CA-CB	-6.24	1.43	1.53
1	A	351	LEU	C-O	6.24	1.32	1.24
1	C	453	HIS	C-O	6.24	1.31	1.24
1	E	453	HIS	C-O	6.23	1.31	1.24
1	B	333	TYR	C-O	6.23	1.32	1.24
1	D	266	GLY	N-CA	6.23	1.53	1.45
1	F	96	TRP	C-O	6.23	1.31	1.24
1	A	191	ASN	CA-CB	-6.23	1.43	1.53
1	F	266	GLY	N-CA	6.22	1.53	1.45
1	D	242	PRO	C-O	6.22	1.32	1.24
1	B	259	LEU	C-N	-6.21	1.24	1.33
1	E	242	PRO	C-O	6.21	1.32	1.24
1	F	191	ASN	CA-CB	-6.21	1.43	1.53
1	C	96	TRP	C-O	6.21	1.31	1.24
1	F	216	LYS	CA-CB	-6.21	1.43	1.53
1	A	259	LEU	C-N	-6.21	1.24	1.33
1	B	453	HIS	C-O	6.21	1.31	1.24
1	A	453	HIS	C-O	6.20	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	ASN	C-O	6.19	1.31	1.24
1	F	351	LEU	C-O	6.19	1.32	1.24
1	D	259	LEU	C-N	-6.19	1.24	1.33
1	D	191	ASN	CA-CB	-6.19	1.43	1.53
1	A	242	PRO	C-O	6.18	1.31	1.24
1	B	191	ASN	CA-CB	-6.18	1.43	1.53
1	E	216	LYS	CA-CB	-6.18	1.43	1.53
1	E	264	TYR	CA-C	6.18	1.60	1.52
1	C	242	PRO	C-O	6.17	1.31	1.24
1	B	216	LYS	CA-CB	-6.17	1.43	1.53
1	C	91	ASN	C-O	6.17	1.31	1.24
1	A	216	LYS	CA-CB	-6.16	1.43	1.53
1	D	216	LYS	CA-CB	-6.16	1.43	1.53
1	E	91	ASN	C-O	6.16	1.31	1.24
1	E	259	LEU	C-N	-6.16	1.24	1.33
1	A	91	ASN	C-O	6.15	1.31	1.24
1	E	191	ASN	CA-CB	-6.15	1.43	1.53
1	D	453	HIS	C-O	6.15	1.31	1.24
1	B	91	ASN	C-O	6.15	1.31	1.24
1	B	113	GLY	N-CA	6.15	1.54	1.45
1	F	242	PRO	C-O	6.15	1.31	1.24
1	D	264	TYR	CA-C	6.14	1.60	1.52
1	E	329	GLU	C-O	-6.14	1.16	1.24
1	F	91	ASN	C-O	6.14	1.31	1.24
1	F	453	HIS	C-O	6.14	1.31	1.24
1	B	242	PRO	C-O	6.14	1.31	1.24
1	C	259	LEU	C-N	-6.12	1.25	1.33
1	C	264	TYR	CA-C	6.12	1.60	1.52
1	C	216	LYS	CA-CB	-6.11	1.43	1.53
1	A	264	TYR	CA-C	6.11	1.59	1.52
1	E	266	GLY	C-O	6.10	1.29	1.23
1	F	584	VAL	N-CA	6.10	1.54	1.46
1	E	113	GLY	N-CA	6.10	1.54	1.45
1	B	247	HIS	CD2-NE2	6.10	1.44	1.37
1	E	247	HIS	CD2-NE2	6.10	1.44	1.37
1	F	113	GLY	N-CA	6.09	1.54	1.45
1	F	247	HIS	CD2-NE2	6.09	1.44	1.37
1	B	329	GLU	C-O	-6.09	1.16	1.24
1	B	264	TYR	CA-C	6.09	1.59	1.52
1	D	247	HIS	CD2-NE2	6.08	1.44	1.37
1	D	329	GLU	C-O	-6.08	1.16	1.24
1	A	113	GLY	N-CA	6.08	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLU	C-O	-6.08	1.16	1.24
1	F	266	GLY	C-O	6.08	1.29	1.23
1	C	113	GLY	N-CA	6.08	1.54	1.45
1	F	264	TYR	CA-C	6.07	1.59	1.52
1	D	113	GLY	N-CA	6.07	1.54	1.45
1	D	169	SER	C-O	6.06	1.31	1.23
1	E	583	TYR	CA-CB	6.06	1.62	1.53
1	D	584	VAL	N-CA	6.06	1.54	1.46
1	A	247	HIS	CD2-NE2	6.05	1.44	1.37
1	D	583	TYR	CA-CB	6.05	1.62	1.53
1	F	329	GLU	C-O	-6.05	1.16	1.24
1	A	583	TYR	CA-CB	6.04	1.62	1.53
1	F	583	TYR	CA-CB	6.04	1.62	1.53
1	A	266	GLY	C-O	6.04	1.29	1.23
1	A	584	VAL	N-CA	6.04	1.54	1.46
1	B	584	VAL	N-CA	6.04	1.54	1.46
1	B	266	GLY	C-O	6.03	1.29	1.23
1	B	311	HIS	ND1-CE1	6.03	1.38	1.32
1	A	232	ASP	N-CA	6.02	1.53	1.46
1	C	329	GLU	C-O	-6.02	1.16	1.24
1	C	247	HIS	CD2-NE2	6.02	1.44	1.37
1	B	232	ASP	N-CA	6.02	1.53	1.46
1	B	272	PRO	N-CA	-6.01	1.39	1.47
1	A	311	HIS	ND1-CE1	6.01	1.38	1.32
1	E	584	VAL	N-CA	6.01	1.54	1.46
1	F	272	PRO	N-CA	-6.01	1.39	1.47
1	B	235	ARG	C-O	6.01	1.31	1.24
1	B	583	TYR	CA-CB	6.01	1.62	1.53
1	D	232	ASP	N-CA	6.01	1.53	1.46
1	D	266	GLY	C-O	6.01	1.29	1.23
1	E	235	ARG	C-O	6.01	1.31	1.24
1	C	583	TYR	CA-CB	6.00	1.62	1.53
1	F	177	ARG	C-O	6.00	1.31	1.24
1	C	232	ASP	N-CA	6.00	1.53	1.46
1	F	232	ASP	N-CA	6.00	1.53	1.46
1	C	266	GLY	C-O	5.99	1.28	1.23
1	D	311	HIS	ND1-CE1	5.99	1.38	1.32
1	C	169	SER	C-O	5.99	1.31	1.23
1	E	373	THR	CB-OG1	5.99	1.53	1.43
1	C	235	ARG	C-O	5.99	1.31	1.24
1	D	373	THR	CB-OG1	5.99	1.53	1.43
1	C	584	VAL	N-CA	5.99	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	375	THR	N-CA	5.99	1.53	1.46
1	D	272	PRO	N-CA	-5.99	1.39	1.47
1	E	3	LEU	CA-C	5.99	1.60	1.53
1	E	311	HIS	ND1-CE1	5.99	1.38	1.32
1	A	169	SER	C-O	5.98	1.31	1.23
1	B	177	ARG	C-O	5.98	1.31	1.24
1	C	3	LEU	CA-C	5.98	1.60	1.53
1	E	232	ASP	N-CA	5.97	1.53	1.46
1	A	3	LEU	CA-C	5.96	1.60	1.53
1	A	235	ARG	C-O	5.96	1.31	1.24
1	C	311	HIS	ND1-CE1	5.96	1.38	1.32
1	D	375	THR	N-CA	5.96	1.53	1.46
1	A	373	THR	CB-OG1	5.96	1.53	1.43
1	B	373	THR	CB-OG1	5.96	1.53	1.43
1	D	3	LEU	CA-C	5.96	1.60	1.53
1	A	272	PRO	N-CA	-5.96	1.39	1.47
1	F	235	ARG	C-O	5.96	1.31	1.24
1	E	169	SER	C-O	5.96	1.31	1.23
1	F	3	LEU	CA-C	5.96	1.60	1.53
1	E	375	THR	N-CA	5.95	1.53	1.46
1	F	373	THR	CB-OG1	5.95	1.53	1.43
1	C	375	THR	N-CA	5.94	1.53	1.46
1	A	375	THR	N-CA	5.93	1.53	1.46
1	B	3	LEU	CA-C	5.93	1.60	1.53
1	C	373	THR	CB-OG1	5.93	1.53	1.43
1	B	169	SER	C-O	5.93	1.31	1.23
1	B	375	THR	N-CA	5.93	1.53	1.46
1	A	177	ARG	C-O	5.92	1.31	1.24
1	F	311	HIS	ND1-CE1	5.92	1.38	1.32
1	E	632	ASP	N-CA	5.92	1.53	1.46
1	C	177	ARG	C-O	5.92	1.31	1.24
1	C	497	GLU	CA-CB	-5.92	1.43	1.53
1	B	632	ASP	N-CA	5.91	1.53	1.46
1	C	279	ASP	CA-CB	-5.91	1.44	1.53
1	D	235	ARG	C-O	5.91	1.31	1.24
1	E	272	PRO	N-CA	-5.91	1.39	1.47
1	D	177	ARG	C-O	5.91	1.31	1.24
1	F	169	SER	C-O	5.91	1.31	1.23
1	E	386	TYR	C-O	5.90	1.30	1.24
1	E	279	ASP	CA-CB	-5.90	1.44	1.53
1	C	369	GLU	C-N	-5.89	1.26	1.33
1	C	499	ARG	CZ-NH2	5.89	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	279	ASP	CA-CB	-5.89	1.44	1.53
1	D	386	TYR	C-O	5.89	1.30	1.24
1	E	177	ARG	C-O	5.89	1.31	1.24
1	A	279	ASP	CA-CB	-5.88	1.44	1.53
1	C	272	PRO	N-CA	-5.88	1.39	1.47
1	F	386	TYR	C-O	5.88	1.30	1.24
1	B	279	ASP	CA-CB	-5.88	1.44	1.53
1	D	564	ILE	C-N	-5.87	1.26	1.33
1	D	369	GLU	C-N	-5.87	1.26	1.33
1	D	632	ASP	N-CA	5.87	1.53	1.46
1	C	386	TYR	C-O	5.87	1.30	1.24
1	F	482	LEU	C-O	5.86	1.30	1.23
1	C	632	ASP	N-CA	5.86	1.53	1.46
1	A	632	ASP	N-CA	5.86	1.53	1.46
1	B	386	TYR	C-O	5.86	1.30	1.24
1	F	279	ASP	CA-CB	-5.86	1.44	1.53
1	D	645	VAL	CA-C	-5.85	1.45	1.52
1	A	386	TYR	C-O	5.85	1.30	1.24
1	B	499	ARG	CZ-NH2	5.84	1.41	1.33
1	C	482	LEU	C-O	5.84	1.30	1.23
1	D	567	ARG	CD-NE	5.84	1.54	1.46
1	F	369	GLU	C-N	-5.84	1.26	1.33
1	A	369	GLU	C-N	-5.84	1.26	1.33
1	E	564	ILE	C-N	-5.84	1.26	1.33
1	E	567	ARG	CD-NE	5.83	1.54	1.46
1	F	499	ARG	CZ-NH2	5.83	1.41	1.33
1	E	169	SER	CA-CB	5.83	1.63	1.53
1	A	499	ARG	CZ-NH2	5.83	1.41	1.33
1	B	645	VAL	CA-C	-5.83	1.45	1.52
1	A	567	ARG	CD-NE	5.83	1.54	1.46
1	E	578	MET	N-CA	5.83	1.53	1.45
1	B	567	ARG	CD-NE	5.83	1.54	1.46
1	C	564	ILE	C-N	-5.83	1.26	1.33
1	E	369	GLU	C-N	-5.83	1.26	1.33
1	D	451	ARG	N-CA	5.82	1.53	1.46
1	F	578	MET	N-CA	5.82	1.53	1.45
1	B	169	SER	CA-CB	5.82	1.63	1.53
1	F	567	ARG	CD-NE	5.82	1.54	1.46
1	D	499	ARG	CZ-NH2	5.82	1.41	1.33
1	D	578	MET	N-CA	5.82	1.53	1.45
1	A	645	VAL	CA-C	-5.82	1.45	1.52
1	D	482	LEU	C-O	5.82	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	482	LEU	C-O	5.82	1.30	1.23
1	F	632	ASP	N-CA	5.82	1.53	1.46
1	B	369	GLU	C-N	-5.81	1.26	1.33
1	A	482	LEU	C-O	5.81	1.30	1.23
1	E	499	ARG	CZ-NH2	5.81	1.41	1.33
1	A	564	ILE	C-N	-5.81	1.26	1.33
1	D	169	SER	CA-CB	5.81	1.63	1.53
1	E	497	GLU	CA-CB	-5.81	1.43	1.53
1	B	578	MET	N-CA	5.80	1.53	1.45
1	A	169	SER	CA-CB	5.80	1.63	1.53
1	F	169	SER	CA-CB	5.80	1.63	1.53
1	F	497	GLU	CA-CB	-5.80	1.43	1.53
1	C	169	SER	CA-CB	5.80	1.63	1.53
1	C	645	VAL	CA-C	-5.80	1.45	1.52
1	F	645	VAL	CA-C	-5.79	1.45	1.52
1	A	578	MET	N-CA	5.79	1.53	1.45
1	C	578	MET	N-CA	5.79	1.53	1.45
1	E	645	VAL	CA-C	-5.79	1.45	1.52
1	F	627	GLU	N-CA	5.79	1.53	1.46
1	C	567	ARG	CD-NE	5.78	1.54	1.46
1	F	564	ILE	C-N	-5.78	1.26	1.33
1	B	503	ILE	C-N	-5.78	1.25	1.33
1	F	203	PHE	C-O	5.78	1.31	1.24
1	A	497	GLU	CA-CB	-5.77	1.43	1.53
1	B	497	GLU	CA-CB	-5.77	1.43	1.53
1	C	451	ARG	N-CA	5.77	1.53	1.46
1	C	627	GLU	N-CA	5.77	1.53	1.46
1	F	129	GLY	C-N	-5.77	1.26	1.33
1	D	272	PRO	C-O	5.77	1.31	1.24
1	F	451	ARG	N-CA	5.77	1.53	1.46
1	B	564	ILE	C-N	-5.77	1.26	1.33
1	D	203	PHE	C-O	5.76	1.31	1.24
1	D	627	GLU	N-CA	5.76	1.53	1.46
1	B	482	LEU	C-O	5.76	1.30	1.23
1	E	503	ILE	C-N	-5.76	1.25	1.33
1	A	627	GLU	N-CA	5.75	1.53	1.46
1	D	497	GLU	CA-CB	-5.75	1.43	1.53
1	E	451	ARG	N-CA	5.75	1.53	1.46
1	A	203	PHE	C-O	5.75	1.31	1.24
1	A	451	ARG	N-CA	5.75	1.53	1.46
1	C	272	PRO	C-O	5.75	1.31	1.24
1	C	203	PHE	C-O	5.75	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	174	LYS	N-CA	5.75	1.53	1.46
1	E	627	GLU	N-CA	5.75	1.53	1.46
1	B	627	GLU	N-CA	5.74	1.53	1.46
1	E	129	GLY	C-N	-5.74	1.26	1.33
1	F	272	PRO	C-O	5.74	1.31	1.24
1	C	129	GLY	C-N	-5.73	1.26	1.33
1	B	129	GLY	C-N	-5.73	1.26	1.33
1	A	272	PRO	C-O	5.73	1.31	1.24
1	A	129	GLY	C-N	-5.73	1.26	1.33
1	B	174	LYS	N-CA	5.72	1.53	1.46
1	A	503	ILE	C-N	-5.72	1.25	1.33
1	B	203	PHE	C-O	5.72	1.31	1.24
1	D	326	ASP	CA-CB	-5.71	1.44	1.53
1	B	272	PRO	C-O	5.71	1.31	1.24
1	E	203	PHE	C-O	5.71	1.31	1.24
1	F	634	ARG	C-O	5.71	1.31	1.24
1	C	174	LYS	N-CA	5.70	1.53	1.46
1	C	503	ILE	C-N	-5.70	1.25	1.33
1	B	451	ARG	N-CA	5.70	1.52	1.46
1	E	326	ASP	CA-CB	-5.70	1.44	1.53
1	F	503	ILE	C-N	-5.70	1.25	1.33
1	D	634	ARG	C-O	5.70	1.31	1.24
1	C	634	ARG	C-O	5.69	1.31	1.24
1	E	272	PRO	C-O	5.69	1.31	1.24
1	A	174	LYS	N-CA	5.69	1.53	1.46
1	A	326	ASP	CA-CB	-5.69	1.44	1.53
1	C	326	ASP	CA-CB	-5.69	1.44	1.53
1	D	129	GLY	C-N	-5.68	1.26	1.33
1	E	143	HIS	CD2-NE2	5.67	1.44	1.37
1	E	174	LYS	N-CA	5.67	1.53	1.46
1	A	634	ARG	C-O	5.67	1.31	1.24
1	B	143	HIS	CD2-NE2	5.67	1.44	1.37
1	D	503	ILE	C-N	-5.67	1.25	1.33
1	F	143	HIS	CD2-NE2	5.67	1.44	1.37
1	F	326	ASP	CA-CB	-5.67	1.44	1.53
1	B	634	ARG	C-O	5.66	1.31	1.24
1	B	326	ASP	CA-CB	-5.66	1.44	1.53
1	D	174	LYS	N-CA	5.66	1.53	1.46
1	E	606	HIS	CA-CB	5.65	1.64	1.53
1	C	270	VAL	N-CA	5.65	1.53	1.46
1	A	606	HIS	CA-CB	5.64	1.64	1.53
1	A	143	HIS	CD2-NE2	5.64	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	143	HIS	CD2-NE2	5.63	1.44	1.37
1	D	143	HIS	CD2-NE2	5.63	1.44	1.37
1	C	606	HIS	CA-CB	5.63	1.64	1.53
1	E	634	ARG	C-O	5.63	1.31	1.24
1	D	606	HIS	CA-CB	5.62	1.64	1.53
1	B	143	HIS	C-N	-5.62	1.25	1.33
1	F	606	HIS	CA-CB	5.62	1.64	1.53
1	B	606	HIS	CA-CB	5.62	1.64	1.53
1	D	343	LEU	C-N	-5.62	1.25	1.33
1	E	541	GLU	C-N	-5.62	1.26	1.34
1	C	410	GLY	C-N	-5.61	1.25	1.33
1	D	143	HIS	C-N	-5.61	1.25	1.33
1	B	343	LEU	C-N	-5.60	1.25	1.33
1	E	410	GLY	C-N	-5.60	1.25	1.33
1	D	541	GLU	C-N	-5.60	1.26	1.34
1	B	541	GLU	C-N	-5.60	1.26	1.34
1	C	541	GLU	C-N	-5.60	1.26	1.34
1	A	270	VAL	N-CA	5.59	1.53	1.46
1	F	343	LEU	C-N	-5.59	1.25	1.33
1	E	270	VAL	N-CA	5.59	1.53	1.46
1	F	489	ASN	CA-CB	-5.59	1.46	1.54
1	A	541	GLU	C-N	-5.59	1.26	1.34
1	D	440	GLY	N-CA	5.58	1.53	1.45
1	A	456	ASN	CA-CB	-5.58	1.44	1.53
1	B	440	GLY	N-CA	5.58	1.53	1.45
1	D	456	ASN	CA-CB	-5.58	1.44	1.53
1	F	456	ASN	CA-CB	-5.58	1.44	1.53
1	A	143	HIS	C-N	-5.58	1.25	1.33
1	A	343	LEU	C-N	-5.58	1.25	1.33
1	C	456	ASN	CA-CB	-5.58	1.44	1.53
1	E	456	ASN	CA-CB	-5.58	1.44	1.53
1	B	456	ASN	CA-CB	-5.58	1.44	1.53
1	D	270	VAL	N-CA	5.58	1.53	1.46
1	C	343	LEU	C-N	-5.57	1.25	1.33
1	F	541	GLU	C-N	-5.57	1.26	1.34
1	A	410	GLY	C-N	-5.56	1.25	1.33
1	E	143	HIS	C-N	-5.56	1.25	1.33
1	F	143	HIS	C-N	-5.56	1.25	1.33
1	B	489	ASN	CA-CB	-5.56	1.46	1.54
1	B	270	VAL	N-CA	5.56	1.53	1.46
1	D	410	GLY	C-N	-5.56	1.25	1.33
1	F	410	GLY	C-N	-5.56	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	ALA	CA-C	-5.55	1.45	1.52
1	F	76	ASN	C-O	5.55	1.30	1.24
1	D	499	ARG	C-O	5.55	1.31	1.24
1	E	343	LEU	C-N	-5.55	1.25	1.33
1	C	499	ARG	C-O	5.54	1.31	1.24
1	D	103	ALA	CA-C	-5.54	1.45	1.52
1	F	270	VAL	N-CA	5.54	1.53	1.46
1	A	440	GLY	N-CA	5.54	1.53	1.45
1	D	489	ASN	CA-CB	-5.54	1.46	1.54
1	B	76	ASN	C-O	5.53	1.30	1.24
1	A	76	ASN	C-O	5.52	1.30	1.24
1	A	174	LYS	C-O	5.52	1.30	1.23
1	B	410	GLY	C-N	-5.52	1.25	1.33
1	C	143	HIS	C-N	-5.52	1.25	1.33
1	E	174	LYS	C-O	5.52	1.30	1.23
1	C	440	GLY	N-CA	5.52	1.53	1.45
1	A	489	ASN	CA-CB	-5.51	1.46	1.54
1	B	174	LYS	C-O	5.51	1.30	1.23
1	F	440	GLY	N-CA	5.51	1.53	1.45
1	A	499	ARG	C-O	5.51	1.30	1.24
1	B	647	VAL	CA-CB	-5.51	1.47	1.54
1	C	76	ASN	C-O	5.51	1.30	1.24
1	C	103	ALA	CA-C	-5.51	1.45	1.52
1	B	499	ARG	C-O	5.51	1.30	1.24
1	F	647	VAL	CA-CB	-5.51	1.47	1.54
1	C	174	LYS	C-O	5.51	1.30	1.23
1	C	96	TRP	CA-CB	-5.50	1.44	1.53
1	D	174	LYS	C-O	5.50	1.30	1.23
1	A	103	ALA	CA-C	-5.50	1.45	1.52
1	F	174	LYS	C-O	5.50	1.30	1.23
1	E	489	ASN	CA-CB	-5.49	1.46	1.54
1	E	499	ARG	C-O	5.49	1.30	1.24
1	A	96	TRP	CA-CB	-5.49	1.44	1.53
1	F	499	ARG	C-O	5.48	1.30	1.24
1	C	435	ASN	CA-CB	-5.48	1.44	1.53
1	D	647	VAL	CA-CB	-5.48	1.47	1.54
1	E	96	TRP	CA-CB	-5.48	1.44	1.53
1	E	647	VAL	CA-CB	-5.48	1.47	1.54
1	E	440	GLY	N-CA	5.48	1.53	1.45
1	F	103	ALA	CA-C	-5.47	1.45	1.52
1	A	647	VAL	CA-CB	-5.47	1.47	1.54
1	E	76	ASN	C-O	5.47	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	TRP	CA-CB	-5.47	1.44	1.53
1	D	401	TYR	N-CA	5.46	1.52	1.45
1	C	193	HIS	ND1-CE1	5.46	1.38	1.32
1	E	103	ALA	CA-C	-5.46	1.45	1.52
1	C	489	ASN	CA-CB	-5.46	1.46	1.54
1	C	647	VAL	CA-CB	-5.46	1.47	1.54
1	F	193	HIS	ND1-CE1	5.46	1.38	1.32
1	F	96	TRP	CA-CB	-5.45	1.44	1.53
1	B	401	TYR	N-CA	5.45	1.52	1.45
1	C	401	TYR	N-CA	5.44	1.52	1.45
1	D	96	TRP	CA-CB	-5.44	1.44	1.53
1	E	84	LEU	CA-C	-5.44	1.45	1.52
1	B	84	LEU	CA-C	-5.44	1.45	1.52
1	F	401	TYR	N-CA	5.43	1.52	1.45
1	A	84	LEU	CA-C	-5.43	1.45	1.52
1	C	330	SER	CB-OG	-5.43	1.31	1.42
1	B	435	ASN	CA-CB	-5.43	1.44	1.53
1	B	592	ASP	C-N	-5.43	1.26	1.33
1	E	435	ASN	CA-CB	-5.43	1.44	1.53
1	C	84	LEU	CA-C	-5.42	1.45	1.52
1	D	435	ASN	CA-CB	-5.42	1.44	1.53
1	E	330	SER	CB-OG	-5.42	1.31	1.42
1	E	285	HIS	CA-C	-5.42	1.46	1.52
1	D	76	ASN	C-O	5.42	1.30	1.24
1	A	435	ASN	CA-CB	-5.42	1.44	1.53
1	F	330	SER	CB-OG	-5.41	1.31	1.42
1	D	330	SER	CB-OG	-5.41	1.31	1.42
1	E	592	ASP	C-N	-5.41	1.26	1.33
1	A	330	SER	CB-OG	-5.41	1.31	1.42
1	F	84	LEU	CA-C	-5.41	1.45	1.52
1	C	293	GLU	CA-CB	-5.41	1.44	1.53
1	F	236	LEU	N-CA	5.41	1.52	1.46
1	E	401	TYR	N-CA	5.40	1.52	1.45
1	A	401	TYR	N-CA	5.40	1.52	1.45
1	B	330	SER	CB-OG	-5.40	1.31	1.42
1	E	393	LYS	C-O	-5.40	1.17	1.24
1	D	84	LEU	CA-C	-5.40	1.45	1.52
1	F	293	GLU	CA-CB	-5.40	1.44	1.53
1	B	293	GLU	CA-CB	-5.39	1.44	1.53
1	E	193	HIS	ND1-CE1	5.39	1.38	1.32
1	E	377	ASP	C-N	-5.39	1.27	1.33
1	A	193	HIS	ND1-CE1	5.39	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	89	VAL	CA-CB	-5.39	1.47	1.54
1	B	236	LEU	N-CA	5.39	1.52	1.46
1	D	393	LYS	C-O	-5.38	1.17	1.24
1	F	447	GLU	CA-C	-5.38	1.46	1.52
1	B	457	HIS	CG-ND1	-5.38	1.32	1.38
1	A	293	GLU	CA-CB	-5.38	1.44	1.53
1	B	285	HIS	CA-C	-5.38	1.46	1.52
1	E	89	VAL	CA-CB	-5.38	1.47	1.54
1	F	592	ASP	C-N	-5.38	1.26	1.33
1	C	336	ASN	C-N	-5.38	1.28	1.34
1	D	447	GLU	CA-C	-5.37	1.46	1.52
1	F	377	ASP	C-N	-5.37	1.27	1.33
1	F	435	ASN	CA-CB	-5.37	1.44	1.53
1	E	336	ASN	C-N	-5.37	1.28	1.34
1	C	447	GLU	CA-C	-5.37	1.46	1.52
1	D	457	HIS	CG-ND1	-5.37	1.32	1.38
1	A	377	ASP	C-N	-5.36	1.27	1.33
1	A	592	ASP	C-N	-5.36	1.26	1.33
1	E	293	GLU	CA-CB	-5.36	1.44	1.53
1	B	393	LYS	C-O	-5.36	1.17	1.24
1	D	377	ASP	C-N	-5.36	1.27	1.33
1	C	236	LEU	N-CA	5.36	1.52	1.46
1	E	457	HIS	CG-ND1	-5.36	1.32	1.38
1	C	592	ASP	C-N	-5.36	1.26	1.33
1	B	447	GLU	CA-C	-5.36	1.46	1.52
1	C	377	ASP	C-N	-5.36	1.27	1.33
1	D	592	ASP	C-N	-5.36	1.26	1.33
1	D	336	ASN	C-N	-5.36	1.28	1.34
1	E	447	GLU	CA-C	-5.35	1.46	1.52
1	A	393	LYS	C-O	-5.35	1.17	1.24
1	D	293	GLU	CA-CB	-5.35	1.44	1.53
1	A	236	LEU	N-CA	5.35	1.52	1.46
1	A	285	HIS	CA-C	-5.35	1.46	1.52
1	F	650	VAL	CA-CB	-5.35	1.47	1.54
1	A	336	ASN	C-N	-5.34	1.28	1.34
1	E	650	VAL	CA-CB	-5.34	1.47	1.54
1	A	89	VAL	CA-CB	-5.34	1.47	1.54
1	F	89	VAL	CA-CB	-5.34	1.47	1.54
1	A	447	GLU	CA-C	-5.34	1.46	1.52
1	D	236	LEU	N-CA	5.33	1.52	1.46
1	F	179	GLN	N-CA	5.33	1.53	1.46
1	B	89	VAL	CA-CB	-5.33	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	650	VAL	CA-CB	-5.33	1.47	1.54
1	D	193	HIS	ND1-CE1	5.33	1.37	1.32
1	D	285	HIS	CA-C	-5.33	1.46	1.52
1	E	236	LEU	N-CA	5.33	1.52	1.46
1	D	89	VAL	CA-CB	-5.33	1.47	1.54
1	D	179	GLN	N-CA	5.33	1.53	1.46
1	B	377	ASP	C-N	-5.33	1.27	1.33
1	F	393	LYS	C-O	-5.33	1.17	1.24
1	B	650	VAL	CA-CB	-5.32	1.47	1.54
1	F	205	TRP	CA-C	-5.32	1.45	1.52
1	F	285	HIS	CA-C	-5.32	1.46	1.52
1	D	620	ARG	N-CA	5.32	1.54	1.45
1	A	650	VAL	CA-CB	-5.32	1.47	1.54
1	D	205	TRP	CA-C	-5.32	1.45	1.52
1	E	179	GLN	N-CA	5.32	1.53	1.46
1	F	620	ARG	N-CA	5.32	1.54	1.45
1	E	205	TRP	CA-C	-5.32	1.45	1.52
1	A	205	TRP	CA-C	-5.32	1.45	1.52
1	A	457	HIS	CG-ND1	-5.32	1.32	1.38
1	C	393	LYS	C-O	-5.31	1.17	1.24
1	D	450	ALA	C-O	5.31	1.30	1.24
1	E	620	ARG	N-CA	5.31	1.54	1.45
1	F	457	HIS	CG-ND1	-5.31	1.32	1.38
1	B	179	GLN	N-CA	5.31	1.53	1.46
1	B	205	TRP	CA-C	-5.31	1.45	1.52
1	C	285	HIS	CA-C	-5.30	1.46	1.52
1	F	336	ASN	C-N	-5.30	1.28	1.34
1	A	620	ARG	N-CA	5.30	1.54	1.45
1	B	336	ASN	C-N	-5.29	1.28	1.34
1	C	205	TRP	CA-C	-5.29	1.45	1.52
1	B	193	HIS	ND1-CE1	5.29	1.37	1.32
1	A	179	GLN	N-CA	5.29	1.53	1.46
1	B	626	LEU	C-O	5.29	1.31	1.24
1	F	450	ALA	C-O	5.28	1.30	1.24
1	D	650	VAL	CA-CB	-5.28	1.47	1.54
1	B	450	ALA	C-O	5.28	1.30	1.24
1	A	450	ALA	C-O	5.27	1.30	1.24
1	B	620	ARG	N-CA	5.27	1.54	1.45
1	F	268	PHE	N-CA	5.26	1.51	1.45
1	B	374	ALA	CA-C	-5.26	1.45	1.52
1	C	620	ARG	N-CA	5.26	1.54	1.45
1	B	390	ILE	CA-C	5.26	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	457	HIS	CG-ND1	-5.26	1.32	1.38
1	D	276	HIS	ND1-CE1	5.25	1.37	1.32
1	C	179	GLN	N-CA	5.25	1.52	1.46
1	C	450	ALA	C-O	5.25	1.30	1.24
1	D	36	ASN	C-O	5.25	1.30	1.24
1	D	626	LEU	C-O	5.25	1.30	1.24
1	E	114	GLU	CA-CB	-5.25	1.45	1.53
1	E	299	ALA	N-CA	5.25	1.52	1.46
1	F	374	ALA	CA-C	-5.25	1.45	1.52
1	D	268	PHE	N-CA	5.24	1.51	1.45
1	C	629	ARG	NE-CZ	5.24	1.38	1.33
1	D	390	ILE	CA-C	5.24	1.58	1.52
1	E	450	ALA	C-O	5.23	1.30	1.24
1	C	276	HIS	ND1-CE1	5.23	1.37	1.32
1	C	487	ASP	C-O	5.23	1.30	1.24
1	B	103	ALA	N-CA	5.23	1.52	1.46
1	A	390	ILE	CA-C	5.22	1.58	1.52
1	A	626	LEU	C-O	5.22	1.30	1.24
1	C	626	LEU	C-O	5.22	1.30	1.24
1	D	374	ALA	CA-C	-5.22	1.45	1.52
1	E	268	PHE	N-CA	5.22	1.51	1.45
1	F	626	LEU	C-O	5.22	1.30	1.24
1	A	374	ALA	CA-C	-5.22	1.45	1.52
1	C	114	GLU	CA-CB	-5.21	1.45	1.53
1	D	629	ARG	NE-CZ	5.21	1.38	1.33
1	F	276	HIS	ND1-CE1	5.21	1.37	1.32
1	A	629	ARG	NE-CZ	5.21	1.38	1.33
1	A	114	GLU	CA-CB	-5.21	1.45	1.53
1	B	629	ARG	NE-CZ	5.21	1.38	1.33
1	C	390	ILE	CA-C	5.21	1.58	1.52
1	F	629	ARG	NE-CZ	5.21	1.38	1.33
1	A	276	HIS	ND1-CE1	5.21	1.37	1.32
1	A	299	ALA	N-CA	5.21	1.52	1.46
1	C	299	ALA	N-CA	5.21	1.52	1.46
1	E	626	LEU	C-O	5.21	1.30	1.24
1	F	390	ILE	CA-C	5.21	1.58	1.52
1	F	487	ASP	C-O	5.21	1.30	1.24
1	D	299	ALA	N-CA	5.20	1.52	1.46
1	F	299	ALA	N-CA	5.20	1.52	1.46
1	B	299	ALA	N-CA	5.20	1.52	1.46
1	E	103	ALA	N-CA	5.20	1.52	1.46
1	D	487	ASP	C-O	5.20	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	390	ILE	CA-C	5.20	1.58	1.52
1	A	268	PHE	N-CA	5.20	1.51	1.45
1	B	268	PHE	N-CA	5.20	1.51	1.45
1	C	374	ALA	CA-C	-5.20	1.45	1.52
1	A	103	ALA	N-CA	5.20	1.52	1.46
1	A	36	ASN	C-O	5.19	1.30	1.24
1	B	387	MET	CA-CB	-5.19	1.45	1.53
1	C	387	MET	CA-CB	-5.19	1.45	1.53
1	F	36	ASN	C-O	5.19	1.30	1.24
1	D	114	GLU	CA-CB	-5.19	1.45	1.53
1	E	139	GLN	CA-CB	-5.19	1.45	1.53
1	E	374	ALA	CA-C	-5.19	1.45	1.52
1	A	487	ASP	C-O	5.19	1.30	1.24
1	B	114	GLU	CA-CB	-5.19	1.45	1.53
1	C	152	ASP	N-CA	5.19	1.52	1.46
1	B	152	ASP	N-CA	5.18	1.52	1.46
1	C	572	LYS	C-N	-5.18	1.27	1.33
1	F	103	ALA	N-CA	5.18	1.52	1.46
1	C	36	ASN	C-O	5.18	1.30	1.24
1	D	387	MET	CA-CB	-5.18	1.45	1.53
1	C	268	PHE	N-CA	5.18	1.51	1.45
1	E	572	LYS	C-N	-5.18	1.27	1.33
1	F	114	GLU	CA-CB	-5.18	1.45	1.53
1	B	276	HIS	ND1-CE1	5.17	1.37	1.32
1	A	387	MET	CA-CB	-5.17	1.45	1.53
1	D	103	ALA	N-CA	5.17	1.52	1.46
1	E	36	ASN	C-O	5.17	1.30	1.24
1	B	572	LYS	C-N	-5.17	1.27	1.33
1	E	494	THR	C-O	5.17	1.30	1.23
1	E	629	ARG	NE-CZ	5.16	1.38	1.33
1	E	102	ASN	C-O	5.16	1.30	1.24
1	F	387	MET	CA-CB	-5.16	1.45	1.53
1	F	139	GLN	CA-CB	-5.16	1.45	1.53
1	D	152	ASP	N-CA	5.15	1.52	1.46
1	A	152	ASP	N-CA	5.15	1.52	1.46
1	C	103	ALA	N-CA	5.15	1.52	1.46
1	C	139	GLN	CA-CB	-5.15	1.45	1.53
1	D	494	THR	C-O	5.15	1.30	1.23
1	D	124	ILE	C-N	-5.15	1.26	1.33
1	F	572	LYS	C-N	-5.15	1.27	1.33
1	A	139	GLN	CA-CB	-5.14	1.45	1.53
1	E	387	MET	CA-CB	-5.14	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	650	VAL	C-O	5.14	1.29	1.24
1	B	36	ASN	C-O	5.14	1.30	1.24
1	B	102	ASN	C-O	5.14	1.29	1.24
1	A	572	LYS	C-N	-5.14	1.27	1.33
1	B	395	THR	C-O	-5.14	1.18	1.24
1	B	101	SER	CA-CB	-5.13	1.45	1.53
1	B	487	ASP	C-O	5.13	1.30	1.24
1	A	494	THR	C-O	5.13	1.30	1.23
1	B	139	GLN	CA-CB	-5.13	1.45	1.53
1	E	124	ILE	C-N	-5.13	1.26	1.33
1	A	124	ILE	C-N	-5.13	1.26	1.33
1	E	276	HIS	ND1-CE1	5.13	1.37	1.32
1	F	152	ASP	N-CA	5.13	1.52	1.46
1	F	124	ILE	C-N	-5.12	1.26	1.33
1	F	494	THR	C-O	5.12	1.30	1.23
1	B	361	PHE	C-O	5.12	1.30	1.24
1	C	102	ASN	C-O	5.12	1.29	1.24
1	A	329	GLU	C-N	-5.12	1.26	1.33
1	C	124	ILE	C-N	-5.12	1.26	1.33
1	E	487	ASP	C-O	5.12	1.30	1.24
1	B	124	ILE	C-N	-5.12	1.26	1.33
1	F	329	GLU	C-N	-5.12	1.26	1.33
1	E	152	ASP	N-CA	5.11	1.52	1.46
1	A	650	VAL	C-O	5.11	1.29	1.24
1	C	329	GLU	C-N	-5.11	1.26	1.33
1	B	329	GLU	C-N	-5.11	1.26	1.33
1	B	190	MET	N-CA	5.11	1.52	1.46
1	B	650	VAL	C-O	5.11	1.29	1.24
1	E	361	PHE	C-O	5.11	1.30	1.24
1	F	650	VAL	C-O	5.11	1.29	1.24
1	C	101	SER	CA-CB	-5.11	1.45	1.53
1	E	329	GLU	C-N	-5.11	1.26	1.33
1	B	225	HIS	N-CA	5.10	1.52	1.46
1	D	190	MET	N-CA	5.10	1.52	1.46
1	D	361	PHE	C-O	5.10	1.30	1.24
1	A	102	ASN	C-O	5.10	1.29	1.24
1	D	572	LYS	C-N	-5.10	1.27	1.33
1	C	190	MET	N-CA	5.09	1.52	1.46
1	D	102	ASN	C-O	5.09	1.29	1.24
1	D	139	GLN	CA-CB	-5.09	1.46	1.53
1	A	361	PHE	C-O	5.09	1.30	1.24
1	C	494	THR	C-O	5.09	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	282	GLY	C-O	5.09	1.30	1.23
1	A	101	SER	CA-CB	-5.09	1.45	1.53
1	C	650	VAL	C-O	5.09	1.29	1.24
1	B	494	THR	C-O	5.09	1.30	1.23
1	A	190	MET	N-CA	5.09	1.52	1.46
1	D	329	GLU	C-N	-5.09	1.26	1.33
1	E	101	SER	CA-CB	-5.09	1.45	1.53
1	D	243	VAL	C-N	-5.08	1.26	1.33
1	B	136	PRO	C-O	5.08	1.29	1.23
1	D	101	SER	CA-CB	-5.08	1.45	1.53
1	C	361	PHE	C-O	5.08	1.30	1.24
1	C	395	THR	C-O	-5.08	1.18	1.24
1	B	212	HIS	N-CA	5.08	1.52	1.46
1	C	524	LYS	CA-C	-5.08	1.46	1.52
1	F	478	PHE	CA-CB	5.08	1.59	1.52
1	D	225	HIS	N-CA	5.07	1.52	1.46
1	A	212	HIS	N-CA	5.07	1.52	1.46
1	C	212	HIS	N-CA	5.07	1.52	1.46
1	C	225	HIS	N-CA	5.07	1.52	1.46
1	A	395	THR	C-O	-5.07	1.18	1.24
1	E	212	HIS	N-CA	5.07	1.52	1.46
1	F	190	MET	N-CA	5.07	1.52	1.46
1	A	225	HIS	N-CA	5.06	1.52	1.46
1	C	136	PRO	C-O	5.06	1.29	1.23
1	D	395	THR	C-O	-5.06	1.18	1.24
1	E	282	GLY	C-O	5.06	1.30	1.23
1	D	181	VAL	CA-CB	-5.06	1.47	1.54
1	D	212	HIS	N-CA	5.06	1.52	1.46
1	F	225	HIS	N-CA	5.06	1.52	1.46
1	A	136	PRO	C-O	5.06	1.29	1.23
1	B	208	SER	CB-OG	5.06	1.52	1.42
1	C	357	PRO	N-CA	-5.06	1.40	1.47
1	E	190	MET	N-CA	5.06	1.52	1.46
1	F	146	THR	CA-CB	5.06	1.61	1.53
1	A	181	VAL	CA-CB	-5.05	1.47	1.54
1	F	101	SER	CA-CB	-5.05	1.45	1.53
1	E	395	THR	C-O	-5.05	1.18	1.24
1	C	206	GLU	CA-CB	-5.05	1.45	1.53
1	C	208	SER	CB-OG	5.05	1.52	1.42
1	E	357	PRO	N-CA	-5.05	1.40	1.47
1	A	208	SER	CB-OG	5.05	1.52	1.42
1	D	208	SER	CB-OG	5.05	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	GLY	C-O	5.05	1.30	1.23
1	B	243	VAL	C-N	-5.05	1.26	1.33
1	B	282	GLY	C-O	5.05	1.30	1.23
1	E	491	ILE	C-N	-5.05	1.26	1.33
1	E	478	PHE	CA-CB	5.04	1.59	1.52
1	D	567	ARG	C-O	5.04	1.30	1.24
1	E	181	VAL	CA-CB	-5.04	1.47	1.54
1	E	208	SER	CB-OG	5.04	1.52	1.42
1	E	243	VAL	C-N	-5.04	1.26	1.33
1	B	357	PRO	N-CA	-5.04	1.40	1.47
1	F	212	HIS	N-CA	5.04	1.52	1.46
1	C	282	GLY	C-O	5.04	1.30	1.23
1	D	206	GLU	CA-CB	-5.04	1.45	1.53
1	F	361	PHE	C-O	5.04	1.30	1.24
1	E	136	PRO	C-O	5.03	1.29	1.23
1	E	225	HIS	N-CA	5.03	1.52	1.46
1	F	206	GLU	CA-CB	-5.03	1.45	1.53
1	A	243	VAL	C-N	-5.03	1.26	1.33
1	C	478	PHE	CA-CB	5.03	1.59	1.52
1	C	567	ARG	C-O	5.03	1.30	1.24
1	D	211	TYR	N-CA	5.03	1.52	1.46
1	E	650	VAL	C-O	5.03	1.29	1.24
1	C	491	ILE	C-N	-5.03	1.26	1.33
1	F	181	VAL	CA-CB	-5.03	1.47	1.54
1	F	208	SER	CB-OG	5.03	1.52	1.42
1	A	357	PRO	N-CA	-5.03	1.40	1.47
1	A	478	PHE	CA-CB	5.03	1.59	1.52
1	B	394	HIS	CA-C	-5.03	1.46	1.52
1	F	102	ASN	C-O	5.03	1.29	1.24
1	B	181	VAL	CA-CB	-5.02	1.47	1.54
1	B	206	GLU	CA-CB	-5.02	1.45	1.53
1	D	136	PRO	C-O	5.02	1.29	1.23
1	E	286	VAL	C-N	-5.02	1.27	1.33
1	E	206	GLU	CA-CB	-5.02	1.45	1.53
1	B	580	PHE	C-N	-5.02	1.26	1.33
1	F	491	ILE	C-N	-5.02	1.26	1.33
1	D	357	PRO	N-CA	-5.02	1.40	1.47
1	A	580	PHE	C-N	-5.01	1.26	1.33
1	F	136	PRO	C-O	5.01	1.29	1.23
1	A	206	GLU	CA-CB	-5.01	1.45	1.53
1	A	491	ILE	C-N	-5.01	1.26	1.33
1	B	643	LYS	C-O	5.01	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	211	TYR	N-CA	5.01	1.52	1.46
1	F	567	ARG	C-O	5.01	1.30	1.24
1	B	478	PHE	CA-CB	5.01	1.59	1.52
1	C	181	VAL	CA-CB	-5.00	1.47	1.54
1	D	580	PHE	C-N	-5.00	1.26	1.33

All (11003) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	390	ILE	N-CA-C	-25.99	89.46	111.81
1	B	390	ILE	N-CA-C	-25.99	89.46	111.81
1	D	390	ILE	N-CA-C	-25.98	89.46	111.81
1	F	390	ILE	N-CA-C	-25.98	89.47	111.81
1	A	390	ILE	N-CA-C	-25.97	89.47	111.81
1	C	390	ILE	N-CA-C	-25.96	89.49	111.81
1	F	458	ASN	CA-CB-CG	25.79	138.39	112.60
1	D	458	ASN	CA-CB-CG	25.79	138.38	112.60
1	E	458	ASN	CA-CB-CG	25.77	138.38	112.60
1	A	458	ASN	CA-CB-CG	25.76	138.36	112.60
1	C	458	ASN	CA-CB-CG	25.74	138.34	112.60
1	B	458	ASN	CA-CB-CG	25.72	138.32	112.60
1	E	99	PHE	CA-CB-CG	25.15	138.95	113.80
1	A	99	PHE	CA-CB-CG	25.14	138.94	113.80
1	D	99	PHE	CA-CB-CG	25.14	138.94	113.80
1	C	99	PHE	CA-CB-CG	25.14	138.94	113.80
1	F	99	PHE	CA-CB-CG	25.13	138.93	113.80
1	B	99	PHE	CA-CB-CG	25.09	138.89	113.80
1	C	279	ASP	CA-CB-CG	24.78	137.38	112.60
1	F	279	ASP	CA-CB-CG	24.77	137.37	112.60
1	A	279	ASP	CA-CB-CG	24.76	137.36	112.60
1	E	279	ASP	CA-CB-CG	24.75	137.34	112.60
1	D	279	ASP	CA-CB-CG	24.73	137.33	112.60
1	B	279	ASP	CA-CB-CG	24.72	137.32	112.60
1	F	628	ARG	NE-CZ-NH2	-24.09	97.52	119.20
1	D	408	PHE	CA-CB-CG	24.08	137.88	113.80
1	C	408	PHE	CA-CB-CG	24.07	137.87	113.80
1	E	628	ARG	NE-CZ-NH2	-24.07	97.54	119.20
1	B	408	PHE	CA-CB-CG	24.05	137.85	113.80
1	C	628	ARG	NE-CZ-NH2	-24.05	97.56	119.20
1	D	628	ARG	NE-CZ-NH2	-24.05	97.56	119.20
1	A	628	ARG	NE-CZ-NH2	-24.04	97.56	119.20
1	A	408	PHE	CA-CB-CG	24.04	137.84	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	408	PHE	CA-CB-CG	24.04	137.84	113.80
1	B	628	ARG	NE-CZ-NH2	-24.00	97.60	119.20
1	E	408	PHE	CA-CB-CG	24.00	137.79	113.80
1	E	299	ALA	CB-CA-C	23.32	149.96	110.79
1	B	299	ALA	CB-CA-C	23.30	149.94	110.79
1	D	299	ALA	CB-CA-C	23.30	149.94	110.79
1	A	299	ALA	CB-CA-C	23.30	149.93	110.79
1	C	299	ALA	CB-CA-C	23.30	149.93	110.79
1	F	299	ALA	CB-CA-C	23.29	149.92	110.79
1	C	1	ASP	CA-CB-CG	22.50	135.10	112.60
1	E	1	ASP	CA-CB-CG	22.49	135.09	112.60
1	D	1	ASP	CA-CB-CG	22.49	135.09	112.60
1	F	1	ASP	CA-CB-CG	22.48	135.08	112.60
1	A	1	ASP	CA-CB-CG	22.47	135.07	112.60
1	B	1	ASP	CA-CB-CG	22.47	135.07	112.60
1	D	7	ASN	CA-CB-CG	22.41	135.01	112.60
1	F	7	ASN	CA-CB-CG	22.40	135.00	112.60
1	B	7	ASN	CA-CB-CG	22.40	135.00	112.60
1	A	7	ASN	CA-CB-CG	22.38	134.98	112.60
1	C	7	ASN	CA-CB-CG	22.36	134.97	112.60
1	E	7	ASN	CA-CB-CG	22.33	134.93	112.60
1	B	232	ASP	CA-CB-CG	21.95	134.54	112.60
1	F	232	ASP	CA-CB-CG	21.93	134.53	112.60
1	C	232	ASP	CA-CB-CG	21.92	134.52	112.60
1	E	232	ASP	CA-CB-CG	21.92	134.52	112.60
1	A	232	ASP	CA-CB-CG	21.90	134.50	112.60
1	D	232	ASP	CA-CB-CG	21.89	134.49	112.60
1	C	390	ILE	CA-C-O	-20.23	98.07	120.32
1	F	390	ILE	CA-C-O	-20.21	98.09	120.32
1	A	390	ILE	CA-C-O	-20.20	98.10	120.32
1	D	390	ILE	CA-C-O	-20.20	98.10	120.32
1	B	390	ILE	CA-C-O	-20.20	98.10	120.32
1	E	390	ILE	CA-C-O	-20.19	98.11	120.32
1	F	644	HIS	CA-C-O	-20.09	97.56	120.66
1	E	644	HIS	CA-C-O	-20.07	97.58	120.66
1	A	644	HIS	CA-C-O	-20.07	97.58	120.66
1	B	644	HIS	CA-C-O	-20.06	97.59	120.66
1	C	644	HIS	CA-C-O	-20.06	97.59	120.66
1	D	644	HIS	CA-C-O	-20.04	97.62	120.66
1	A	649	ILE	O-C-N	20.02	144.80	123.18
1	B	649	ILE	O-C-N	20.01	144.79	123.18
1	F	649	ILE	O-C-N	20.01	144.79	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	649	ILE	O-C-N	20.00	144.78	123.18
1	C	649	ILE	O-C-N	19.99	144.77	123.18
1	E	649	ILE	O-C-N	19.98	144.76	123.18
1	F	489	ASN	N-CA-C	-19.27	89.31	113.97
1	D	489	ASN	N-CA-C	-19.25	89.33	113.97
1	B	489	ASN	N-CA-C	-19.24	89.34	113.97
1	E	489	ASN	N-CA-C	-19.24	89.34	113.97
1	A	489	ASN	N-CA-C	-19.23	89.35	113.97
1	C	489	ASN	N-CA-C	-19.22	89.37	113.97
1	E	367	VAL	O-C-N	-19.19	102.52	121.90
1	A	367	VAL	O-C-N	-19.16	102.55	121.90
1	F	367	VAL	O-C-N	-19.16	102.55	121.90
1	D	367	VAL	O-C-N	-19.15	102.56	121.90
1	B	367	VAL	O-C-N	-19.14	102.57	121.90
1	B	48	ASP	CA-CB-CG	19.13	131.73	112.60
1	C	48	ASP	CA-CB-CG	19.13	131.73	112.60
1	C	367	VAL	O-C-N	-19.12	102.58	121.90
1	F	48	ASP	CA-CB-CG	19.12	131.72	112.60
1	E	48	ASP	CA-CB-CG	19.11	131.71	112.60
1	A	48	ASP	CA-CB-CG	19.09	131.69	112.60
1	D	48	ASP	CA-CB-CG	19.05	131.65	112.60
1	C	326	ASP	CA-CB-CG	19.03	131.63	112.60
1	E	326	ASP	CA-CB-CG	19.01	131.61	112.60
1	B	326	ASP	CA-CB-CG	19.01	131.61	112.60
1	A	326	ASP	CA-CB-CG	18.99	131.59	112.60
1	D	326	ASP	CA-CB-CG	18.98	131.58	112.60
1	F	326	ASP	CA-CB-CG	18.97	131.57	112.60
1	E	169	SER	N-CA-C	18.96	139.35	112.04
1	B	169	SER	N-CA-C	18.95	139.32	112.04
1	F	169	SER	N-CA-C	18.95	139.32	112.04
1	A	169	SER	N-CA-C	18.94	139.31	112.04
1	C	169	SER	N-CA-C	18.94	139.32	112.04
1	D	169	SER	N-CA-C	18.94	139.31	112.04
1	E	487	ASP	N-CA-C	18.87	131.93	111.36
1	D	487	ASP	N-CA-C	18.87	131.93	111.36
1	A	487	ASP	N-CA-C	18.86	131.92	111.36
1	B	487	ASP	N-CA-C	18.85	131.91	111.36
1	C	487	ASP	N-CA-C	18.84	131.90	111.36
1	F	512	VAL	CA-C-O	18.84	131.43	119.19
1	C	512	VAL	CA-C-O	18.82	131.43	119.19
1	B	512	VAL	CA-C-O	18.82	131.42	119.19
1	F	487	ASP	N-CA-C	18.82	131.87	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	512	VAL	CA-C-O	18.81	131.42	119.19
1	A	512	VAL	CA-C-O	18.81	131.42	119.19
1	E	512	VAL	CA-C-O	18.73	131.37	119.19
1	E	273	ASP	CA-CB-CG	18.64	131.24	112.60
1	C	273	ASP	CA-CB-CG	18.62	131.22	112.60
1	C	76	ASN	OD1-CG-ND2	18.61	141.21	122.60
1	F	273	ASP	CA-CB-CG	18.61	131.21	112.60
1	D	76	ASN	OD1-CG-ND2	18.60	141.20	122.60
1	A	273	ASP	CA-CB-CG	18.60	131.20	112.60
1	F	76	ASN	OD1-CG-ND2	18.60	141.20	122.60
1	B	273	ASP	CA-CB-CG	18.59	131.19	112.60
1	D	273	ASP	CA-CB-CG	18.59	131.19	112.60
1	A	76	ASN	OD1-CG-ND2	18.59	141.19	122.60
1	E	76	ASN	OD1-CG-ND2	18.58	141.18	122.60
1	B	76	ASN	OD1-CG-ND2	18.55	141.15	122.60
1	F	246	LEU	CA-C-O	-18.46	100.00	121.05
1	D	452	VAL	O-C-N	18.45	142.71	122.97
1	B	246	LEU	CA-C-O	-18.45	100.02	121.05
1	E	246	LEU	CA-C-O	-18.45	100.02	121.05
1	D	246	LEU	CA-C-O	-18.44	100.03	121.05
1	A	246	LEU	CA-C-O	-18.44	100.03	121.05
1	C	246	LEU	CA-C-O	-18.42	100.06	121.05
1	B	452	VAL	O-C-N	18.41	142.67	122.97
1	E	452	VAL	O-C-N	18.41	142.67	122.97
1	A	452	VAL	O-C-N	18.38	142.63	122.97
1	F	452	VAL	O-C-N	18.36	142.62	122.97
1	C	452	VAL	O-C-N	18.36	142.62	122.97
1	E	61	ASN	CA-CB-CG	-18.14	94.46	112.60
1	F	61	ASN	CA-CB-CG	-18.14	94.46	112.60
1	C	61	ASN	CA-CB-CG	-18.13	94.47	112.60
1	B	61	ASN	CA-CB-CG	-18.12	94.48	112.60
1	A	61	ASN	CA-CB-CG	-18.12	94.48	112.60
1	D	61	ASN	CA-CB-CG	-18.10	94.50	112.60
1	E	620	ARG	CA-CB-CG	17.84	149.79	114.10
1	F	620	ARG	CA-CB-CG	17.83	149.76	114.10
1	A	620	ARG	CA-CB-CG	17.83	149.76	114.10
1	C	620	ARG	CA-CB-CG	17.82	149.74	114.10
1	D	620	ARG	CA-CB-CG	17.82	149.74	114.10
1	B	620	ARG	CA-CB-CG	17.82	149.74	114.10
1	C	345	ASN	OD1-CG-ND2	17.66	140.25	122.60
1	B	331	SER	CA-C-O	-17.62	99.44	121.46
1	B	345	ASN	OD1-CG-ND2	17.62	140.22	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	331	SER	CA-C-O	-17.62	99.44	121.46
1	A	331	SER	CA-C-O	-17.61	99.45	121.46
1	E	331	SER	CA-C-O	-17.60	99.46	121.46
1	A	345	ASN	OD1-CG-ND2	17.60	140.20	122.60
1	F	345	ASN	OD1-CG-ND2	17.59	140.19	122.60
1	C	331	SER	CA-C-O	-17.59	99.48	121.46
1	D	345	ASN	OD1-CG-ND2	17.58	140.18	122.60
1	D	331	SER	CA-C-O	-17.57	99.50	121.46
1	E	345	ASN	OD1-CG-ND2	17.54	140.14	122.60
1	F	302	HIS	O-C-N	17.42	143.25	122.17
1	B	302	HIS	O-C-N	17.41	143.24	122.17
1	D	302	HIS	O-C-N	17.41	143.24	122.17
1	E	302	HIS	O-C-N	17.40	143.23	122.17
1	A	302	HIS	O-C-N	17.40	143.22	122.17
1	C	302	HIS	O-C-N	17.36	143.17	122.17
1	F	126	SER	CA-C-O	17.33	140.57	121.16
1	C	126	SER	CA-C-O	17.33	140.56	121.16
1	B	126	SER	CA-C-O	17.32	140.56	121.16
1	A	126	SER	CA-C-O	17.32	140.56	121.16
1	D	126	SER	CA-C-O	17.32	140.56	121.16
1	E	126	SER	CA-C-O	17.32	140.56	121.16
1	C	390	ILE	O-C-N	17.26	149.43	122.16
1	A	390	ILE	O-C-N	17.25	149.41	122.16
1	F	390	ILE	O-C-N	17.25	149.41	122.16
1	B	390	ILE	O-C-N	17.24	149.40	122.16
1	B	486	GLU	CA-C-N	17.24	144.77	120.29
1	B	486	GLU	C-N-CA	17.24	144.77	120.29
1	C	486	GLU	CA-C-N	17.23	144.75	120.29
1	C	486	GLU	C-N-CA	17.23	144.75	120.29
1	D	390	ILE	O-C-N	17.22	149.38	122.16
1	F	486	GLU	CA-C-N	17.22	144.75	120.29
1	F	486	GLU	C-N-CA	17.22	144.75	120.29
1	F	285	HIS	CA-C-O	-17.22	103.30	121.55
1	E	390	ILE	O-C-N	17.22	149.37	122.16
1	C	285	HIS	CA-C-O	-17.22	103.30	121.55
1	D	285	HIS	CA-C-O	-17.21	103.30	121.55
1	A	285	HIS	CA-C-O	-17.21	103.31	121.55
1	D	486	GLU	CA-C-N	17.21	144.73	120.29
1	D	486	GLU	C-N-CA	17.21	144.73	120.29
1	E	486	GLU	CA-C-N	17.21	144.72	120.29
1	E	486	GLU	C-N-CA	17.21	144.72	120.29
1	A	486	GLU	CA-C-N	17.21	144.72	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	486	GLU	C-N-CA	17.21	144.72	120.29
1	B	285	HIS	CA-C-O	-17.19	103.33	121.55
1	E	285	HIS	CA-C-O	-17.18	103.34	121.55
1	C	645	VAL	CA-C-O	-17.16	101.45	120.67
1	E	645	VAL	CA-C-O	-17.16	101.45	120.67
1	A	645	VAL	CA-C-O	-17.16	101.45	120.67
1	B	645	VAL	CA-C-O	-17.16	101.46	120.67
1	F	645	VAL	CA-C-O	-17.15	101.46	120.67
1	D	645	VAL	CA-C-O	-17.14	101.47	120.67
1	B	461	THR	CA-C-O	17.02	141.03	121.11
1	F	461	THR	CA-C-O	16.99	140.99	121.11
1	C	461	THR	CA-C-O	16.99	140.98	121.11
1	A	461	THR	CA-C-O	16.98	140.98	121.11
1	E	461	THR	CA-C-O	16.96	140.96	121.11
1	D	461	THR	CA-C-O	16.95	140.94	121.11
1	C	329	GLU	CA-C-N	16.67	153.38	121.54
1	C	329	GLU	C-N-CA	16.67	153.38	121.54
1	A	329	GLU	CA-C-N	16.66	153.37	121.54
1	A	329	GLU	C-N-CA	16.66	153.37	121.54
1	B	329	GLU	CA-C-N	16.66	153.37	121.54
1	B	329	GLU	C-N-CA	16.66	153.37	121.54
1	D	329	GLU	CA-C-N	16.66	153.35	121.54
1	D	329	GLU	C-N-CA	16.66	153.35	121.54
1	E	329	GLU	CA-C-N	16.66	153.35	121.54
1	E	329	GLU	C-N-CA	16.66	153.35	121.54
1	F	329	GLU	CA-C-N	16.62	153.29	121.54
1	F	329	GLU	C-N-CA	16.62	153.29	121.54
1	C	206	GLU	CA-C-O	-16.56	101.52	121.56
1	B	206	GLU	CA-C-O	-16.56	101.53	121.56
1	A	206	GLU	CA-C-O	-16.54	101.54	121.56
1	E	206	GLU	CA-C-O	-16.54	101.55	121.56
1	D	206	GLU	CA-C-O	-16.54	101.55	121.56
1	F	206	GLU	CA-C-O	-16.52	101.56	121.56
1	C	17	LEU	CA-C-O	-16.46	103.54	120.82
1	B	17	LEU	CA-C-O	-16.45	103.55	120.82
1	A	17	LEU	CA-C-O	-16.44	103.56	120.82
1	D	17	LEU	CA-C-O	-16.43	103.57	120.82
1	E	17	LEU	CA-C-O	-16.42	103.58	120.82
1	F	17	LEU	CA-C-O	-16.41	103.58	120.82
1	F	305	ILE	CA-C-O	-16.38	100.68	121.48
1	B	305	ILE	CA-C-O	-16.37	100.69	121.48
1	A	305	ILE	CA-C-O	-16.37	100.69	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	305	ILE	CA-C-O	-16.36	100.70	121.48
1	D	316	ARG	CD-NE-CZ	16.36	147.30	124.40
1	C	305	ILE	CA-C-O	-16.34	100.72	121.48
1	D	305	ILE	CA-C-O	-16.34	100.73	121.48
1	F	316	ARG	CD-NE-CZ	16.34	147.27	124.40
1	C	316	ARG	CD-NE-CZ	16.33	147.27	124.40
1	A	316	ARG	CD-NE-CZ	16.33	147.27	124.40
1	E	316	ARG	CD-NE-CZ	16.32	147.25	124.40
1	B	316	ARG	CD-NE-CZ	16.31	147.23	124.40
1	E	460	PHE	O-C-N	16.06	141.56	123.25
1	C	460	PHE	O-C-N	16.05	141.54	123.25
1	F	460	PHE	O-C-N	16.05	141.54	123.25
1	B	77	THR	CA-C-O	-16.04	100.69	119.61
1	A	460	PHE	O-C-N	16.02	141.52	123.25
1	B	460	PHE	O-C-N	16.02	141.51	123.25
1	F	77	THR	CA-C-O	-16.02	100.71	119.61
1	D	77	THR	CA-C-O	-16.01	100.72	119.61
1	D	460	PHE	O-C-N	16.01	141.50	123.25
1	A	77	THR	CA-C-O	-16.00	100.72	119.61
1	E	77	THR	CA-C-O	-16.00	100.73	119.61
1	C	77	THR	CA-C-O	-16.00	100.73	119.61
1	B	354	GLN	OE1-CD-NE2	-15.91	106.69	122.60
1	D	354	GLN	OE1-CD-NE2	-15.91	106.69	122.60
1	D	522	SER	N-CA-C	15.90	136.68	109.96
1	E	522	SER	N-CA-C	15.89	136.65	109.96
1	C	522	SER	N-CA-C	15.88	136.65	109.96
1	F	354	GLN	OE1-CD-NE2	-15.88	106.72	122.60
1	E	78	ARG	NE-CZ-NH2	15.88	133.49	119.20
1	A	354	GLN	OE1-CD-NE2	-15.88	106.72	122.60
1	A	522	SER	N-CA-C	15.87	136.62	109.96
1	F	78	ARG	NE-CZ-NH2	15.87	133.48	119.20
1	C	354	GLN	OE1-CD-NE2	-15.87	106.73	122.60
1	B	522	SER	N-CA-C	15.86	136.60	109.96
1	F	522	SER	N-CA-C	15.85	136.59	109.96
1	B	78	ARG	NE-CZ-NH2	15.84	133.46	119.20
1	A	78	ARG	NE-CZ-NH2	15.84	133.45	119.20
1	C	78	ARG	NE-CZ-NH2	15.83	133.45	119.20
1	D	78	ARG	NE-CZ-NH2	15.83	133.45	119.20
1	E	354	GLN	OE1-CD-NE2	-15.83	106.77	122.60
1	C	309	ASP	CA-CB-CG	-15.82	96.78	112.60
1	B	92	GLN	OE1-CD-NE2	15.81	138.41	122.60
1	B	25	THR	CA-CB-OG1	-15.81	85.89	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	25	THR	CA-CB-OG1	-15.79	85.91	109.60
1	D	92	GLN	OE1-CD-NE2	15.79	138.39	122.60
1	E	25	THR	CA-CB-OG1	-15.79	85.91	109.60
1	A	25	THR	CA-CB-OG1	-15.79	85.92	109.60
1	A	309	ASP	CA-CB-CG	-15.78	96.82	112.60
1	C	92	GLN	OE1-CD-NE2	15.78	138.38	122.60
1	E	309	ASP	CA-CB-CG	-15.78	96.82	112.60
1	F	25	THR	CA-CB-OG1	-15.78	85.93	109.60
1	D	25	THR	CA-CB-OG1	-15.77	85.94	109.60
1	F	309	ASP	CA-CB-CG	-15.77	96.83	112.60
1	F	92	GLN	OE1-CD-NE2	15.76	138.36	122.60
1	D	309	ASP	CA-CB-CG	-15.76	96.84	112.60
1	B	309	ASP	CA-CB-CG	-15.76	96.84	112.60
1	A	92	GLN	OE1-CD-NE2	15.75	138.35	122.60
1	E	92	GLN	OE1-CD-NE2	15.72	138.32	122.60
1	B	207	ASP	CA-CB-CG	15.60	128.20	112.60
1	A	207	ASP	CA-CB-CG	15.57	128.17	112.60
1	C	207	ASP	CA-CB-CG	15.56	128.16	112.60
1	D	207	ASP	CA-CB-CG	15.56	128.16	112.60
1	E	207	ASP	CA-CB-CG	15.55	128.15	112.60
1	F	207	ASP	CA-CB-CG	15.54	128.15	112.60
1	E	193	HIS	CA-CB-CG	15.48	129.28	113.80
1	F	606	HIS	CA-CB-CG	-15.48	98.32	113.80
1	D	193	HIS	CA-CB-CG	15.46	129.25	113.80
1	A	606	HIS	CA-CB-CG	-15.45	98.35	113.80
1	D	606	HIS	CA-CB-CG	-15.45	98.35	113.80
1	E	75	PHE	CA-C-O	-15.45	100.80	119.18
1	E	606	HIS	CA-CB-CG	-15.45	98.35	113.80
1	B	606	HIS	CA-CB-CG	-15.45	98.35	113.80
1	F	75	PHE	CA-C-O	-15.44	100.81	119.18
1	D	75	PHE	CA-C-O	-15.44	100.81	119.18
1	B	75	PHE	CA-C-O	-15.44	100.81	119.18
1	A	193	HIS	CA-CB-CG	15.43	129.23	113.80
1	C	193	HIS	CA-CB-CG	15.43	129.23	113.80
1	C	75	PHE	CA-C-O	-15.43	100.82	119.18
1	A	75	PHE	CA-C-O	-15.43	100.82	119.18
1	F	193	HIS	CA-CB-CG	15.42	129.22	113.80
1	C	606	HIS	CA-CB-CG	-15.42	98.38	113.80
1	B	193	HIS	CA-CB-CG	15.40	129.21	113.80
1	B	439	SER	CA-C-O	-15.39	103.92	120.24
1	F	439	SER	CA-C-O	-15.39	103.93	120.24
1	D	439	SER	CA-C-O	-15.38	103.94	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	439	SER	CA-C-O	-15.37	103.95	120.24
1	A	439	SER	CA-C-O	-15.37	103.95	120.24
1	C	247	HIS	CA-C-O	-15.36	103.49	121.46
1	D	247	HIS	CA-C-O	-15.36	103.49	121.46
1	B	205	TRP	CA-C-O	-15.34	103.17	120.81
1	B	247	HIS	CA-C-O	-15.34	103.51	121.46
1	C	205	TRP	CA-C-O	-15.34	103.17	120.81
1	E	247	HIS	CA-C-O	-15.34	103.51	121.46
1	A	247	HIS	CA-C-O	-15.34	103.52	121.46
1	A	205	TRP	CA-C-O	-15.33	103.18	120.81
1	E	439	SER	CA-C-O	-15.32	104.00	120.24
1	E	205	TRP	CA-C-O	-15.31	103.20	120.81
1	D	205	TRP	CA-C-O	-15.31	103.20	120.81
1	F	205	TRP	CA-C-O	-15.30	103.21	120.81
1	F	247	HIS	CA-C-O	-15.30	103.56	121.46
1	B	244	ASP	CA-CB-CG	15.29	127.89	112.60
1	D	494	THR	N-CA-C	15.28	132.43	112.26
1	E	72	TYR	O-C-N	15.28	140.83	123.42
1	E	494	THR	N-CA-C	15.27	132.42	112.26
1	B	494	THR	N-CA-C	15.27	132.41	112.26
1	A	244	ASP	CA-CB-CG	15.27	127.87	112.60
1	D	244	ASP	CA-CB-CG	15.27	127.86	112.60
1	C	494	THR	N-CA-C	15.26	132.40	112.26
1	F	494	THR	N-CA-C	15.26	132.40	112.26
1	C	244	ASP	CA-CB-CG	15.25	127.85	112.60
1	A	494	THR	N-CA-C	15.25	132.39	112.26
1	E	244	ASP	CA-CB-CG	15.24	127.84	112.60
1	F	244	ASP	CA-CB-CG	15.21	127.81	112.60
1	D	257	ALA	O-C-N	15.21	134.92	121.39
1	B	257	ALA	O-C-N	15.20	134.92	121.39
1	A	257	ALA	O-C-N	15.19	134.91	121.39
1	E	257	ALA	O-C-N	15.19	134.91	121.39
1	F	257	ALA	O-C-N	15.15	134.88	121.39
1	B	80	ARG	CD-NE-CZ	-15.14	103.20	124.40
1	F	80	ARG	CD-NE-CZ	-15.14	103.20	124.40
1	D	247	HIS	N-CA-CB	15.14	135.72	111.20
1	E	80	ARG	CD-NE-CZ	-15.14	103.21	124.40
1	A	80	ARG	CD-NE-CZ	-15.13	103.22	124.40
1	B	247	HIS	N-CA-CB	15.13	135.71	111.20
1	C	80	ARG	CD-NE-CZ	-15.13	103.22	124.40
1	C	257	ALA	O-C-N	15.13	134.85	121.39
1	A	247	HIS	N-CA-CB	15.11	135.67	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	247	HIS	N-CA-CB	15.10	135.66	111.20
1	D	80	ARG	CD-NE-CZ	-15.08	103.29	124.40
1	F	247	HIS	N-CA-CB	15.07	135.62	111.20
1	E	247	HIS	N-CA-CB	15.07	135.61	111.20
1	C	388	ASP	CA-C-O	-15.04	104.53	121.07
1	C	290	GLU	CB-CG-CD	15.04	138.16	112.60
1	A	290	GLU	CB-CG-CD	15.03	138.16	112.60
1	F	290	GLU	CB-CG-CD	15.03	138.16	112.60
1	D	290	GLU	CB-CG-CD	15.03	138.15	112.60
1	B	290	GLU	CB-CG-CD	15.02	138.14	112.60
1	E	290	GLU	CB-CG-CD	15.01	138.12	112.60
1	A	388	ASP	CA-C-O	-15.00	104.57	121.07
1	E	388	ASP	CA-C-O	-14.99	104.58	121.07
1	D	388	ASP	CA-C-O	-14.98	104.59	121.07
1	F	80	ARG	NE-CZ-NH2	-14.98	105.72	119.20
1	B	388	ASP	CA-C-O	-14.97	104.60	121.07
1	C	281	ASP	O-C-N	14.97	141.52	122.95
1	F	388	ASP	CA-C-O	-14.97	104.60	121.07
1	E	80	ARG	NE-CZ-NH2	-14.95	105.74	119.20
1	B	281	ASP	O-C-N	14.95	141.48	122.95
1	A	281	ASP	O-C-N	14.94	141.47	122.95
1	E	260	THR	CA-CB-OG1	-14.94	87.19	109.60
1	A	80	ARG	NE-CZ-NH2	-14.94	105.76	119.20
1	C	260	THR	CA-CB-OG1	-14.93	87.20	109.60
1	F	281	ASP	O-C-N	14.92	141.45	122.95
1	B	80	ARG	NE-CZ-NH2	-14.91	105.78	119.20
1	C	80	ARG	NE-CZ-NH2	-14.91	105.78	119.20
1	B	260	THR	CA-CB-OG1	-14.91	87.24	109.60
1	A	260	THR	CA-CB-OG1	-14.90	87.24	109.60
1	D	281	ASP	O-C-N	14.90	141.43	122.95
1	D	260	THR	CA-CB-OG1	-14.90	87.25	109.60
1	E	281	ASP	O-C-N	14.90	141.42	122.95
1	F	260	THR	CA-CB-OG1	-14.90	87.26	109.60
1	D	80	ARG	NE-CZ-NH2	-14.88	105.81	119.20
1	E	322	GLU	CA-CB-CG	14.81	143.71	114.10
1	A	322	GLU	CA-CB-CG	14.80	143.69	114.10
1	B	322	GLU	CA-CB-CG	14.80	143.69	114.10
1	D	322	GLU	CA-CB-CG	14.80	143.69	114.10
1	C	322	GLU	CA-CB-CG	14.79	143.69	114.10
1	F	322	GLU	CA-CB-CG	14.78	143.67	114.10
1	F	395	THR	CA-C-O	-14.76	104.69	120.63
1	E	395	THR	CA-C-O	-14.73	104.72	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	79	GLN	CG-CD-NE2	-14.71	94.33	116.40
1	C	79	GLN	CG-CD-NE2	-14.71	94.34	116.40
1	A	395	THR	CA-C-O	-14.71	104.75	120.63
1	D	395	THR	CA-C-O	-14.71	104.75	120.63
1	E	311	HIS	CA-CB-CG	-14.71	99.09	113.80
1	B	79	GLN	CG-CD-NE2	-14.69	94.37	116.40
1	B	395	THR	CA-C-O	-14.69	104.77	120.63
1	C	395	THR	CA-C-O	-14.69	104.77	120.63
1	A	79	GLN	CG-CD-NE2	-14.68	94.38	116.40
1	F	79	GLN	CG-CD-NE2	-14.68	94.38	116.40
1	A	311	HIS	CA-CB-CG	-14.67	99.13	113.80
1	D	311	HIS	CA-CB-CG	-14.67	99.13	113.80
1	F	311	HIS	CA-CB-CG	-14.67	99.13	113.80
1	C	311	HIS	CA-CB-CG	-14.67	99.13	113.80
1	B	311	HIS	CA-CB-CG	-14.66	99.14	113.80
1	D	79	GLN	CG-CD-NE2	-14.66	94.41	116.40
1	B	360	LYS	CA-C-O	-14.62	102.17	119.27
1	B	132	ILE	N-CA-C	14.60	129.22	109.80
1	A	360	LYS	CA-C-O	-14.60	102.19	119.27
1	F	360	LYS	CA-C-O	-14.60	102.19	119.27
1	B	387	MET	N-CA-CB	14.59	131.94	110.06
1	E	360	LYS	CA-C-O	-14.59	102.21	119.27
1	A	132	ILE	N-CA-C	14.58	129.19	109.80
1	C	132	ILE	N-CA-C	14.58	129.19	109.80
1	D	387	MET	N-CA-CB	14.57	131.92	110.06
1	A	387	MET	N-CA-CB	14.57	131.91	110.06
1	D	132	ILE	N-CA-C	14.57	129.18	109.80
1	E	132	ILE	N-CA-C	14.57	129.18	109.80
1	F	132	ILE	N-CA-C	14.57	129.18	109.80
1	C	213	LEU	CA-C-O	-14.56	104.45	121.05
1	C	360	LYS	CA-C-O	-14.56	102.24	119.27
1	C	387	MET	N-CA-CB	14.56	131.90	110.06
1	D	360	LYS	CA-C-O	-14.55	102.24	119.27
1	F	387	MET	N-CA-CB	14.55	131.89	110.06
1	E	213	LEU	CA-C-O	-14.53	104.48	121.05
1	E	387	MET	N-CA-CB	14.53	131.86	110.06
1	B	213	LEU	CA-C-O	-14.53	104.48	121.05
1	A	213	LEU	CA-C-O	-14.52	104.50	121.05
1	D	213	LEU	CA-C-O	-14.51	104.51	121.05
1	F	213	LEU	CA-C-O	-14.50	104.52	121.05
1	A	556	SER	N-CA-C	-14.32	88.62	109.96
1	D	556	SER	N-CA-C	-14.32	88.62	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	556	SER	N-CA-C	-14.32	88.63	109.96
1	B	556	SER	N-CA-C	-14.31	88.63	109.96
1	E	556	SER	N-CA-C	-14.31	88.64	109.96
1	F	556	SER	N-CA-C	-14.31	88.64	109.96
1	B	92	GLN	CB-CG-CD	-14.29	88.31	112.60
1	A	92	GLN	CB-CG-CD	-14.29	88.31	112.60
1	E	92	GLN	CB-CG-CD	-14.29	88.31	112.60
1	C	92	GLN	CB-CG-CD	-14.29	88.31	112.60
1	E	577	GLY	CA-C-O	-14.29	112.93	122.22
1	D	92	GLN	CB-CG-CD	-14.28	88.32	112.60
1	F	92	GLN	CB-CG-CD	-14.28	88.33	112.60
1	C	460	PHE	CA-C-O	-14.22	105.97	121.33
1	B	460	PHE	CA-C-O	-14.22	105.97	121.33
1	A	460	PHE	CA-C-O	-14.22	105.97	121.33
1	E	460	PHE	CA-C-O	-14.21	105.98	121.33
1	D	460	PHE	CA-C-O	-14.21	105.99	121.33
1	F	460	PHE	CA-C-O	-14.21	105.99	121.33
1	C	577	GLY	CA-C-O	-14.21	112.99	122.22
1	A	577	GLY	CA-C-O	-14.20	112.99	122.22
1	F	577	GLY	CA-C-O	-14.18	113.00	122.22
1	D	72	TYR	O-C-N	14.17	140.87	123.44
1	D	577	GLY	CA-C-O	-14.17	113.01	122.22
1	A	72	TYR	O-C-N	14.16	140.86	123.44
1	F	72	TYR	O-C-N	14.15	140.84	123.44
1	B	72	TYR	O-C-N	14.14	140.83	123.44
1	B	577	GLY	CA-C-O	-14.14	113.03	122.22
1	C	72	TYR	O-C-N	14.11	140.79	123.44
1	B	25	THR	OG1-CB-CG2	14.09	137.48	109.30
1	F	25	THR	OG1-CB-CG2	14.09	137.47	109.30
1	A	25	THR	OG1-CB-CG2	14.07	137.44	109.30
1	D	25	THR	OG1-CB-CG2	14.06	137.43	109.30
1	C	25	THR	OG1-CB-CG2	14.06	137.42	109.30
1	D	554	ASP	CA-C-N	14.06	144.56	122.49
1	D	554	ASP	C-N-CA	14.06	144.56	122.49
1	E	25	THR	OG1-CB-CG2	14.06	137.42	109.30
1	F	554	ASP	CA-C-N	14.06	144.56	122.49
1	F	554	ASP	C-N-CA	14.06	144.56	122.49
1	B	554	ASP	CA-C-N	14.06	144.56	122.49
1	B	554	ASP	C-N-CA	14.06	144.56	122.49
1	F	290	GLU	CA-C-O	-14.05	104.58	121.02
1	E	290	GLU	CA-C-O	-14.05	104.58	121.02
1	A	554	ASP	CA-C-N	14.05	144.54	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	554	ASP	C-N-CA	14.05	144.54	122.49
1	C	290	GLU	CA-C-O	-14.04	104.59	121.02
1	D	290	GLU	CA-C-O	-14.04	104.59	121.02
1	B	290	GLU	CA-C-O	-14.04	104.59	121.02
1	C	554	ASP	CA-C-N	14.04	144.53	122.49
1	C	554	ASP	C-N-CA	14.04	144.53	122.49
1	E	554	ASP	CA-C-N	14.04	144.53	122.49
1	E	554	ASP	C-N-CA	14.04	144.53	122.49
1	A	290	GLU	CA-C-O	-14.02	104.61	121.02
1	F	483	CYS	CA-C-O	-14.02	100.85	121.46
1	F	10	LYS	CG-CD-CE	14.02	143.55	111.30
1	E	10	LYS	CG-CD-CE	14.02	143.53	111.30
1	B	10	LYS	CG-CD-CE	14.01	143.52	111.30
1	D	10	LYS	CG-CD-CE	14.01	143.52	111.30
1	A	10	LYS	CG-CD-CE	14.01	143.52	111.30
1	D	483	CYS	CA-C-O	-14.00	100.88	121.46
1	C	10	LYS	CG-CD-CE	14.00	143.50	111.30
1	B	483	CYS	CA-C-O	-14.00	100.88	121.46
1	E	483	CYS	CA-C-O	-14.00	100.88	121.46
1	A	483	CYS	CA-C-O	-13.99	100.89	121.46
1	C	483	CYS	CA-C-O	-13.98	100.91	121.46
1	F	9	GLN	O-C-N	13.78	138.07	121.95
1	D	9	GLN	O-C-N	13.75	138.04	121.95
1	F	299	ALA	N-CA-C	-13.74	94.63	111.40
1	B	299	ALA	N-CA-C	-13.74	94.64	111.40
1	C	9	GLN	O-C-N	13.73	138.02	121.95
1	D	299	ALA	N-CA-C	-13.73	94.65	111.40
1	A	9	GLN	O-C-N	13.73	138.01	121.95
1	E	299	ALA	N-CA-C	-13.72	94.66	111.40
1	B	219	LEU	CB-CA-C	13.72	132.42	110.88
1	D	219	LEU	CB-CA-C	13.72	132.42	110.88
1	A	219	LEU	CB-CA-C	13.71	132.41	110.88
1	B	9	GLN	O-C-N	13.71	138.00	121.95
1	E	9	GLN	O-C-N	13.71	138.00	121.95
1	F	219	LEU	CB-CA-C	13.71	132.41	110.88
1	A	299	ALA	N-CA-C	-13.71	94.67	111.40
1	C	219	LEU	CB-CA-C	13.71	132.40	110.88
1	C	299	ALA	N-CA-C	-13.71	94.68	111.40
1	E	219	LEU	CB-CA-C	13.70	132.39	110.88
1	E	72	TYR	CA-C-O	-13.69	103.44	120.14
1	C	155	TYR	N-CA-CB	13.68	131.49	110.28
1	E	155	TYR	N-CA-CB	13.68	131.48	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	155	TYR	N-CA-CB	13.67	131.47	110.28
1	F	155	TYR	N-CA-CB	13.67	131.46	110.28
1	D	155	TYR	N-CA-CB	13.65	131.44	110.28
1	B	155	TYR	N-CA-CB	13.65	131.43	110.28
1	D	235	ARG	NH1-CZ-NH2	13.64	137.03	119.30
1	B	235	ARG	NH1-CZ-NH2	13.61	137.00	119.30
1	A	235	ARG	NH1-CZ-NH2	13.59	136.97	119.30
1	C	235	ARG	NH1-CZ-NH2	13.58	136.95	119.30
1	D	163	PRO	O-C-N	13.58	139.86	122.89
1	F	235	ARG	NH1-CZ-NH2	13.58	136.95	119.30
1	E	163	PRO	O-C-N	13.57	139.85	122.89
1	E	235	ARG	NH1-CZ-NH2	13.56	136.93	119.30
1	C	163	PRO	O-C-N	13.56	139.84	122.89
1	A	163	PRO	O-C-N	13.54	139.82	122.89
1	B	163	PRO	O-C-N	13.54	139.82	122.89
1	C	644	HIS	CA-CB-CG	13.54	127.34	113.80
1	F	163	PRO	O-C-N	13.54	139.81	122.89
1	B	644	HIS	CA-CB-CG	13.53	127.33	113.80
1	F	644	HIS	CA-CB-CG	13.53	127.33	113.80
1	A	644	HIS	CA-CB-CG	13.51	127.31	113.80
1	D	644	HIS	CA-CB-CG	13.51	127.31	113.80
1	D	532	ASP	CA-CB-CG	13.48	126.08	112.60
1	E	644	HIS	CA-CB-CG	13.47	127.28	113.80
1	E	532	ASP	CA-CB-CG	13.47	126.07	112.60
1	A	532	ASP	CA-CB-CG	13.46	126.06	112.60
1	C	532	ASP	CA-CB-CG	13.46	126.06	112.60
1	B	532	ASP	CA-CB-CG	13.44	126.04	112.60
1	F	532	ASP	CA-CB-CG	13.42	126.02	112.60
1	B	111	ASN	OD1-CG-ND2	13.30	135.90	122.60
1	F	111	ASN	OD1-CG-ND2	13.29	135.89	122.60
1	D	111	ASN	OD1-CG-ND2	13.28	135.88	122.60
1	C	111	ASN	OD1-CG-ND2	13.25	135.85	122.60
1	E	111	ASN	OD1-CG-ND2	13.25	135.85	122.60
1	A	111	ASN	OD1-CG-ND2	13.24	135.84	122.60
1	C	92	GLN	CA-CB-CG	13.24	140.58	114.10
1	B	92	GLN	CA-CB-CG	13.23	140.57	114.10
1	F	92	GLN	CA-CB-CG	13.23	140.56	114.10
1	A	92	GLN	CA-CB-CG	13.22	140.55	114.10
1	E	92	GLN	CA-CB-CG	13.22	140.54	114.10
1	E	49	HIS	CA-CB-CG	-13.21	100.59	113.80
1	D	92	GLN	CA-CB-CG	13.21	140.51	114.10
1	B	637	ASP	CA-CB-CG	13.19	125.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	49	HIS	CA-CB-CG	-13.19	100.61	113.80
1	A	49	HIS	CA-CB-CG	-13.18	100.62	113.80
1	B	49	HIS	CA-CB-CG	-13.18	100.62	113.80
1	F	49	HIS	CA-CB-CG	-13.18	100.62	113.80
1	D	174	LYS	N-CA-C	-13.16	91.68	110.24
1	E	174	LYS	N-CA-C	-13.16	91.69	110.24
1	A	637	ASP	CA-CB-CG	13.16	125.76	112.60
1	F	174	LYS	N-CA-C	-13.16	91.69	110.24
1	B	174	LYS	N-CA-C	-13.15	91.69	110.24
1	D	637	ASP	CA-CB-CG	13.15	125.75	112.60
1	C	637	ASP	CA-CB-CG	13.15	125.75	112.60
1	A	174	LYS	N-CA-C	-13.14	91.70	110.24
1	E	637	ASP	CA-CB-CG	13.14	125.74	112.60
1	F	642	ILE	CA-C-O	-13.14	106.30	120.76
1	D	49	HIS	CA-CB-CG	-13.14	100.66	113.80
1	B	642	ILE	CA-C-O	-13.13	106.31	120.76
1	F	637	ASP	CA-CB-CG	13.13	125.73	112.60
1	C	174	LYS	N-CA-C	-13.12	91.73	110.24
1	E	642	ILE	CA-C-O	-13.12	106.33	120.76
1	A	642	ILE	CA-C-O	-13.12	106.33	120.76
1	D	642	ILE	CA-C-O	-13.12	106.33	120.76
1	C	642	ILE	CA-C-O	-13.10	106.35	120.76
1	C	69	ARG	NE-CZ-NH2	13.09	130.98	119.20
1	D	238	ASN	OD1-CG-ND2	13.08	135.68	122.60
1	C	413	VAL	O-C-N	13.07	136.92	122.67
1	D	69	ARG	NE-CZ-NH2	13.07	130.97	119.20
1	E	124	ILE	CA-C-O	-13.07	107.31	121.17
1	E	69	ARG	NE-CZ-NH2	13.07	130.96	119.20
1	D	413	VAL	O-C-N	13.06	136.91	122.67
1	B	413	VAL	O-C-N	13.06	136.91	122.67
1	F	413	VAL	O-C-N	13.06	136.91	122.67
1	C	238	ASN	OD1-CG-ND2	13.06	135.66	122.60
1	A	413	VAL	O-C-N	13.06	136.90	122.67
1	F	69	ARG	NE-CZ-NH2	13.05	130.95	119.20
1	E	413	VAL	O-C-N	13.05	136.90	122.67
1	A	238	ASN	OD1-CG-ND2	13.05	135.65	122.60
1	F	238	ASN	OD1-CG-ND2	13.05	135.65	122.60
1	B	124	ILE	CA-C-O	-13.05	107.34	121.17
1	D	124	ILE	CA-C-O	-13.05	107.34	121.17
1	F	124	ILE	CA-C-O	-13.04	107.34	121.17
1	A	124	ILE	CA-C-O	-13.04	107.35	121.17
1	A	69	ARG	NE-CZ-NH2	13.04	130.93	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	238	ASN	OD1-CG-ND2	13.03	135.63	122.60
1	C	124	ILE	CA-C-O	-13.02	107.37	121.17
1	E	238	ASN	OD1-CG-ND2	13.02	135.62	122.60
1	C	310	GLY	O-C-N	12.99	136.02	122.51
1	E	238	ASN	CB-CG-OD1	-12.98	94.84	120.80
1	B	69	ARG	NE-CZ-NH2	12.98	130.88	119.20
1	C	238	ASN	CB-CG-OD1	-12.98	94.84	120.80
1	F	345	ASN	CA-C-O	-12.98	107.37	121.00
1	A	238	ASN	CB-CG-OD1	-12.97	94.86	120.80
1	F	238	ASN	CB-CG-OD1	-12.97	94.86	120.80
1	D	238	ASN	CB-CG-OD1	-12.96	94.87	120.80
1	B	238	ASN	CB-CG-OD1	-12.95	94.90	120.80
1	D	310	GLY	O-C-N	12.95	135.98	122.51
1	B	345	ASN	CA-C-O	-12.94	107.41	121.00
1	C	212	HIS	CA-C-O	-12.94	105.95	120.32
1	A	310	GLY	O-C-N	12.94	135.97	122.51
1	D	212	HIS	CA-C-O	-12.94	105.96	120.32
1	F	212	HIS	CA-C-O	-12.94	105.96	120.32
1	A	212	HIS	CA-C-O	-12.93	105.97	120.32
1	A	345	ASN	CA-C-O	-12.93	107.42	121.00
1	C	345	ASN	CA-C-O	-12.93	107.42	121.00
1	E	310	GLY	O-C-N	12.92	135.95	122.51
1	B	310	GLY	O-C-N	12.92	135.95	122.51
1	E	345	ASN	CA-C-O	-12.92	107.43	121.00
1	E	212	HIS	CA-C-O	-12.92	105.98	120.32
1	B	212	HIS	CA-C-O	-12.91	105.99	120.32
1	F	310	GLY	O-C-N	12.91	135.94	122.51
1	D	345	ASN	CA-C-O	-12.90	107.45	121.00
1	C	361	PHE	CA-CB-CG	-12.88	100.92	113.80
1	D	314	ASP	CA-C-O	-12.88	107.52	121.56
1	D	310	GLY	N-CA-C	-12.88	94.89	116.01
1	F	361	PHE	CA-CB-CG	-12.87	100.93	113.80
1	B	361	PHE	CA-CB-CG	-12.86	100.94	113.80
1	C	310	GLY	N-CA-C	-12.86	94.91	116.01
1	A	310	GLY	N-CA-C	-12.85	94.93	116.01
1	B	310	GLY	N-CA-C	-12.85	94.93	116.01
1	E	310	GLY	N-CA-C	-12.85	94.93	116.01
1	F	314	ASP	CA-C-O	-12.85	107.55	121.56
1	F	310	GLY	N-CA-C	-12.85	94.94	116.01
1	B	152	ASP	CA-CB-CG	12.84	125.44	112.60
1	E	361	PHE	CA-CB-CG	-12.84	100.96	113.80
1	A	314	ASP	CA-C-O	-12.84	107.57	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	361	PHE	CA-CB-CG	-12.84	100.96	113.80
1	C	314	ASP	CA-C-O	-12.84	107.57	121.56
1	B	314	ASP	CA-C-O	-12.82	107.58	121.56
1	E	314	ASP	CA-C-O	-12.82	107.58	121.56
1	D	361	PHE	CA-CB-CG	-12.82	100.98	113.80
1	E	152	ASP	CA-CB-CG	12.81	125.41	112.60
1	F	152	ASP	CA-CB-CG	12.80	125.40	112.60
1	A	152	ASP	CA-CB-CG	12.80	125.40	112.60
1	D	152	ASP	CA-CB-CG	12.79	125.39	112.60
1	C	152	ASP	CA-CB-CG	12.79	125.39	112.60
1	E	279	ASP	CB-CA-C	12.79	128.58	110.16
1	C	279	ASP	CB-CA-C	12.77	128.55	110.16
1	B	279	ASP	CB-CA-C	12.76	128.54	110.16
1	D	279	ASP	CB-CA-C	12.75	128.53	110.16
1	A	279	ASP	CB-CA-C	12.75	128.52	110.16
1	F	279	ASP	CB-CA-C	12.75	128.52	110.16
1	D	395	THR	O-C-N	12.65	135.53	122.12
1	A	395	THR	O-C-N	12.64	135.52	122.12
1	F	395	THR	O-C-N	12.63	135.51	122.12
1	C	395	THR	O-C-N	12.63	135.51	122.12
1	E	395	THR	O-C-N	12.63	135.51	122.12
1	B	631	PRO	CA-C-O	-12.63	101.43	119.74
1	D	631	PRO	CA-C-O	-12.62	101.44	119.74
1	C	631	PRO	CA-C-O	-12.61	101.45	119.74
1	F	631	PRO	CA-C-O	-12.61	101.45	119.74
1	E	480	ILE	CA-CB-CG2	12.60	131.93	110.50
1	A	631	PRO	CA-C-O	-12.60	101.47	119.74
1	A	480	ILE	CA-CB-CG2	12.59	131.91	110.50
1	C	480	ILE	CA-CB-CG2	12.59	131.91	110.50
1	B	395	THR	O-C-N	12.59	135.47	122.12
1	C	109	ARG	NE-CZ-NH2	-12.59	107.87	119.20
1	E	631	PRO	CA-C-O	-12.59	101.49	119.74
1	F	480	ILE	CA-CB-CG2	12.58	131.89	110.50
1	D	480	ILE	CA-CB-CG2	12.58	131.88	110.50
1	B	109	ARG	NE-CZ-NH2	-12.57	107.89	119.20
1	B	480	ILE	CA-CB-CG2	12.56	131.85	110.50
1	D	452	VAL	CA-C-O	-12.55	106.94	121.75
1	F	109	ARG	NE-CZ-NH2	-12.55	107.90	119.20
1	A	109	ARG	NE-CZ-NH2	-12.55	107.91	119.20
1	E	109	ARG	NE-CZ-NH2	-12.54	107.91	119.20
1	D	109	ARG	NE-CZ-NH2	-12.54	107.91	119.20
1	E	612	HIS	CA-CB-CG	12.54	126.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	452	VAL	CA-C-O	-12.54	106.95	121.75
1	D	612	HIS	CA-CB-CG	12.54	126.33	113.80
1	C	612	HIS	CA-CB-CG	12.52	126.32	113.80
1	A	452	VAL	CA-C-O	-12.52	106.98	121.75
1	B	174	LYS	CB-CA-C	12.52	129.85	109.70
1	C	452	VAL	CA-C-O	-12.52	106.98	121.75
1	E	453	HIS	CA-CB-CG	-12.52	101.28	113.80
1	F	453	HIS	CA-CB-CG	-12.51	101.29	113.80
1	C	174	LYS	CB-CA-C	12.51	129.84	109.70
1	B	453	HIS	CA-CB-CG	-12.51	101.29	113.80
1	E	174	LYS	CB-CA-C	12.51	129.84	109.70
1	F	612	HIS	CA-CB-CG	12.51	126.31	113.80
1	A	174	LYS	CB-CA-C	12.50	129.83	109.70
1	B	612	HIS	CA-CB-CG	12.50	126.30	113.80
1	A	453	HIS	CA-CB-CG	-12.50	101.30	113.80
1	A	612	HIS	CA-CB-CG	12.50	126.30	113.80
1	B	50	GLY	N-CA-C	12.50	131.73	113.48
1	F	174	LYS	CB-CA-C	12.50	129.83	109.70
1	C	453	HIS	CA-CB-CG	-12.50	101.30	113.80
1	E	452	VAL	CA-C-O	-12.50	107.00	121.75
1	F	452	VAL	CA-C-O	-12.49	107.01	121.75
1	D	174	LYS	CB-CA-C	12.49	129.81	109.70
1	D	453	HIS	CA-CB-CG	-12.49	101.31	113.80
1	F	50	GLY	N-CA-C	12.49	131.71	113.48
1	D	50	GLY	N-CA-C	12.47	131.69	113.48
1	D	72	TYR	CA-C-O	-12.47	103.38	120.21
1	A	50	GLY	N-CA-C	12.46	131.67	113.48
1	C	50	GLY	N-CA-C	12.46	131.67	113.48
1	F	491	ILE	CA-C-O	-12.45	105.22	120.78
1	E	50	GLY	N-CA-C	12.44	131.65	113.48
1	A	72	TYR	CA-C-O	-12.44	103.41	120.21
1	A	491	ILE	CA-C-O	-12.43	105.24	120.78
1	F	72	TYR	CA-C-O	-12.43	103.43	120.21
1	D	491	ILE	CA-C-O	-12.43	105.24	120.78
1	C	72	TYR	CA-C-O	-12.43	103.43	120.21
1	B	491	ILE	CA-C-O	-12.42	105.25	120.78
1	C	491	ILE	CA-C-O	-12.42	105.26	120.78
1	E	491	ILE	CA-C-O	-12.42	105.26	120.78
1	B	72	TYR	CA-C-O	-12.40	103.47	120.21
1	D	243	VAL	CB-CA-C	-12.25	94.72	111.63
1	A	243	VAL	CB-CA-C	-12.24	94.73	111.63
1	F	243	VAL	CB-CA-C	-12.24	94.73	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	243	VAL	CB-CA-C	-12.24	94.74	111.63
1	C	243	VAL	CB-CA-C	-12.23	94.75	111.63
1	E	243	VAL	CB-CA-C	-12.23	94.75	111.63
1	D	68	GLN	OE1-CD-NE2	-12.23	110.37	122.60
1	E	56	LEU	CA-C-O	-12.23	107.47	120.55
1	E	68	GLN	OE1-CD-NE2	-12.22	110.38	122.60
1	E	393	LYS	N-CA-CB	12.22	129.04	110.22
1	B	443	ILE	CA-C-O	-12.22	106.90	120.71
1	C	443	ILE	CA-C-O	-12.22	106.90	120.71
1	A	393	LYS	N-CA-CB	12.21	129.03	110.22
1	D	393	LYS	N-CA-CB	12.21	129.03	110.22
1	C	435	ASN	CA-CB-CG	12.21	124.81	112.60
1	F	393	LYS	N-CA-CB	12.21	129.02	110.22
1	A	443	ILE	CA-C-O	-12.20	106.92	120.71
1	B	56	LEU	CA-C-O	-12.21	107.49	120.55
1	C	56	LEU	CA-C-O	-12.20	107.49	120.55
1	B	393	LYS	N-CA-CB	12.20	129.01	110.22
1	F	443	ILE	CA-C-O	-12.20	106.92	120.71
1	A	68	GLN	OE1-CD-NE2	-12.20	110.40	122.60
1	F	309	ASP	CA-C-N	-12.20	105.80	122.63
1	F	309	ASP	C-N-CA	-12.20	105.80	122.63
1	A	56	LEU	CA-C-O	-12.19	107.50	120.55
1	C	68	GLN	OE1-CD-NE2	-12.19	110.41	122.60
1	E	443	ILE	CA-C-O	-12.19	106.94	120.71
1	D	443	ILE	CA-C-O	-12.19	106.94	120.71
1	A	309	ASP	CA-C-N	-12.18	105.82	122.63
1	A	309	ASP	C-N-CA	-12.18	105.82	122.63
1	C	393	LYS	N-CA-CB	12.18	128.98	110.22
1	E	309	ASP	CA-C-N	-12.18	105.82	122.63
1	E	309	ASP	C-N-CA	-12.18	105.82	122.63
1	F	56	LEU	CA-C-O	-12.18	107.51	120.55
1	F	68	GLN	OE1-CD-NE2	-12.18	110.42	122.60
1	B	68	GLN	OE1-CD-NE2	-12.18	110.42	122.60
1	D	309	ASP	CA-C-N	-12.18	105.83	122.63
1	D	309	ASP	C-N-CA	-12.18	105.83	122.63
1	B	435	ASN	CA-CB-CG	12.17	124.77	112.60
1	C	309	ASP	CA-C-N	-12.17	105.83	122.63
1	C	309	ASP	C-N-CA	-12.17	105.83	122.63
1	D	56	LEU	CA-C-O	-12.17	107.52	120.55
1	D	435	ASN	CA-CB-CG	12.17	124.77	112.60
1	B	309	ASP	CA-C-N	-12.16	105.85	122.63
1	B	309	ASP	C-N-CA	-12.16	105.85	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	435	ASN	CA-CB-CG	12.16	124.76	112.60
1	A	435	ASN	CA-CB-CG	12.15	124.75	112.60
1	C	422	LEU	CB-CA-C	12.14	131.70	111.31
1	F	422	LEU	CB-CA-C	12.13	131.70	111.31
1	D	422	LEU	CB-CA-C	12.12	131.67	111.31
1	A	422	LEU	CB-CA-C	12.12	131.67	111.31
1	B	422	LEU	CB-CA-C	12.12	131.67	111.31
1	E	422	LEU	CB-CA-C	12.11	131.66	111.31
1	F	411	MET	CA-CB-CG	-12.11	89.89	114.10
1	F	435	ASN	CA-CB-CG	12.11	124.70	112.60
1	C	411	MET	CA-CB-CG	-12.10	89.91	114.10
1	D	411	MET	CA-CB-CG	-12.09	89.92	114.10
1	A	411	MET	CA-CB-CG	-12.08	89.94	114.10
1	B	411	MET	CA-CB-CG	-12.08	89.94	114.10
1	F	510	GLN	CA-C-O	-12.08	106.98	121.11
1	C	510	GLN	CA-C-O	-12.07	106.98	121.11
1	E	411	MET	CA-CB-CG	-12.07	89.97	114.10
1	B	215	ARG	NE-CZ-NH1	-12.06	109.44	121.50
1	B	632	ASP	O-C-N	12.06	137.38	123.27
1	F	215	ARG	NE-CZ-NH1	-12.06	109.44	121.50
1	F	632	ASP	O-C-N	12.06	137.38	123.27
1	E	215	ARG	NE-CZ-NH1	-12.05	109.45	121.50
1	C	632	ASP	O-C-N	12.05	137.37	123.27
1	A	215	ARG	NE-CZ-NH1	-12.04	109.46	121.50
1	D	510	GLN	CA-C-O	-12.04	107.02	121.11
1	D	632	ASP	O-C-N	12.04	137.36	123.27
1	B	510	GLN	CA-C-O	-12.04	107.02	121.11
1	A	510	GLN	CA-C-O	-12.04	107.02	121.11
1	D	296	ILE	O-C-N	12.04	134.34	121.94
1	E	632	ASP	O-C-N	12.04	137.36	123.27
1	D	482	LEU	CA-C-O	-12.04	103.79	120.52
1	A	632	ASP	O-C-N	12.03	137.34	123.27
1	E	510	GLN	CA-C-O	-12.02	107.04	121.11
1	F	482	LEU	CA-C-O	-12.02	103.81	120.52
1	D	215	ARG	NE-CZ-NH1	-12.01	109.49	121.50
1	A	482	LEU	CA-C-O	-12.01	103.83	120.52
1	C	482	LEU	CA-C-O	-12.01	103.83	120.52
1	C	215	ARG	NE-CZ-NH1	-12.00	109.50	121.50
1	E	482	LEU	CA-C-O	-12.00	103.84	120.52
1	E	395	THR	CA-CB-OG1	-12.00	91.60	109.60
1	A	296	ILE	O-C-N	11.99	134.29	121.94
1	B	296	ILE	O-C-N	11.99	134.29	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	296	ILE	O-C-N	11.99	134.29	121.94
1	B	482	LEU	CA-C-O	-11.99	103.86	120.52
1	B	395	THR	CA-CB-OG1	-11.98	91.63	109.60
1	C	296	ILE	O-C-N	11.97	134.28	121.94
1	F	395	THR	CA-CB-OG1	-11.97	91.64	109.60
1	C	395	THR	CA-CB-OG1	-11.97	91.65	109.60
1	D	632	ASP	CA-CB-CG	11.97	124.57	112.60
1	A	395	THR	CA-CB-OG1	-11.96	91.66	109.60
1	E	632	ASP	CA-CB-CG	11.96	124.56	112.60
1	B	276	HIS	CA-CB-CG	-11.96	101.84	113.80
1	C	632	ASP	CA-CB-CG	11.95	124.55	112.60
1	D	395	THR	CA-CB-OG1	-11.95	91.67	109.60
1	F	276	HIS	CA-CB-CG	-11.95	101.85	113.80
1	F	632	ASP	CA-CB-CG	11.95	124.55	112.60
1	A	632	ASP	CA-CB-CG	11.94	124.54	112.60
1	E	296	ILE	O-C-N	11.94	134.24	121.94
1	D	276	HIS	CA-CB-CG	-11.93	101.87	113.80
1	B	632	ASP	CA-CB-CG	11.93	124.53	112.60
1	E	275	ILE	CB-CA-C	-11.93	98.46	111.59
1	C	275	ILE	CB-CA-C	-11.93	98.47	111.59
1	A	276	HIS	CA-CB-CG	-11.93	101.88	113.80
1	E	276	HIS	CA-CB-CG	-11.92	101.88	113.80
1	D	275	ILE	CB-CA-C	-11.91	98.49	111.59
1	A	275	ILE	CB-CA-C	-11.91	98.49	111.59
1	F	275	ILE	CB-CA-C	-11.91	98.49	111.59
1	C	551	HIS	CB-CA-C	-11.90	90.56	109.72
1	D	163	PRO	CB-CA-C	-11.90	91.20	110.96
1	D	551	HIS	CB-CA-C	-11.90	90.56	109.72
1	E	551	HIS	CB-CA-C	-11.90	90.56	109.72
1	F	163	PRO	CB-CA-C	-11.90	91.20	110.96
1	A	551	HIS	CB-CA-C	-11.90	90.56	109.72
1	E	163	PRO	CB-CA-C	-11.90	91.21	110.96
1	F	551	HIS	CB-CA-C	-11.90	90.57	109.72
1	B	275	ILE	CB-CA-C	-11.89	98.51	111.59
1	C	308	SER	O-C-N	11.89	136.14	122.22
1	B	163	PRO	CB-CA-C	-11.89	91.22	110.96
1	B	308	SER	O-C-N	11.89	136.13	122.22
1	C	276	HIS	CA-CB-CG	-11.89	101.91	113.80
1	A	163	PRO	CB-CA-C	-11.89	91.22	110.96
1	B	551	HIS	CB-CA-C	-11.89	90.58	109.72
1	E	308	SER	O-C-N	11.88	136.12	122.22
1	C	163	PRO	CB-CA-C	-11.87	91.25	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	308	SER	O-C-N	11.87	136.11	122.22
1	A	308	SER	O-C-N	11.87	136.11	122.22
1	F	308	SER	O-C-N	11.85	136.09	122.22
1	B	7	ASN	N-CA-CB	11.84	130.51	110.49
1	F	373	THR	N-CA-CB	-11.84	92.54	111.01
1	F	551	HIS	N-CA-C	11.84	126.34	108.46
1	A	551	HIS	N-CA-C	11.84	126.34	108.46
1	D	551	HIS	N-CA-C	11.84	126.34	108.46
1	B	114	GLU	N-CA-C	-11.84	98.40	111.07
1	C	7	ASN	N-CA-CB	11.84	130.50	110.49
1	C	551	HIS	N-CA-C	11.84	126.33	108.46
1	B	551	HIS	N-CA-C	11.83	126.33	108.46
1	F	40	LEU	N-CA-CB	-11.83	91.99	110.92
1	E	7	ASN	N-CA-CB	11.83	130.48	110.49
1	F	7	ASN	N-CA-CB	11.83	130.48	110.49
1	A	7	ASN	N-CA-CB	11.82	130.47	110.49
1	A	373	THR	N-CA-CB	-11.82	92.56	111.01
1	C	114	GLU	N-CA-C	-11.82	98.42	111.07
1	B	588	ASP	CA-CB-CG	11.82	124.42	112.60
1	D	40	LEU	N-CA-CB	-11.82	92.01	110.92
1	E	114	GLU	N-CA-C	-11.82	98.42	111.07
1	D	7	ASN	N-CA-CB	11.81	130.46	110.49
1	E	373	THR	N-CA-CB	-11.81	92.58	111.01
1	A	40	LEU	N-CA-CB	-11.81	92.02	110.92
1	C	588	ASP	CA-CB-CG	11.81	124.41	112.60
1	D	350	MET	CA-C-O	-11.81	107.90	120.42
1	E	551	HIS	N-CA-C	11.81	126.30	108.46
1	F	588	ASP	CA-CB-CG	11.81	124.41	112.60
1	A	588	ASP	CA-CB-CG	11.81	124.41	112.60
1	A	350	MET	CA-C-O	-11.81	107.91	120.42
1	B	40	LEU	N-CA-CB	-11.80	92.03	110.92
1	C	373	THR	N-CA-CB	-11.80	92.60	111.01
1	D	373	THR	N-CA-CB	-11.80	92.59	111.01
1	B	373	THR	N-CA-CB	-11.80	92.60	111.01
1	C	40	LEU	N-CA-CB	-11.80	92.04	110.92
1	C	350	MET	CA-C-O	-11.80	107.91	120.42
1	E	350	MET	CA-C-O	-11.80	107.91	120.42
1	E	588	ASP	CA-CB-CG	11.80	124.40	112.60
1	A	114	GLU	N-CA-C	-11.80	98.44	111.07
1	D	588	ASP	CA-CB-CG	11.80	124.40	112.60
1	E	40	LEU	N-CA-CB	-11.79	92.05	110.92
1	F	350	MET	CA-C-O	-11.79	107.92	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	114	GLU	N-CA-C	-11.79	98.46	111.07
1	D	114	GLU	N-CA-C	-11.78	98.46	111.07
1	E	488	ASN	N-CA-CB	11.78	125.88	114.10
1	B	488	ASN	N-CA-CB	11.77	125.87	114.10
1	C	488	ASN	N-CA-CB	11.77	125.87	114.10
1	B	350	MET	CA-C-O	-11.76	107.95	120.42
1	D	488	ASN	N-CA-CB	11.76	125.86	114.10
1	A	488	ASN	N-CA-CB	11.74	125.84	114.10
1	B	182	ALA	CA-C-O	11.74	133.00	120.55
1	F	358	HIS	CA-CB-CG	-11.74	102.06	113.80
1	F	488	ASN	N-CA-CB	11.74	125.84	114.10
1	E	358	HIS	CA-CB-CG	-11.73	102.07	113.80
1	B	358	HIS	CA-CB-CG	-11.73	102.07	113.80
1	C	358	HIS	CA-CB-CG	-11.72	102.08	113.80
1	C	608	GLN	CB-CG-CD	11.72	132.53	112.60
1	E	182	ALA	CA-C-O	11.72	132.98	120.55
1	A	358	HIS	CA-CB-CG	-11.72	102.08	113.80
1	D	331	SER	O-C-N	11.72	138.31	122.72
1	F	279	ASP	N-CA-CB	-11.72	91.00	109.51
1	A	331	SER	O-C-N	11.72	138.30	122.72
1	C	112	GLU	N-CA-C	11.71	124.05	111.28
1	A	608	GLN	CB-CG-CD	11.71	132.50	112.60
1	C	182	ALA	CA-C-O	11.71	132.96	120.55
1	D	279	ASP	N-CA-CB	-11.71	91.01	109.51
1	C	331	SER	O-C-N	11.70	138.29	122.72
1	F	608	GLN	CB-CG-CD	11.71	132.50	112.60
1	B	608	GLN	CB-CG-CD	11.70	132.49	112.60
1	D	358	HIS	CA-CB-CG	-11.70	102.10	113.80
1	F	182	ALA	CA-C-O	11.70	132.95	120.55
1	B	331	SER	O-C-N	11.70	138.28	122.72
1	A	279	ASP	N-CA-CB	-11.70	91.03	109.51
1	B	279	ASP	N-CA-CB	-11.70	91.03	109.51
1	E	331	SER	O-C-N	11.69	138.27	122.72
1	F	331	SER	O-C-N	11.70	138.27	122.72
1	A	182	ALA	CA-C-O	11.69	132.94	120.55
1	C	279	ASP	N-CA-CB	-11.69	91.04	109.51
1	E	608	GLN	CB-CG-CD	11.69	132.47	112.60
1	D	182	ALA	CA-C-O	11.69	132.94	120.55
1	C	303	GLY	N-CA-C	-11.69	100.57	114.48
1	A	112	GLU	N-CA-C	11.69	124.02	111.28
1	B	112	GLU	N-CA-C	11.68	124.01	111.28
1	D	112	GLU	N-CA-C	11.68	124.02	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	303	GLY	N-CA-C	-11.68	100.58	114.48
1	F	303	GLY	N-CA-C	-11.68	100.58	114.48
1	A	303	GLY	N-CA-C	-11.68	100.58	114.48
1	E	112	GLU	N-CA-C	11.68	124.01	111.28
1	E	279	ASP	N-CA-CB	-11.68	91.06	109.51
1	D	608	GLN	CB-CG-CD	11.66	132.43	112.60
1	D	303	GLY	N-CA-C	-11.66	100.60	114.48
1	F	112	GLU	N-CA-C	11.66	123.99	111.28
1	B	303	GLY	N-CA-C	-11.66	100.61	114.48
1	B	445	ASP	CA-CB-CG	11.66	124.26	112.60
1	C	445	ASP	CA-CB-CG	11.66	124.26	112.60
1	A	445	ASP	CA-CB-CG	11.64	124.24	112.60
1	C	226	GLN	OE1-CD-NE2	11.63	134.24	122.60
1	D	445	ASP	CA-CB-CG	11.62	124.22	112.60
1	E	445	ASP	CA-CB-CG	11.61	124.21	112.60
1	F	445	ASP	CA-CB-CG	11.61	124.21	112.60
1	B	608	GLN	O-C-N	11.60	137.39	122.19
1	D	226	GLN	OE1-CD-NE2	11.60	134.20	122.60
1	F	608	GLN	O-C-N	11.60	137.39	122.19
1	D	608	GLN	O-C-N	11.60	137.38	122.19
1	C	608	GLN	O-C-N	11.60	137.38	122.19
1	E	181	VAL	CA-C-N	11.59	135.81	120.28
1	E	181	VAL	C-N-CA	11.59	135.81	120.28
1	A	608	GLN	O-C-N	11.59	137.37	122.19
1	E	608	GLN	O-C-N	11.58	137.36	122.19
1	A	226	GLN	OE1-CD-NE2	11.57	134.17	122.60
1	C	181	VAL	CA-C-N	11.57	135.78	120.28
1	C	181	VAL	C-N-CA	11.57	135.78	120.28
1	D	181	VAL	CA-C-N	11.56	135.77	120.28
1	D	181	VAL	C-N-CA	11.56	135.77	120.28
1	A	181	VAL	CA-C-N	11.56	135.77	120.28
1	A	181	VAL	C-N-CA	11.56	135.77	120.28
1	F	181	VAL	CA-C-N	11.56	135.76	120.28
1	F	181	VAL	C-N-CA	11.56	135.76	120.28
1	B	226	GLN	OE1-CD-NE2	11.54	134.14	122.60
1	F	226	GLN	OE1-CD-NE2	11.54	134.15	122.60
1	B	181	VAL	CA-C-N	11.54	135.75	120.28
1	B	181	VAL	C-N-CA	11.54	135.75	120.28
1	E	226	GLN	OE1-CD-NE2	11.53	134.13	122.60
1	E	22	TYR	CA-C-O	-11.53	105.42	119.59
1	C	16	HIS	CA-CB-CG	-11.52	102.28	113.80
1	E	16	HIS	CA-CB-CG	-11.52	102.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	416	VAL	CB-CA-C	11.51	128.47	110.28
1	C	416	VAL	CB-CA-C	11.51	128.47	110.28
1	E	416	VAL	CB-CA-C	11.51	128.46	110.28
1	F	416	VAL	CB-CA-C	11.51	128.46	110.28
1	D	16	HIS	CA-CB-CG	-11.50	102.30	113.80
1	A	16	HIS	CA-CB-CG	-11.50	102.30	113.80
1	B	416	VAL	CB-CA-C	11.50	128.45	110.28
1	D	416	VAL	CB-CA-C	11.50	128.44	110.28
1	F	16	HIS	CA-CB-CG	-11.49	102.31	113.80
1	C	22	TYR	CA-C-O	-11.48	105.46	119.59
1	D	22	TYR	CA-C-O	-11.48	105.47	119.59
1	A	22	TYR	CA-C-O	-11.48	105.47	119.59
1	F	22	TYR	CA-C-O	-11.48	105.47	119.59
1	B	22	TYR	CA-C-O	-11.47	105.48	119.59
1	D	364	PRO	CA-C-O	-11.45	103.96	120.56
1	C	364	PRO	CA-C-O	-11.44	103.97	120.56
1	B	16	HIS	CA-CB-CG	-11.44	102.36	113.80
1	B	364	PRO	CA-C-O	-11.43	103.98	120.56
1	F	364	PRO	CA-C-O	-11.43	103.98	120.56
1	A	364	PRO	CA-C-O	-11.43	103.99	120.56
1	E	364	PRO	CA-C-O	-11.43	103.99	120.56
1	C	230	ARG	CA-C-O	-11.42	108.68	120.90
1	F	302	HIS	CA-C-O	-11.41	108.34	120.55
1	E	230	ARG	CA-C-O	-11.41	108.70	120.90
1	C	450	ALA	CA-C-O	11.40	133.02	120.70
1	B	302	HIS	CA-C-O	-11.40	108.35	120.55
1	A	450	ALA	CA-C-O	11.39	133.00	120.70
1	F	230	ARG	CA-C-O	-11.39	108.71	120.90
1	C	25	THR	N-CA-CB	11.39	126.57	110.17
1	F	25	THR	N-CA-CB	11.39	126.57	110.17
1	A	230	ARG	CA-C-O	-11.38	108.72	120.90
1	D	25	THR	N-CA-CB	11.38	126.56	110.17
1	D	230	ARG	CA-C-O	-11.38	108.72	120.90
1	B	450	ALA	CA-C-O	11.38	132.99	120.70
1	E	302	HIS	CA-C-O	-11.38	108.37	120.55
1	A	302	HIS	CA-C-O	-11.38	108.37	120.55
1	A	25	THR	N-CA-CB	11.38	126.55	110.17
1	E	228	THR	CA-CB-OG1	-11.38	92.53	109.60
1	D	302	HIS	CA-C-O	-11.38	108.38	120.55
1	B	230	ARG	CA-C-O	-11.37	108.73	120.90
1	E	25	THR	N-CA-CB	11.37	126.55	110.17
1	B	228	THR	CA-CB-OG1	-11.37	92.55	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	450	ALA	CA-C-O	11.36	132.97	120.70
1	B	25	THR	N-CA-CB	11.36	126.53	110.17
1	C	302	HIS	CA-C-O	-11.36	108.39	120.55
1	F	228	THR	CA-CB-OG1	-11.36	92.56	109.60
1	A	228	THR	CA-CB-OG1	-11.36	92.56	109.60
1	C	228	THR	CA-CB-OG1	-11.36	92.56	109.60
1	E	450	ALA	CA-C-O	11.36	132.97	120.70
1	D	228	THR	CA-CB-OG1	-11.35	92.57	109.60
1	F	217	GLY	N-CA-C	-11.35	86.29	113.18
1	F	450	ALA	CA-C-O	11.34	132.94	120.70
1	D	217	GLY	N-CA-C	-11.33	86.32	113.18
1	F	173	THR	N-CA-CB	11.33	126.90	110.58
1	B	217	GLY	N-CA-C	-11.33	86.33	113.18
1	A	217	GLY	N-CA-C	-11.33	86.33	113.18
1	D	173	THR	N-CA-CB	11.33	126.89	110.58
1	C	217	GLY	N-CA-C	-11.32	86.35	113.18
1	E	173	THR	N-CA-CB	11.31	126.87	110.58
1	E	217	GLY	N-CA-C	-11.31	86.37	113.18
1	B	311	HIS	CA-C-O	-11.31	107.79	120.69
1	F	311	HIS	CA-C-O	-11.31	107.80	120.69
1	F	399	PRO	CB-CA-C	11.31	124.72	110.92
1	A	173	THR	N-CA-CB	11.31	126.86	110.58
1	C	311	HIS	CA-C-O	-11.30	107.81	120.69
1	D	625	PRO	N-CA-CB	-11.29	90.17	102.60
1	F	625	PRO	N-CA-CB	-11.29	90.18	102.60
1	C	173	THR	N-CA-CB	11.29	126.84	110.58
1	E	625	PRO	N-CA-CB	-11.29	90.18	102.60
1	B	173	THR	N-CA-CB	11.29	126.83	110.58
1	E	248	TRP	CA-C-O	-11.29	105.32	119.31
1	A	399	PRO	CB-CA-C	11.28	124.68	110.92
1	C	399	PRO	CB-CA-C	11.28	124.68	110.92
1	D	311	HIS	CA-C-O	-11.28	107.83	120.69
1	A	625	PRO	N-CA-CB	-11.28	90.19	102.60
1	D	399	PRO	CB-CA-C	11.28	124.68	110.92
1	E	399	PRO	CB-CA-C	11.28	124.68	110.92
1	B	52	ALA	N-CA-CB	11.27	126.33	109.98
1	B	625	PRO	N-CA-CB	-11.27	90.20	102.60
1	F	248	TRP	CA-C-O	-11.27	105.33	119.31
1	B	399	PRO	CB-CA-C	11.27	124.67	110.92
1	E	311	HIS	CA-C-O	-11.27	107.84	120.69
1	A	311	HIS	CA-C-O	-11.27	107.84	120.69
1	C	248	TRP	CA-C-O	-11.27	105.34	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	625	PRO	N-CA-CB	-11.27	90.21	102.60
1	D	52	ALA	N-CA-CB	11.27	126.31	109.98
1	A	248	TRP	CA-C-O	-11.26	105.35	119.31
1	B	248	TRP	CA-C-O	-11.26	105.35	119.31
1	E	52	ALA	N-CA-CB	11.25	126.30	109.98
1	F	52	ALA	N-CA-CB	11.25	126.30	109.98
1	A	52	ALA	N-CA-CB	11.25	126.29	109.98
1	C	52	ALA	N-CA-CB	11.24	126.28	109.98
1	D	248	TRP	CA-C-O	-11.24	105.37	119.31
1	C	501	PHE	N-CA-CB	-11.22	93.28	110.44
1	D	337	VAL	CA-CB-CG2	11.21	129.46	110.40
1	F	501	PHE	N-CA-CB	-11.21	93.29	110.44
1	E	337	VAL	CA-CB-CG2	11.21	129.45	110.40
1	A	501	PHE	N-CA-CB	-11.21	93.30	110.44
1	F	337	VAL	CA-CB-CG2	11.21	129.45	110.40
1	B	337	VAL	CA-CB-CG2	11.20	129.44	110.40
1	D	457	HIS	CA-C-O	-11.20	108.97	121.40
1	A	337	VAL	CA-CB-CG2	11.19	129.43	110.40
1	B	501	PHE	N-CA-CB	-11.19	93.31	110.44
1	D	501	PHE	N-CA-CB	-11.19	93.31	110.44
1	F	305	ILE	O-C-N	11.19	135.44	122.69
1	C	337	VAL	CA-CB-CG2	11.19	129.41	110.40
1	C	488	ASN	N-CA-C	-11.18	96.51	113.51
1	F	488	ASN	N-CA-C	-11.17	96.53	113.51
1	A	488	ASN	N-CA-C	-11.17	96.53	113.51
1	E	501	PHE	N-CA-CB	-11.17	93.35	110.44
1	B	457	HIS	CA-C-O	-11.16	109.01	121.40
1	D	488	ASN	N-CA-C	-11.16	96.54	113.51
1	E	488	ASN	N-CA-C	-11.16	96.55	113.51
1	B	488	ASN	N-CA-C	-11.16	96.55	113.51
1	C	457	HIS	CA-C-O	-11.16	109.01	121.40
1	A	457	HIS	CA-C-O	-11.15	109.02	121.40
1	D	270	VAL	CA-C-O	-11.15	106.84	120.78
1	D	45	ILE	O-C-N	11.14	134.39	121.80
1	A	270	VAL	CA-C-O	-11.14	106.85	120.78
1	B	270	VAL	CA-C-O	-11.14	106.85	120.78
1	F	270	VAL	CA-C-O	-11.14	106.86	120.78
1	E	305	ILE	O-C-N	11.14	135.39	122.69
1	A	45	ILE	O-C-N	11.13	134.38	121.80
1	B	305	ILE	O-C-N	11.13	135.38	122.69
1	E	45	ILE	O-C-N	11.13	134.38	121.80
1	E	270	VAL	CA-C-O	-11.13	106.87	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	45	ILE	O-C-N	11.13	134.38	121.80
1	F	457	HIS	CA-C-O	-11.13	109.05	121.40
1	C	270	VAL	CA-C-O	-11.13	106.87	120.78
1	C	305	ILE	O-C-N	11.13	135.38	122.69
1	A	305	ILE	O-C-N	11.12	135.37	122.69
1	C	45	ILE	O-C-N	11.12	134.36	121.80
1	E	457	HIS	CA-C-O	-11.12	109.06	121.40
1	B	45	ILE	O-C-N	11.11	134.36	121.80
1	B	377	ASP	CA-C-O	-11.11	108.69	119.80
1	D	305	ILE	O-C-N	11.10	135.35	122.69
1	D	377	ASP	CA-C-O	-11.10	108.70	119.80
1	D	122	SER	O-C-N	11.09	134.79	122.15
1	E	377	ASP	CA-C-O	-11.09	108.71	119.80
1	C	17	LEU	O-C-N	11.08	133.49	122.07
1	E	17	LEU	O-C-N	11.08	133.49	122.07
1	E	628	ARG	NE-CZ-NH1	11.08	132.58	121.50
1	A	377	ASP	CA-C-O	-11.08	108.72	119.80
1	D	17	LEU	O-C-N	11.08	133.48	122.07
1	C	155	TYR	O-C-N	11.07	135.89	122.27
1	E	64	ARG	CD-NE-CZ	11.07	139.90	124.40
1	E	155	TYR	O-C-N	11.07	135.89	122.27
1	B	17	LEU	O-C-N	11.07	133.47	122.07
1	F	64	ARG	CD-NE-CZ	11.07	139.90	124.40
1	A	17	LEU	O-C-N	11.07	133.47	122.07
1	B	64	ARG	CD-NE-CZ	11.07	139.89	124.40
1	D	64	ARG	CD-NE-CZ	11.07	139.90	124.40
1	C	377	ASP	CA-C-O	-11.06	108.74	119.80
1	B	122	SER	O-C-N	11.06	134.76	122.15
1	B	155	TYR	O-C-N	11.06	135.88	122.27
1	C	122	SER	O-C-N	11.06	134.76	122.15
1	A	64	ARG	CD-NE-CZ	11.06	139.88	124.40
1	C	64	ARG	CD-NE-CZ	11.06	139.88	124.40
1	D	155	TYR	O-C-N	11.06	135.87	122.27
1	E	122	SER	O-C-N	11.06	134.75	122.15
1	E	448	ILE	CA-C-O	-11.05	108.02	120.84
1	F	448	ILE	CA-C-O	-11.05	108.02	120.84
1	A	628	ARG	NE-CZ-NH1	11.05	132.55	121.50
1	B	496	ASP	N-CA-C	-11.05	87.26	110.80
1	D	448	ILE	CA-C-O	-11.05	108.02	120.84
1	D	628	ARG	NE-CZ-NH1	11.05	132.55	121.50
1	F	17	LEU	O-C-N	11.05	133.45	122.07
1	E	496	ASP	N-CA-C	-11.05	87.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	377	ASP	CA-C-O	-11.05	108.75	119.80
1	C	628	ARG	NE-CZ-NH1	11.04	132.54	121.50
1	A	155	TYR	O-C-N	11.04	135.85	122.27
1	A	122	SER	O-C-N	11.04	134.74	122.15
1	A	448	ILE	CA-C-O	-11.04	108.03	120.84
1	F	183	TYR	O-C-N	11.03	134.78	122.20
1	A	496	ASP	N-CA-C	-11.03	87.30	110.80
1	B	448	ILE	CA-C-O	-11.03	108.05	120.84
1	C	496	ASP	N-CA-C	-11.03	87.31	110.80
1	D	496	ASP	N-CA-C	-11.03	87.31	110.80
1	F	628	ARG	NE-CZ-NH1	11.03	132.53	121.50
1	C	448	ILE	CA-C-O	-11.03	108.05	120.84
1	A	183	TYR	O-C-N	11.03	134.77	122.20
1	E	183	TYR	O-C-N	11.03	134.77	122.20
1	F	496	ASP	N-CA-C	-11.03	87.31	110.80
1	F	122	SER	O-C-N	11.02	134.71	122.15
1	B	628	ARG	NE-CZ-NH1	11.00	132.50	121.50
1	C	183	TYR	O-C-N	11.00	134.74	122.20
1	B	183	TYR	O-C-N	10.99	134.73	122.20
1	D	183	TYR	O-C-N	10.99	134.73	122.20
1	D	314	ASP	O-C-N	10.99	135.82	122.86
1	F	155	TYR	O-C-N	10.99	135.78	122.27
1	C	306	THR	CA-CB-OG1	-10.97	93.14	109.60
1	F	306	THR	CA-CB-OG1	-10.97	93.14	109.60
1	D	306	THR	CA-CB-OG1	-10.97	93.15	109.60
1	B	306	THR	CA-CB-OG1	-10.96	93.16	109.60
1	A	306	THR	CA-CB-OG1	-10.96	93.17	109.60
1	E	306	THR	CA-CB-OG1	-10.96	93.17	109.60
1	F	314	ASP	O-C-N	10.95	135.78	122.86
1	F	70	HIS	CA-C-O	-10.95	109.77	121.38
1	A	314	ASP	O-C-N	10.95	135.78	122.86
1	D	70	HIS	CA-C-O	-10.94	109.78	121.38
1	A	70	HIS	CA-C-O	-10.93	109.80	121.38
1	B	31	LYS	CA-C-O	-10.93	108.11	120.24
1	C	314	ASP	O-C-N	10.93	135.75	122.86
1	B	314	ASP	O-C-N	10.92	135.75	122.86
1	D	31	LYS	CA-C-O	-10.92	108.12	120.24
1	A	31	LYS	CA-C-O	-10.92	108.12	120.24
1	C	70	HIS	CA-C-O	-10.92	109.81	121.38
1	F	581	ASN	N-CA-CB	-10.92	93.41	110.55
1	C	31	LYS	CA-C-O	-10.92	108.12	120.24
1	E	44	SER	O-C-N	10.91	137.10	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	314	ASP	O-C-N	10.91	135.73	122.86
1	A	581	ASN	N-CA-CB	-10.90	93.43	110.55
1	F	31	LYS	CA-C-O	-10.90	108.14	120.24
1	C	581	ASN	N-CA-CB	-10.90	93.44	110.55
1	B	70	HIS	CA-C-O	-10.89	109.83	121.38
1	D	581	ASN	N-CA-CB	-10.89	93.45	110.55
1	B	581	ASN	N-CA-CB	-10.89	93.45	110.55
1	E	534	PRO	CB-CA-C	-10.89	93.59	111.56
1	C	534	PRO	CB-CA-C	-10.89	93.60	111.56
1	F	147	ASN	CA-CB-CG	-10.89	101.71	112.60
1	E	70	HIS	CA-C-O	-10.89	109.84	121.38
1	E	31	LYS	CA-C-O	-10.88	108.16	120.24
1	A	534	PRO	CB-CA-C	-10.88	93.61	111.56
1	F	534	PRO	CB-CA-C	-10.88	93.60	111.56
1	B	44	SER	O-C-N	10.88	137.06	122.59
1	B	534	PRO	CB-CA-C	-10.88	93.61	111.56
1	B	5	THR	CA-C-N	10.88	142.73	121.41
1	B	5	THR	C-N-CA	10.88	142.73	121.41
1	E	147	ASN	CA-CB-CG	-10.88	101.72	112.60
1	A	44	SER	O-C-N	10.88	137.05	122.59
1	A	147	ASN	CA-CB-CG	-10.87	101.73	112.60
1	F	44	SER	O-C-N	10.87	137.05	122.59
1	D	44	SER	O-C-N	10.87	137.04	122.59
1	D	534	PRO	CB-CA-C	-10.87	93.63	111.56
1	C	291	ILE	N-CA-CB	10.87	123.26	110.55
1	E	581	ASN	N-CA-CB	-10.87	93.49	110.55
1	C	147	ASN	CA-CB-CG	-10.86	101.74	112.60
1	E	5	THR	CA-C-N	10.86	142.70	121.41
1	E	5	THR	C-N-CA	10.86	142.70	121.41
1	C	44	SER	O-C-N	10.86	137.03	122.59
1	B	147	ASN	CA-CB-CG	-10.86	101.74	112.60
1	F	291	ILE	N-CA-CB	10.86	123.25	110.55
1	F	191	ASN	OD1-CG-ND2	10.85	133.45	122.60
1	F	242	PRO	N-CA-CB	-10.85	91.86	103.25
1	A	5	THR	CA-C-N	10.85	142.67	121.41
1	A	5	THR	C-N-CA	10.85	142.67	121.41
1	A	291	ILE	N-CA-CB	10.85	123.24	110.55
1	C	191	ASN	OD1-CG-ND2	10.85	133.45	122.60
1	D	5	THR	CA-C-N	10.84	142.65	121.41
1	D	5	THR	C-N-CA	10.84	142.65	121.41
1	E	242	PRO	N-CA-CB	-10.84	91.87	103.25
1	F	5	THR	CA-C-N	10.84	142.65	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	5	THR	C-N-CA	10.84	142.65	121.41
1	B	291	ILE	N-CA-CB	10.83	123.22	110.55
1	C	242	PRO	N-CA-CB	-10.83	91.88	103.25
1	D	191	ASN	OD1-CG-ND2	10.83	133.43	122.60
1	E	65	LEU	CA-C-O	-10.83	108.36	121.36
1	D	291	ILE	N-CA-CB	10.83	123.22	110.55
1	C	5	THR	CA-C-N	10.83	142.63	121.41
1	C	5	THR	C-N-CA	10.83	142.63	121.41
1	A	191	ASN	OD1-CG-ND2	10.83	133.43	122.60
1	A	242	PRO	N-CA-CB	-10.83	91.88	103.25
1	E	291	ILE	N-CA-CB	10.83	123.22	110.55
1	E	191	ASN	OD1-CG-ND2	10.83	133.43	122.60
1	D	242	PRO	N-CA-CB	-10.82	91.88	103.25
1	D	635	VAL	N-CA-C	10.82	121.52	111.45
1	B	242	PRO	N-CA-CB	-10.82	91.89	103.25
1	D	147	ASN	CA-CB-CG	-10.82	101.78	112.60
1	B	191	ASN	OD1-CG-ND2	10.82	133.42	122.60
1	D	494	THR	CA-C-O	-10.81	107.47	120.55
1	E	42	ASP	CA-CB-CG	10.81	123.41	112.60
1	F	174	LYS	CA-CB-CG	10.81	135.73	114.10
1	E	494	THR	CA-C-O	-10.81	107.47	120.55
1	B	174	LYS	CA-CB-CG	10.81	135.72	114.10
1	F	494	THR	CA-C-O	-10.81	107.47	120.55
1	A	494	THR	CA-C-O	-10.81	107.47	120.55
1	A	635	VAL	N-CA-C	10.80	121.50	111.45
1	C	65	LEU	CA-C-O	-10.80	108.40	121.36
1	D	65	LEU	CA-C-O	-10.80	108.40	121.36
1	F	42	ASP	CA-CB-CG	10.80	123.40	112.60
1	D	529	THR	CA-CB-OG1	-10.80	93.40	109.60
1	A	65	LEU	CA-C-O	-10.79	108.41	121.36
1	A	174	LYS	CA-CB-CG	10.79	135.68	114.10
1	D	174	LYS	CA-CB-CG	10.79	135.68	114.10
1	C	635	VAL	N-CA-C	10.79	121.48	111.45
1	F	65	LEU	CA-C-O	-10.79	108.42	121.36
1	E	174	LYS	CA-CB-CG	10.79	135.67	114.10
1	F	529	THR	CA-CB-OG1	-10.78	93.42	109.60
1	C	361	PHE	N-CA-CB	-10.78	94.80	110.65
1	A	42	ASP	CA-CB-CG	10.78	123.38	112.60
1	F	59	GLU	CA-C-O	-10.78	108.28	120.24
1	B	65	LEU	CA-C-O	-10.78	108.43	121.36
1	C	174	LYS	CA-CB-CG	10.78	135.66	114.10
1	B	59	GLU	CA-C-O	-10.78	108.28	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	361	PHE	N-CA-CB	-10.78	94.81	110.65
1	A	361	PHE	N-CA-CB	-10.77	94.81	110.65
1	A	529	THR	CA-CB-OG1	-10.77	93.44	109.60
1	C	529	THR	CA-CB-OG1	-10.77	93.44	109.60
1	D	42	ASP	CA-CB-CG	10.77	123.37	112.60
1	B	494	THR	CA-C-O	-10.77	107.52	120.55
1	D	361	PHE	N-CA-CB	-10.77	94.83	110.65
1	E	635	VAL	N-CA-C	10.77	121.46	111.45
1	C	494	THR	CA-C-O	-10.76	107.53	120.55
1	C	42	ASP	CA-CB-CG	10.76	123.36	112.60
1	E	529	THR	CA-CB-OG1	-10.76	93.46	109.60
1	F	361	PHE	N-CA-CB	-10.76	94.84	110.65
1	B	361	PHE	N-CA-CB	-10.75	94.84	110.65
1	B	42	ASP	CA-CB-CG	10.75	123.35	112.60
1	E	59	GLU	CA-C-O	-10.75	108.31	120.24
1	A	59	GLU	CA-C-O	-10.75	108.31	120.24
1	C	200	ASP	CA-CB-CG	10.75	123.35	112.60
1	B	529	THR	CA-CB-OG1	-10.75	93.48	109.60
1	C	59	GLU	CA-C-O	-10.74	108.32	120.24
1	D	123	VAL	CA-C-N	10.74	134.09	120.56
1	D	123	VAL	C-N-CA	10.74	134.09	120.56
1	D	59	GLU	CA-C-O	-10.74	108.32	120.24
1	F	123	VAL	CA-C-N	10.73	134.08	120.56
1	F	123	VAL	C-N-CA	10.73	134.08	120.56
1	F	90	LEU	N-CA-CB	-10.73	92.36	110.49
1	D	200	ASP	CA-CB-CG	10.72	123.32	112.60
1	C	123	VAL	CA-C-N	10.72	134.07	120.56
1	C	123	VAL	C-N-CA	10.72	134.07	120.56
1	A	200	ASP	CA-CB-CG	10.72	123.32	112.60
1	E	123	VAL	CA-C-N	10.71	134.06	120.56
1	E	123	VAL	C-N-CA	10.71	134.06	120.56
1	A	90	LEU	N-CA-CB	-10.71	92.39	110.49
1	C	90	LEU	N-CA-CB	-10.71	92.39	110.49
1	B	90	LEU	N-CA-CB	-10.71	92.39	110.49
1	B	200	ASP	CA-CB-CG	10.71	123.31	112.60
1	A	123	VAL	CA-C-N	10.70	134.05	120.56
1	A	123	VAL	C-N-CA	10.70	134.05	120.56
1	D	90	LEU	N-CA-CB	-10.70	92.40	110.49
1	E	90	LEU	N-CA-CB	-10.70	92.40	110.49
1	B	123	VAL	CA-C-N	10.69	134.03	120.56
1	B	123	VAL	C-N-CA	10.69	134.03	120.56
1	E	554	ASP	CA-C-O	10.69	138.69	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	200	ASP	CA-CB-CG	10.69	123.29	112.60
1	D	554	ASP	CA-C-O	10.68	138.69	120.85
1	D	235	ARG	NE-CZ-NH1	-10.68	110.82	121.50
1	E	200	ASP	CA-CB-CG	10.68	123.28	112.60
1	C	554	ASP	CA-C-O	10.67	138.67	120.85
1	A	554	ASP	CA-C-O	10.66	138.66	120.85
1	D	252	ILE	N-CA-C	-10.66	90.84	107.15
1	F	554	ASP	CA-C-O	10.66	138.65	120.85
1	F	85	MET	N-CA-CB	10.65	126.71	110.30
1	F	252	ILE	N-CA-C	-10.65	90.85	107.15
1	B	554	ASP	CA-C-O	10.65	138.63	120.85
1	B	632	ASP	CA-C-O	-10.65	108.95	120.24
1	B	85	MET	N-CA-CB	10.65	126.70	110.30
1	C	177	ARG	NE-CZ-NH2	10.65	128.78	119.20
1	D	85	MET	N-CA-CB	10.65	126.70	110.30
1	E	252	ILE	N-CA-C	-10.65	90.86	107.15
1	A	235	ARG	NE-CZ-NH1	-10.64	110.86	121.50
1	B	235	ARG	NE-CZ-NH1	-10.64	110.86	121.50
1	D	180	ARG	CD-NE-CZ	10.64	139.30	124.40
1	D	365	PRO	CA-C-N	-10.64	110.96	122.67
1	D	365	PRO	C-N-CA	-10.64	110.96	122.67
1	C	252	ILE	N-CA-C	-10.64	90.87	107.15
1	A	85	MET	N-CA-CB	10.63	126.68	110.30
1	A	252	ILE	N-CA-C	-10.63	90.88	107.15
1	B	500	TRP	CA-CB-CG	10.63	133.81	113.60
1	F	235	ARG	NE-CZ-NH1	-10.63	110.86	121.50
1	B	365	PRO	CA-C-N	-10.63	110.97	122.67
1	B	365	PRO	C-N-CA	-10.63	110.97	122.67
1	C	85	MET	N-CA-CB	10.63	126.67	110.30
1	F	632	ASP	CA-C-O	-10.63	108.97	120.24
1	C	180	ARG	CD-NE-CZ	10.63	139.28	124.40
1	C	556	SER	N-CA-CB	10.63	126.30	109.51
1	E	85	MET	N-CA-CB	10.63	126.67	110.30
1	B	252	ILE	N-CA-C	-10.63	90.89	107.15
1	F	500	TRP	CA-CB-CG	10.62	133.78	113.60
1	F	556	SER	N-CA-CB	10.62	126.29	109.51
1	A	177	ARG	NE-CZ-NH2	10.62	128.75	119.20
1	D	500	TRP	CA-CB-CG	10.62	133.77	113.60
1	D	556	SER	N-CA-CB	10.62	126.29	109.51
1	F	177	ARG	NE-CZ-NH2	10.62	128.75	119.20
1	A	500	TRP	CA-CB-CG	10.61	133.76	113.60
1	C	500	TRP	CA-CB-CG	10.61	133.76	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	500	TRP	CA-CB-CG	10.61	133.76	113.60
1	D	632	ASP	CA-C-O	-10.61	109.00	120.24
1	F	180	ARG	CD-NE-CZ	10.61	139.25	124.40
1	A	180	ARG	CD-NE-CZ	10.60	139.24	124.40
1	A	632	ASP	CA-C-O	-10.60	109.00	120.24
1	A	556	SER	N-CA-CB	10.60	126.26	109.51
1	C	235	ARG	NE-CZ-NH1	-10.60	110.90	121.50
1	E	235	ARG	NE-CZ-NH1	-10.60	110.90	121.50
1	F	365	PRO	CA-C-N	-10.60	111.01	122.67
1	F	365	PRO	C-N-CA	-10.60	111.01	122.67
1	A	365	PRO	CA-C-N	-10.60	111.01	122.67
1	A	365	PRO	C-N-CA	-10.60	111.01	122.67
1	C	632	ASP	CA-C-O	-10.60	109.00	120.24
1	D	177	ARG	NE-CZ-NH2	10.60	128.74	119.20
1	E	632	ASP	CA-C-O	-10.59	109.01	120.24
1	E	545	ASN	CA-CB-CG	10.59	123.19	112.60
1	B	545	ASN	CA-CB-CG	10.59	123.19	112.60
1	C	365	PRO	CA-C-N	-10.59	111.02	122.67
1	C	365	PRO	C-N-CA	-10.59	111.02	122.67
1	B	581	ASN	CA-C-O	-10.59	108.68	120.32
1	E	177	ARG	NE-CZ-NH2	10.58	128.73	119.20
1	E	556	SER	N-CA-CB	10.58	126.23	109.51
1	B	177	ARG	NE-CZ-NH2	10.58	128.72	119.20
1	D	581	ASN	CA-C-O	-10.58	108.68	120.32
1	A	545	ASN	CA-CB-CG	10.57	123.17	112.60
1	B	556	SER	N-CA-CB	10.57	126.21	109.51
1	C	330	SER	O-C-N	10.57	136.65	122.59
1	F	581	ASN	CA-C-O	-10.57	108.69	120.32
1	E	180	ARG	CD-NE-CZ	10.57	139.20	124.40
1	C	545	ASN	CA-CB-CG	10.57	123.17	112.60
1	D	330	SER	O-C-N	10.57	136.64	122.59
1	E	365	PRO	CA-C-N	-10.56	111.05	122.67
1	E	365	PRO	C-N-CA	-10.56	111.05	122.67
1	C	245	GLU	O-C-N	-10.56	111.23	123.06
1	F	545	ASN	CA-CB-CG	10.56	123.16	112.60
1	B	180	ARG	CD-NE-CZ	10.56	139.18	124.40
1	C	581	ASN	CA-C-O	-10.56	108.71	120.32
1	E	581	ASN	CA-C-O	-10.56	108.70	120.32
1	B	80	ARG	O-C-N	10.55	133.48	122.09
1	A	330	SER	O-C-N	10.55	136.62	122.59
1	A	581	ASN	CA-C-O	-10.55	108.72	120.32
1	E	245	GLU	O-C-N	-10.55	111.25	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	330	SER	O-C-N	10.54	136.61	122.59
1	D	545	ASN	CA-CB-CG	10.54	123.14	112.60
1	A	333	TYR	N-CA-C	-10.54	100.09	113.16
1	C	333	TYR	N-CA-C	-10.54	100.09	113.16
1	D	333	TYR	N-CA-C	-10.54	100.09	113.16
1	B	56	LEU	N-CA-C	-10.54	98.55	111.40
1	C	364	PRO	O-C-N	10.54	133.89	121.46
1	E	497	GLU	N-CA-C	-10.54	99.60	111.82
1	E	333	TYR	N-CA-C	-10.53	100.10	113.16
1	E	330	SER	O-C-N	10.53	136.60	122.59
1	C	56	LEU	N-CA-C	-10.53	98.55	111.40
1	A	80	ARG	O-C-N	10.53	133.46	122.09
1	D	80	ARG	O-C-N	10.53	133.46	122.09
1	E	56	LEU	N-CA-C	-10.53	98.56	111.40
1	F	80	ARG	O-C-N	10.53	133.46	122.09
1	E	80	ARG	O-C-N	10.53	133.46	122.09
1	A	56	LEU	N-CA-C	-10.52	98.56	111.40
1	B	333	TYR	N-CA-C	-10.52	100.11	113.16
1	D	109	ARG	O-C-N	-10.52	107.84	122.04
1	F	245	GLU	O-C-N	-10.52	111.28	123.06
1	F	333	TYR	N-CA-C	-10.52	100.12	113.16
1	A	245	GLU	O-C-N	-10.52	111.28	123.06
1	D	364	PRO	O-C-N	10.52	133.87	121.46
1	B	245	GLU	O-C-N	-10.51	111.29	123.06
1	B	109	ARG	O-C-N	-10.51	107.86	122.04
1	D	497	GLU	N-CA-C	-10.51	99.63	111.82
1	F	364	PRO	O-C-N	10.51	133.86	121.46
1	B	411	MET	N-CA-C	10.51	133.18	110.80
1	A	364	PRO	O-C-N	10.50	133.85	121.46
1	D	245	GLU	O-C-N	-10.50	111.30	123.06
1	A	109	ARG	O-C-N	-10.50	107.87	122.04
1	B	364	PRO	O-C-N	10.50	133.85	121.46
1	A	497	GLU	N-CA-C	-10.50	99.64	111.82
1	D	56	LEU	N-CA-C	-10.50	98.59	111.40
1	F	330	SER	O-C-N	10.50	136.55	122.59
1	D	411	MET	N-CA-C	10.50	133.16	110.80
1	F	497	GLU	N-CA-C	-10.49	99.65	111.82
1	A	411	MET	N-CA-C	10.49	133.14	110.80
1	E	109	ARG	O-C-N	-10.49	107.88	122.04
1	C	80	ARG	O-C-N	10.49	133.42	122.09
1	C	109	ARG	O-C-N	-10.49	107.88	122.04
1	F	56	LEU	N-CA-C	-10.49	98.61	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	238	ASN	CA-CB-CG	-10.49	102.11	112.60
1	B	497	GLU	N-CA-C	-10.48	99.66	111.82
1	F	411	MET	N-CA-C	10.48	133.13	110.80
1	C	411	MET	N-CA-C	10.48	133.13	110.80
1	C	238	ASN	CA-CB-CG	-10.48	102.12	112.60
1	E	364	PRO	O-C-N	10.48	133.82	121.46
1	F	109	ARG	O-C-N	-10.47	107.90	122.04
1	E	411	MET	N-CA-C	10.47	133.10	110.80
1	D	512	VAL	CB-CA-C	10.47	121.63	110.53
1	F	508	PHE	CA-C-N	-10.46	108.85	122.77
1	F	508	PHE	C-N-CA	-10.46	108.85	122.77
1	A	238	ASN	CA-CB-CG	-10.46	102.14	112.60
1	A	508	PHE	CA-C-N	-10.45	108.87	122.77
1	A	508	PHE	C-N-CA	-10.45	108.87	122.77
1	B	238	ASN	CA-CB-CG	-10.45	102.15	112.60
1	C	508	PHE	CA-C-N	-10.45	108.87	122.77
1	C	508	PHE	C-N-CA	-10.45	108.87	122.77
1	D	508	PHE	CA-C-N	-10.46	108.86	122.77
1	D	508	PHE	C-N-CA	-10.46	108.86	122.77
1	E	508	PHE	CA-C-N	-10.45	108.87	122.77
1	E	508	PHE	C-N-CA	-10.45	108.87	122.77
1	F	83	ALA	N-CA-CB	10.44	125.47	110.12
1	B	508	PHE	CA-C-N	-10.44	108.89	122.77
1	B	508	PHE	C-N-CA	-10.44	108.89	122.77
1	D	238	ASN	CA-CB-CG	-10.44	102.17	112.60
1	C	543	ALA	O-C-N	10.43	133.36	122.09
1	E	238	ASN	CA-CB-CG	-10.43	102.17	112.60
1	B	83	ALA	N-CA-CB	10.43	125.45	110.12
1	A	83	ALA	N-CA-CB	10.42	125.44	110.12
1	B	496	ASP	N-CA-CB	10.42	128.10	110.49
1	D	543	ALA	O-C-N	10.42	133.34	122.09
1	D	496	ASP	N-CA-CB	10.42	128.10	110.49
1	F	496	ASP	N-CA-CB	10.42	128.10	110.49
1	E	496	ASP	N-CA-CB	10.42	128.09	110.49
1	A	512	VAL	CB-CA-C	10.41	121.57	110.53
1	B	543	ALA	O-C-N	10.41	133.34	122.09
1	E	83	ALA	N-CA-CB	10.41	125.43	110.12
1	E	512	VAL	CB-CA-C	10.41	121.56	110.53
1	A	496	ASP	N-CA-CB	10.41	128.08	110.49
1	C	277	PHE	CB-CA-C	-10.41	95.17	110.16
1	D	83	ALA	N-CA-CB	10.41	125.42	110.12
1	C	512	VAL	CB-CA-C	10.40	121.56	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	284	ALA	CA-C-N	10.40	136.46	120.75
1	E	284	ALA	C-N-CA	10.40	136.46	120.75
1	F	512	VAL	CB-CA-C	10.40	121.56	110.53
1	A	543	ALA	O-C-N	10.40	133.32	122.09
1	B	512	VAL	CB-CA-C	10.40	121.56	110.53
1	C	83	ALA	N-CA-CB	10.40	125.41	110.12
1	B	284	ALA	CA-C-N	10.40	136.45	120.75
1	B	284	ALA	C-N-CA	10.40	136.45	120.75
1	C	284	ALA	CA-C-N	10.40	136.46	120.75
1	C	284	ALA	C-N-CA	10.40	136.46	120.75
1	E	306	THR	CA-C-O	-10.40	109.05	120.38
1	C	496	ASP	N-CA-CB	10.39	128.05	110.49
1	B	306	THR	CA-C-O	-10.39	109.06	120.38
1	A	284	ALA	CA-C-N	10.39	136.44	120.75
1	A	284	ALA	C-N-CA	10.39	136.44	120.75
1	F	277	PHE	CB-CA-C	-10.38	95.21	110.16
1	D	277	PHE	CB-CA-C	-10.38	95.21	110.16
1	A	306	THR	CA-C-O	-10.38	109.07	120.38
1	B	277	PHE	CB-CA-C	-10.38	95.21	110.16
1	F	284	ALA	CA-C-N	10.38	136.42	120.75
1	F	284	ALA	C-N-CA	10.38	136.42	120.75
1	E	543	ALA	O-C-N	10.38	133.30	122.09
1	A	277	PHE	CB-CA-C	-10.38	95.22	110.16
1	D	284	ALA	CA-C-N	10.38	136.42	120.75
1	D	284	ALA	C-N-CA	10.38	136.42	120.75
1	F	543	ALA	O-C-N	10.37	133.29	122.09
1	F	147	ASN	OD1-CG-ND2	10.37	132.97	122.60
1	D	3	LEU	CA-C-O	10.37	133.78	121.65
1	C	11	GLN	O-C-N	10.36	132.86	122.09
1	D	306	THR	CA-C-O	-10.36	109.09	120.38
1	E	277	PHE	CB-CA-C	-10.36	95.25	110.16
1	C	306	THR	CA-C-O	-10.35	109.10	120.38
1	B	3	LEU	CA-C-O	10.34	133.75	121.65
1	F	306	THR	CA-C-O	-10.34	109.11	120.38
1	A	3	LEU	CA-C-O	10.33	133.74	121.65
1	C	499	ARG	NE-CZ-NH2	10.33	128.50	119.20
1	B	91	ASN	CB-CG-ND2	-10.33	100.91	116.40
1	C	3	LEU	CA-C-O	10.33	133.73	121.65
1	C	91	ASN	CB-CG-ND2	-10.33	100.91	116.40
1	E	91	ASN	CB-CG-ND2	-10.33	100.91	116.40
1	B	499	ARG	NE-CZ-NH2	10.32	128.49	119.20
1	D	91	ASN	CB-CG-ND2	-10.32	100.92	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	ASN	CB-CG-ND2	-10.32	100.92	116.40
1	E	3	LEU	CA-C-O	10.32	133.73	121.65
1	E	561	SER	CA-C-N	10.32	134.94	120.29
1	E	561	SER	C-N-CA	10.32	134.94	120.29
1	D	499	ARG	NE-CZ-NH2	10.31	128.48	119.20
1	F	91	ASN	CB-CG-ND2	-10.31	100.93	116.40
1	A	499	ARG	NE-CZ-NH2	10.31	128.48	119.20
1	F	3	LEU	CA-C-O	10.31	133.72	121.65
1	B	390	ILE	N-CA-CB	10.31	128.90	110.86
1	E	390	ILE	N-CA-CB	10.30	128.89	110.86
1	A	11	GLN	O-C-N	10.30	132.80	122.09
1	C	561	SER	CA-C-N	10.30	134.92	120.29
1	C	561	SER	C-N-CA	10.30	134.92	120.29
1	A	390	ILE	N-CA-CB	10.29	128.87	110.86
1	B	147	ASN	OD1-CG-ND2	10.29	132.89	122.60
1	F	499	ARG	NE-CZ-NH2	10.29	128.46	119.20
1	B	11	GLN	O-C-N	10.29	132.79	122.09
1	C	390	ILE	N-CA-CB	10.29	128.86	110.86
1	E	499	ARG	NE-CZ-NH2	10.29	128.46	119.20
1	B	561	SER	CA-C-N	10.28	134.89	120.29
1	B	561	SER	C-N-CA	10.28	134.89	120.29
1	A	147	ASN	OD1-CG-ND2	10.28	132.88	122.60
1	A	561	SER	CA-C-N	10.28	134.89	120.29
1	A	561	SER	C-N-CA	10.28	134.89	120.29
1	D	25	THR	CB-CA-C	-10.28	90.63	109.54
1	F	390	ILE	N-CA-CB	10.28	128.85	110.86
1	E	147	ASN	OD1-CG-ND2	10.28	132.88	122.60
1	D	390	ILE	N-CA-CB	10.28	128.84	110.86
1	D	147	ASN	OD1-CG-ND2	10.27	132.87	122.60
1	E	11	GLN	O-C-N	10.27	132.77	122.09
1	A	25	THR	CB-CA-C	-10.27	90.64	109.54
1	F	25	THR	CB-CA-C	-10.27	90.65	109.54
1	B	25	THR	CB-CA-C	-10.26	90.66	109.54
1	D	561	SER	CA-C-N	10.26	134.86	120.29
1	D	561	SER	C-N-CA	10.26	134.86	120.29
1	B	49	HIS	N-CA-C	-10.26	100.72	113.23
1	E	25	THR	CB-CA-C	-10.26	90.67	109.54
1	C	25	THR	CB-CA-C	-10.26	90.67	109.54
1	F	183	TYR	CA-C-O	-10.26	108.72	120.20
1	E	49	HIS	N-CA-C	-10.25	100.72	113.23
1	F	11	GLN	O-C-N	10.25	132.75	122.09
1	F	561	SER	CA-C-N	10.25	134.84	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	561	SER	C-N-CA	10.25	134.84	120.29
1	B	247	HIS	O-C-N	10.24	136.84	123.11
1	C	247	HIS	O-C-N	10.24	136.84	123.11
1	D	11	GLN	O-C-N	10.24	132.74	122.09
1	E	183	TYR	CA-C-O	-10.24	108.73	120.20
1	D	109	ARG	CA-C-O	10.24	129.63	119.08
1	F	49	HIS	N-CA-C	-10.24	100.74	113.23
1	F	226	GLN	CA-CB-CG	-10.24	93.62	114.10
1	A	183	TYR	CA-C-O	-10.24	108.74	120.20
1	C	49	HIS	N-CA-C	-10.23	100.74	113.23
1	A	226	GLN	CA-CB-CG	-10.23	93.64	114.10
1	A	49	HIS	N-CA-C	-10.23	100.75	113.23
1	F	247	HIS	O-C-N	10.23	136.82	123.11
1	A	247	HIS	O-C-N	10.22	136.81	123.11
1	C	226	GLN	CA-CB-CG	-10.22	93.65	114.10
1	D	226	GLN	CA-CB-CG	-10.22	93.65	114.10
1	F	643	LYS	CA-CB-CG	10.22	134.54	114.10
1	A	643	LYS	CA-CB-CG	10.22	134.53	114.10
1	B	183	TYR	CA-C-O	-10.22	108.76	120.20
1	D	247	HIS	O-C-N	10.22	136.80	123.11
1	E	226	GLN	CA-CB-CG	-10.22	93.66	114.10
1	F	307	ASP	CA-C-N	10.22	135.00	120.28
1	F	307	ASP	C-N-CA	10.22	135.00	120.28
1	B	226	GLN	CA-CB-CG	-10.21	93.67	114.10
1	B	307	ASP	CA-C-N	10.21	134.99	120.28
1	B	307	ASP	C-N-CA	10.21	134.99	120.28
1	D	643	LYS	CA-CB-CG	10.21	134.53	114.10
1	C	147	ASN	OD1-CG-ND2	10.21	132.81	122.60
1	E	247	HIS	O-C-N	10.21	136.79	123.11
1	E	643	LYS	CA-CB-CG	10.21	134.52	114.10
1	D	307	ASP	CA-C-N	10.21	134.98	120.28
1	D	307	ASP	C-N-CA	10.21	134.98	120.28
1	E	302	HIS	N-CA-CB	10.21	125.24	110.13
1	B	643	LYS	CA-CB-CG	10.20	134.51	114.10
1	D	183	TYR	CA-C-O	-10.20	108.77	120.20
1	C	216	LYS	N-CA-C	-10.20	94.76	109.96
1	D	302	HIS	N-CA-CB	10.20	125.23	110.13
1	A	109	ARG	CA-C-O	10.20	129.59	119.08
1	A	216	LYS	N-CA-C	-10.20	94.76	109.96
1	D	216	LYS	N-CA-C	-10.20	94.76	109.96
1	E	528	VAL	N-CA-CB	-10.20	100.45	112.39
1	D	49	HIS	N-CA-C	-10.20	100.79	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	LYS	N-CA-C	-10.20	94.77	109.96
1	C	643	LYS	CA-CB-CG	10.20	134.50	114.10
1	C	302	HIS	N-CA-CB	10.20	125.22	110.13
1	A	307	ASP	CA-C-N	10.20	134.96	120.28
1	A	307	ASP	C-N-CA	10.20	134.96	120.28
1	C	109	ARG	CA-C-O	10.19	129.58	119.08
1	C	183	TYR	CA-C-O	-10.19	108.79	120.20
1	F	216	LYS	N-CA-C	-10.19	94.78	109.96
1	E	216	LYS	N-CA-C	-10.19	94.78	109.96
1	A	302	HIS	N-CA-CB	10.18	125.20	110.13
1	B	109	ARG	CA-C-O	10.18	129.56	119.08
1	F	109	ARG	CA-C-O	10.18	129.56	119.08
1	C	307	ASP	CA-C-N	10.18	134.94	120.28
1	C	307	ASP	C-N-CA	10.18	134.94	120.28
1	C	77	THR	N-CA-CB	10.17	128.49	110.18
1	E	77	THR	N-CA-CB	10.17	128.49	110.18
1	D	528	VAL	N-CA-CB	-10.17	100.49	112.39
1	B	77	THR	N-CA-CB	10.17	128.48	110.18
1	A	528	VAL	N-CA-CB	-10.17	100.50	112.39
1	B	302	HIS	N-CA-CB	10.16	125.17	110.13
1	D	25	THR	O-C-N	10.16	134.85	122.86
1	E	307	ASP	CA-C-N	10.16	134.91	120.28
1	E	307	ASP	C-N-CA	10.16	134.91	120.28
1	A	77	THR	N-CA-CB	10.16	128.46	110.18
1	B	25	THR	O-C-N	10.16	134.84	122.86
1	F	77	THR	N-CA-CB	10.16	128.46	110.18
1	E	109	ARG	CA-C-O	10.15	129.54	119.08
1	F	302	HIS	N-CA-CB	10.15	125.16	110.13
1	B	528	VAL	N-CA-CB	-10.15	100.51	112.39
1	F	528	VAL	N-CA-CB	-10.15	100.52	112.39
1	C	528	VAL	N-CA-CB	-10.14	100.52	112.39
1	D	579	GLU	CA-C-O	10.14	131.48	120.32
1	B	572	LYS	CA-C-N	10.14	144.34	121.53
1	B	572	LYS	C-N-CA	10.14	144.34	121.53
1	C	427	ASP	CA-CB-CG	-10.13	102.47	112.60
1	E	427	ASP	CA-CB-CG	-10.13	102.47	112.60
1	A	427	ASP	CA-CB-CG	-10.12	102.48	112.60
1	F	427	ASP	CA-CB-CG	-10.12	102.48	112.60
1	D	77	THR	N-CA-CB	10.12	128.40	110.18
1	B	427	ASP	CA-CB-CG	-10.12	102.48	112.60
1	C	572	LYS	CA-C-N	10.12	144.30	121.53
1	C	572	LYS	C-N-CA	10.12	144.30	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	THR	O-C-N	10.11	134.79	122.86
1	C	616	TYR	CA-C-O	-10.11	111.21	119.71
1	C	25	THR	O-C-N	10.11	134.79	122.86
1	E	579	GLU	CA-C-O	10.11	131.44	120.32
1	F	25	THR	O-C-N	10.11	134.79	122.86
1	A	572	LYS	CA-C-N	10.11	144.27	121.53
1	A	572	LYS	C-N-CA	10.11	144.27	121.53
1	B	579	GLU	CA-C-O	10.11	131.44	120.32
1	D	572	LYS	CA-C-N	10.10	144.26	121.53
1	D	572	LYS	C-N-CA	10.10	144.26	121.53
1	E	572	LYS	CA-C-N	10.10	144.26	121.53
1	E	572	LYS	C-N-CA	10.10	144.26	121.53
1	D	427	ASP	CA-CB-CG	-10.10	102.50	112.60
1	A	579	GLU	CA-C-O	10.10	131.43	120.32
1	F	572	LYS	CA-C-N	10.10	144.25	121.53
1	F	572	LYS	C-N-CA	10.10	144.25	121.53
1	E	109	ARG	NH1-CZ-NH2	10.09	132.42	119.30
1	C	67	GLU	CB-CG-CD	-10.08	95.46	112.60
1	C	109	ARG	NH1-CZ-NH2	10.08	132.41	119.30
1	E	67	GLU	CB-CG-CD	-10.08	95.46	112.60
1	A	67	GLU	CB-CG-CD	-10.08	95.46	112.60
1	F	67	GLU	CB-CG-CD	-10.08	95.47	112.60
1	E	616	TYR	CA-C-O	-10.07	111.25	119.71
1	D	67	GLU	CB-CG-CD	-10.07	95.48	112.60
1	B	67	GLU	CB-CG-CD	-10.06	95.49	112.60
1	A	616	TYR	CA-C-O	-10.06	111.26	119.71
1	D	294	SER	O-C-N	10.06	137.07	122.28
1	A	294	SER	O-C-N	10.06	137.06	122.28
1	F	294	SER	O-C-N	10.06	137.06	122.28
1	F	579	GLU	CA-C-O	10.06	131.38	120.32
1	A	109	ARG	NH1-CZ-NH2	10.05	132.37	119.30
1	B	294	SER	O-C-N	10.05	137.06	122.28
1	D	616	TYR	CA-C-O	-10.05	111.26	119.71
1	E	25	THR	O-C-N	10.05	134.72	122.86
1	E	294	SER	O-C-N	10.05	137.06	122.28
1	F	109	ARG	NH1-CZ-NH2	10.05	132.37	119.30
1	F	616	TYR	CA-C-O	-10.05	111.27	119.71
1	B	109	ARG	NH1-CZ-NH2	10.05	132.36	119.30
1	C	294	SER	O-C-N	10.05	137.05	122.28
1	E	441	GLU	N-CA-C	10.05	125.93	108.75
1	C	579	GLU	CA-C-O	10.04	131.37	120.32
1	A	441	GLU	N-CA-C	10.04	125.92	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	423	ILE	CB-CA-C	10.04	126.14	110.28
1	C	441	GLU	N-CA-C	10.04	125.92	108.75
1	F	423	ILE	CB-CA-C	10.04	126.14	110.28
1	C	423	ILE	CB-CA-C	10.04	126.14	110.28
1	B	441	GLU	N-CA-C	10.03	125.91	108.75
1	E	171	THR	N-CA-C	10.03	132.17	110.80
1	E	423	ILE	CB-CA-C	10.03	126.13	110.28
1	F	441	GLU	N-CA-C	10.03	125.91	108.75
1	D	109	ARG	NH1-CZ-NH2	10.03	132.34	119.30
1	A	423	ILE	CB-CA-C	10.03	126.12	110.28
1	D	423	ILE	CB-CA-C	10.02	126.11	110.28
1	F	171	THR	N-CA-C	10.02	132.15	110.80
1	D	441	GLU	N-CA-C	10.02	125.88	108.75
1	B	171	THR	N-CA-C	10.02	132.13	110.80
1	B	616	TYR	CA-C-O	-10.01	111.30	119.71
1	C	171	THR	N-CA-C	10.01	132.12	110.80
1	A	171	THR	N-CA-C	10.00	132.10	110.80
1	E	89	VAL	CB-CA-C	9.99	127.68	111.29
1	C	497	GLU	N-CA-C	-9.99	99.64	112.23
1	F	191	ASN	CB-CG-OD1	-9.99	100.82	120.80
1	B	271	ARG	CA-C-N	9.99	129.75	119.56
1	B	271	ARG	C-N-CA	9.99	129.75	119.56
1	E	191	ASN	CB-CG-OD1	-9.99	100.82	120.80
1	B	89	VAL	CB-CA-C	9.99	127.67	111.29
1	D	85	MET	N-CA-C	-9.99	99.65	112.23
1	D	171	THR	N-CA-C	9.99	132.07	110.80
1	E	226	GLN	CB-CA-C	9.99	126.68	110.90
1	D	191	ASN	CB-CG-OD1	-9.98	100.83	120.80
1	A	89	VAL	CB-CA-C	9.98	127.66	111.29
1	C	89	VAL	CB-CA-C	9.98	127.66	111.29
1	D	574	LYS	CB-CG-CD	9.98	134.26	111.30
1	A	191	ASN	CB-CG-OD1	-9.98	100.85	120.80
1	C	271	ARG	CA-C-N	9.97	129.73	119.56
1	C	271	ARG	C-N-CA	9.97	129.73	119.56
1	F	89	VAL	CB-CA-C	9.97	127.65	111.29
1	F	226	GLN	CB-CA-C	9.97	126.66	110.90
1	B	574	LYS	CB-CG-CD	9.97	134.24	111.30
1	C	191	ASN	CB-CG-OD1	-9.97	100.85	120.80
1	D	226	GLN	CB-CA-C	9.97	126.66	110.90
1	F	271	ARG	CA-C-N	9.97	129.73	119.56
1	F	271	ARG	C-N-CA	9.97	129.73	119.56
1	B	191	ASN	CB-CG-OD1	-9.97	100.86	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	GLN	CB-CA-C	9.96	126.64	110.90
1	B	226	GLN	CB-CA-C	9.96	126.64	110.90
1	D	89	VAL	CB-CA-C	9.96	127.63	111.29
1	F	85	MET	N-CA-C	-9.96	99.68	112.23
1	F	574	LYS	CB-CG-CD	9.96	134.21	111.30
1	C	226	GLN	CB-CA-C	9.96	126.63	110.90
1	A	574	LYS	CB-CG-CD	9.96	134.20	111.30
1	D	271	ARG	CA-C-N	9.96	129.71	119.56
1	D	271	ARG	C-N-CA	9.96	129.71	119.56
1	E	574	LYS	CB-CG-CD	9.95	134.19	111.30
1	C	574	LYS	CB-CG-CD	9.95	134.19	111.30
1	D	629	ARG	CA-CB-CG	9.95	134.01	114.10
1	F	376	ARG	CA-C-O	-9.95	109.91	120.55
1	F	489	ASN	N-CA-CB	9.95	124.50	110.67
1	A	271	ARG	CA-C-N	9.95	129.70	119.56
1	A	271	ARG	C-N-CA	9.95	129.70	119.56
1	A	85	MET	N-CA-C	-9.94	99.70	112.23
1	B	85	MET	N-CA-C	-9.94	99.70	112.23
1	E	85	MET	N-CA-C	-9.94	99.70	112.23
1	F	629	ARG	CA-CB-CG	9.94	133.98	114.10
1	B	376	ARG	CA-C-O	-9.94	109.92	120.55
1	C	85	MET	N-CA-C	-9.94	99.71	112.23
1	F	386	TYR	CA-C-O	-9.94	110.14	121.07
1	A	376	ARG	CA-C-O	-9.93	109.92	120.55
1	A	629	ARG	CA-CB-CG	9.93	133.96	114.10
1	D	386	TYR	CA-C-O	-9.93	110.15	121.07
1	B	109	ARG	CD-NE-CZ	-9.93	110.50	124.40
1	E	629	ARG	CA-CB-CG	9.93	133.96	114.10
1	D	489	ASN	N-CA-CB	9.93	124.47	110.67
1	E	386	TYR	CA-C-O	-9.93	110.15	121.07
1	D	8	ALA	O-C-N	-9.92	109.39	122.59
1	D	109	ARG	CD-NE-CZ	-9.92	110.51	124.40
1	B	8	ALA	O-C-N	-9.92	109.40	122.59
1	C	386	TYR	CA-C-O	-9.92	110.16	121.07
1	C	489	ASN	N-CA-CB	9.92	124.46	110.67
1	A	109	ARG	CD-NE-CZ	-9.92	110.52	124.40
1	A	386	TYR	CA-C-O	-9.92	110.16	121.07
1	C	376	ARG	CA-C-O	-9.92	109.94	120.55
1	C	629	ARG	CA-CB-CG	9.92	133.93	114.10
1	B	629	ARG	CA-CB-CG	9.91	133.93	114.10
1	F	572	LYS	CA-C-O	-9.91	110.49	120.70
1	E	8	ALA	O-C-N	-9.91	109.41	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	8	ALA	O-C-N	-9.91	109.41	122.59
1	D	436	ALA	CA-C-O	-9.91	109.24	120.24
1	F	109	ARG	CD-NE-CZ	-9.91	110.53	124.40
1	A	8	ALA	O-C-N	-9.90	109.42	122.59
1	A	489	ASN	N-CA-CB	9.90	124.43	110.67
1	D	260	THR	CA-C-O	-9.90	109.97	121.16
1	D	376	ARG	CA-C-O	-9.90	109.96	120.55
1	B	386	TYR	CA-C-O	-9.90	110.18	121.07
1	E	489	ASN	N-CA-CB	9.90	124.43	110.67
1	C	400	PRO	O-C-N	9.89	134.58	122.71
1	C	109	ARG	CD-NE-CZ	-9.89	110.55	124.40
1	E	109	ARG	CD-NE-CZ	-9.89	110.55	124.40
1	F	260	THR	CA-C-O	-9.89	109.98	121.16
1	C	260	THR	CA-C-O	-9.89	109.98	121.16
1	E	271	ARG	CA-C-N	9.89	129.65	119.56
1	E	271	ARG	C-N-CA	9.89	129.65	119.56
1	A	260	THR	CA-C-O	-9.89	109.98	121.16
1	E	376	ARG	CA-C-O	-9.88	109.97	120.55
1	B	489	ASN	N-CA-CB	9.88	124.41	110.67
1	B	572	LYS	CA-C-O	-9.88	110.52	120.70
1	C	8	ALA	O-C-N	-9.88	109.45	122.59
1	E	572	LYS	CA-C-O	-9.88	110.52	120.70
1	C	572	LYS	CA-C-O	-9.88	110.53	120.70
1	C	285	HIS	CA-CB-CG	-9.88	103.92	113.80
1	E	260	THR	CA-C-O	-9.88	110.00	121.16
1	E	436	ALA	CA-C-O	-9.88	109.28	120.24
1	A	285	HIS	CA-CB-CG	-9.87	103.93	113.80
1	A	572	LYS	CA-C-O	-9.87	110.53	120.70
1	F	400	PRO	O-C-N	9.87	134.55	122.71
1	E	400	PRO	O-C-N	9.87	134.55	122.71
1	B	285	HIS	CA-CB-CG	-9.86	103.94	113.80
1	C	335	SER	CA-C-O	-9.86	107.97	120.00
1	B	260	THR	CA-C-O	-9.86	110.02	121.16
1	C	652	HIS	CA-CB-CG	-9.86	103.94	113.80
1	E	335	SER	CA-C-O	-9.86	107.97	120.00
1	E	383	LEU	CA-C-O	-9.86	108.63	119.97
1	F	335	SER	CA-C-O	-9.86	107.97	120.00
1	F	383	LEU	CA-C-O	-9.86	108.63	119.97
1	C	436	ALA	CA-C-O	-9.86	109.30	120.24
1	A	400	PRO	O-C-N	9.85	134.53	122.71
1	A	436	ALA	CA-C-O	-9.85	109.31	120.24
1	B	400	PRO	O-C-N	9.85	134.53	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	ALA	N-CA-CB	-9.85	93.85	110.49
1	B	317	GLN	CA-CB-CG	-9.85	94.41	114.10
1	C	22	TYR	O-C-N	9.85	134.97	122.37
1	F	285	HIS	CA-CB-CG	-9.85	103.95	113.80
1	D	285	HIS	CA-CB-CG	-9.85	103.95	113.80
1	D	383	LEU	CA-C-O	-9.85	108.65	119.97
1	F	22	TYR	O-C-N	9.85	134.97	122.37
1	D	400	PRO	O-C-N	9.84	134.52	122.71
1	A	335	SER	CA-C-O	-9.84	108.00	120.00
1	C	103	ALA	N-CA-CB	-9.84	93.86	110.49
1	D	273	ASP	CB-CA-C	9.84	130.00	110.42
1	E	285	HIS	CA-CB-CG	-9.84	103.96	113.80
1	B	652	HIS	CA-CB-CG	-9.84	103.96	113.80
1	D	652	HIS	CA-CB-CG	-9.84	103.96	113.80
1	E	22	TYR	O-C-N	9.84	134.96	122.37
1	A	317	GLN	CA-CB-CG	-9.83	94.43	114.10
1	F	273	ASP	CB-CA-C	9.83	129.99	110.42
1	A	652	HIS	CA-CB-CG	-9.83	103.97	113.80
1	F	317	GLN	CA-CB-CG	-9.83	94.44	114.10
1	A	103	ALA	N-CA-CB	-9.83	93.88	110.49
1	B	22	TYR	O-C-N	9.83	134.95	122.37
1	B	335	SER	CA-C-O	-9.83	108.01	120.00
1	C	273	ASP	CB-CA-C	9.83	129.98	110.42
1	E	317	GLN	CA-CB-CG	-9.83	94.44	114.10
1	D	572	LYS	CA-C-O	-9.83	110.58	120.70
1	E	273	ASP	CB-CA-C	9.83	129.98	110.42
1	A	22	TYR	O-C-N	9.83	134.95	122.37
1	A	273	ASP	CB-CA-C	9.83	129.98	110.42
1	A	383	LEU	CA-C-O	-9.83	108.67	119.97
1	C	317	GLN	CA-CB-CG	-9.83	94.45	114.10
1	D	317	GLN	CA-CB-CG	-9.83	94.44	114.10
1	F	652	HIS	CA-CB-CG	-9.83	103.97	113.80
1	B	273	ASP	CB-CA-C	9.82	129.97	110.42
1	B	436	ALA	CA-C-O	-9.82	109.34	120.24
1	D	335	SER	CA-C-O	-9.82	108.02	120.00
1	F	103	ALA	N-CA-CB	-9.81	93.90	110.49
1	E	103	ALA	N-CA-CB	-9.81	93.91	110.49
1	B	383	LEU	CA-C-O	-9.81	108.69	119.97
1	C	383	LEU	CA-C-O	-9.81	108.69	119.97
1	D	22	TYR	O-C-N	9.81	134.93	122.37
1	D	103	ALA	N-CA-CB	-9.81	93.91	110.49
1	F	436	ALA	CA-C-O	-9.81	109.35	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	652	HIS	CA-CB-CG	-9.81	103.99	113.80
1	F	145	PHE	CA-C-O	-9.80	106.50	120.51
1	A	145	PHE	CA-C-O	-9.77	106.53	120.51
1	B	145	PHE	CA-C-O	-9.77	106.53	120.51
1	E	145	PHE	CA-C-O	-9.77	106.55	120.51
1	C	502	CYS	N-CA-CB	9.76	124.80	110.06
1	C	145	PHE	CA-C-O	-9.76	106.55	120.51
1	D	502	CYS	N-CA-CB	9.76	124.80	110.06
1	F	357	PRO	CA-C-O	-9.76	102.84	120.60
1	B	357	PRO	CA-C-O	-9.75	102.85	120.60
1	A	502	CYS	N-CA-CB	9.75	124.78	110.06
1	F	287	HIS	N-CA-CB	-9.75	94.20	110.39
1	C	287	HIS	N-CA-CB	-9.75	94.21	110.39
1	F	502	CYS	N-CA-CB	9.75	124.78	110.06
1	A	287	HIS	N-CA-CB	-9.74	94.22	110.39
1	D	357	PRO	CA-C-O	-9.74	102.86	120.60
1	A	357	PRO	CA-C-O	-9.74	102.87	120.60
1	D	145	PHE	CA-C-O	-9.74	106.58	120.51
1	C	357	PRO	CA-C-O	-9.74	102.87	120.60
1	D	287	HIS	N-CA-CB	-9.73	94.23	110.39
1	E	357	PRO	CA-C-O	-9.73	102.89	120.60
1	E	287	HIS	N-CA-CB	-9.73	94.24	110.39
1	B	502	CYS	N-CA-CB	9.73	124.75	110.06
1	E	502	CYS	N-CA-CB	9.73	124.75	110.06
1	B	287	HIS	N-CA-CB	-9.72	94.25	110.39
1	D	63	HIS	N-CA-CB	9.72	126.92	110.49
1	F	63	HIS	N-CA-CB	9.72	126.91	110.49
1	E	63	HIS	N-CA-CB	9.71	126.91	110.49
1	A	63	HIS	N-CA-CB	9.71	126.91	110.49
1	C	63	HIS	N-CA-CB	9.70	126.89	110.49
1	B	63	HIS	N-CA-CB	9.68	126.85	110.49
1	D	243	VAL	N-CA-C	9.68	122.90	109.55
1	D	224	HIS	CA-C-O	9.67	131.30	119.31
1	F	243	VAL	N-CA-C	9.67	122.89	109.55
1	A	243	VAL	N-CA-C	9.66	122.89	109.55
1	B	631	PRO	O-C-N	9.66	134.31	122.23
1	E	297	HIS	CA-CB-CG	-9.66	104.14	113.80
1	C	297	HIS	CA-CB-CG	-9.66	104.14	113.80
1	F	644	HIS	O-C-N	9.66	135.05	123.27
1	D	297	HIS	CA-CB-CG	-9.66	104.14	113.80
1	B	644	HIS	O-C-N	9.65	135.05	123.27
1	B	243	VAL	N-CA-C	9.65	122.87	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	243	VAL	N-CA-C	9.65	122.87	109.55
1	C	224	HIS	CA-C-O	9.65	131.28	119.31
1	C	644	HIS	O-C-N	9.65	135.04	123.27
1	E	224	HIS	CA-C-O	9.65	131.28	119.31
1	E	416	VAL	CA-C-O	9.64	130.94	120.43
1	A	297	HIS	CA-CB-CG	-9.64	104.16	113.80
1	C	243	VAL	N-CA-C	9.64	122.85	109.55
1	B	416	VAL	CA-C-O	9.64	130.93	120.43
1	A	644	HIS	O-C-N	9.63	135.02	123.27
1	D	631	PRO	O-C-N	9.63	134.27	122.23
1	F	416	VAL	CA-C-O	9.63	130.93	120.43
1	A	224	HIS	CA-C-O	9.63	131.25	119.31
1	D	149	GLU	CG-CD-OE2	-9.63	96.26	118.40
1	E	644	HIS	O-C-N	9.62	135.01	123.27
1	B	149	GLU	CG-CD-OE2	-9.62	96.27	118.40
1	C	149	GLU	CG-CD-OE2	-9.62	96.27	118.40
1	D	416	VAL	CA-C-O	9.62	130.92	120.43
1	A	149	GLU	CG-CD-OE2	-9.62	96.27	118.40
1	A	416	VAL	CA-C-O	9.62	130.91	120.43
1	B	297	HIS	CA-CB-CG	-9.62	104.18	113.80
1	B	224	HIS	CA-C-O	9.62	131.24	119.31
1	C	631	PRO	O-C-N	9.62	134.25	122.23
1	E	149	GLU	CG-CD-OE2	-9.62	96.28	118.40
1	F	149	GLU	CG-CD-OE2	-9.62	96.28	118.40
1	F	297	HIS	CA-CB-CG	-9.61	104.19	113.80
1	E	631	PRO	O-C-N	9.61	134.24	122.23
1	A	631	PRO	O-C-N	9.60	134.23	122.23
1	F	224	HIS	CA-C-O	9.60	131.21	119.31
1	C	416	VAL	CA-C-O	9.59	130.89	120.43
1	D	520	GLU	CA-C-O	-9.59	110.34	120.70
1	F	266	GLY	CA-C-O	-9.59	114.29	122.16
1	D	644	HIS	O-C-N	9.59	134.97	123.27
1	F	631	PRO	O-C-N	9.58	134.21	122.23
1	C	117	TYR	N-CA-CB	9.58	123.90	110.01
1	C	266	GLY	CA-C-O	-9.57	114.31	122.16
1	E	117	TYR	N-CA-CB	9.56	123.87	110.01
1	E	266	GLY	CA-C-O	-9.56	114.32	122.16
1	A	266	GLY	CA-C-O	-9.56	114.32	122.16
1	D	117	TYR	N-CA-CB	9.56	123.87	110.01
1	A	117	TYR	N-CA-CB	9.55	123.86	110.01
1	F	117	TYR	N-CA-CB	9.54	123.85	110.01
1	B	117	TYR	N-CA-CB	9.54	123.84	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	520	GLU	CA-C-O	-9.54	110.40	120.70
1	A	520	GLU	CA-C-O	-9.53	110.41	120.70
1	B	520	GLU	CA-C-O	-9.53	110.41	120.70
1	E	520	GLU	CA-C-O	-9.53	110.41	120.70
1	F	520	GLU	CA-C-O	-9.53	110.41	120.70
1	B	266	GLY	CA-C-O	-9.53	114.35	122.16
1	D	266	GLY	CA-C-O	-9.52	114.35	122.16
1	D	31	LYS	N-CA-CB	9.52	124.38	110.20
1	C	122	SER	CA-CB-OG	-9.52	92.07	111.10
1	F	31	LYS	N-CA-CB	9.52	124.38	110.20
1	D	510	GLN	O-C-N	9.51	134.94	123.24
1	B	122	SER	CA-CB-OG	-9.51	92.09	111.10
1	E	31	LYS	N-CA-CB	9.50	124.36	110.20
1	F	151	ILE	CB-CG1-CD1	9.50	133.75	113.80
1	A	31	LYS	N-CA-CB	9.50	124.35	110.20
1	C	31	LYS	N-CA-CB	9.50	124.35	110.20
1	D	122	SER	CA-CB-OG	-9.50	92.11	111.10
1	A	122	SER	CA-CB-OG	-9.49	92.11	111.10
1	A	151	ILE	CB-CG1-CD1	9.49	133.74	113.80
1	B	31	LYS	N-CA-CB	9.49	124.34	110.20
1	B	151	ILE	CB-CG1-CD1	9.49	133.74	113.80
1	C	151	ILE	CB-CG1-CD1	9.49	133.74	113.80
1	F	122	SER	CA-CB-OG	-9.49	92.11	111.10
1	E	630	ILE	CA-C-O	9.49	132.67	119.95
1	E	151	ILE	CB-CG1-CD1	9.49	133.73	113.80
1	E	510	GLN	O-C-N	9.49	134.91	123.24
1	B	630	ILE	CA-C-O	9.48	132.66	119.95
1	E	122	SER	CA-CB-OG	-9.48	92.13	111.10
1	E	277	PHE	CA-C-O	-9.48	109.79	120.70
1	C	630	ILE	CA-C-O	9.48	132.65	119.95
1	D	151	ILE	CB-CG1-CD1	9.48	133.71	113.80
1	F	630	ILE	CA-C-O	9.48	132.65	119.95
1	C	357	PRO	CA-C-N	-9.48	105.23	122.38
1	C	357	PRO	C-N-CA	-9.48	105.23	122.38
1	A	630	ILE	CA-C-O	9.47	132.65	119.95
1	D	162	LYS	CA-C-N	9.47	131.12	120.98
1	D	162	LYS	C-N-CA	9.47	131.12	120.98
1	A	510	GLN	O-C-N	9.47	134.89	123.24
1	F	510	GLN	O-C-N	9.46	134.88	123.24
1	C	286	VAL	CA-C-O	9.46	130.47	120.25
1	A	357	PRO	CA-C-N	-9.46	105.26	122.38
1	A	357	PRO	C-N-CA	-9.46	105.26	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	286	VAL	CA-C-O	9.46	130.47	120.25
1	F	286	VAL	CA-C-O	9.46	130.47	120.25
1	E	349	VAL	CB-CA-C	-9.46	99.65	112.04
1	D	277	PHE	CA-C-O	-9.45	109.83	120.70
1	E	414	ASN	O-C-N	9.46	133.19	122.32
1	F	357	PRO	CA-C-N	-9.46	105.27	122.38
1	F	357	PRO	C-N-CA	-9.46	105.27	122.38
1	F	478	PHE	CA-C-O	-9.45	110.77	120.98
1	B	510	GLN	O-C-N	9.45	134.87	123.24
1	C	510	GLN	O-C-N	9.45	134.87	123.24
1	D	357	PRO	CA-C-N	-9.45	105.27	122.38
1	D	357	PRO	C-N-CA	-9.45	105.27	122.38
1	C	349	VAL	CB-CA-C	-9.45	99.66	112.04
1	B	349	VAL	CB-CA-C	-9.45	99.66	112.04
1	B	467	SER	N-CA-C	9.45	125.14	109.46
1	E	593	THR	CA-CB-OG1	-9.45	95.43	109.60
1	B	162	LYS	CA-C-N	9.44	131.09	120.98
1	B	162	LYS	C-N-CA	9.44	131.09	120.98
1	D	286	VAL	CA-C-O	9.44	130.45	120.25
1	D	593	THR	CA-CB-OG1	-9.44	95.43	109.60
1	D	630	ILE	CA-C-O	9.44	132.60	119.95
1	A	162	LYS	CA-C-N	9.44	131.08	120.98
1	A	162	LYS	C-N-CA	9.44	131.08	120.98
1	A	373	THR	CA-CB-OG1	-9.44	95.44	109.60
1	B	357	PRO	CA-C-N	-9.44	105.30	122.38
1	B	357	PRO	C-N-CA	-9.44	105.30	122.38
1	E	373	THR	CA-CB-OG1	-9.44	95.44	109.60
1	D	123	VAL	CB-CA-C	9.44	124.05	111.97
1	E	357	PRO	CA-C-N	-9.44	105.30	122.38
1	E	357	PRO	C-N-CA	-9.44	105.30	122.38
1	A	95	GLU	CB-CG-CD	9.43	128.64	112.60
1	A	277	PHE	CA-C-O	-9.43	109.85	120.70
1	A	286	VAL	CA-C-O	9.43	130.44	120.25
1	A	478	PHE	CA-C-O	-9.43	110.79	120.98
1	B	373	THR	CA-CB-OG1	-9.43	95.45	109.60
1	E	95	GLU	CB-CG-CD	9.43	128.63	112.60
1	F	349	VAL	CB-CA-C	-9.43	99.68	112.04
1	C	95	GLU	CB-CG-CD	9.43	128.63	112.60
1	C	593	THR	CA-CB-OG1	-9.43	95.45	109.60
1	F	95	GLU	CB-CG-CD	9.43	128.63	112.60
1	F	162	LYS	CA-C-N	9.43	131.07	120.98
1	F	162	LYS	C-N-CA	9.43	131.07	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	123	VAL	CB-CA-C	9.43	124.04	111.97
1	C	277	PHE	CA-C-O	-9.43	109.86	120.70
1	C	373	THR	CA-CB-OG1	-9.43	95.46	109.60
1	D	95	GLU	CB-CG-CD	9.43	128.63	112.60
1	F	373	THR	CA-CB-OG1	-9.43	95.46	109.60
1	D	373	THR	CA-CB-OG1	-9.43	95.46	109.60
1	A	593	THR	CA-CB-OG1	-9.42	95.46	109.60
1	D	349	VAL	CB-CA-C	-9.42	99.69	112.04
1	E	123	VAL	CB-CA-C	9.42	124.03	111.97
1	A	349	VAL	CB-CA-C	-9.42	99.70	112.04
1	B	95	GLU	CB-CG-CD	9.42	128.61	112.60
1	A	414	ASN	O-C-N	9.42	133.15	122.32
1	B	277	PHE	CA-C-O	-9.42	109.87	120.70
1	E	553	LEU	CA-C-N	-9.41	107.89	123.33
1	C	478	PHE	CA-C-O	-9.41	110.81	120.98
1	E	478	PHE	CA-C-O	-9.41	110.81	120.98
1	E	553	LEU	C-N-CA	-9.41	107.89	123.33
1	F	593	THR	CA-CB-OG1	-9.41	95.48	109.60
1	A	467	SER	N-CA-C	9.41	125.08	109.46
1	D	478	PHE	CA-C-O	-9.41	110.82	120.98
1	C	228	THR	OG1-CB-CG2	9.41	128.12	109.30
1	C	400	PRO	CA-C-O	-9.41	108.76	122.31
1	D	414	ASN	O-C-N	9.41	133.14	122.32
1	F	277	PHE	CA-C-O	-9.41	109.88	120.70
1	F	344	HIS	CB-CG-CD2	9.41	143.43	131.20
1	F	467	SER	N-CA-C	9.41	125.08	109.46
1	C	162	LYS	CA-C-N	9.41	131.04	120.98
1	C	162	LYS	C-N-CA	9.41	131.04	120.98
1	B	593	THR	CA-CB-OG1	-9.40	95.49	109.60
1	C	414	ASN	O-C-N	9.40	133.13	122.32
1	F	123	VAL	CB-CA-C	9.40	124.01	111.97
1	D	467	SER	N-CA-C	9.40	125.07	109.46
1	D	553	LEU	CA-C-N	-9.40	107.91	123.33
1	D	553	LEU	C-N-CA	-9.40	107.91	123.33
1	F	414	ASN	O-C-N	9.40	133.13	122.32
1	A	123	VAL	CB-CA-C	9.40	124.00	111.97
1	A	553	LEU	CA-C-N	-9.40	107.92	123.33
1	A	553	LEU	C-N-CA	-9.40	107.92	123.33
1	B	123	VAL	CB-CA-C	9.40	124.00	111.97
1	C	467	SER	N-CA-C	9.40	125.06	109.46
1	B	478	PHE	CA-C-O	-9.39	110.83	120.98
1	E	344	HIS	CB-CG-CD2	9.39	143.41	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	414	ASN	O-C-N	9.39	133.12	122.32
1	B	344	HIS	CB-CG-CD2	9.39	143.40	131.20
1	E	467	SER	N-CA-C	9.39	125.05	109.46
1	E	228	THR	OG1-CB-CG2	9.39	128.07	109.30
1	B	170	PHE	N-CA-CB	9.39	126.35	110.49
1	B	400	PRO	CA-C-O	-9.39	108.79	122.31
1	F	228	THR	OG1-CB-CG2	9.38	128.07	109.30
1	D	228	THR	OG1-CB-CG2	9.38	128.07	109.30
1	A	228	THR	OG1-CB-CG2	9.38	128.06	109.30
1	B	33	ILE	CA-C-O	9.38	131.46	121.05
1	B	553	LEU	CA-C-N	-9.38	107.94	123.33
1	B	553	LEU	C-N-CA	-9.38	107.94	123.33
1	E	286	VAL	CA-C-O	9.38	130.38	120.25
1	F	553	LEU	CA-C-N	-9.38	107.94	123.33
1	F	553	LEU	C-N-CA	-9.38	107.94	123.33
1	E	162	LYS	CA-C-N	9.38	131.02	120.98
1	E	162	LYS	C-N-CA	9.38	131.02	120.98
1	A	344	HIS	CB-CG-CD2	9.38	143.39	131.20
1	B	635	VAL	N-CA-C	9.38	121.52	111.58
1	C	170	PHE	N-CA-CB	9.38	126.34	110.49
1	D	344	HIS	CB-CG-CD2	9.38	143.39	131.20
1	F	635	VAL	N-CA-C	9.37	121.52	111.58
1	B	228	THR	OG1-CB-CG2	9.37	128.05	109.30
1	A	170	PHE	N-CA-CB	9.37	126.33	110.49
1	C	344	HIS	CB-CG-CD2	9.37	143.38	131.20
1	C	553	LEU	CA-C-N	-9.37	107.97	123.33
1	C	553	LEU	C-N-CA	-9.37	107.97	123.33
1	D	636	ILE	N-CA-C	-9.37	101.06	110.62
1	F	170	PHE	N-CA-CB	9.37	126.32	110.49
1	A	33	ILE	CA-C-O	9.36	131.44	121.05
1	A	400	PRO	CA-C-O	-9.36	108.83	122.31
1	A	636	ILE	N-CA-C	-9.36	101.07	110.62
1	E	400	PRO	CA-C-O	-9.36	108.83	122.31
1	B	636	ILE	N-CA-C	-9.36	101.07	110.62
1	C	33	ILE	CA-C-O	9.36	131.44	121.05
1	E	170	PHE	N-CA-CB	9.36	126.31	110.49
1	C	162	LYS	CB-CA-C	9.36	122.05	109.42
1	D	162	LYS	CB-CA-C	9.35	122.05	109.42
1	B	295	ARG	CD-NE-CZ	-9.35	111.31	124.40
1	C	474	ARG	CB-CG-CD	9.35	132.80	111.30
1	D	170	PHE	N-CA-CB	9.35	126.29	110.49
1	F	400	PRO	CA-C-O	-9.35	108.85	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	636	ILE	N-CA-C	-9.35	101.09	110.62
1	F	295	ARG	CD-NE-CZ	-9.35	111.32	124.40
1	F	636	ILE	N-CA-C	-9.35	101.09	110.62
1	A	474	ARG	CB-CG-CD	9.34	132.79	111.30
1	D	319	LYS	N-CA-C	-9.34	101.88	113.18
1	B	162	LYS	CB-CA-C	9.34	122.03	109.42
1	E	33	ILE	CA-C-O	9.34	131.42	121.05
1	D	33	ILE	CA-C-O	9.34	131.41	121.05
1	F	162	LYS	CB-CA-C	9.34	122.03	109.42
1	F	237	SER	CA-C-O	-9.34	107.33	119.10
1	C	636	ILE	N-CA-C	-9.34	101.10	110.62
1	D	4	GLY	CA-C-O	9.34	136.81	120.57
1	E	295	ARG	CD-NE-CZ	-9.34	111.33	124.40
1	F	474	ARG	CB-CG-CD	9.34	132.77	111.30
1	A	162	LYS	CB-CA-C	9.33	122.02	109.42
1	D	400	PRO	CA-C-O	-9.33	108.87	122.31
1	F	475	LEU	CA-C-O	-9.33	110.71	121.16
1	B	319	LYS	N-CA-C	-9.33	101.89	113.18
1	F	33	ILE	CA-C-O	9.33	131.41	121.05
1	B	237	SER	CA-C-O	-9.33	107.35	119.10
1	B	474	ARG	CB-CG-CD	9.33	132.76	111.30
1	D	52	ALA	CA-C-O	-9.33	111.29	120.90
1	D	474	ARG	CB-CG-CD	9.33	132.76	111.30
1	E	162	LYS	CB-CA-C	9.33	122.01	109.42
1	C	237	SER	CA-C-O	-9.33	107.35	119.10
1	C	295	ARG	CD-NE-CZ	-9.33	111.34	124.40
1	C	4	GLY	CA-C-O	9.32	136.79	120.57
1	C	475	LEU	CA-C-O	-9.32	110.72	121.16
1	E	474	ARG	CB-CG-CD	9.32	132.74	111.30
1	E	475	LEU	CA-C-O	-9.32	110.72	121.16
1	A	295	ARG	CD-NE-CZ	-9.32	111.35	124.40
1	B	410	GLY	N-CA-C	-9.32	91.09	113.18
1	D	295	ARG	CD-NE-CZ	-9.32	111.35	124.40
1	F	4	GLY	CA-C-O	9.32	136.79	120.57
1	A	319	LYS	N-CA-C	-9.32	101.91	113.18
1	A	475	LEU	CA-C-O	-9.32	110.72	121.16
1	D	475	LEU	CA-C-O	-9.31	110.73	121.16
1	E	4	GLY	CA-C-O	9.31	136.78	120.57
1	B	4	GLY	CA-C-O	9.31	136.77	120.57
1	E	253	ARG	NE-CZ-NH1	-9.31	112.19	121.50
1	F	253	ARG	NE-CZ-NH1	-9.31	112.19	121.50
1	F	410	GLY	N-CA-C	-9.31	91.11	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	319	LYS	N-CA-C	-9.31	101.92	113.18
1	A	4	GLY	CA-C-O	9.31	136.76	120.57
1	A	237	SER	CA-C-O	-9.31	107.37	119.10
1	A	410	GLY	N-CA-C	-9.31	91.12	113.18
1	B	475	LEU	CA-C-O	-9.30	110.74	121.16
1	D	410	GLY	N-CA-C	-9.30	91.13	113.18
1	E	237	SER	CA-C-O	-9.30	107.38	119.10
1	D	151	ILE	O-C-N	9.30	131.41	121.83
1	A	253	ARG	NE-CZ-NH1	-9.30	112.20	121.50
1	D	237	SER	CA-C-O	-9.30	107.38	119.10
1	C	319	LYS	N-CA-C	-9.30	101.93	113.18
1	E	52	ALA	CA-C-O	-9.30	111.32	120.90
1	E	319	LYS	N-CA-C	-9.30	101.93	113.18
1	B	253	ARG	NE-CZ-NH1	-9.29	112.20	121.50
1	C	410	GLY	N-CA-C	-9.30	91.15	113.18
1	E	410	GLY	N-CA-C	-9.29	91.17	113.18
1	B	151	ILE	O-C-N	9.29	131.39	121.83
1	C	253	ARG	NE-CZ-NH1	-9.29	112.21	121.50
1	C	151	ILE	O-C-N	9.28	131.39	121.83
1	E	536	PHE	O-C-N	9.28	131.68	122.03
1	D	253	ARG	NE-CZ-NH1	-9.28	112.22	121.50
1	A	52	ALA	CA-C-O	-9.28	111.34	120.90
1	F	536	PHE	O-C-N	9.28	131.68	122.03
1	C	527	SER	N-CA-CB	9.27	125.02	110.46
1	F	52	ALA	CA-C-O	-9.27	111.35	120.90
1	B	527	SER	N-CA-CB	9.27	125.01	110.46
1	E	636	ILE	O-C-N	9.27	130.86	121.87
1	B	312	THR	CA-CB-OG1	-9.26	95.70	109.60
1	E	527	SER	N-CA-CB	9.26	125.00	110.46
1	A	151	ILE	O-C-N	9.26	131.37	121.83
1	C	536	PHE	O-C-N	9.26	131.66	122.03
1	F	322	GLU	CA-C-O	-9.26	108.73	120.31
1	A	527	SER	N-CA-CB	9.26	125.00	110.46
1	F	151	ILE	O-C-N	9.25	131.36	121.83
1	A	536	PHE	O-C-N	9.25	131.65	122.03
1	F	312	THR	CA-CB-OG1	-9.25	95.72	109.60
1	F	527	SER	N-CA-CB	9.25	124.99	110.46
1	C	52	ALA	CA-C-O	-9.25	111.37	120.90
1	D	643	LYS	CA-C-N	-9.25	107.75	122.73
1	D	643	LYS	C-N-CA	-9.25	107.75	122.73
1	E	151	ILE	O-C-N	9.25	131.36	121.83
1	E	312	THR	CA-CB-OG1	-9.25	95.72	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	536	PHE	O-C-N	9.25	131.65	122.03
1	B	461	THR	O-C-N	-9.24	111.87	123.24
1	D	322	GLU	CA-C-O	-9.24	108.75	120.31
1	D	389	ASN	OD1-CG-ND2	-9.24	113.36	122.60
1	B	536	PHE	O-C-N	9.24	131.64	122.03
1	A	312	THR	CA-CB-OG1	-9.24	95.74	109.60
1	A	643	LYS	CA-C-N	-9.24	107.76	122.73
1	A	643	LYS	C-N-CA	-9.24	107.76	122.73
1	B	322	GLU	CA-C-O	-9.24	108.76	120.31
1	C	643	LYS	CA-C-N	-9.24	107.76	122.73
1	C	643	LYS	C-N-CA	-9.24	107.76	122.73
1	D	527	SER	N-CA-CB	9.24	124.97	110.46
1	B	389	ASN	OD1-CG-ND2	-9.24	113.36	122.60
1	E	389	ASN	OD1-CG-ND2	-9.24	113.36	122.60
1	B	298	GLU	N-CA-C	-9.23	102.02	113.38
1	A	322	GLU	CA-C-O	-9.23	108.77	120.31
1	D	636	ILE	O-C-N	9.23	130.82	121.87
1	E	643	LYS	CA-C-N	-9.23	107.78	122.73
1	E	643	LYS	C-N-CA	-9.23	107.78	122.73
1	B	52	ALA	CA-C-O	-9.23	111.40	120.90
1	F	643	LYS	CA-C-N	-9.23	107.78	122.73
1	F	643	LYS	C-N-CA	-9.23	107.78	122.73
1	B	636	ILE	O-C-N	9.22	130.82	121.87
1	C	389	ASN	OD1-CG-ND2	-9.22	113.38	122.60
1	D	312	THR	CA-CB-OG1	-9.22	95.76	109.60
1	E	322	GLU	CA-C-O	-9.22	108.78	120.31
1	F	461	THR	O-C-N	-9.22	111.90	123.24
1	A	636	ILE	O-C-N	9.22	130.81	121.87
1	C	312	THR	CA-CB-OG1	-9.22	95.77	109.60
1	D	298	GLU	N-CA-C	-9.22	102.04	113.38
1	A	298	GLU	N-CA-C	-9.22	102.05	113.38
1	A	461	THR	O-C-N	-9.21	111.91	123.24
1	B	643	LYS	CA-C-N	-9.21	107.80	122.73
1	B	643	LYS	C-N-CA	-9.21	107.80	122.73
1	E	461	THR	O-C-N	-9.21	111.91	123.24
1	F	360	LYS	O-C-N	9.21	135.08	122.46
1	F	298	GLU	N-CA-C	-9.21	102.05	113.38
1	F	389	ASN	OD1-CG-ND2	-9.21	113.39	122.60
1	B	360	LYS	O-C-N	9.21	135.07	122.46
1	C	298	GLU	N-CA-C	-9.21	102.06	113.38
1	E	360	LYS	O-C-N	9.21	135.07	122.46
1	C	636	ILE	O-C-N	9.20	130.80	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	636	ILE	O-C-N	9.21	130.80	121.87
1	A	360	LYS	O-C-N	9.20	135.07	122.46
1	E	298	GLU	N-CA-C	-9.20	102.06	113.38
1	B	486	GLU	O-C-N	-9.20	110.18	122.97
1	C	208	SER	N-CA-C	-9.20	100.64	112.23
1	A	389	ASN	OD1-CG-ND2	-9.20	113.40	122.60
1	C	322	GLU	CA-C-O	-9.20	108.81	120.31
1	D	360	LYS	O-C-N	9.19	135.05	122.46
1	D	461	THR	O-C-N	-9.19	111.93	123.24
1	C	360	LYS	O-C-N	9.19	135.05	122.46
1	F	208	SER	N-CA-C	-9.19	100.65	112.23
1	F	486	GLU	O-C-N	-9.19	110.20	122.97
1	B	208	SER	N-CA-C	-9.19	100.66	112.23
1	D	274	ASN	CA-CB-CG	9.19	121.79	112.60
1	F	432	SER	N-CA-C	9.19	123.70	108.73
1	F	617	PRO	N-CA-C	9.19	125.60	113.57
1	B	281	ASP	CA-C-O	-9.18	110.45	120.92
1	C	461	THR	O-C-N	-9.18	111.94	123.24
1	C	617	PRO	N-CA-C	9.18	125.60	113.57
1	D	432	SER	N-CA-C	9.18	123.70	108.73
1	E	617	PRO	N-CA-C	9.18	125.60	113.57
1	D	617	PRO	N-CA-C	9.18	125.59	113.57
1	A	432	SER	N-CA-C	9.18	123.69	108.73
1	E	432	SER	N-CA-C	9.18	123.69	108.73
1	B	227	LEU	N-CA-C	-9.17	101.28	111.28
1	C	281	ASP	CA-C-O	-9.17	110.46	120.92
1	B	617	PRO	N-CA-C	9.17	125.58	113.57
1	F	274	ASN	CA-CB-CG	9.17	121.77	112.60
1	A	281	ASP	CA-C-O	-9.17	110.47	120.92
1	C	486	GLU	O-C-N	-9.17	110.23	122.97
1	E	486	GLU	O-C-N	-9.17	110.23	122.97
1	B	432	SER	N-CA-C	9.16	123.67	108.73
1	E	274	ASN	CA-CB-CG	9.16	121.76	112.60
1	E	281	ASP	CA-C-O	-9.16	110.47	120.92
1	F	227	LEU	N-CA-C	-9.16	101.29	111.28
1	A	208	SER	N-CA-C	-9.16	100.69	112.23
1	F	281	ASP	CA-C-O	-9.16	110.47	120.92
1	A	486	GLU	O-C-N	-9.16	110.24	122.97
1	A	617	PRO	N-CA-C	9.16	125.57	113.57
1	E	208	SER	N-CA-C	-9.16	100.69	112.23
1	F	332	LYS	CA-CB-CG	-9.16	95.78	114.10
1	C	227	LEU	N-CA-C	-9.16	101.30	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	221	PHE	CA-C-N	9.16	132.90	120.54
1	F	221	PHE	C-N-CA	9.16	132.90	120.54
1	D	221	PHE	CA-C-N	9.16	132.90	120.54
1	D	221	PHE	C-N-CA	9.16	132.90	120.54
1	A	227	LEU	N-CA-C	-9.15	101.30	111.28
1	C	432	SER	N-CA-C	9.15	123.64	108.73
1	D	281	ASP	CA-C-O	-9.15	110.49	120.92
1	B	221	PHE	CA-C-N	9.15	132.89	120.54
1	B	221	PHE	C-N-CA	9.15	132.89	120.54
1	D	208	SER	N-CA-C	-9.15	100.70	112.23
1	B	274	ASN	CA-CB-CG	9.14	121.75	112.60
1	D	332	LYS	CA-CB-CG	-9.14	95.81	114.10
1	A	332	LYS	CA-CB-CG	-9.14	95.82	114.10
1	D	486	GLU	O-C-N	-9.14	110.26	122.97
1	E	227	LEU	N-CA-C	-9.14	101.32	111.28
1	B	497	GLU	CA-C-O	-9.14	109.46	119.97
1	F	237	SER	N-CA-C	-9.14	101.90	112.87
1	D	227	LEU	N-CA-C	-9.14	101.32	111.28
1	C	332	LYS	CA-CB-CG	-9.13	95.83	114.10
1	A	221	PHE	CA-C-N	9.13	132.87	120.54
1	A	221	PHE	C-N-CA	9.13	132.87	120.54
1	C	221	PHE	CA-C-N	9.13	132.87	120.54
1	C	221	PHE	C-N-CA	9.13	132.87	120.54
1	A	274	ASN	CA-CB-CG	9.13	121.73	112.60
1	C	237	SER	N-CA-C	-9.13	101.92	112.87
1	E	332	LYS	CA-CB-CG	-9.13	95.85	114.10
1	B	332	LYS	CA-CB-CG	-9.13	95.85	114.10
1	E	237	SER	N-CA-C	-9.12	101.92	112.87
1	D	104	ALA	N-CA-C	-9.12	91.38	110.80
1	D	403	HIS	CA-C-O	9.12	130.29	120.90
1	E	334	SER	CB-CA-C	-9.12	95.02	109.70
1	A	237	SER	N-CA-C	-9.11	101.93	112.87
1	B	104	ALA	N-CA-C	-9.11	91.40	110.80
1	B	237	SER	N-CA-C	-9.11	101.94	112.87
1	C	403	HIS	CA-C-O	9.11	130.28	120.90
1	C	621	PRO	CA-C-N	-9.11	110.43	123.00
1	C	621	PRO	C-N-CA	-9.11	110.43	123.00
1	D	237	SER	N-CA-C	-9.11	101.94	112.87
1	D	497	GLU	CA-C-O	-9.11	109.49	119.97
1	A	104	ALA	N-CA-C	-9.11	91.40	110.80
1	A	497	GLU	CA-C-O	-9.11	109.50	119.97
1	F	621	PRO	CA-C-N	-9.11	110.44	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	621	PRO	C-N-CA	-9.11	110.44	123.00
1	C	423	ILE	N-CA-CB	-9.10	96.83	111.58
1	D	621	PRO	CA-C-N	-9.10	110.44	123.00
1	D	621	PRO	C-N-CA	-9.10	110.44	123.00
1	E	104	ALA	N-CA-C	-9.10	91.41	110.80
1	E	221	PHE	CA-C-N	9.10	132.83	120.54
1	E	221	PHE	C-N-CA	9.10	132.83	120.54
1	E	621	PRO	CA-C-N	-9.10	110.44	123.00
1	E	621	PRO	C-N-CA	-9.10	110.44	123.00
1	E	423	ILE	N-CA-CB	-9.10	96.84	111.58
1	F	497	GLU	CA-C-O	-9.10	109.50	119.97
1	C	334	SER	CB-CA-C	-9.10	95.05	109.70
1	A	334	SER	CB-CA-C	-9.10	95.05	109.70
1	A	621	PRO	CA-C-N	-9.10	110.44	123.00
1	A	621	PRO	C-N-CA	-9.10	110.44	123.00
1	D	334	SER	CB-CA-C	-9.10	95.05	109.70
1	B	383	LEU	N-CA-CB	9.09	124.38	110.28
1	C	104	ALA	N-CA-C	-9.09	91.43	110.80
1	C	383	LEU	N-CA-CB	9.09	124.38	110.28
1	F	334	SER	CB-CA-C	-9.09	95.06	109.70
1	C	274	ASN	CA-CB-CG	9.09	121.69	112.60
1	F	104	ALA	N-CA-C	-9.09	91.44	110.80
1	F	403	HIS	CA-C-O	9.09	130.26	120.90
1	F	423	ILE	N-CA-CB	-9.09	96.86	111.58
1	A	383	LEU	N-CA-CB	9.09	124.36	110.28
1	A	423	ILE	N-CA-CB	-9.09	96.86	111.58
1	D	423	ILE	N-CA-CB	-9.09	96.86	111.58
1	B	621	PRO	CA-C-N	-9.08	110.47	123.00
1	B	621	PRO	C-N-CA	-9.08	110.47	123.00
1	B	334	SER	CB-CA-C	-9.08	95.08	109.70
1	A	403	HIS	CA-C-O	9.08	130.25	120.90
1	B	403	HIS	CA-C-O	9.08	130.25	120.90
1	F	383	LEU	N-CA-CB	9.08	124.36	110.28
1	B	423	ILE	N-CA-CB	-9.08	96.88	111.58
1	C	313	ILE	CA-CB-CG2	9.08	125.93	110.50
1	D	643	LYS	CB-CA-C	-9.08	91.71	109.68
1	B	313	ILE	CA-CB-CG2	9.07	125.93	110.50
1	A	313	ILE	CA-CB-CG2	9.07	125.92	110.50
1	D	383	LEU	N-CA-CB	9.07	124.34	110.28
1	E	101	SER	CB-CA-C	9.07	125.34	110.92
1	E	497	GLU	CA-C-O	-9.07	109.54	119.97
1	E	643	LYS	CB-CA-C	-9.07	91.72	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	530	VAL	N-CA-CB	-9.07	98.51	111.21
1	A	643	LYS	CB-CA-C	-9.07	91.73	109.68
1	E	383	LEU	N-CA-CB	9.07	124.33	110.28
1	B	643	LYS	CB-CA-C	-9.06	91.73	109.68
1	C	643	LYS	CB-CA-C	-9.06	91.74	109.68
1	D	8	ALA	CA-C-N	9.06	136.12	122.17
1	D	8	ALA	C-N-CA	9.06	136.12	122.17
1	D	313	ILE	CA-CB-CG2	9.06	125.91	110.50
1	F	313	ILE	CA-CB-CG2	9.06	125.90	110.50
1	F	101	SER	CB-CA-C	9.06	125.32	110.92
1	A	101	SER	CB-CA-C	9.06	125.32	110.92
1	B	101	SER	CB-CA-C	9.06	125.32	110.92
1	C	101	SER	CB-CA-C	9.06	125.32	110.92
1	D	101	SER	CB-CA-C	9.05	125.31	110.92
1	D	130	ASP	N-CA-C	9.05	121.08	111.03
1	F	643	LYS	CB-CA-C	-9.06	91.75	109.68
1	E	130	ASP	N-CA-C	9.05	121.08	111.03
1	E	251	ILE	O-C-N	9.05	133.84	122.52
1	B	8	ALA	CA-C-N	9.05	136.11	122.17
1	B	8	ALA	C-N-CA	9.05	136.11	122.17
1	D	396	ASP	N-CA-CB	-9.05	96.59	110.44
1	E	403	HIS	CA-C-O	9.05	130.22	120.90
1	E	313	ILE	CA-CB-CG2	9.05	125.89	110.50
1	A	421	GLU	CA-C-N	-9.05	110.27	122.85
1	A	421	GLU	C-N-CA	-9.05	110.27	122.85
1	C	365	PRO	CA-C-O	-9.05	109.55	122.31
1	D	530	VAL	N-CA-CB	-9.05	98.54	111.21
1	A	8	ALA	CA-C-N	9.05	136.10	122.17
1	A	8	ALA	C-N-CA	9.05	136.10	122.17
1	D	251	ILE	O-C-N	9.05	133.83	122.52
1	F	564	ILE	CA-C-O	9.05	132.07	119.95
1	C	8	ALA	CA-C-N	9.04	136.10	122.17
1	C	8	ALA	C-N-CA	9.04	136.10	122.17
1	A	251	ILE	O-C-N	9.04	133.82	122.52
1	B	421	GLU	CA-C-N	-9.04	110.28	122.85
1	B	421	GLU	C-N-CA	-9.04	110.28	122.85
1	D	365	PRO	CA-C-O	-9.04	109.56	122.31
1	D	421	GLU	CA-C-N	-9.04	110.28	122.85
1	D	421	GLU	C-N-CA	-9.04	110.28	122.85
1	E	8	ALA	CA-C-N	9.04	136.10	122.17
1	E	8	ALA	C-N-CA	9.04	136.10	122.17
1	A	130	ASP	N-CA-C	9.04	121.06	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	PRO	CA-C-O	-9.04	109.57	122.31
1	B	130	ASP	N-CA-C	9.04	121.06	111.03
1	E	530	VAL	N-CA-CB	-9.04	98.56	111.21
1	B	564	ILE	CA-C-O	9.04	132.06	119.95
1	E	396	ASP	N-CA-CB	-9.04	96.61	110.44
1	E	421	GLU	CA-C-N	-9.04	110.29	122.85
1	E	421	GLU	C-N-CA	-9.04	110.29	122.85
1	B	365	PRO	CA-C-O	-9.03	109.57	122.31
1	C	530	VAL	N-CA-CB	-9.04	98.56	111.21
1	C	564	ILE	CA-C-O	9.03	132.06	119.95
1	E	564	ILE	CA-C-O	9.04	132.06	119.95
1	A	530	VAL	N-CA-CB	-9.03	98.57	111.21
1	B	457	HIS	O-C-N	9.03	134.79	122.78
1	F	421	GLU	CA-C-N	-9.03	110.30	122.85
1	F	421	GLU	C-N-CA	-9.03	110.30	122.85
1	A	396	ASP	N-CA-CB	-9.03	96.63	110.44
1	A	564	ILE	CA-C-O	9.03	132.05	119.95
1	C	396	ASP	N-CA-CB	-9.03	96.62	110.44
1	C	251	ILE	O-C-N	9.03	133.80	122.52
1	D	457	HIS	O-C-N	9.03	134.78	122.78
1	E	365	PRO	CA-C-O	-9.02	109.59	122.31
1	F	365	PRO	CA-C-O	-9.02	109.59	122.31
1	C	421	GLU	CA-C-N	-9.02	110.31	122.85
1	C	421	GLU	C-N-CA	-9.02	110.31	122.85
1	F	8	ALA	CA-C-N	9.02	136.06	122.17
1	F	8	ALA	C-N-CA	9.02	136.06	122.17
1	F	211	TYR	CA-C-O	-9.02	111.66	121.31
1	F	251	ILE	O-C-N	9.02	133.80	122.52
1	F	396	ASP	N-CA-CB	-9.02	96.64	110.44
1	B	530	VAL	N-CA-CB	-9.02	98.59	111.21
1	D	564	ILE	CA-C-O	9.02	132.03	119.95
1	F	75	PHE	O-C-N	9.02	135.21	122.41
1	C	211	TYR	CA-C-O	-9.01	111.67	121.31
1	F	130	ASP	N-CA-C	9.01	121.03	111.03
1	A	211	TYR	CA-C-O	-9.01	111.67	121.31
1	B	211	TYR	CA-C-O	-9.00	111.68	121.31
1	B	251	ILE	O-C-N	9.00	133.77	122.52
1	E	73	SER	CA-C-O	-9.00	110.67	121.56
1	F	73	SER	CA-C-O	-9.00	110.67	121.56
1	B	396	ASP	N-CA-CB	-9.00	96.67	110.44
1	A	457	HIS	O-C-N	8.99	134.74	122.78
1	C	130	ASP	N-CA-C	8.99	121.01	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	73	SER	CA-C-O	-8.99	110.68	121.56
1	E	75	PHE	O-C-N	8.99	135.18	122.41
1	C	650	VAL	N-CA-C	8.99	121.42	108.48
1	E	211	TYR	CA-C-O	-8.99	111.69	121.31
1	B	546	ALA	O-C-N	8.99	133.06	122.19
1	A	73	SER	CA-C-O	-8.99	110.69	121.56
1	D	75	PHE	O-C-N	8.98	135.17	122.41
1	D	481	PHE	O-C-N	-8.98	113.00	123.06
1	A	650	VAL	N-CA-C	8.98	121.41	108.48
1	B	650	VAL	N-CA-C	8.98	121.41	108.48
1	C	75	PHE	O-C-N	8.98	135.16	122.41
1	B	467	SER	CA-C-O	-8.98	110.40	120.54
1	B	651	HIS	CA-C-O	-8.98	110.85	120.46
1	C	546	ALA	O-C-N	8.98	133.05	122.19
1	D	467	SER	CA-C-O	-8.98	110.40	120.54
1	B	75	PHE	O-C-N	8.97	135.15	122.41
1	C	73	SER	CA-C-O	-8.97	110.70	121.56
1	D	211	TYR	CA-C-O	-8.97	111.71	121.31
1	E	642	ILE	N-CA-C	-8.97	95.17	108.45
1	A	75	PHE	O-C-N	8.97	135.15	122.41
1	C	465	THR	O-C-N	8.97	133.45	123.22
1	B	148	SER	O-C-N	8.97	134.51	122.49
1	D	546	ALA	O-C-N	8.97	133.04	122.19
1	D	465	THR	O-C-N	8.97	133.44	123.22
1	E	148	SER	O-C-N	8.96	134.50	122.49
1	F	650	VAL	N-CA-C	8.96	121.39	108.48
1	F	651	HIS	CA-C-O	-8.97	110.87	120.46
1	E	650	VAL	N-CA-C	8.96	121.39	108.48
1	B	3	LEU	N-CA-C	-8.96	98.97	111.52
1	B	481	PHE	O-C-N	-8.96	113.02	123.06
1	F	642	ILE	N-CA-C	-8.96	95.19	108.45
1	D	650	VAL	N-CA-C	8.96	121.38	108.48
1	A	642	ILE	N-CA-C	-8.96	95.19	108.45
1	C	173	THR	O-C-N	8.96	134.20	122.38
1	C	457	HIS	O-C-N	8.96	134.69	122.78
1	C	642	ILE	N-CA-C	-8.96	95.19	108.45
1	C	651	HIS	CA-C-O	-8.96	110.88	120.46
1	D	73	SER	CA-C-O	-8.96	110.72	121.56
1	E	457	HIS	O-C-N	8.96	134.69	122.78
1	F	457	HIS	O-C-N	8.96	134.69	122.78
1	F	546	ALA	O-C-N	8.96	133.03	122.19
1	B	642	ILE	N-CA-C	-8.96	95.20	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	651	HIS	CA-C-O	-8.96	110.88	120.46
1	E	546	ALA	O-C-N	8.95	133.02	122.19
1	F	148	SER	O-C-N	8.95	134.49	122.49
1	F	65	LEU	N-CA-CB	-8.95	95.83	110.41
1	C	581	ASN	OD1-CG-ND2	8.95	131.54	122.60
1	A	467	SER	CA-C-O	-8.94	110.43	120.54
1	A	546	ALA	O-C-N	8.94	133.01	122.19
1	A	651	HIS	CA-C-O	-8.94	110.89	120.46
1	C	3	LEU	N-CA-C	-8.94	99.00	111.52
1	C	65	LEU	N-CA-CB	-8.94	95.83	110.41
1	C	467	SER	CA-C-O	-8.94	110.44	120.54
1	D	146	THR	CA-CB-OG1	-8.94	96.19	109.60
1	D	148	SER	O-C-N	8.94	134.47	122.49
1	E	465	THR	O-C-N	8.94	133.41	123.22
1	F	190	MET	CA-C-N	-8.94	108.30	120.28
1	F	190	MET	C-N-CA	-8.94	108.30	120.28
1	A	148	SER	O-C-N	8.94	134.47	122.49
1	F	360	LYS	N-CA-C	-8.94	102.14	113.23
1	E	65	LEU	N-CA-CB	-8.94	95.84	110.41
1	E	467	SER	CA-C-O	-8.94	110.44	120.54
1	E	651	HIS	CA-C-O	-8.94	110.90	120.46
1	F	465	THR	O-C-N	8.94	133.41	123.22
1	A	3	LEU	N-CA-C	-8.93	99.01	111.52
1	A	465	THR	O-C-N	8.93	133.40	123.22
1	B	173	THR	O-C-N	8.93	134.17	122.38
1	B	465	THR	O-C-N	8.93	133.40	123.22
1	C	190	MET	CA-C-N	-8.93	108.31	120.28
1	C	190	MET	C-N-CA	-8.93	108.31	120.28
1	F	3	LEU	N-CA-C	-8.93	99.02	111.52
1	A	481	PHE	O-C-N	-8.93	113.06	123.06
1	D	190	MET	CA-C-N	-8.93	108.31	120.28
1	D	190	MET	C-N-CA	-8.93	108.31	120.28
1	E	190	MET	CA-C-N	-8.93	108.31	120.28
1	F	173	THR	O-C-N	8.93	134.17	122.38
1	A	65	LEU	N-CA-CB	-8.93	95.86	110.41
1	B	65	LEU	N-CA-CB	-8.93	95.86	110.41
1	B	190	MET	CA-C-N	-8.93	108.31	120.28
1	B	190	MET	C-N-CA	-8.93	108.31	120.28
1	D	642	ILE	N-CA-C	-8.93	95.23	108.45
1	E	190	MET	C-N-CA	-8.93	108.31	120.28
1	F	467	SER	CA-C-O	-8.93	110.45	120.54
1	A	173	THR	O-C-N	8.93	134.16	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	MET	CA-C-N	-8.93	108.32	120.28
1	A	190	MET	C-N-CA	-8.93	108.32	120.28
1	D	3	LEU	N-CA-C	-8.93	99.02	111.52
1	E	3	LEU	N-CA-C	-8.93	99.02	111.52
1	D	65	LEU	N-CA-CB	-8.93	95.86	110.41
1	F	254	GLU	N-CA-C	8.92	124.75	107.98
1	A	180	ARG	NE-CZ-NH2	-8.92	111.17	119.20
1	E	581	ASN	OD1-CG-ND2	8.92	131.52	122.60
1	A	360	LYS	N-CA-C	-8.92	102.17	113.23
1	C	148	SER	O-C-N	8.92	134.44	122.49
1	E	389	ASN	CB-CG-ND2	8.92	129.77	116.40
1	B	180	ARG	NE-CZ-NH2	-8.91	111.18	119.20
1	E	481	PHE	O-C-N	-8.91	113.08	123.06
1	F	389	ASN	CB-CG-ND2	8.91	129.77	116.40
1	D	78	ARG	NE-CZ-NH1	-8.91	112.59	121.50
1	B	360	LYS	N-CA-C	-8.91	102.19	113.23
1	E	180	ARG	NE-CZ-NH2	-8.91	111.18	119.20
1	B	146	THR	CA-CB-OG1	-8.90	96.24	109.60
1	C	146	THR	CA-CB-OG1	-8.90	96.24	109.60
1	D	173	THR	O-C-N	8.90	134.13	122.38
1	F	180	ARG	NE-CZ-NH2	-8.90	111.19	119.20
1	C	216	LYS	O-C-N	8.90	134.85	123.01
1	E	360	LYS	N-CA-C	-8.90	102.19	113.23
1	C	389	ASN	CB-CG-ND2	8.90	129.75	116.40
1	A	389	ASN	CB-CG-ND2	8.90	129.75	116.40
1	B	389	ASN	CB-CG-ND2	8.90	129.75	116.40
1	A	146	THR	CA-CB-OG1	-8.89	96.26	109.60
1	C	360	LYS	N-CA-C	-8.89	102.20	113.23
1	D	216	LYS	O-C-N	8.89	134.84	123.01
1	E	146	THR	CA-CB-OG1	-8.89	96.26	109.60
1	A	254	GLU	N-CA-C	8.89	124.70	107.98
1	D	389	ASN	CB-CG-ND2	8.89	129.74	116.40
1	E	78	ARG	NE-CZ-NH1	-8.89	112.61	121.50
1	E	254	GLU	N-CA-C	8.89	124.70	107.98
1	F	481	PHE	O-C-N	-8.89	113.10	123.06
1	A	581	ASN	OD1-CG-ND2	8.89	131.49	122.60
1	D	180	ARG	NE-CZ-NH2	-8.89	111.20	119.20
1	F	298	GLU	CA-C-O	8.89	129.28	119.15
1	C	78	ARG	NE-CZ-NH1	-8.88	112.62	121.50
1	C	180	ARG	NE-CZ-NH2	-8.88	111.20	119.20
1	C	254	GLU	N-CA-C	8.88	124.68	107.98
1	C	446	VAL	O-C-N	8.88	132.20	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	481	PHE	O-C-N	-8.89	113.11	123.06
1	F	78	ARG	NE-CZ-NH1	-8.88	112.62	121.50
1	B	216	LYS	O-C-N	8.88	134.82	123.01
1	B	254	GLU	N-CA-C	8.88	124.68	107.98
1	D	254	GLU	N-CA-C	8.88	124.68	107.98
1	E	446	VAL	O-C-N	8.88	132.20	123.14
1	F	216	LYS	O-C-N	8.88	134.82	123.01
1	A	446	VAL	O-C-N	8.88	132.20	123.14
1	C	385	LYS	N-CA-CB	8.88	122.94	110.07
1	E	173	THR	O-C-N	8.88	134.09	122.38
1	E	216	LYS	O-C-N	8.88	134.81	123.01
1	B	581	ASN	OD1-CG-ND2	8.87	131.47	122.60
1	D	446	VAL	O-C-N	8.87	132.19	123.14
1	A	78	ARG	NE-CZ-NH1	-8.87	112.63	121.50
1	B	446	VAL	O-C-N	8.87	132.19	123.14
1	D	360	LYS	N-CA-C	-8.87	102.23	113.23
1	F	446	VAL	O-C-N	8.87	132.19	123.14
1	D	581	ASN	OD1-CG-ND2	8.87	131.47	122.60
1	E	298	GLU	CA-C-O	8.87	129.26	119.15
1	A	216	LYS	O-C-N	8.86	134.80	123.01
1	F	146	THR	CA-CB-OG1	-8.86	96.31	109.60
1	A	385	LYS	N-CA-CB	8.86	122.91	110.07
1	A	298	GLU	CA-C-O	8.85	129.24	119.15
1	D	385	LYS	N-CA-CB	8.85	122.91	110.07
1	D	298	GLU	CA-C-O	8.85	129.24	119.15
1	B	298	GLU	CA-C-O	8.85	129.24	119.15
1	B	78	ARG	NE-CZ-NH1	-8.84	112.66	121.50
1	B	385	LYS	N-CA-CB	8.84	122.89	110.07
1	E	385	LYS	N-CA-CB	8.84	122.89	110.07
1	F	581	ASN	OD1-CG-ND2	8.84	131.44	122.60
1	E	218	GLU	CB-CG-CD	8.84	127.62	112.60
1	F	218	GLU	CB-CG-CD	8.84	127.62	112.60
1	F	385	LYS	N-CA-CB	8.84	122.88	110.07
1	A	218	GLU	CB-CG-CD	8.83	127.61	112.60
1	C	298	GLU	CA-C-O	8.83	129.21	119.15
1	D	462	TYR	O-C-N	8.82	133.27	123.22
1	C	218	GLU	CB-CG-CD	8.81	127.58	112.60
1	C	530	VAL	CA-CB-CG2	-8.81	95.42	110.40
1	B	241	ASP	N-CA-CB	-8.81	95.58	110.11
1	C	216	LYS	CA-CB-CG	8.81	131.71	114.10
1	C	650	VAL	CA-C-N	-8.81	110.61	123.11
1	C	650	VAL	C-N-CA	-8.81	110.61	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	216	LYS	CA-CB-CG	8.81	131.71	114.10
1	D	650	VAL	CA-C-N	-8.81	110.61	123.11
1	D	650	VAL	C-N-CA	-8.81	110.61	123.11
1	F	241	ASP	N-CA-CB	-8.81	95.58	110.11
1	D	218	GLU	CB-CG-CD	8.80	127.57	112.60
1	B	218	GLU	CB-CG-CD	8.80	127.56	112.60
1	C	261	SER	CA-C-O	-8.80	110.81	121.11
1	F	216	LYS	CA-CB-CG	8.80	131.70	114.10
1	A	216	LYS	CA-CB-CG	8.79	131.69	114.10
1	A	650	VAL	CA-C-N	-8.80	110.62	123.11
1	A	650	VAL	C-N-CA	-8.80	110.62	123.11
1	B	650	VAL	CA-C-N	-8.79	110.62	123.11
1	B	650	VAL	C-N-CA	-8.79	110.62	123.11
1	F	80	ARG	NH1-CZ-NH2	8.79	130.73	119.30
1	E	650	VAL	CA-C-N	-8.79	110.63	123.11
1	E	650	VAL	C-N-CA	-8.79	110.63	123.11
1	F	61	ASN	CB-CG-ND2	8.79	129.59	116.40
1	F	462	TYR	O-C-N	8.79	133.24	123.22
1	B	150	VAL	CA-CB-CG2	-8.79	95.46	110.40
1	B	261	SER	CA-C-O	-8.79	110.83	121.11
1	F	650	VAL	CA-C-N	-8.79	110.63	123.11
1	F	650	VAL	C-N-CA	-8.79	110.63	123.11
1	A	530	VAL	CA-CB-CG2	-8.79	95.46	110.40
1	E	530	VAL	CA-CB-CG2	-8.79	95.46	110.40
1	F	530	VAL	CA-CB-CG2	-8.79	95.47	110.40
1	A	241	ASP	N-CA-CB	-8.78	95.62	110.11
1	A	462	TYR	O-C-N	8.78	133.23	123.22
1	D	530	VAL	CA-CB-CG2	-8.78	95.47	110.40
1	F	292	THR	CA-CB-OG1	-8.78	96.43	109.60
1	F	471	ASP	CA-C-O	-8.78	111.24	120.55
1	A	261	SER	CA-C-O	-8.78	110.84	121.11
1	B	530	VAL	CA-CB-CG2	-8.78	95.48	110.40
1	E	471	ASP	CA-C-O	-8.78	111.24	120.55
1	D	216	LYS	CA-CB-CG	8.78	131.66	114.10
1	A	292	THR	CA-CB-OG1	-8.78	96.44	109.60
1	B	216	LYS	CA-CB-CG	8.78	131.65	114.10
1	E	241	ASP	N-CA-CB	-8.78	95.63	110.11
1	C	61	ASN	CB-CG-ND2	8.78	129.56	116.40
1	E	173	THR	CB-CA-C	-8.78	97.79	111.83
1	B	292	THR	CA-CB-OG1	-8.77	96.44	109.60
1	E	578	MET	N-CA-C	-8.77	95.99	109.24
1	A	61	ASN	CB-CG-ND2	8.77	129.56	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	173	THR	CB-CA-C	-8.77	97.80	111.83
1	C	241	ASP	N-CA-CB	-8.77	95.64	110.11
1	C	462	TYR	O-C-N	8.77	133.22	123.22
1	D	150	VAL	CA-CB-CG2	-8.77	95.49	110.40
1	F	330	SER	N-CA-CB	8.77	125.31	110.49
1	D	412	VAL	O-C-N	8.77	133.11	123.03
1	D	61	ASN	CB-CG-ND2	8.77	129.55	116.40
1	E	61	ASN	CB-CG-ND2	8.77	129.55	116.40
1	F	127	LYS	CG-CD-CE	8.77	131.46	111.30
1	F	388	ASP	CA-CB-CG	8.77	121.37	112.60
1	A	127	LYS	CG-CD-CE	8.76	131.46	111.30
1	B	61	ASN	CB-CG-ND2	8.76	129.54	116.40
1	D	127	LYS	CG-CD-CE	8.76	131.46	111.30
1	D	241	ASP	N-CA-CB	-8.76	95.65	110.11
1	B	127	LYS	CG-CD-CE	8.76	131.45	111.30
1	F	173	THR	CB-CA-C	-8.76	97.81	111.83
1	B	368	MET	N-CA-CB	-8.76	96.70	110.46
1	D	261	SER	CA-C-O	-8.76	110.86	121.11
1	D	292	THR	CA-CB-OG1	-8.76	96.46	109.60
1	E	261	SER	CA-C-O	-8.76	110.86	121.11
1	F	150	VAL	CA-CB-CG2	-8.76	95.51	110.40
1	E	292	THR	CA-CB-OG1	-8.76	96.46	109.60
1	F	578	MET	N-CA-C	-8.76	96.01	109.24
1	B	462	TYR	O-C-N	8.76	133.20	123.22
1	B	616	TYR	CA-C-N	8.76	128.47	119.19
1	B	616	TYR	C-N-CA	8.76	128.47	119.19
1	C	471	ASP	CA-C-O	-8.76	111.27	120.55
1	D	173	THR	CB-CA-C	-8.76	97.82	111.83
1	E	127	LYS	CG-CD-CE	8.76	131.44	111.30
1	E	150	VAL	CA-CB-CG2	-8.76	95.51	110.40
1	E	238	ASN	CB-CG-ND2	8.76	129.54	116.40
1	F	261	SER	CA-C-O	-8.76	110.86	121.11
1	F	528	VAL	O-C-N	8.76	130.98	122.05
1	F	553	LEU	N-CA-CB	-8.76	97.00	111.53
1	A	173	THR	CB-CA-C	-8.75	97.82	111.83
1	D	569	LEU	CA-C-O	-8.75	107.99	120.51
1	E	412	VAL	O-C-N	8.75	133.10	123.03
1	F	569	LEU	CA-C-O	-8.75	107.99	120.51
1	C	292	THR	CA-CB-OG1	-8.75	96.47	109.60
1	A	150	VAL	CA-CB-CG2	-8.75	95.52	110.40
1	C	330	SER	N-CA-CB	8.75	125.28	110.49
1	D	471	ASP	CA-C-O	-8.75	111.27	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	578	MET	N-CA-C	-8.75	96.03	109.24
1	F	585	ALA	N-CA-C	-8.75	94.64	108.90
1	B	578	MET	N-CA-C	-8.75	96.03	109.24
1	D	528	VAL	O-C-N	8.75	130.97	122.05
1	A	412	VAL	O-C-N	8.75	133.09	123.03
1	C	150	VAL	CA-CB-CG2	-8.75	95.53	110.40
1	D	80	ARG	NH1-CZ-NH2	8.75	130.67	119.30
1	E	569	LEU	CA-C-O	-8.75	108.00	120.51
1	A	578	MET	N-CA-C	-8.74	96.04	109.24
1	B	173	THR	CB-CA-C	-8.74	97.84	111.83
1	B	569	LEU	CA-C-O	-8.74	108.01	120.51
1	E	462	TYR	O-C-N	8.74	133.19	123.22
1	F	412	VAL	O-C-N	8.74	133.09	123.03
1	D	165	THR	CA-CB-OG1	-8.74	96.49	109.60
1	D	368	MET	N-CA-CB	-8.74	96.73	110.46
1	A	80	ARG	NH1-CZ-NH2	8.74	130.66	119.30
1	A	215	ARG	CD-NE-CZ	-8.74	112.16	124.40
1	A	569	LEU	CA-C-O	-8.74	108.01	120.51
1	B	528	VAL	O-C-N	8.74	130.97	122.05
1	C	127	LYS	CG-CD-CE	8.74	131.40	111.30
1	C	165	THR	CA-CB-OG1	-8.74	96.49	109.60
1	C	368	MET	N-CA-CB	-8.74	96.74	110.46
1	C	553	LEU	N-CA-CB	-8.74	97.02	111.53
1	C	388	ASP	CA-CB-CG	8.74	121.34	112.60
1	C	569	LEU	CA-C-O	-8.74	108.01	120.51
1	C	578	MET	N-CA-C	-8.74	96.04	109.24
1	A	528	VAL	O-C-N	8.74	130.96	122.05
1	A	585	ALA	N-CA-C	-8.74	94.66	108.90
1	D	215	ARG	CD-NE-CZ	-8.74	112.17	124.40
1	E	215	ARG	CD-NE-CZ	-8.74	112.17	124.40
1	F	616	TYR	CA-C-N	8.74	128.45	119.19
1	F	616	TYR	C-N-CA	8.74	128.45	119.19
1	A	388	ASP	CA-CB-CG	8.73	121.33	112.60
1	B	215	ARG	CD-NE-CZ	-8.73	112.17	124.40
1	B	471	ASP	CA-C-O	-8.73	111.29	120.55
1	F	214	ASP	CA-C-N	-8.73	106.60	122.50
1	F	214	ASP	C-N-CA	-8.73	106.60	122.50
1	F	297	HIS	ND1-CG-CD2	8.73	114.83	106.10
1	C	585	ALA	N-CA-C	-8.73	94.67	108.90
1	E	368	MET	N-CA-CB	-8.73	96.75	110.46
1	E	528	VAL	O-C-N	8.73	130.96	122.05
1	F	215	ARG	CD-NE-CZ	-8.73	112.17	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	471	ASP	CA-C-O	-8.73	111.30	120.55
1	B	585	ALA	N-CA-C	-8.73	94.67	108.90
1	A	553	LEU	N-CA-CB	-8.73	97.04	111.53
1	C	616	TYR	CA-C-N	8.73	128.44	119.19
1	C	616	TYR	C-N-CA	8.73	128.44	119.19
1	E	165	THR	CA-CB-OG1	-8.73	96.50	109.60
1	E	585	ALA	N-CA-C	-8.73	94.67	108.90
1	D	553	LEU	N-CA-CB	-8.73	97.04	111.53
1	F	165	THR	CA-CB-OG1	-8.73	96.50	109.60
1	A	330	SER	N-CA-CB	8.73	125.24	110.49
1	A	368	MET	N-CA-CB	-8.73	96.76	110.46
1	A	616	TYR	CA-C-N	8.73	128.44	119.19
1	A	616	TYR	C-N-CA	8.73	128.44	119.19
1	D	585	ALA	N-CA-C	-8.73	94.67	108.90
1	E	388	ASP	CA-CB-CG	8.73	121.33	112.60
1	F	368	MET	N-CA-CB	-8.73	96.76	110.46
1	A	165	THR	CA-CB-OG1	-8.72	96.51	109.60
1	C	238	ASN	CB-CG-ND2	8.72	129.49	116.40
1	C	497	GLU	CA-C-O	-8.72	109.50	119.79
1	D	388	ASP	CA-CB-CG	8.72	121.33	112.60
1	B	62	ASP	N-CA-C	-8.72	102.81	113.19
1	E	553	LEU	N-CA-CB	-8.72	97.05	111.53
1	A	238	ASN	CB-CG-ND2	8.72	129.48	116.40
1	B	553	LEU	N-CA-CB	-8.72	97.05	111.53
1	C	215	ARG	CD-NE-CZ	-8.72	112.19	124.40
1	D	330	SER	N-CA-CB	8.72	125.23	110.49
1	D	616	TYR	CA-C-N	8.72	128.43	119.19
1	D	616	TYR	C-N-CA	8.72	128.43	119.19
1	E	302	HIS	CB-CA-C	-8.72	96.14	110.79
1	F	302	HIS	CB-CA-C	-8.72	96.14	110.79
1	B	84	LEU	N-CA-CB	-8.72	96.30	110.42
1	B	302	HIS	CB-CA-C	-8.72	96.15	110.79
1	C	214	ASP	CA-C-N	-8.72	106.63	122.50
1	C	214	ASP	C-N-CA	-8.72	106.63	122.50
1	E	80	ARG	NH1-CZ-NH2	8.72	130.63	119.30
1	F	238	ASN	CB-CG-ND2	8.72	129.48	116.40
1	D	214	ASP	CA-C-N	-8.72	106.64	122.50
1	D	214	ASP	C-N-CA	-8.72	106.64	122.50
1	E	214	ASP	CA-C-N	-8.71	106.64	122.50
1	E	214	ASP	C-N-CA	-8.71	106.64	122.50
1	A	214	ASP	CA-C-N	-8.71	106.64	122.50
1	A	214	ASP	C-N-CA	-8.71	106.64	122.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	80	ARG	NH1-CZ-NH2	8.71	130.62	119.30
1	B	165	THR	CA-CB-OG1	-8.71	96.53	109.60
1	B	297	HIS	ND1-CG-CD2	8.71	114.81	106.10
1	B	330	SER	N-CA-CB	8.71	125.21	110.49
1	B	238	ASN	CB-CG-ND2	8.71	129.46	116.40
1	A	84	LEU	N-CA-CB	-8.71	96.31	110.42
1	F	62	ASP	N-CA-C	-8.71	102.83	113.19
1	A	62	ASP	N-CA-C	-8.70	102.83	113.19
1	C	80	ARG	NH1-CZ-NH2	8.70	130.62	119.30
1	C	412	VAL	O-C-N	8.71	133.04	123.03
1	E	616	TYR	CA-C-N	8.71	128.42	119.19
1	E	616	TYR	C-N-CA	8.71	128.42	119.19
1	D	302	HIS	CB-CA-C	-8.70	96.17	110.79
1	E	330	SER	N-CA-CB	8.70	125.20	110.49
1	A	302	HIS	CB-CA-C	-8.70	96.17	110.79
1	C	528	VAL	O-C-N	8.70	130.93	122.05
1	B	214	ASP	CA-C-N	-8.70	106.67	122.50
1	B	214	ASP	C-N-CA	-8.70	106.67	122.50
1	D	238	ASN	CB-CG-ND2	8.70	129.44	116.40
1	F	84	LEU	N-CA-CB	-8.70	96.33	110.42
1	E	84	LEU	N-CA-CB	-8.69	96.34	110.42
1	C	84	LEU	N-CA-CB	-8.69	96.34	110.42
1	B	388	ASP	CA-CB-CG	8.69	121.29	112.60
1	A	297	HIS	ND1-CG-CD2	8.69	114.79	106.10
1	B	412	VAL	O-C-N	8.69	133.02	123.03
1	D	84	LEU	N-CA-CB	-8.69	96.35	110.42
1	E	62	ASP	N-CA-C	-8.69	102.85	113.19
1	E	297	HIS	ND1-CG-CD2	8.69	114.78	106.10
1	C	62	ASP	N-CA-C	-8.68	102.86	113.19
1	D	297	HIS	ND1-CG-CD2	8.68	114.78	106.10
1	C	302	HIS	CB-CA-C	-8.68	96.21	110.79
1	F	23	GLU	CB-CA-C	-8.68	96.87	109.45
1	D	62	ASP	N-CA-C	-8.67	102.87	113.19
1	B	23	GLU	CB-CA-C	-8.66	96.89	109.45
1	F	249	ASP	CA-C-O	-8.66	108.95	119.43
1	A	362	ASN	CB-CA-C	8.65	124.74	112.11
1	D	23	GLU	CB-CA-C	-8.65	96.90	109.45
1	A	23	GLU	CB-CA-C	-8.65	96.91	109.45
1	D	249	ASP	CA-C-O	-8.65	108.97	119.43
1	F	362	ASN	CB-CA-C	8.65	124.73	112.11
1	B	631	PRO	CA-C-N	-8.64	110.58	122.77
1	B	631	PRO	C-N-CA	-8.64	110.58	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	23	GLU	CB-CA-C	-8.64	96.92	109.45
1	C	249	ASP	CA-C-O	-8.64	108.97	119.43
1	D	270	VAL	CB-CA-C	8.64	125.47	111.29
1	E	362	ASN	CB-CA-C	8.64	124.73	112.11
1	C	297	HIS	ND1-CG-CD2	8.64	114.74	106.10
1	D	362	ASN	CB-CA-C	8.64	124.73	112.11
1	C	362	ASN	CB-CA-C	8.64	124.72	112.11
1	B	249	ASP	CA-C-O	-8.64	108.98	119.43
1	B	270	VAL	CB-CA-C	8.64	125.45	111.29
1	C	248	TRP	O-C-N	8.63	134.37	122.46
1	F	298	GLU	CA-C-N	-8.63	106.30	120.71
1	F	298	GLU	C-N-CA	-8.63	106.30	120.71
1	A	248	TRP	O-C-N	8.63	134.37	122.46
1	A	249	ASP	CA-C-O	-8.63	108.99	119.43
1	A	298	GLU	CA-C-N	-8.63	106.30	120.71
1	A	298	GLU	C-N-CA	-8.63	106.30	120.71
1	C	270	VAL	CB-CA-C	8.63	125.44	111.29
1	C	298	GLU	CA-C-N	-8.62	106.31	120.71
1	C	298	GLU	C-N-CA	-8.62	106.31	120.71
1	E	298	GLU	CA-C-N	-8.62	106.31	120.71
1	E	298	GLU	C-N-CA	-8.62	106.31	120.71
1	A	270	VAL	CB-CA-C	8.62	125.43	111.29
1	D	631	PRO	CA-C-N	-8.62	110.61	122.77
1	D	631	PRO	C-N-CA	-8.62	110.61	122.77
1	F	248	TRP	O-C-N	8.62	134.36	122.46
1	B	298	GLU	CA-C-N	-8.62	106.31	120.71
1	B	298	GLU	C-N-CA	-8.62	106.31	120.71
1	B	362	ASN	CB-CA-C	8.62	124.69	112.11
1	D	298	GLU	CA-C-N	-8.62	106.32	120.71
1	D	298	GLU	C-N-CA	-8.62	106.32	120.71
1	E	23	GLU	CB-CA-C	-8.62	96.95	109.45
1	E	270	VAL	CB-CA-C	8.62	125.42	111.29
1	E	248	TRP	O-C-N	8.61	134.35	122.46
1	C	384	HIS	O-C-N	8.61	134.64	122.41
1	D	167	ASN	CA-CB-CG	8.61	121.21	112.60
1	F	270	VAL	CB-CA-C	8.61	125.41	111.29
1	D	248	TRP	O-C-N	8.61	134.34	122.46
1	D	384	HIS	O-C-N	8.61	134.63	122.41
1	E	631	PRO	CA-C-N	-8.60	110.64	122.77
1	E	631	PRO	C-N-CA	-8.60	110.64	122.77
1	F	384	HIS	O-C-N	8.60	134.63	122.41
1	A	631	PRO	CA-C-N	-8.60	110.65	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	631	PRO	C-N-CA	-8.60	110.65	122.77
1	B	167	ASN	CA-CB-CG	8.60	121.20	112.60
1	C	631	PRO	CA-C-N	-8.60	110.64	122.77
1	C	631	PRO	C-N-CA	-8.60	110.64	122.77
1	B	248	TRP	O-C-N	8.60	134.33	122.46
1	E	127	LYS	CA-C-O	8.60	130.10	120.90
1	E	249	ASP	CA-C-O	-8.60	109.03	119.43
1	B	127	LYS	CA-C-O	8.60	130.10	120.90
1	D	562	CYS	CB-CA-C	-8.60	96.24	110.85
1	E	384	HIS	O-C-N	8.60	134.62	122.41
1	F	127	LYS	CA-C-O	8.60	130.10	120.90
1	A	562	CYS	CB-CA-C	-8.59	96.25	110.85
1	E	167	ASN	CA-CB-CG	8.59	121.19	112.60
1	B	562	CYS	CB-CA-C	-8.59	96.25	110.85
1	B	69	ARG	CB-CG-CD	8.59	131.04	111.30
1	F	167	ASN	CA-CB-CG	8.59	121.19	112.60
1	A	384	HIS	O-C-N	8.58	134.60	122.41
1	B	298	GLU	CB-CG-CD	-8.58	98.01	112.60
1	E	562	CYS	CB-CA-C	-8.58	96.26	110.85
1	F	562	CYS	CB-CA-C	-8.58	96.26	110.85
1	A	167	ASN	CA-CB-CG	8.58	121.18	112.60
1	A	127	LYS	CA-C-O	8.57	130.07	120.90
1	C	562	CYS	CB-CA-C	-8.57	96.27	110.85
1	E	195	VAL	N-CA-CB	8.57	121.54	110.57
1	C	167	ASN	CA-CB-CG	8.57	121.17	112.60
1	F	631	PRO	CA-C-N	-8.57	110.68	122.77
1	F	631	PRO	C-N-CA	-8.57	110.68	122.77
1	A	69	ARG	CB-CG-CD	8.56	131.00	111.30
1	C	195	VAL	N-CA-CB	8.56	121.53	110.57
1	C	69	ARG	CB-CG-CD	8.56	130.99	111.30
1	B	122	SER	CA-C-N	-8.56	109.77	120.56
1	B	122	SER	C-N-CA	-8.56	109.77	120.56
1	D	298	GLU	CB-CG-CD	-8.56	98.05	112.60
1	E	69	ARG	CB-CG-CD	8.56	130.99	111.30
1	E	122	SER	CA-C-N	-8.56	109.78	120.56
1	E	122	SER	C-N-CA	-8.56	109.78	120.56
1	F	298	GLU	CB-CG-CD	-8.56	98.05	112.60
1	D	127	LYS	CA-C-O	8.56	130.06	120.90
1	B	384	HIS	O-C-N	8.56	134.56	122.41
1	C	298	GLU	CB-CG-CD	-8.56	98.05	112.60
1	C	127	LYS	CA-C-O	8.56	130.06	120.90
1	C	607	ALA	N-CA-C	-8.55	101.29	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	298	GLU	CB-CG-CD	-8.55	98.06	112.60
1	F	195	VAL	N-CA-CB	8.55	121.52	110.57
1	E	607	ALA	N-CA-C	-8.55	101.30	112.41
1	A	298	GLU	CB-CG-CD	-8.55	98.07	112.60
1	D	69	ARG	CB-CG-CD	8.55	130.96	111.30
1	F	69	ARG	CB-CG-CD	8.54	130.95	111.30
1	E	190	MET	O-C-N	8.54	133.34	122.23
1	F	607	ALA	N-CA-C	-8.54	101.31	112.41
1	A	195	VAL	N-CA-CB	8.54	121.50	110.57
1	D	607	ALA	N-CA-C	-8.54	101.31	112.41
1	F	218	GLU	CG-CD-OE2	-8.54	98.76	118.40
1	A	607	ALA	N-CA-C	-8.54	101.31	112.41
1	F	190	MET	O-C-N	8.53	133.32	122.23
1	B	218	GLU	CG-CD-OE2	-8.53	98.78	118.40
1	D	190	MET	O-C-N	8.53	133.32	122.23
1	D	195	VAL	N-CA-CB	8.53	121.49	110.57
1	E	218	GLU	CG-CD-OE2	-8.53	98.78	118.40
1	A	190	MET	O-C-N	8.53	133.31	122.23
1	A	388	ASP	N-CA-CB	8.53	122.78	109.82
1	B	195	VAL	N-CA-CB	8.53	121.48	110.57
1	B	511	LYS	N-CA-CB	8.53	124.31	110.41
1	C	218	GLU	CG-CD-OE2	-8.53	98.79	118.40
1	F	179	GLN	N-CA-C	-8.53	92.64	110.80
1	F	556	SER	O-C-N	8.53	134.35	123.01
1	D	218	GLU	CG-CD-OE2	-8.52	98.80	118.40
1	B	190	MET	O-C-N	8.52	133.31	122.23
1	C	122	SER	CA-C-N	-8.52	109.82	120.56
1	C	122	SER	C-N-CA	-8.52	109.82	120.56
1	D	122	SER	CA-C-N	-8.52	109.82	120.56
1	D	122	SER	C-N-CA	-8.52	109.82	120.56
1	E	384	HIS	CA-C-O	-8.52	109.04	119.18
1	D	388	ASP	N-CA-CB	8.52	122.77	109.82
1	F	388	ASP	N-CA-CB	8.52	122.77	109.82
1	A	122	SER	CA-C-N	-8.52	109.83	120.56
1	A	122	SER	C-N-CA	-8.52	109.83	120.56
1	A	218	GLU	CG-CD-OE2	-8.52	98.81	118.40
1	B	213	LEU	O-C-N	8.52	133.06	123.01
1	C	384	HIS	CA-C-O	-8.52	109.04	119.18
1	E	179	GLN	N-CA-C	-8.52	92.66	110.80
1	E	430	GLN	CA-C-O	8.52	130.76	120.28
1	B	230	ARG	N-CA-CB	8.52	122.63	109.94
1	B	430	GLN	CA-C-O	8.52	130.75	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	607	ALA	N-CA-C	-8.52	101.34	112.41
1	C	64	ARG	NE-CZ-NH2	-8.52	111.54	119.20
1	D	511	LYS	N-CA-CB	8.52	124.29	110.41
1	F	430	GLN	CA-C-O	8.52	130.76	120.28
1	E	388	ASP	N-CA-CB	8.51	122.76	109.82
1	C	388	ASP	N-CA-CB	8.51	122.76	109.82
1	E	367	VAL	CA-C-O	8.51	129.92	120.64
1	F	384	HIS	CA-C-O	-8.51	109.05	119.18
1	A	179	GLN	N-CA-C	-8.51	92.67	110.80
1	B	388	ASP	N-CA-CB	8.51	122.75	109.82
1	C	190	MET	O-C-N	8.51	133.29	122.23
1	C	357	PRO	N-CD-CG	-8.51	90.44	103.20
1	C	556	SER	O-C-N	8.51	134.33	123.01
1	D	179	GLN	N-CA-C	-8.51	92.67	110.80
1	A	384	HIS	CA-C-O	-8.51	109.06	119.18
1	B	179	GLN	N-CA-C	-8.51	92.68	110.80
1	B	556	SER	O-C-N	8.51	134.33	123.01
1	F	122	SER	CA-C-N	-8.51	109.84	120.56
1	F	122	SER	C-N-CA	-8.51	109.84	120.56
1	A	230	ARG	N-CA-CB	8.51	122.61	109.94
1	C	57	MET	O-C-N	8.51	131.14	122.12
1	C	179	GLN	N-CA-C	-8.50	92.69	110.80
1	C	230	ARG	N-CA-CB	8.50	122.61	109.94
1	C	430	GLN	CA-C-O	8.50	130.74	120.28
1	D	384	HIS	CA-C-O	-8.50	109.06	119.18
1	C	511	LYS	N-CA-CB	8.50	124.27	110.41
1	D	492	THR	CA-C-O	8.50	132.66	120.51
1	D	556	SER	O-C-N	8.50	134.31	123.01
1	F	57	MET	O-C-N	8.50	131.13	122.12
1	A	511	LYS	N-CA-CB	8.50	124.26	110.41
1	C	213	LEU	O-C-N	8.50	133.04	123.01
1	F	511	LYS	N-CA-CB	8.50	124.26	110.41
1	B	433	LEU	N-CA-CB	-8.50	98.25	110.57
1	D	357	PRO	N-CD-CG	-8.50	90.45	103.20
1	D	43	THR	N-CA-CB	-8.49	96.14	110.49
1	D	591	LYS	N-CA-C	-8.49	103.06	113.50
1	E	357	PRO	N-CD-CG	-8.49	90.46	103.20
1	E	492	THR	CA-C-O	8.49	132.66	120.51
1	A	357	PRO	N-CD-CG	-8.49	90.46	103.20
1	D	312	THR	CA-CB-CG2	8.49	124.94	110.50
1	E	230	ARG	N-CA-CB	8.49	122.59	109.94
1	B	247	HIS	CA-C-N	-8.49	106.28	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	247	HIS	C-N-CA	-8.49	106.28	121.14
1	C	492	THR	CA-C-O	8.49	132.65	120.51
1	D	433	LEU	N-CA-CB	-8.49	98.26	110.57
1	E	57	MET	O-C-N	8.49	131.12	122.12
1	A	367	VAL	CA-C-O	8.49	129.89	120.64
1	A	430	GLN	CA-C-O	8.49	130.72	120.28
1	B	116	VAL	N-CA-CB	8.49	119.93	110.51
1	C	433	LEU	N-CA-CB	-8.49	98.27	110.57
1	D	430	GLN	CA-C-O	8.49	130.72	120.28
1	F	357	PRO	N-CD-CG	-8.49	90.47	103.20
1	F	433	LEU	N-CA-CB	-8.49	98.26	110.57
1	B	367	VAL	CA-C-O	8.48	129.89	120.64
1	A	64	ARG	NE-CZ-NH2	-8.48	111.56	119.20
1	B	492	THR	CA-C-O	8.48	132.64	120.51
1	D	390	ILE	CB-CA-C	-8.48	101.79	111.55
1	F	492	THR	CA-C-O	8.48	132.64	120.51
1	A	116	VAL	N-CA-CB	8.48	119.92	110.51
1	A	312	THR	CA-CB-CG2	8.48	124.92	110.50
1	A	556	SER	O-C-N	8.48	134.29	123.01
1	B	57	MET	O-C-N	8.48	131.11	122.12
1	D	57	MET	O-C-N	8.48	131.11	122.12
1	D	367	VAL	CA-C-O	8.48	129.88	120.64
1	F	247	HIS	CA-C-N	-8.48	106.30	121.14
1	F	247	HIS	C-N-CA	-8.48	106.30	121.14
1	A	433	LEU	N-CA-CB	-8.48	98.28	110.57
1	E	511	LYS	N-CA-CB	8.48	124.23	110.41
1	F	43	THR	N-CA-CB	-8.48	96.16	110.49
1	C	247	HIS	CA-C-N	-8.48	106.31	121.14
1	C	247	HIS	C-N-CA	-8.48	106.31	121.14
1	D	213	LEU	O-C-N	8.48	133.01	123.01
1	D	230	ARG	N-CA-CB	8.48	122.57	109.94
1	E	43	THR	N-CA-CB	-8.48	96.17	110.49
1	E	390	ILE	CB-CA-C	-8.48	101.80	111.55
1	E	483	CYS	N-CA-CB	-8.48	99.91	109.49
1	F	230	ARG	N-CA-CB	8.48	122.57	109.94
1	A	43	THR	N-CA-CB	-8.47	96.17	110.49
1	A	57	MET	O-C-N	8.47	131.10	122.12
1	C	312	THR	CA-CB-CG2	8.47	124.91	110.50
1	E	312	THR	CA-CB-CG2	8.47	124.90	110.50
1	E	433	LEU	N-CA-CB	-8.47	98.28	110.57
1	A	492	THR	CA-C-O	8.47	132.62	120.51
1	C	43	THR	N-CA-CB	-8.47	96.17	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	LEU	O-C-N	8.47	133.00	123.01
1	B	390	ILE	CB-CA-C	-8.47	101.81	111.55
1	C	427	ASP	N-CA-CB	-8.47	96.17	110.49
1	E	247	HIS	CA-C-N	-8.47	106.32	121.14
1	E	247	HIS	C-N-CA	-8.47	106.32	121.14
1	E	556	SER	O-C-N	8.47	134.28	123.01
1	F	312	THR	CA-CB-CG2	8.47	124.90	110.50
1	F	390	ILE	CB-CA-C	-8.47	101.81	111.55
1	E	64	ARG	NE-CZ-NH2	-8.47	111.58	119.20
1	B	312	THR	CA-CB-CG2	8.47	124.89	110.50
1	B	384	HIS	CA-C-O	-8.47	109.10	119.18
1	E	116	VAL	N-CA-CB	8.47	119.91	110.51
1	F	632	ASP	N-CA-CB	8.47	124.06	110.77
1	A	427	ASP	N-CA-CB	-8.47	96.18	110.49
1	C	632	ASP	CB-CG-OD2	8.46	137.87	118.40
1	E	427	ASP	N-CA-CB	-8.46	96.19	110.49
1	F	632	ASP	CB-CG-OD2	8.46	137.87	118.40
1	A	247	HIS	CA-C-N	-8.46	106.33	121.14
1	A	247	HIS	C-N-CA	-8.46	106.33	121.14
1	B	632	ASP	CB-CG-OD2	8.46	137.86	118.40
1	F	213	LEU	O-C-N	8.46	133.00	123.01
1	A	632	ASP	CB-CG-OD2	8.46	137.86	118.40
1	F	116	VAL	N-CA-CB	8.46	119.90	110.51
1	A	390	ILE	CB-CA-C	-8.46	101.82	111.55
1	A	591	LYS	N-CA-C	-8.46	103.10	113.50
1	B	43	THR	N-CA-CB	-8.46	96.20	110.49
1	B	273	ASP	CA-C-O	8.46	132.61	120.51
1	C	116	VAL	N-CA-CB	8.46	119.90	110.51
1	C	591	LYS	N-CA-C	-8.46	103.09	113.50
1	D	64	ARG	NE-CZ-NH2	-8.46	111.59	119.20
1	D	632	ASP	CB-CG-OD2	8.46	137.85	118.40
1	F	483	CYS	N-CA-CB	-8.46	99.93	109.49
1	F	591	LYS	N-CA-C	-8.46	103.10	113.50
1	B	427	ASP	N-CA-CB	-8.45	96.20	110.49
1	D	606	HIS	CB-CA-C	-8.46	94.04	110.10
1	F	427	ASP	N-CA-CB	-8.46	96.20	110.49
1	F	606	HIS	CB-CA-C	-8.46	94.03	110.10
1	B	64	ARG	NE-CZ-NH2	-8.45	111.59	119.20
1	E	194	HIS	N-CA-CB	8.45	122.53	109.94
1	E	213	LEU	O-C-N	8.45	132.98	123.01
1	E	632	ASP	CB-CG-OD2	8.45	137.84	118.40
1	F	218	GLU	OE1-CD-OE2	8.45	143.18	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	357	PRO	N-CD-CG	-8.45	90.53	103.20
1	C	632	ASP	N-CA-CB	8.45	124.03	110.77
1	F	367	VAL	CA-C-O	8.45	129.85	120.64
1	C	442	ASN	CB-CA-C	8.45	122.80	110.04
1	D	116	VAL	N-CA-CB	8.45	119.89	110.51
1	D	247	HIS	CA-C-N	-8.45	106.36	121.14
1	D	247	HIS	C-N-CA	-8.45	106.36	121.14
1	D	427	ASP	N-CA-CB	-8.45	96.22	110.49
1	E	591	LYS	N-CA-C	-8.45	103.11	113.50
1	A	606	HIS	CB-CA-C	-8.45	94.05	110.10
1	A	632	ASP	N-CA-CB	8.44	124.03	110.77
1	B	423	ILE	CB-CG1-CD1	-8.45	96.06	113.80
1	C	194	HIS	N-CA-CB	8.45	122.52	109.94
1	C	606	HIS	CB-CA-C	-8.44	94.06	110.10
1	F	64	ARG	NE-CZ-NH2	-8.45	111.60	119.20
1	A	483	CYS	N-CA-CB	-8.44	99.95	109.49
1	B	606	HIS	CB-CA-C	-8.44	94.06	110.10
1	D	194	HIS	N-CA-CB	8.44	122.52	109.94
1	E	437	VAL	CA-C-O	-8.44	110.76	121.48
1	F	194	HIS	N-CA-CB	8.44	122.52	109.94
1	E	177	ARG	N-CA-C	8.44	128.78	110.80
1	F	177	ARG	N-CA-C	8.44	128.78	110.80
1	E	273	ASP	CA-C-O	8.44	132.58	120.51
1	B	194	HIS	N-CA-CB	8.44	122.51	109.94
1	B	632	ASP	N-CA-CB	8.44	124.02	110.77
1	C	177	ARG	N-CA-C	8.44	128.77	110.80
1	D	177	ARG	N-CA-C	8.44	128.78	110.80
1	A	423	ILE	CB-CG1-CD1	-8.44	96.08	113.80
1	E	423	ILE	CB-CG1-CD1	-8.44	96.08	113.80
1	B	218	GLU	OE1-CD-OE2	8.44	143.14	122.90
1	E	497	GLU	N-CA-CB	8.44	123.36	110.28
1	E	606	HIS	CB-CA-C	-8.44	94.07	110.10
1	E	632	ASP	N-CA-CB	8.44	124.02	110.77
1	F	423	ILE	CB-CG1-CD1	-8.44	96.08	113.80
1	A	177	ARG	N-CA-C	8.43	128.76	110.80
1	B	591	LYS	N-CA-C	-8.43	103.13	113.50
1	C	437	VAL	CA-C-O	-8.43	110.77	121.48
1	D	483	CYS	N-CA-CB	-8.43	99.96	109.49
1	D	632	ASP	N-CA-CB	8.43	124.01	110.77
1	B	483	CYS	N-CA-CB	-8.43	99.97	109.49
1	C	390	ILE	CB-CA-C	-8.43	101.86	111.55
1	B	177	ARG	N-CA-C	8.43	128.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	423	ILE	CB-CG1-CD1	-8.43	96.10	113.80
1	A	194	HIS	N-CA-CB	8.43	122.49	109.94
1	C	483	CYS	N-CA-CB	-8.43	99.97	109.49
1	D	273	ASP	CA-C-O	8.43	132.56	120.51
1	F	437	VAL	CA-C-O	-8.43	110.78	121.48
1	F	442	ASN	CB-CA-C	8.43	122.76	110.04
1	F	546	ALA	N-CA-C	-8.43	101.06	112.94
1	A	218	GLU	OE1-CD-OE2	8.42	143.12	122.90
1	C	423	ILE	CB-CG1-CD1	-8.42	96.11	113.80
1	B	442	ASN	CB-CA-C	8.42	122.76	110.04
1	C	497	GLU	N-CA-CB	8.42	123.27	110.30
1	E	442	ASN	CB-CA-C	8.42	122.76	110.04
1	A	273	ASP	CA-C-O	8.42	132.55	120.51
1	C	367	VAL	CA-C-O	8.42	129.82	120.64
1	D	546	ALA	N-CA-C	-8.42	101.07	112.94
1	D	218	GLU	OE1-CD-OE2	8.42	143.10	122.90
1	D	437	VAL	CA-C-O	-8.42	110.79	121.48
1	E	218	GLU	OE1-CD-OE2	8.42	143.10	122.90
1	E	294	SER	CA-C-N	-8.42	109.00	120.28
1	E	294	SER	C-N-CA	-8.42	109.00	120.28
1	F	497	GLU	N-CA-CB	8.42	123.33	110.28
1	A	442	ASN	CB-CA-C	8.41	122.75	110.04
1	C	55	THR	CA-C-O	8.41	128.40	119.14
1	C	218	GLU	OE1-CD-OE2	8.41	143.10	122.90
1	C	273	ASP	CA-C-O	8.41	132.54	120.51
1	E	55	THR	CA-C-O	8.41	128.40	119.14
1	A	437	VAL	CA-C-O	-8.41	110.80	121.48
1	B	321	ILE	CA-C-O	-8.41	110.27	120.78
1	D	442	ASN	CB-CA-C	8.41	122.74	110.04
1	B	635	VAL	CB-CA-C	-8.41	101.34	111.94
1	E	175	LYS	CA-CB-CG	8.41	130.92	114.10
1	F	635	VAL	CA-C-O	-8.41	111.13	120.46
1	B	175	LYS	CA-CB-CG	8.41	130.91	114.10
1	B	546	ALA	N-CA-C	-8.41	101.08	112.94
1	B	294	SER	CA-C-N	-8.41	109.02	120.28
1	B	294	SER	C-N-CA	-8.41	109.02	120.28
1	D	434	ILE	CA-C-O	-8.41	111.72	120.71
1	A	294	SER	CA-C-N	-8.40	109.02	120.28
1	A	294	SER	C-N-CA	-8.40	109.02	120.28
1	D	296	ILE	CB-CG1-CD1	-8.40	96.15	113.80
1	D	497	GLU	N-CA-CB	8.40	123.31	110.28
1	A	497	GLU	N-CA-CB	8.40	123.30	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	296	ILE	CB-CG1-CD1	-8.40	96.16	113.80
1	F	55	THR	CA-C-O	8.40	128.38	119.14
1	B	635	VAL	CA-C-O	-8.40	111.14	120.46
1	C	321	ILE	CA-C-O	-8.40	110.28	120.78
1	C	490	GLY	CA-C-O	8.40	127.75	119.27
1	D	412	VAL	CA-C-O	-8.40	111.66	120.64
1	A	546	ALA	N-CA-C	-8.39	101.10	112.94
1	B	55	THR	CA-C-O	8.39	128.37	119.14
1	E	434	ILE	CA-C-O	-8.39	111.73	120.71
1	F	294	SER	CA-C-N	-8.39	109.03	120.28
1	F	294	SER	C-N-CA	-8.39	109.03	120.28
1	F	296	ILE	CB-CG1-CD1	-8.39	96.17	113.80
1	F	490	GLY	CA-C-O	8.39	127.75	119.27
1	F	635	VAL	CB-CA-C	-8.39	101.36	111.94
1	E	257	ALA	CA-C-O	-8.39	111.13	119.69
1	E	296	ILE	CB-CG1-CD1	-8.39	96.18	113.80
1	A	490	GLY	CA-C-O	8.39	127.74	119.27
1	B	235	ARG	NE-CZ-NH2	-8.39	111.65	119.20
1	D	235	ARG	NE-CZ-NH2	-8.39	111.65	119.20
1	D	294	SER	CA-C-N	-8.39	109.04	120.28
1	D	294	SER	C-N-CA	-8.39	109.04	120.28
1	E	177	ARG	CD-NE-CZ	-8.39	112.66	124.40
1	E	546	ALA	N-CA-C	-8.39	101.11	112.94
1	A	296	ILE	CB-CG1-CD1	-8.39	96.19	113.80
1	A	55	THR	CA-C-O	8.38	128.36	119.14
1	B	497	GLU	N-CA-CB	8.38	123.28	110.28
1	C	294	SER	CA-C-N	-8.38	109.05	120.28
1	C	294	SER	C-N-CA	-8.38	109.05	120.28
1	D	490	GLY	CA-C-O	8.38	127.74	119.27
1	A	175	LYS	CA-CB-CG	8.38	130.87	114.10
1	C	235	ARG	NE-CZ-NH2	-8.38	111.66	119.20
1	C	296	ILE	CB-CG1-CD1	-8.38	96.20	113.80
1	F	321	ILE	CA-C-O	-8.38	110.30	120.78
1	C	546	ALA	N-CA-C	-8.38	101.12	112.94
1	E	577	GLY	O-C-N	8.38	131.59	122.87
1	A	321	ILE	CA-C-O	-8.38	110.31	120.78
1	F	577	GLY	O-C-N	8.38	131.58	122.87
1	F	273	ASP	CA-C-O	8.38	132.49	120.51
1	C	175	LYS	CA-CB-CG	8.38	130.85	114.10
1	F	177	ARG	CD-NE-CZ	-8.37	112.68	124.40
1	A	412	VAL	CA-C-O	-8.37	111.68	120.64
1	B	177	ARG	CD-NE-CZ	-8.37	112.68	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	437	VAL	CA-C-O	-8.37	110.85	121.48
1	D	175	LYS	CA-CB-CG	8.37	130.85	114.10
1	D	177	ARG	CD-NE-CZ	-8.37	112.68	124.40
1	F	175	LYS	CA-CB-CG	8.37	130.84	114.10
1	D	55	THR	CA-C-O	8.37	128.35	119.14
1	E	321	ILE	CA-C-O	-8.37	110.32	120.78
1	E	412	VAL	CA-C-O	-8.37	111.69	120.64
1	B	490	GLY	CA-C-O	8.36	127.72	119.27
1	D	257	ALA	CA-C-O	-8.37	111.16	119.69
1	A	177	ARG	CD-NE-CZ	-8.36	112.69	124.40
1	D	321	ILE	CA-C-O	-8.36	110.33	120.78
1	A	235	ARG	NE-CZ-NH2	-8.36	111.67	119.20
1	A	434	ILE	CA-C-O	-8.36	111.76	120.71
1	B	577	GLY	O-C-N	8.36	131.57	122.87
1	C	434	ILE	CA-C-O	-8.36	111.76	120.71
1	F	405	ASN	O-C-N	8.36	131.06	122.03
1	F	434	ILE	CA-C-O	-8.36	111.77	120.71
1	A	577	GLY	O-C-N	8.36	131.56	122.87
1	C	484	PRO	O-C-N	8.36	133.92	122.64
1	E	490	GLY	CA-C-O	8.36	127.71	119.27
1	F	206	GLU	CB-CG-CD	-8.36	98.40	112.60
1	B	434	ILE	CA-C-O	-8.35	111.77	120.71
1	A	257	ALA	CA-C-O	-8.35	111.17	119.69
1	C	177	ARG	CD-NE-CZ	-8.35	112.71	124.40
1	E	235	ARG	NE-CZ-NH2	-8.35	111.68	119.20
1	E	623	GLY	CA-C-O	8.35	127.30	118.95
1	B	412	VAL	CA-C-O	-8.35	111.70	120.64
1	B	484	PRO	O-C-N	8.35	133.91	122.64
1	F	363	LEU	N-CA-C	-8.35	99.17	110.36
1	C	412	VAL	CA-C-O	-8.35	111.71	120.64
1	C	505	LEU	N-CA-CB	-8.35	99.49	110.59
1	F	153	LYS	O-C-N	8.35	132.54	122.27
1	F	484	PRO	O-C-N	8.35	133.91	122.64
1	B	623	GLY	CA-C-O	8.35	127.30	118.95
1	D	484	PRO	O-C-N	8.35	133.91	122.64
1	E	429	PHE	CA-C-N	-8.35	108.31	122.33
1	E	429	PHE	C-N-CA	-8.35	108.31	122.33
1	B	257	ALA	CA-C-O	-8.35	111.18	119.69
1	D	206	GLU	CB-CG-CD	-8.35	98.41	112.60
1	F	429	PHE	CA-C-N	-8.35	108.31	122.33
1	F	429	PHE	C-N-CA	-8.35	108.31	122.33
1	F	505	LEU	N-CA-CB	-8.34	99.49	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	ARG	NH1-CZ-NH2	8.34	130.14	119.30
1	C	253	ARG	NH1-CZ-NH2	8.34	130.14	119.30
1	C	577	GLY	O-C-N	8.34	131.54	122.87
1	F	235	ARG	NE-CZ-NH2	-8.34	111.69	119.20
1	A	206	GLU	CB-CG-CD	-8.34	98.43	112.60
1	F	412	VAL	CA-C-O	-8.34	111.72	120.64
1	B	505	LEU	N-CA-CB	-8.34	99.50	110.59
1	A	429	PHE	CA-C-N	-8.33	108.33	122.33
1	A	429	PHE	C-N-CA	-8.33	108.33	122.33
1	B	429	PHE	CA-C-N	-8.33	108.33	122.33
1	B	429	PHE	C-N-CA	-8.33	108.33	122.33
1	D	298	GLU	CG-CD-OE2	-8.33	99.24	118.40
1	D	429	PHE	CA-C-N	-8.33	108.33	122.33
1	D	429	PHE	C-N-CA	-8.33	108.33	122.33
1	D	577	GLY	O-C-N	8.33	131.53	122.87
1	E	206	GLU	CB-CG-CD	-8.33	98.44	112.60
1	E	253	ARG	NH1-CZ-NH2	8.33	130.13	119.30
1	F	253	ARG	NH1-CZ-NH2	8.33	130.13	119.30
1	A	484	PRO	O-C-N	8.33	133.88	122.64
1	A	505	LEU	N-CA-CB	-8.33	99.52	110.59
1	B	206	GLU	CB-CG-CD	-8.33	98.44	112.60
1	E	505	LEU	N-CA-CB	-8.33	99.51	110.59
1	B	298	GLU	CG-CD-OE2	-8.33	99.25	118.40
1	C	206	GLU	CB-CG-CD	-8.33	98.44	112.60
1	A	363	LEU	N-CA-C	-8.32	99.21	110.36
1	F	257	ALA	CA-C-O	-8.32	111.20	119.69
1	B	253	ARG	NH1-CZ-NH2	8.32	130.12	119.30
1	C	298	GLU	CG-CD-OE2	-8.32	99.26	118.40
1	C	429	PHE	CA-C-N	-8.32	108.35	122.33
1	C	429	PHE	C-N-CA	-8.32	108.35	122.33
1	A	153	LYS	O-C-N	8.32	132.50	122.27
1	A	298	GLU	CG-CD-OE2	-8.32	99.27	118.40
1	A	405	ASN	O-C-N	8.32	131.02	122.03
1	D	253	ARG	NH1-CZ-NH2	8.32	130.12	119.30
1	E	298	GLU	CG-CD-OE2	-8.32	99.26	118.40
1	C	153	LYS	O-C-N	8.32	132.50	122.27
1	C	405	ASN	O-C-N	8.32	131.01	122.03
1	C	363	LEU	N-CA-C	-8.32	99.22	110.36
1	A	623	GLY	CA-C-O	8.31	127.27	118.95
1	C	323	LEU	CA-C-O	-8.31	110.89	120.20
1	B	323	LEU	CA-C-O	-8.31	110.89	120.20
1	B	363	LEU	N-CA-C	-8.31	99.22	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	405	ASN	O-C-N	8.31	131.01	122.03
1	D	623	GLY	CA-C-O	8.31	127.26	118.95
1	E	363	LEU	N-CA-C	-8.31	99.22	110.36
1	F	298	GLU	CG-CD-OE2	-8.31	99.29	118.40
1	D	216	LYS	CA-C-N	-8.31	105.13	121.41
1	D	216	LYS	C-N-CA	-8.31	105.13	121.41
1	F	216	LYS	CA-C-N	-8.31	105.12	121.41
1	F	216	LYS	C-N-CA	-8.31	105.12	121.41
1	B	153	LYS	O-C-N	8.31	132.49	122.27
1	C	257	ALA	CA-C-O	-8.31	111.22	119.69
1	B	216	LYS	CA-C-N	-8.30	105.13	121.41
1	B	216	LYS	C-N-CA	-8.30	105.13	121.41
1	D	363	LEU	N-CA-C	-8.30	99.23	110.36
1	D	505	LEU	N-CA-CB	-8.30	99.55	110.59
1	E	405	ASN	O-C-N	8.30	130.99	122.03
1	A	216	LYS	CA-C-N	-8.29	105.15	121.41
1	A	216	LYS	C-N-CA	-8.29	105.15	121.41
1	B	250	ARG	NH1-CZ-NH2	8.29	130.08	119.30
1	C	75	PHE	N-CA-CB	8.29	123.48	110.46
1	C	216	LYS	CA-C-N	-8.29	105.15	121.41
1	C	216	LYS	C-N-CA	-8.29	105.15	121.41
1	D	405	ASN	O-C-N	8.29	130.99	122.03
1	E	484	PRO	O-C-N	8.29	133.84	122.64
1	D	250	ARG	NH1-CZ-NH2	8.29	130.08	119.30
1	D	471	ASP	O-C-N	8.29	130.91	122.12
1	D	645	VAL	N-CA-CB	-8.29	97.84	111.44
1	F	323	LEU	CA-C-O	-8.29	110.91	120.20
1	A	323	LEU	CA-C-O	-8.29	110.92	120.20
1	C	443	ILE	CB-CA-C	8.29	121.19	110.91
1	E	153	LYS	O-C-N	8.29	132.47	122.27
1	C	250	ARG	NH1-CZ-NH2	8.29	130.07	119.30
1	E	189	GLY	O-C-N	8.29	133.48	122.70
1	C	518	THR	CA-C-O	-8.29	110.36	120.89
1	D	545	ASN	CA-C-O	-8.29	108.66	120.51
1	E	645	VAL	N-CA-CB	-8.29	97.85	111.44
1	B	189	GLY	O-C-N	8.29	133.47	122.70
1	D	153	LYS	O-C-N	8.29	132.46	122.27
1	F	471	ASP	O-C-N	8.29	130.90	122.12
1	E	216	LYS	CA-C-N	-8.28	105.17	121.41
1	E	216	LYS	C-N-CA	-8.28	105.17	121.41
1	F	75	PHE	N-CA-CB	8.29	123.47	110.46
1	F	645	VAL	N-CA-CB	-8.28	97.85	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	75	PHE	N-CA-CB	8.28	123.46	110.46
1	F	518	THR	CA-C-O	-8.28	110.37	120.89
1	D	518	THR	CA-C-O	-8.28	110.37	120.89
1	B	645	VAL	N-CA-CB	-8.28	97.86	111.44
1	C	545	ASN	CA-C-O	-8.28	108.67	120.51
1	E	323	LEU	CA-C-O	-8.28	110.93	120.20
1	F	623	GLY	CA-C-O	8.28	127.23	118.95
1	C	645	VAL	N-CA-CB	-8.28	97.87	111.44
1	B	471	ASP	O-C-N	8.28	130.89	122.12
1	D	472	GLY	O-C-N	8.28	133.46	122.70
1	A	250	ARG	NH1-CZ-NH2	8.27	130.05	119.30
1	C	471	ASP	O-C-N	8.27	130.89	122.12
1	E	518	THR	CA-C-O	-8.27	110.38	120.89
1	A	75	PHE	N-CA-CB	8.27	123.44	110.46
1	D	316	ARG	CB-CG-CD	8.27	130.32	111.30
1	D	323	LEU	CA-C-O	-8.27	110.94	120.20
1	F	189	GLY	O-C-N	8.27	133.45	122.70
1	A	645	VAL	N-CA-CB	-8.27	97.88	111.44
1	C	426	PHE	CA-C-N	8.27	137.33	121.54
1	C	426	PHE	C-N-CA	8.27	137.33	121.54
1	A	189	GLY	O-C-N	8.27	133.44	122.70
1	C	370	HIS	CA-CB-CG	8.26	122.06	113.80
1	A	426	PHE	CA-C-N	8.26	137.31	121.54
1	A	426	PHE	C-N-CA	8.26	137.31	121.54
1	A	545	ASN	CA-C-O	-8.26	108.70	120.51
1	D	189	GLY	O-C-N	8.26	133.44	122.70
1	D	426	PHE	CA-C-N	8.26	137.31	121.54
1	D	426	PHE	C-N-CA	8.26	137.31	121.54
1	B	426	PHE	CA-C-N	8.26	137.31	121.54
1	B	426	PHE	C-N-CA	8.26	137.31	121.54
1	C	316	ARG	CB-CG-CD	8.26	130.29	111.30
1	D	370	HIS	CA-CB-CG	8.26	122.06	113.80
1	E	471	ASP	O-C-N	8.26	130.87	122.12
1	A	518	THR	CA-C-O	-8.26	110.41	120.89
1	B	75	PHE	N-CA-CB	8.26	123.42	110.46
1	B	443	ILE	CB-CA-C	8.26	121.15	110.91
1	C	199	MET	N-CA-C	-8.26	93.22	110.80
1	C	623	GLY	CA-C-O	8.26	127.20	118.95
1	E	75	PHE	N-CA-CB	8.26	123.42	110.46
1	E	370	HIS	CA-CB-CG	8.26	122.06	113.80
1	F	453	HIS	N-CA-CB	-8.26	96.75	110.37
1	A	316	ARG	CB-CG-CD	8.25	130.28	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250	ARG	N-CA-C	8.25	121.57	109.69
1	C	250	ARG	N-CA-C	8.25	121.57	109.69
1	E	374	ALA	O-C-N	8.25	133.39	122.33
1	E	545	ASN	CA-C-O	-8.25	108.71	120.51
1	D	374	ALA	O-C-N	8.25	133.39	122.33
1	E	308	SER	CA-C-O	-8.25	110.78	120.10
1	F	316	ARG	CB-CG-CD	8.25	130.28	111.30
1	F	426	PHE	CA-C-N	8.25	137.30	121.54
1	F	426	PHE	C-N-CA	8.25	137.30	121.54
1	F	545	ASN	CA-C-O	-8.25	108.71	120.51
1	C	155	TYR	CA-C-O	-8.25	110.48	119.97
1	B	316	ARG	CB-CG-CD	8.25	130.27	111.30
1	C	588	ASP	N-CA-C	8.25	123.49	107.98
1	E	250	ARG	N-CA-C	8.25	121.57	109.69
1	E	316	ARG	CB-CG-CD	8.25	130.28	111.30
1	E	426	PHE	CA-C-N	8.25	137.29	121.54
1	E	426	PHE	C-N-CA	8.25	137.29	121.54
1	B	576	GLU	CA-CB-CG	-8.25	97.60	114.10
1	F	199	MET	N-CA-C	-8.25	93.23	110.80
1	F	443	ILE	CB-CA-C	8.25	121.14	110.91
1	C	374	ALA	O-C-N	8.24	133.38	122.33
1	C	472	GLY	O-C-N	8.24	133.42	122.70
1	C	189	GLY	O-C-N	8.24	133.41	122.70
1	F	405	ASN	CA-C-O	-8.24	112.41	120.90
1	A	443	ILE	CB-CA-C	8.24	121.13	110.91
1	B	370	HIS	CA-CB-CG	8.24	122.04	113.80
1	D	443	ILE	CB-CA-C	8.24	121.13	110.91
1	E	250	ARG	NH1-CZ-NH2	8.24	130.01	119.30
1	E	576	GLU	CA-CB-CG	-8.24	97.62	114.10
1	A	471	ASP	O-C-N	8.24	130.85	122.12
1	A	199	MET	N-CA-C	-8.24	93.26	110.80
1	B	199	MET	N-CA-C	-8.24	93.26	110.80
1	B	545	ASN	CA-C-O	-8.24	108.73	120.51
1	B	588	ASP	N-CA-C	8.24	123.47	107.98
1	D	250	ARG	N-CA-C	8.24	121.55	109.69
1	E	268	PHE	O-C-N	-8.24	114.63	121.38
1	F	250	ARG	NH1-CZ-NH2	8.24	130.01	119.30
1	B	268	PHE	O-C-N	-8.23	114.63	121.38
1	A	250	ARG	N-CA-C	8.23	121.55	109.69
1	B	453	HIS	N-CA-CB	-8.23	96.78	110.37
1	B	518	THR	CA-C-O	-8.23	110.43	120.89
1	C	453	HIS	N-CA-CB	-8.23	96.78	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	453	HIS	N-CA-CB	-8.23	96.78	110.37
1	E	199	MET	N-CA-C	-8.23	93.26	110.80
1	A	453	HIS	N-CA-CB	-8.23	96.79	110.37
1	A	472	GLY	O-C-N	8.23	133.40	122.70
1	A	576	GLU	CA-CB-CG	-8.23	97.64	114.10
1	C	576	GLU	CA-CB-CG	-8.23	97.64	114.10
1	E	155	TYR	CA-C-O	-8.23	110.51	119.97
1	F	370	HIS	CA-CB-CG	8.23	122.03	113.80
1	F	472	GLY	O-C-N	8.23	133.40	122.70
1	F	566	ASP	CA-C-N	-8.23	108.43	120.28
1	F	566	ASP	C-N-CA	-8.23	108.43	120.28
1	A	370	HIS	CA-CB-CG	8.23	122.03	113.80
1	A	588	ASP	N-CA-C	8.23	123.45	107.98
1	B	554	ASP	CB-CA-C	8.23	125.17	111.51
1	C	250	ARG	CD-NE-CZ	8.23	135.92	124.40
1	D	199	MET	N-CA-C	-8.23	93.28	110.80
1	D	576	GLU	CA-CB-CG	-8.23	97.64	114.10
1	C	405	ASN	CA-C-O	-8.22	112.43	120.90
1	D	123	VAL	O-C-N	-8.22	113.85	121.91
1	E	443	ILE	CB-CA-C	8.22	121.11	110.91
1	E	566	ASP	CA-C-N	-8.22	108.44	120.28
1	E	566	ASP	C-N-CA	-8.22	108.44	120.28
1	E	588	ASP	N-CA-C	8.22	123.44	107.98
1	F	576	GLU	CA-CB-CG	-8.22	97.65	114.10
1	F	588	ASP	N-CA-C	8.22	123.44	107.98
1	A	374	ALA	O-C-N	8.22	133.35	122.33
1	B	308	SER	CA-C-O	-8.22	110.81	120.10
1	E	453	HIS	N-CA-CB	-8.22	96.80	110.37
1	C	554	ASP	CB-CA-C	8.22	125.15	111.51
1	D	554	ASP	CB-CA-C	8.22	125.15	111.51
1	F	123	VAL	O-C-N	-8.22	113.86	121.91
1	F	250	ARG	N-CA-C	8.22	121.52	109.69
1	F	554	ASP	CB-CA-C	8.22	125.15	111.51
1	A	453	HIS	CA-C-N	-8.22	109.01	122.81
1	A	453	HIS	C-N-CA	-8.22	109.01	122.81
1	A	554	ASP	CB-CA-C	8.21	125.15	111.51
1	B	453	HIS	CA-C-N	-8.22	109.01	122.81
1	B	453	HIS	C-N-CA	-8.22	109.01	122.81
1	C	123	VAL	O-C-N	-8.22	113.86	121.91
1	D	588	ASP	N-CA-C	8.22	123.42	107.98
1	F	268	PHE	O-C-N	-8.21	114.64	121.38
1	A	566	ASP	CA-C-N	-8.21	108.45	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	SER	CA-C-O	-8.21	110.82	120.10
1	A	405	ASN	CA-C-O	-8.21	112.44	120.90
1	A	566	ASP	C-N-CA	-8.21	108.45	120.28
1	B	472	GLY	O-C-N	8.21	133.37	122.70
1	C	453	HIS	CA-C-N	-8.21	109.02	122.81
1	C	453	HIS	C-N-CA	-8.21	109.02	122.81
1	D	250	ARG	CD-NE-CZ	8.21	135.90	124.40
1	D	268	PHE	O-C-N	-8.21	114.65	121.38
1	D	566	ASP	CA-C-N	-8.21	108.45	120.28
1	D	566	ASP	C-N-CA	-8.21	108.45	120.28
1	E	453	HIS	CA-C-N	-8.21	109.02	122.81
1	E	453	HIS	C-N-CA	-8.21	109.02	122.81
1	D	141	THR	CA-C-N	8.21	128.41	119.87
1	D	141	THR	C-N-CA	8.21	128.41	119.87
1	D	453	HIS	CA-C-N	-8.21	109.02	122.81
1	D	453	HIS	C-N-CA	-8.21	109.02	122.81
1	F	374	ALA	O-C-N	8.21	133.33	122.33
1	F	453	HIS	CA-C-N	-8.21	109.02	122.81
1	F	453	HIS	C-N-CA	-8.21	109.02	122.81
1	B	123	VAL	O-C-N	-8.21	113.87	121.91
1	B	374	ALA	O-C-N	8.20	133.32	122.33
1	B	405	ASN	CA-C-O	-8.20	112.45	120.90
1	B	566	ASP	CA-C-N	-8.21	108.47	120.28
1	B	566	ASP	C-N-CA	-8.21	108.47	120.28
1	C	308	SER	CA-C-O	-8.21	110.83	120.10
1	A	250	ARG	CD-NE-CZ	8.20	135.88	124.40
1	A	268	PHE	O-C-N	-8.20	114.65	121.38
1	D	155	TYR	CA-C-O	-8.20	110.54	119.97
1	B	250	ARG	CD-NE-CZ	8.20	135.88	124.40
1	D	266	GLY	N-CA-C	-8.20	102.20	111.63
1	D	308	SER	CA-C-O	-8.20	110.83	120.10
1	F	155	TYR	CA-C-O	-8.20	110.54	119.97
1	A	155	TYR	CA-C-O	-8.20	110.54	119.97
1	C	268	PHE	O-C-N	-8.20	114.66	121.38
1	E	266	GLY	N-CA-C	-8.20	102.20	111.63
1	E	472	GLY	O-C-N	8.20	133.35	122.70
1	B	452	VAL	CB-CA-C	-8.19	99.10	110.90
1	C	219	LEU	N-CA-C	-8.19	102.31	111.07
1	F	452	VAL	CB-CA-C	-8.19	99.10	110.90
1	B	155	TYR	CA-C-O	-8.19	110.55	119.97
1	C	452	VAL	CB-CA-C	-8.19	99.11	110.90
1	D	51	ALA	N-CA-CB	-8.19	97.59	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	266	GLY	N-CA-C	-8.19	102.22	111.63
1	B	297	HIS	ND1-CE1-NE2	8.19	116.58	108.40
1	D	452	VAL	CB-CA-C	-8.19	99.11	110.90
1	F	308	SER	CA-C-O	-8.19	110.85	120.10
1	F	51	ALA	N-CA-CB	-8.19	97.59	110.28
1	A	51	ALA	N-CA-CB	-8.18	97.60	110.28
1	E	452	VAL	CB-CA-C	-8.18	99.11	110.90
1	F	250	ARG	CD-NE-CZ	8.18	135.86	124.40
1	A	452	VAL	CB-CA-C	-8.18	99.12	110.90
1	C	266	GLY	N-CA-C	-8.18	102.22	111.63
1	C	566	ASP	CA-C-N	-8.18	108.50	120.28
1	C	566	ASP	C-N-CA	-8.18	108.50	120.28
1	E	297	HIS	ND1-CE1-NE2	8.18	116.58	108.40
1	E	554	ASP	CB-CA-C	8.18	125.09	111.51
1	A	123	VAL	O-C-N	-8.18	113.90	121.91
1	D	297	HIS	ND1-CE1-NE2	8.18	116.58	108.40
1	A	266	GLY	N-CA-C	-8.17	102.23	111.63
1	E	250	ARG	CD-NE-CZ	8.17	135.84	124.40
1	A	297	HIS	ND1-CE1-NE2	8.17	116.57	108.40
1	C	345	ASN	CB-CG-ND2	-8.17	104.15	116.40
1	E	219	LEU	N-CA-C	-8.17	102.33	111.07
1	A	141	THR	CA-C-N	8.16	128.36	119.87
1	A	141	THR	C-N-CA	8.16	128.36	119.87
1	C	141	THR	CA-C-N	8.16	128.36	119.87
1	C	141	THR	C-N-CA	8.16	128.36	119.87
1	C	51	ALA	N-CA-CB	-8.16	97.63	110.28
1	C	582	LEU	CB-CA-C	8.16	123.21	109.75
1	A	582	LEU	CB-CA-C	8.16	123.21	109.75
1	E	51	ALA	N-CA-CB	-8.16	97.64	110.28
1	E	582	LEU	CB-CA-C	8.16	123.21	109.75
1	D	405	ASN	CA-C-O	-8.15	112.50	120.90
1	F	141	THR	CA-C-N	8.15	128.35	119.87
1	F	141	THR	C-N-CA	8.15	128.35	119.87
1	E	405	ASN	CA-C-O	-8.15	112.50	120.90
1	B	141	THR	CA-C-N	8.15	128.35	119.87
1	B	141	THR	C-N-CA	8.15	128.35	119.87
1	B	219	LEU	N-CA-C	-8.15	102.35	111.07
1	B	345	ASN	CB-CG-ND2	-8.15	104.17	116.40
1	D	345	ASN	CB-CG-ND2	-8.15	104.17	116.40
1	D	582	LEU	CB-CA-C	8.15	123.20	109.75
1	A	219	LEU	N-CA-C	-8.15	102.35	111.07
1	E	123	VAL	O-C-N	-8.14	113.93	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	345	ASN	CB-CG-ND2	-8.14	104.18	116.40
1	A	345	ASN	CB-CG-ND2	-8.14	104.19	116.40
1	B	51	ALA	N-CA-CB	-8.14	97.66	110.28
1	B	582	LEU	CB-CA-C	8.14	123.18	109.75
1	E	345	ASN	CB-CG-ND2	-8.13	104.20	116.40
1	F	297	HIS	ND1-CE1-NE2	8.13	116.53	108.40
1	E	132	ILE	CA-C-O	-8.13	113.21	121.59
1	C	297	HIS	ND1-CE1-NE2	8.13	116.53	108.40
1	E	316	ARG	NE-CZ-NH1	8.13	129.63	121.50
1	F	422	LEU	CA-C-N	-8.13	110.96	122.75
1	F	422	LEU	C-N-CA	-8.13	110.96	122.75
1	F	266	GLY	N-CA-C	-8.13	102.28	111.63
1	F	582	LEU	CB-CA-C	8.13	123.16	109.75
1	E	141	THR	CA-C-N	8.12	128.32	119.87
1	E	141	THR	C-N-CA	8.12	128.32	119.87
1	E	422	LEU	CA-C-N	-8.12	110.97	122.75
1	E	422	LEU	C-N-CA	-8.12	110.97	122.75
1	F	316	ARG	NE-CZ-NH1	8.12	129.62	121.50
1	C	132	ILE	CA-C-O	-8.12	113.22	121.59
1	D	219	LEU	N-CA-C	-8.12	102.38	111.07
1	F	497	GLU	CA-C-N	-8.12	109.90	122.49
1	F	497	GLU	C-N-CA	-8.12	109.90	122.49
1	E	427	ASP	CB-CG-OD2	8.12	137.08	118.40
1	A	427	ASP	CB-CG-OD2	8.12	137.08	118.40
1	A	422	LEU	CA-C-N	-8.12	110.98	122.75
1	A	422	LEU	C-N-CA	-8.12	110.98	122.75
1	B	316	ARG	NE-CZ-NH1	8.12	129.62	121.50
1	C	18	LEU	CA-C-O	-8.12	108.92	119.80
1	C	427	ASP	CB-CG-OD2	8.12	137.07	118.40
1	D	497	GLU	CA-C-N	-8.12	109.91	122.49
1	D	497	GLU	C-N-CA	-8.12	109.91	122.49
1	A	132	ILE	CA-C-O	-8.11	113.23	121.59
1	A	497	GLU	CA-C-N	-8.11	109.91	122.49
1	A	497	GLU	C-N-CA	-8.11	109.91	122.49
1	C	316	ARG	NE-CZ-NH1	8.11	129.61	121.50
1	B	422	LEU	CA-C-N	-8.11	110.99	122.75
1	B	422	LEU	C-N-CA	-8.11	110.99	122.75
1	F	427	ASP	CB-CG-OD2	8.11	137.06	118.40
1	C	391	PHE	CA-CB-CG	8.11	121.91	113.80
1	D	427	ASP	CB-CG-OD2	8.11	137.06	118.40
1	A	316	ARG	NE-CZ-NH1	8.11	129.61	121.50
1	B	18	LEU	CA-C-O	-8.11	108.93	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	220	PHE	CA-CB-CG	8.11	121.91	113.80
1	C	465	THR	CA-C-O	-8.11	111.38	120.54
1	D	18	LEU	CA-C-O	-8.10	108.94	119.80
1	F	391	PHE	CA-CB-CG	8.10	121.90	113.80
1	E	18	LEU	CA-C-O	-8.10	108.95	119.80
1	E	220	PHE	CA-CB-CG	8.10	121.90	113.80
1	C	422	LEU	CA-C-N	-8.10	111.01	122.75
1	C	422	LEU	C-N-CA	-8.10	111.01	122.75
1	E	497	GLU	CA-C-N	-8.10	109.94	122.49
1	E	497	GLU	C-N-CA	-8.10	109.94	122.49
1	F	219	LEU	N-CA-C	-8.10	102.41	111.07
1	B	427	ASP	CB-CG-OD2	8.10	137.02	118.40
1	B	497	GLU	CA-C-N	-8.10	109.94	122.49
1	B	497	GLU	C-N-CA	-8.10	109.94	122.49
1	C	497	GLU	CA-C-N	-8.10	109.94	122.49
1	C	497	GLU	C-N-CA	-8.10	109.94	122.49
1	A	18	LEU	CA-C-O	-8.09	108.95	119.80
1	A	220	PHE	CA-CB-CG	8.09	121.89	113.80
1	B	132	ILE	CA-C-O	-8.09	113.26	121.59
1	B	465	THR	CA-C-O	-8.09	111.40	120.54
1	D	162	LYS	N-CA-C	-8.09	96.46	109.40
1	D	465	THR	CA-C-O	-8.09	111.40	120.54
1	D	422	LEU	CA-C-N	-8.09	111.03	122.75
1	D	422	LEU	C-N-CA	-8.09	111.03	122.75
1	D	316	ARG	NE-CZ-NH1	8.08	129.58	121.50
1	E	218	GLU	CB-CA-C	-8.08	97.11	110.85
1	F	18	LEU	CA-C-O	-8.08	108.97	119.80
1	F	465	THR	CA-C-O	-8.08	111.41	120.54
1	B	391	PHE	CA-CB-CG	8.08	121.88	113.80
1	B	220	PHE	CA-CB-CG	8.08	121.88	113.80
1	D	220	PHE	CA-CB-CG	8.08	121.88	113.80
1	A	465	THR	CA-C-O	-8.08	111.42	120.54
1	E	455	LEU	O-C-N	8.08	132.20	122.75
1	F	218	GLU	CB-CA-C	-8.08	97.12	110.85
1	F	511	LYS	CA-C-O	8.08	131.05	121.36
1	A	162	LYS	N-CA-C	-8.07	96.48	109.40
1	C	162	LYS	N-CA-C	-8.07	96.48	109.40
1	A	511	LYS	CA-C-O	8.07	131.04	121.36
1	B	550	GLY	CA-C-O	-8.07	106.53	120.57
1	E	465	THR	CA-C-O	-8.07	111.42	120.54
1	D	391	PHE	CA-CB-CG	8.07	121.87	113.80
1	F	132	ILE	CA-C-O	-8.07	113.28	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	391	PHE	CA-CB-CG	8.07	121.87	113.80
1	C	347	ALA	CA-C-O	-8.07	110.99	120.10
1	C	413	VAL	CA-CB-CG2	-8.07	96.69	110.40
1	C	524	LYS	CA-C-O	-8.07	112.39	120.70
1	D	454	ARG	CB-CA-C	8.07	125.31	109.66
1	C	126	SER	N-CA-CB	8.06	121.83	109.97
1	E	162	LYS	N-CA-C	-8.06	96.50	109.40
1	A	550	GLY	CA-C-O	-8.06	106.55	120.57
1	B	511	LYS	CA-C-O	8.06	131.03	121.36
1	D	132	ILE	CA-C-O	-8.06	113.29	121.59
1	E	511	LYS	CA-C-O	8.05	131.03	121.36
1	B	162	LYS	N-CA-C	-8.05	96.52	109.40
1	C	43	THR	N-CA-C	-8.05	93.65	110.80
1	E	391	PHE	CA-CB-CG	8.05	121.85	113.80
1	B	281	ASP	CA-CB-CG	8.05	120.65	112.60
1	B	413	VAL	CA-CB-CG2	-8.05	96.71	110.40
1	B	454	ARG	CB-CA-C	8.05	125.28	109.66
1	C	454	ARG	CB-CA-C	8.05	125.28	109.66
1	C	511	LYS	CA-C-O	8.05	131.02	121.36
1	E	126	SER	N-CA-CB	8.05	121.81	109.97
1	F	126	SER	N-CA-CB	8.05	121.81	109.97
1	F	550	GLY	CA-C-O	-8.05	106.56	120.57
1	A	218	GLU	CB-CA-C	-8.05	97.17	110.85
1	A	454	ARG	CB-CA-C	8.05	125.28	109.66
1	B	126	SER	N-CA-CB	8.05	121.80	109.97
1	C	218	GLU	CB-CA-C	-8.05	97.17	110.85
1	D	511	LYS	CA-C-O	8.05	131.02	121.36
1	D	550	GLY	CA-C-O	-8.05	106.56	120.57
1	E	281	ASP	CA-CB-CG	8.05	120.65	112.60
1	F	162	LYS	N-CA-C	-8.05	96.52	109.40
1	A	413	VAL	CA-CB-CG2	-8.05	96.72	110.40
1	C	281	ASP	CA-CB-CG	8.05	120.65	112.60
1	E	454	ARG	CB-CA-C	8.05	125.27	109.66
1	F	413	VAL	CA-CB-CG2	-8.05	96.72	110.40
1	B	251	ILE	N-CA-C	-8.05	101.28	110.05
1	C	455	LEU	O-C-N	8.05	132.16	122.75
1	A	126	SER	N-CA-CB	8.04	121.80	109.97
1	C	251	ILE	N-CA-C	-8.04	101.28	110.05
1	C	568	MET	CG-SD-CE	8.04	118.60	100.90
1	E	251	ILE	N-CA-C	-8.04	101.28	110.05
1	A	281	ASP	CA-CB-CG	8.04	120.64	112.60
1	C	550	GLY	CA-C-O	-8.04	106.58	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	568	MET	CG-SD-CE	8.04	118.59	100.90
1	F	220	PHE	CA-CB-CG	8.04	121.84	113.80
1	A	635	VAL	CB-CA-C	-8.04	101.39	111.92
1	C	145	PHE	CA-CB-CG	8.04	121.84	113.80
1	D	43	THR	N-CA-C	-8.04	93.68	110.80
1	B	218	GLU	CB-CA-C	-8.04	97.19	110.85
1	D	413	VAL	CA-CB-CG2	-8.04	96.74	110.40
1	E	550	GLY	CA-C-O	-8.04	106.58	120.57
1	F	455	LEU	O-C-N	8.04	132.15	122.75
1	A	568	MET	CG-SD-CE	8.04	118.58	100.90
1	A	251	ILE	N-CA-C	-8.03	101.29	110.05
1	B	455	LEU	O-C-N	8.04	132.15	122.75
1	B	568	MET	CG-SD-CE	8.04	118.58	100.90
1	E	413	VAL	CA-CB-CG2	-8.03	96.74	110.40
1	A	43	THR	N-CA-C	-8.03	93.69	110.80
1	D	218	GLU	CB-CA-C	-8.03	97.19	110.85
1	B	43	THR	N-CA-C	-8.03	93.69	110.80
1	C	215	ARG	N-CA-CB	-8.03	99.89	111.54
1	E	84	LEU	CB-CA-C	8.03	125.37	110.11
1	A	455	LEU	O-C-N	8.03	132.15	122.75
1	B	458	ASN	CA-C-O	-8.03	112.03	120.70
1	E	43	THR	N-CA-C	-8.03	93.70	110.80
1	D	215	ARG	N-CA-CB	-8.03	99.90	111.54
1	D	458	ASN	CA-C-O	-8.03	112.03	120.70
1	E	492	THR	CA-C-N	8.03	138.63	121.45
1	E	492	THR	C-N-CA	8.03	138.63	121.45
1	F	281	ASP	CA-CB-CG	8.03	120.63	112.60
1	C	635	VAL	CB-CA-C	-8.03	101.41	111.92
1	D	369	GLU	O-C-N	8.03	133.83	121.63
1	D	455	LEU	O-C-N	8.03	132.14	122.75
1	E	206	GLU	CG-CD-OE2	-8.03	99.94	118.40
1	F	454	ARG	CB-CA-C	8.03	125.23	109.66
1	E	568	MET	CG-SD-CE	8.03	118.56	100.90
1	F	568	MET	CG-SD-CE	8.03	118.55	100.90
1	A	206	GLU	CG-CD-OE2	-8.02	99.95	118.40
1	A	215	ARG	N-CA-CB	-8.02	99.91	111.54
1	B	347	ALA	CA-C-O	-8.02	111.03	120.10
1	D	126	SER	N-CA-CB	8.02	121.76	109.97
1	D	240	LEU	O-C-N	-8.02	113.53	122.84
1	E	215	ARG	N-CA-CB	-8.02	99.91	111.54
1	E	458	ASN	CA-C-O	-8.02	112.03	120.70
1	D	439	SER	O-C-N	8.02	132.66	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	492	THR	CA-C-N	8.02	138.62	121.45
1	D	492	THR	C-N-CA	8.02	138.62	121.45
1	F	206	GLU	CG-CD-OE2	-8.02	99.95	118.40
1	A	347	ALA	CA-C-O	-8.02	111.04	120.10
1	B	100	ARG	NE-CZ-NH1	8.02	129.52	121.50
1	C	206	GLU	CG-CD-OE2	-8.02	99.96	118.40
1	D	251	ILE	N-CA-C	-8.02	101.31	110.05
1	D	281	ASP	CA-CB-CG	8.02	120.62	112.60
1	E	347	ALA	CA-C-O	-8.02	111.04	120.10
1	F	193	HIS	CE1-NE2-CD2	-8.02	100.98	109.00
1	A	458	ASN	CA-C-O	-8.02	112.04	120.70
1	A	84	LEU	CB-CA-C	8.02	125.34	110.11
1	B	215	ARG	N-CA-CB	-8.02	99.92	111.54
1	B	439	SER	O-C-N	8.02	132.65	123.27
1	F	84	LEU	CB-CA-C	8.02	125.34	110.11
1	C	236	LEU	CB-CA-C	-8.02	98.24	110.90
1	C	635	VAL	CA-C-O	-8.02	111.05	120.83
1	F	251	ILE	N-CA-C	-8.02	101.31	110.05
1	F	651	HIS	O-C-N	8.02	133.23	123.13
1	A	560	ARG	CA-C-O	8.01	131.97	120.51
1	B	145	PHE	CA-CB-CG	8.01	121.81	113.80
1	B	206	GLU	CG-CD-OE2	-8.01	99.97	118.40
1	C	100	ARG	NE-CZ-NH1	8.01	129.51	121.50
1	F	458	ASN	CA-C-O	-8.01	112.05	120.70
1	C	369	GLU	O-C-N	8.01	133.81	121.63
1	D	84	LEU	CB-CA-C	8.01	125.33	110.11
1	E	145	PHE	CA-CB-CG	8.01	121.81	113.80
1	E	193	HIS	CE1-NE2-CD2	-8.01	100.99	109.00
1	F	43	THR	N-CA-C	-8.01	93.73	110.80
1	B	84	LEU	CB-CA-C	8.01	125.33	110.11
1	D	236	LEU	CB-CA-C	-8.01	98.24	110.90
1	E	635	VAL	CA-C-O	-8.01	111.06	120.83
1	B	193	HIS	CE1-NE2-CD2	-8.01	100.99	109.00
1	D	347	ALA	CA-C-O	-8.01	111.05	120.10
1	D	635	VAL	CB-CA-C	-8.01	101.43	111.92
1	A	236	LEU	CB-CA-C	-8.01	98.25	110.90
1	B	492	THR	CA-C-N	8.01	138.58	121.45
1	B	492	THR	C-N-CA	8.01	138.58	121.45
1	C	193	HIS	CE1-NE2-CD2	-8.01	100.99	109.00
1	C	492	THR	CA-C-N	8.01	138.58	121.45
1	C	492	THR	C-N-CA	8.01	138.58	121.45
1	D	206	GLU	CG-CD-OE2	-8.01	99.98	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	3	LEU	N-CA-CB	8.01	124.08	111.91
1	E	560	ARG	CA-C-O	8.01	131.96	120.51
1	F	492	THR	CA-C-N	8.01	138.59	121.45
1	F	492	THR	C-N-CA	8.01	138.59	121.45
1	A	145	PHE	CA-CB-CG	8.00	121.80	113.80
1	C	560	ARG	CA-C-O	8.00	131.95	120.51
1	E	635	VAL	CB-CA-C	-8.00	101.44	111.92
1	F	3	LEU	N-CA-CB	8.00	124.07	111.91
1	F	15	ASN	OD1-CG-ND2	8.00	130.60	122.60
1	A	193	HIS	CE1-NE2-CD2	-8.00	101.00	109.00
1	D	100	ARG	NE-CZ-NH1	8.00	129.50	121.50
1	A	492	THR	CA-C-N	8.00	138.56	121.45
1	A	492	THR	C-N-CA	8.00	138.56	121.45
1	B	560	ARG	CA-C-O	8.00	131.94	120.51
1	D	145	PHE	CA-CB-CG	8.00	121.80	113.80
1	D	193	HIS	CE1-NE2-CD2	-8.00	101.00	109.00
1	F	215	ARG	N-CA-CB	-8.00	99.94	111.54
1	B	369	GLU	O-C-N	7.99	133.78	121.63
1	F	236	LEU	CB-CA-C	-7.99	98.27	110.90
1	B	236	LEU	CB-CA-C	-7.99	98.27	110.90
1	A	3	LEU	N-CA-CB	7.99	124.06	111.91
1	C	84	LEU	CB-CA-C	7.99	125.29	110.11
1	B	38	ASN	OD1-CG-ND2	7.99	130.59	122.60
1	F	145	PHE	CA-CB-CG	7.99	121.79	113.80
1	A	100	ARG	NE-CZ-NH1	7.99	129.49	121.50
1	E	236	LEU	CB-CA-C	-7.99	98.28	110.90
1	C	15	ASN	OD1-CG-ND2	7.99	130.59	122.60
1	F	347	ALA	CA-C-O	-7.98	111.08	120.10
1	F	560	ARG	CA-C-O	7.98	131.93	120.51
1	A	439	SER	O-C-N	7.98	132.61	123.27
1	B	3	LEU	N-CA-CB	7.98	124.04	111.91
1	B	204	TRP	CA-C-O	-7.98	109.77	119.43
1	B	373	THR	CA-CB-CG2	7.98	124.07	110.50
1	D	560	ARG	CA-C-O	7.98	131.92	120.51
1	E	100	ARG	NE-CZ-NH1	7.98	129.48	121.50
1	E	369	GLU	O-C-N	7.98	133.76	121.63
1	C	458	ASN	CA-C-O	-7.98	112.08	120.70
1	D	3	LEU	N-CA-CB	7.98	124.03	111.91
1	D	204	TRP	CA-C-O	-7.98	109.78	119.43
1	C	3	LEU	N-CA-CB	7.98	124.03	111.91
1	D	15	ASN	OD1-CG-ND2	7.98	130.58	122.60
1	A	240	LEU	O-C-N	-7.97	113.59	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	175	LYS	N-CA-C	-7.97	101.58	110.91
1	E	240	LEU	O-C-N	-7.97	113.59	122.84
1	F	439	SER	O-C-N	7.97	132.60	123.27
1	B	651	HIS	O-C-N	7.97	133.18	123.13
1	E	38	ASN	OD1-CG-ND2	7.97	130.57	122.60
1	C	240	LEU	O-C-N	-7.97	113.59	122.84
1	A	635	VAL	CA-C-O	-7.97	111.11	120.83
1	E	15	ASN	OD1-CG-ND2	7.97	130.57	122.60
1	E	204	TRP	CA-C-O	-7.97	109.79	119.43
1	E	414	ASN	CA-C-N	-7.97	109.94	121.26
1	E	414	ASN	C-N-CA	-7.97	109.94	121.26
1	F	240	LEU	O-C-N	-7.97	113.60	122.84
1	A	369	GLU	O-C-N	7.97	133.74	121.63
1	F	100	ARG	NE-CZ-NH1	7.97	129.47	121.50
1	A	651	HIS	O-C-N	7.96	133.17	123.13
1	B	240	LEU	O-C-N	-7.96	113.60	122.84
1	C	439	SER	O-C-N	7.96	132.59	123.27
1	D	336	ASN	CB-CA-C	7.96	123.48	112.09
1	D	373	THR	CA-CB-CG2	7.96	124.04	110.50
1	C	653	LEU	CB-CA-C	7.96	125.23	110.10
1	C	651	HIS	O-C-N	7.96	133.16	123.13
1	E	651	HIS	O-C-N	7.96	133.16	123.13
1	D	651	HIS	O-C-N	7.96	133.16	123.13
1	E	373	THR	CA-CB-CG2	7.96	124.03	110.50
1	D	617	PRO	CB-CA-C	-7.96	100.50	112.11
1	F	556	SER	CB-CA-C	7.96	121.61	110.16
1	B	414	ASN	CA-C-N	-7.95	109.97	121.26
1	B	414	ASN	C-N-CA	-7.95	109.97	121.26
1	B	653	LEU	CB-CA-C	7.95	125.21	110.10
1	E	372	GLU	CA-CB-CG	-7.95	98.19	114.10
1	A	15	ASN	OD1-CG-ND2	7.95	130.55	122.60
1	A	653	LEU	CB-CA-C	7.95	125.21	110.10
1	A	204	TRP	CA-C-O	-7.95	109.81	119.43
1	A	373	THR	CA-CB-CG2	7.95	124.02	110.50
1	C	175	LYS	N-CA-C	-7.95	101.61	110.91
1	C	373	THR	CA-CB-CG2	7.95	124.01	110.50
1	F	147	ASN	CB-CG-OD1	-7.95	104.90	120.80
1	F	653	LEU	CB-CA-C	7.95	125.21	110.10
1	A	556	SER	CB-CA-C	7.95	121.61	110.16
1	D	653	LEU	CB-CA-C	7.95	125.20	110.10
1	B	15	ASN	OD1-CG-ND2	7.95	130.55	122.60
1	E	653	LEU	CB-CA-C	7.95	125.20	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	LYS	N-CA-C	-7.95	101.61	110.91
1	F	414	ASN	CA-C-N	-7.95	109.98	121.26
1	F	414	ASN	C-N-CA	-7.95	109.98	121.26
1	F	617	PRO	CB-CA-C	-7.95	100.51	112.11
1	E	441	GLU	O-C-N	7.94	132.71	123.41
1	A	414	ASN	CA-C-N	-7.94	109.98	121.26
1	A	414	ASN	C-N-CA	-7.94	109.98	121.26
1	B	175	LYS	N-CA-C	-7.94	101.62	110.91
1	D	556	SER	CB-CA-C	7.94	121.60	110.16
1	D	635	VAL	CA-C-O	-7.94	111.14	120.83
1	A	38	ASN	OD1-CG-ND2	7.94	130.54	122.60
1	D	414	ASN	CA-C-N	-7.94	109.98	121.26
1	D	414	ASN	C-N-CA	-7.94	109.98	121.26
1	F	100	ARG	O-C-N	7.94	130.35	122.09
1	E	175	LYS	N-CA-C	-7.94	101.62	110.91
1	A	617	PRO	CB-CA-C	-7.94	100.52	112.11
1	B	617	PRO	CB-CA-C	-7.94	100.52	112.11
1	F	204	TRP	CA-C-O	-7.94	109.83	119.43
1	F	373	THR	CA-CB-CG2	7.94	123.99	110.50
1	C	204	TRP	CA-C-O	-7.94	109.83	119.43
1	C	540	LYS	N-CA-C	-7.93	101.00	111.24
1	C	556	SER	CB-CA-C	7.93	121.59	110.16
1	F	73	SER	N-CA-CB	7.93	123.07	110.85
1	A	372	GLU	CA-CB-CG	-7.93	98.24	114.10
1	A	441	GLU	O-C-N	7.93	132.69	123.41
1	C	336	ASN	CB-CA-C	7.93	123.43	112.09
1	F	175	LYS	N-CA-C	-7.93	101.63	110.91
1	F	372	GLU	CA-CB-CG	-7.93	98.24	114.10
1	D	372	GLU	CA-CB-CG	-7.93	98.24	114.10
1	E	350	MET	O-C-N	7.93	131.19	122.15
1	B	556	SER	CB-CA-C	7.93	121.58	110.16
1	C	466	MET	N-CA-CB	-7.93	97.09	110.49
1	D	441	GLU	O-C-N	7.93	132.69	123.41
1	B	73	SER	N-CA-CB	7.93	123.06	110.85
1	C	414	ASN	CA-C-N	-7.93	110.00	121.26
1	C	414	ASN	C-N-CA	-7.93	110.00	121.26
1	D	147	ASN	CB-CG-OD1	-7.93	104.95	120.80
1	E	617	PRO	CB-CA-C	-7.93	100.54	112.11
1	F	395	THR	N-CA-CB	7.93	121.95	110.06
1	D	133	VAL	O-C-N	-7.92	114.86	123.18
1	E	371	PHE	N-CA-C	7.92	121.01	111.82
1	E	395	THR	N-CA-CB	7.92	121.95	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	556	SER	CB-CA-C	7.92	121.57	110.16
1	A	395	THR	N-CA-CB	7.92	121.94	110.06
1	E	73	SER	N-CA-CB	7.92	123.05	110.85
1	E	147	ASN	CB-CG-OD1	-7.92	104.95	120.80
1	A	336	ASN	CB-CA-C	7.92	123.42	112.09
1	D	38	ASN	OD1-CG-ND2	7.92	130.52	122.60
1	E	540	LYS	N-CA-C	-7.92	101.02	111.24
1	F	38	ASN	OD1-CG-ND2	7.92	130.52	122.60
1	B	336	ASN	CB-CA-C	7.92	123.42	112.09
1	F	466	MET	N-CA-CB	-7.92	97.10	110.49
1	A	73	SER	N-CA-CB	7.92	123.05	110.85
1	B	147	ASN	CB-CG-OD1	-7.92	104.96	120.80
1	B	372	GLU	CA-CB-CG	-7.92	98.26	114.10
1	C	372	GLU	CA-CB-CG	-7.92	98.26	114.10
1	E	439	SER	O-C-N	7.92	132.53	123.27
1	A	147	ASN	CB-CG-OD1	-7.92	104.97	120.80
1	C	387	MET	CG-SD-CE	7.92	118.32	100.90
1	C	415	GLY	CA-C-N	-7.92	111.27	122.75
1	C	415	GLY	C-N-CA	-7.92	111.27	122.75
1	C	617	PRO	CB-CA-C	-7.92	100.55	112.11
1	E	466	MET	N-CA-CB	-7.92	97.11	110.49
1	F	369	GLU	O-C-N	7.92	133.66	121.63
1	D	100	ARG	O-C-N	7.92	130.32	122.09
1	E	100	ARG	O-C-N	7.92	130.32	122.09
1	E	387	MET	CG-SD-CE	7.92	118.31	100.90
1	D	395	THR	N-CA-CB	7.91	121.93	110.06
1	A	350	MET	O-C-N	7.91	131.17	122.15
1	A	466	MET	N-CA-CB	-7.91	97.12	110.49
1	D	73	SER	N-CA-CB	7.91	123.03	110.85
1	F	336	ASN	CB-CA-C	7.91	123.41	112.09
1	A	415	GLY	CA-C-N	-7.91	111.28	122.75
1	A	415	GLY	C-N-CA	-7.91	111.28	122.75
1	B	441	GLU	O-C-N	7.91	132.67	123.41
1	F	387	MET	CG-SD-CE	7.91	118.31	100.90
1	A	387	MET	CG-SD-CE	7.91	118.30	100.90
1	B	466	MET	N-CA-CB	-7.91	97.12	110.49
1	F	68	GLN	O-C-N	7.91	132.38	122.65
1	D	350	MET	O-C-N	7.91	131.16	122.15
1	A	540	LYS	N-CA-C	-7.91	101.04	111.24
1	C	38	ASN	OD1-CG-ND2	7.91	130.51	122.60
1	C	147	ASN	CB-CG-OD1	-7.91	104.99	120.80
1	C	73	SER	N-CA-CB	7.90	123.02	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	133	VAL	O-C-N	-7.90	114.88	123.18
1	A	100	ARG	O-C-N	7.90	130.31	122.09
1	B	68	GLN	O-C-N	7.90	132.37	122.65
1	B	100	ARG	O-C-N	7.90	130.31	122.09
1	B	415	GLY	CA-C-N	-7.90	111.29	122.75
1	B	415	GLY	C-N-CA	-7.90	111.29	122.75
1	C	395	THR	N-CA-CB	7.90	121.91	110.06
1	D	111	ASN	N-CA-CB	-7.90	99.06	110.36
1	D	387	MET	CG-SD-CE	7.90	118.28	100.90
1	B	387	MET	CG-SD-CE	7.90	118.28	100.90
1	C	100	ARG	O-C-N	7.90	130.31	122.09
1	B	83	ALA	O-C-N	7.90	130.49	122.12
1	B	350	MET	O-C-N	7.90	131.15	122.15
1	E	68	GLN	O-C-N	7.90	132.36	122.65
1	B	395	THR	N-CA-CB	7.90	121.90	110.06
1	F	540	LYS	N-CA-C	-7.90	101.06	111.24
1	C	350	MET	O-C-N	7.89	131.15	122.15
1	C	441	GLU	O-C-N	7.89	132.65	123.41
1	D	466	MET	N-CA-CB	-7.89	97.15	110.49
1	E	415	GLY	CA-C-N	-7.89	111.30	122.75
1	E	415	GLY	C-N-CA	-7.89	111.30	122.75
1	A	371	PHE	N-CA-C	7.89	120.97	111.82
1	D	415	GLY	CA-C-N	-7.89	111.31	122.75
1	D	415	GLY	C-N-CA	-7.89	111.31	122.75
1	F	415	GLY	CA-C-N	-7.89	111.31	122.75
1	F	415	GLY	C-N-CA	-7.89	111.31	122.75
1	A	133	VAL	O-C-N	-7.89	114.90	123.18
1	B	133	VAL	O-C-N	-7.89	114.90	123.18
1	D	540	LYS	N-CA-C	-7.89	101.06	111.24
1	E	336	ASN	CB-CA-C	7.89	123.37	112.09
1	E	272	PRO	CA-C-O	-7.88	107.90	119.18
1	A	68	GLN	O-C-N	7.88	132.34	122.65
1	B	540	LYS	N-CA-C	-7.88	101.07	111.24
1	D	68	GLN	O-C-N	7.88	132.34	122.65
1	F	350	MET	O-C-N	7.88	131.13	122.15
1	F	371	PHE	N-CA-C	7.88	120.96	111.82
1	E	256	PHE	CA-CB-CG	7.88	121.68	113.80
1	F	111	ASN	N-CA-CB	-7.88	99.10	110.36
1	A	111	ASN	N-CA-CB	-7.87	99.10	110.36
1	C	133	VAL	O-C-N	-7.87	114.91	123.18
1	D	371	PHE	N-CA-C	7.87	120.95	111.82
1	C	272	PRO	CA-C-O	-7.87	107.92	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	441	GLU	O-C-N	7.87	132.62	123.41
1	C	68	GLN	O-C-N	7.87	132.33	122.65
1	D	272	PRO	CA-C-O	-7.87	107.93	119.18
1	B	111	ASN	N-CA-CB	-7.86	99.11	110.36
1	E	111	ASN	N-CA-CB	-7.86	99.11	110.36
1	C	111	ASN	N-CA-CB	-7.86	99.12	110.36
1	E	83	ALA	O-C-N	7.86	130.45	122.12
1	A	272	PRO	CA-C-O	-7.86	107.94	119.18
1	B	371	PHE	N-CA-C	7.86	120.94	111.82
1	C	371	PHE	N-CA-C	7.86	120.94	111.82
1	B	256	PHE	CA-CB-CG	7.85	121.65	113.80
1	E	469	ASN	CB-CG-OD1	7.85	136.50	120.80
1	A	469	ASN	CB-CG-OD1	7.84	136.49	120.80
1	B	272	PRO	CA-C-O	-7.84	107.97	119.18
1	C	469	ASN	CB-CG-OD1	7.84	136.48	120.80
1	E	133	VAL	O-C-N	-7.84	114.95	123.18
1	A	256	PHE	CA-CB-CG	7.84	121.64	113.80
1	C	83	ALA	O-C-N	7.84	130.43	122.12
1	F	272	PRO	CA-C-O	-7.84	107.97	119.18
1	A	83	ALA	O-C-N	7.84	130.43	122.12
1	F	537	GLN	CA-CB-CG	-7.83	98.43	114.10
1	C	537	GLN	CA-CB-CG	-7.83	98.43	114.10
1	B	469	ASN	CB-CG-OD1	7.83	136.46	120.80
1	D	256	PHE	CA-CB-CG	7.83	121.63	113.80
1	F	469	ASN	CB-CG-OD1	7.83	136.46	120.80
1	C	256	PHE	CA-CB-CG	7.82	121.62	113.80
1	D	469	ASN	CB-CG-OD1	7.82	136.44	120.80
1	E	537	GLN	CA-CB-CG	-7.82	98.46	114.10
1	A	537	GLN	CA-CB-CG	-7.82	98.47	114.10
1	B	25	THR	N-CA-C	7.82	121.52	110.50
1	C	492	THR	CA-CB-CG2	7.82	123.79	110.50
1	F	256	PHE	CA-CB-CG	7.82	121.62	113.80
1	D	614	GLU	N-CA-CB	-7.81	97.29	110.49
1	F	614	GLU	N-CA-CB	-7.81	97.29	110.49
1	F	492	THR	CA-CB-CG2	7.81	123.78	110.50
1	B	537	GLN	CA-CB-CG	-7.81	98.49	114.10
1	F	83	ALA	O-C-N	7.81	130.40	122.12
1	D	537	GLN	CA-CB-CG	-7.80	98.50	114.10
1	E	614	GLU	N-CA-CB	-7.80	97.31	110.49
1	A	492	THR	CA-CB-CG2	7.79	123.75	110.50
1	C	614	GLU	N-CA-CB	-7.79	97.33	110.49
1	E	25	THR	N-CA-C	7.79	121.48	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	614	GLU	N-CA-CB	-7.79	97.33	110.49
1	D	83	ALA	O-C-N	7.79	130.37	122.12
1	B	190	MET	N-CA-C	-7.79	102.11	111.69
1	A	25	THR	N-CA-C	7.78	121.47	110.50
1	B	519	ILE	CA-C-O	7.78	130.37	121.11
1	B	614	GLU	N-CA-CB	-7.78	97.33	110.49
1	E	492	THR	CA-CB-CG2	7.78	123.73	110.50
1	F	609	CYS	CB-CA-C	-7.78	98.18	111.41
1	D	492	THR	CA-CB-CG2	7.78	123.73	110.50
1	B	492	THR	CA-CB-CG2	7.78	123.72	110.50
1	D	609	CYS	CB-CA-C	-7.78	98.19	111.41
1	B	239	TRP	N-CA-C	-7.78	104.28	113.38
1	B	609	CYS	CB-CA-C	-7.78	98.19	111.41
1	E	609	CYS	CB-CA-C	-7.78	98.19	111.41
1	A	519	ILE	CA-C-O	7.77	130.36	121.11
1	C	519	ILE	CA-C-O	7.77	130.36	121.11
1	F	337	VAL	CA-CB-CG1	-7.77	97.19	110.40
1	C	25	THR	N-CA-C	7.77	121.45	110.50
1	E	519	ILE	CA-C-O	7.77	130.36	121.11
1	C	609	CYS	CB-CA-C	-7.77	98.20	111.41
1	D	25	THR	N-CA-C	7.76	121.45	110.50
1	D	337	VAL	CA-CB-CG1	-7.76	97.20	110.40
1	A	609	CYS	CB-CA-C	-7.76	98.21	111.41
1	F	25	THR	N-CA-C	7.76	121.45	110.50
1	D	190	MET	N-CA-C	-7.76	102.14	111.69
1	B	95	GLU	CA-C-O	-7.76	113.14	121.36
1	C	337	VAL	CA-CB-CG1	-7.76	97.21	110.40
1	D	95	GLU	CA-C-O	-7.76	113.14	121.36
1	F	519	ILE	CA-C-O	7.76	130.34	121.11
1	B	337	VAL	CA-CB-CG1	-7.76	97.21	110.40
1	C	294	SER	CA-CB-OG	-7.76	95.59	111.10
1	E	335	SER	O-C-N	7.75	133.68	122.28
1	B	578	MET	O-C-N	7.75	132.55	123.17
1	E	239	TRP	N-CA-C	-7.75	104.31	113.38
1	E	337	VAL	CA-CB-CG1	-7.75	97.22	110.40
1	E	525	ASP	CA-CB-CG	7.75	120.35	112.60
1	E	612	HIS	CA-C-O	-7.75	111.11	120.65
1	B	294	SER	CA-CB-OG	-7.75	95.59	111.10
1	D	91	ASN	CB-CG-OD1	7.75	136.30	120.80
1	E	294	SER	CA-CB-OG	-7.75	95.60	111.10
1	F	27	TYR	CA-C-N	7.75	129.53	119.84
1	F	27	TYR	C-N-CA	7.75	129.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	91	ASN	CB-CG-OD1	7.75	136.30	120.80
1	A	294	SER	CA-CB-OG	-7.75	95.60	111.10
1	F	190	MET	N-CA-C	-7.75	102.16	111.69
1	D	612	HIS	CA-C-O	-7.75	111.12	120.65
1	A	239	TRP	N-CA-C	-7.75	104.32	113.38
1	A	337	VAL	CA-CB-CG1	-7.75	97.23	110.40
1	D	525	ASP	CA-CB-CG	7.75	120.35	112.60
1	B	612	HIS	CA-C-O	-7.75	111.12	120.65
1	F	294	SER	CA-CB-OG	-7.74	95.61	111.10
1	A	190	MET	N-CA-C	-7.74	102.17	111.69
1	E	483	CYS	CB-CA-C	-7.74	96.77	110.47
1	F	257	ALA	N-CA-C	-7.74	97.01	109.40
1	F	335	SER	O-C-N	7.74	133.66	122.28
1	D	27	TYR	CA-C-N	7.74	129.52	119.84
1	D	27	TYR	C-N-CA	7.74	129.52	119.84
1	F	612	HIS	CA-C-O	-7.74	111.13	120.65
1	A	95	GLU	CA-C-O	-7.74	113.16	121.36
1	C	239	TRP	N-CA-C	-7.74	104.33	113.38
1	D	294	SER	CA-CB-OG	-7.74	95.63	111.10
1	E	296	ILE	CA-C-O	7.74	129.57	121.29
1	A	91	ASN	CB-CG-OD1	7.74	136.27	120.80
1	E	91	ASN	CB-CG-OD1	7.74	136.27	120.80
1	F	95	GLU	CA-C-O	-7.74	113.16	121.36
1	C	95	GLU	CA-C-O	-7.73	113.16	121.36
1	F	239	TRP	N-CA-C	-7.73	104.33	113.38
1	F	483	CYS	CB-CA-C	-7.73	96.78	110.47
1	D	239	TRP	N-CA-C	-7.73	104.34	113.38
1	E	95	GLU	CA-C-O	-7.73	113.17	121.36
1	A	335	SER	O-C-N	7.73	133.64	122.28
1	C	230	ARG	N-CA-C	-7.73	101.83	111.11
1	E	190	MET	N-CA-C	-7.73	102.18	111.69
1	A	612	HIS	CA-C-O	-7.73	111.15	120.65
1	B	335	SER	O-C-N	7.73	133.64	122.28
1	B	483	CYS	CB-CA-C	-7.73	96.79	110.47
1	D	519	ILE	CA-C-O	7.73	130.31	121.11
1	B	180	ARG	O-C-N	7.72	132.86	122.59
1	D	639	VAL	N-CA-C	-7.72	97.36	108.17
1	A	525	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	91	ASN	CB-CG-OD1	7.72	136.25	120.80
1	C	525	ASP	CA-CB-CG	7.72	120.32	112.60
1	E	136	PRO	CB-CA-C	-7.72	102.08	111.11
1	F	7	ASN	CA-C-N	-7.72	106.79	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	7	ASN	C-N-CA	-7.72	106.79	121.54
1	A	483	CYS	CB-CA-C	-7.72	96.81	110.47
1	C	91	ASN	CB-CG-OD1	7.72	136.24	120.80
1	E	469	ASN	OD1-CG-ND2	-7.72	114.88	122.60
1	C	335	SER	O-C-N	7.72	133.63	122.28
1	F	578	MET	O-C-N	7.72	132.51	123.17
1	A	257	ALA	N-CA-C	-7.72	97.06	109.40
1	D	335	SER	O-C-N	7.72	133.62	122.28
1	A	7	ASN	CA-C-N	-7.71	106.81	121.54
1	A	7	ASN	C-N-CA	-7.71	106.81	121.54
1	D	305	ILE	N-CA-C	-7.71	97.01	108.97
1	D	351	LEU	CA-C-O	7.71	128.99	119.11
1	E	27	TYR	CA-C-N	7.71	129.48	119.84
1	E	27	TYR	C-N-CA	7.71	129.48	119.84
1	C	7	ASN	CA-C-N	-7.71	106.81	121.54
1	C	7	ASN	C-N-CA	-7.71	106.81	121.54
1	C	180	ARG	O-C-N	7.71	132.85	122.59
1	A	230	ARG	N-CA-C	-7.71	101.86	111.11
1	A	578	MET	O-C-N	7.71	132.50	123.17
1	D	230	ARG	N-CA-C	-7.71	101.86	111.11
1	D	483	CYS	CB-CA-C	-7.71	96.82	110.47
1	E	7	ASN	CA-C-N	-7.71	106.81	121.54
1	E	7	ASN	C-N-CA	-7.71	106.81	121.54
1	E	578	MET	O-C-N	7.71	132.50	123.17
1	A	299	ALA	N-CA-CB	-7.71	98.72	110.13
1	B	299	ALA	N-CA-CB	-7.71	98.72	110.13
1	C	612	HIS	CA-C-O	-7.71	111.17	120.65
1	B	27	TYR	CA-C-N	7.71	129.47	119.84
1	B	27	TYR	C-N-CA	7.71	129.47	119.84
1	C	257	ALA	N-CA-C	-7.71	97.07	109.40
1	C	305	ILE	N-CA-C	-7.71	97.03	108.97
1	C	483	CYS	CB-CA-C	-7.71	96.83	110.47
1	E	230	ARG	N-CA-C	-7.71	101.86	111.11
1	C	469	ASN	OD1-CG-ND2	-7.71	114.89	122.60
1	A	136	PRO	CB-CA-C	-7.70	102.10	111.11
1	C	190	MET	N-CA-C	-7.70	102.22	111.69
1	D	136	PRO	CB-CA-C	-7.70	102.10	111.11
1	E	257	ALA	N-CA-C	-7.70	97.08	109.40
1	F	639	VAL	N-CA-C	-7.70	97.39	108.17
1	B	257	ALA	N-CA-C	-7.70	97.08	109.40
1	A	27	TYR	CA-C-N	7.70	129.47	119.84
1	A	27	TYR	C-N-CA	7.70	129.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	525	ASP	CA-CB-CG	7.70	120.30	112.60
1	B	530	VAL	CA-CB-CG1	7.70	123.49	110.40
1	D	650	VAL	CA-CB-CG1	-7.70	97.31	110.40
1	E	299	ALA	N-CA-CB	-7.70	98.73	110.13
1	E	305	ILE	N-CA-C	-7.70	97.03	108.97
1	C	299	ALA	N-CA-CB	-7.70	98.73	110.13
1	D	7	ASN	CA-C-N	-7.70	106.84	121.54
1	D	7	ASN	C-N-CA	-7.70	106.84	121.54
1	F	49	HIS	N-CA-CB	7.70	125.03	112.63
1	F	650	VAL	CA-CB-CG1	-7.70	97.31	110.40
1	D	257	ALA	N-CA-C	-7.70	97.08	109.40
1	F	299	ALA	N-CA-CB	-7.70	98.74	110.13
1	B	121	VAL	O-C-N	7.70	129.34	121.87
1	D	49	HIS	N-CA-CB	7.69	125.02	112.63
1	F	351	LEU	CA-C-O	7.69	128.96	119.11
1	A	639	VAL	N-CA-C	-7.69	97.40	108.17
1	B	230	ARG	N-CA-C	-7.69	101.88	111.11
1	F	179	GLN	CB-CA-C	7.69	125.73	110.42
1	F	230	ARG	N-CA-C	-7.69	101.88	111.11
1	C	27	TYR	CA-C-N	7.69	129.45	119.84
1	C	27	TYR	C-N-CA	7.69	129.45	119.84
1	D	299	ALA	N-CA-CB	-7.69	98.75	110.13
1	F	136	PRO	CB-CA-C	-7.69	102.11	111.11
1	E	49	HIS	N-CA-CB	7.69	125.01	112.63
1	F	525	ASP	CA-CB-CG	7.69	120.29	112.60
1	A	305	ILE	N-CA-C	-7.69	97.06	108.97
1	B	7	ASN	CA-C-N	-7.69	106.86	121.54
1	B	7	ASN	C-N-CA	-7.69	106.86	121.54
1	F	305	ILE	N-CA-C	-7.69	97.05	108.97
1	B	305	ILE	N-CA-C	-7.69	97.06	108.97
1	C	121	VAL	O-C-N	7.69	129.33	121.87
1	C	578	MET	O-C-N	7.69	132.47	123.17
1	A	351	LEU	CA-C-O	7.68	128.95	119.11
1	B	639	VAL	N-CA-C	-7.68	97.41	108.17
1	C	296	ILE	CA-C-O	7.68	129.51	121.29
1	D	179	GLN	CB-CA-C	7.68	125.71	110.42
1	E	639	VAL	N-CA-C	-7.68	97.41	108.17
1	A	180	ARG	O-C-N	7.68	132.81	122.59
1	E	179	GLN	CB-CA-C	7.68	125.71	110.42
1	B	59	GLU	O-C-N	7.68	132.21	122.23
1	B	136	PRO	CB-CA-C	-7.68	102.12	111.11
1	C	136	PRO	CB-CA-C	-7.68	102.12	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	179	GLN	CB-CA-C	7.68	125.70	110.42
1	C	530	VAL	CA-CB-CG1	7.68	123.45	110.40
1	D	48	ASP	N-CA-CB	7.68	122.21	110.61
1	D	530	VAL	CA-CB-CG1	7.68	123.46	110.40
1	B	179	GLN	CB-CA-C	7.68	125.70	110.42
1	C	351	LEU	CA-C-O	7.68	128.94	119.11
1	A	49	HIS	N-CA-CB	7.68	124.99	112.63
1	A	530	VAL	CA-CB-CG1	7.68	123.45	110.40
1	E	180	ARG	O-C-N	7.68	132.80	122.59
1	F	296	ILE	CA-C-O	7.68	129.50	121.29
1	A	179	GLN	CB-CA-C	7.67	125.69	110.42
1	A	650	VAL	CA-CB-CG1	-7.67	97.35	110.40
1	C	32	ASP	CA-CB-CG	7.67	120.27	112.60
1	D	180	ARG	O-C-N	7.67	132.80	122.59
1	E	234	GLU	CA-C-O	-7.67	112.42	120.55
1	B	49	HIS	N-CA-CB	7.67	124.98	112.63
1	E	125	HIS	CA-CB-CG	-7.67	106.13	113.80
1	E	650	VAL	CA-CB-CG1	-7.67	97.36	110.40
1	F	180	ARG	O-C-N	7.67	132.79	122.59
1	B	296	ILE	CA-C-O	7.67	129.50	121.29
1	C	59	GLU	O-C-N	7.67	132.20	122.23
1	A	296	ILE	CA-C-O	7.67	129.50	121.29
1	C	234	GLU	CA-C-O	-7.67	112.42	120.55
1	C	639	VAL	N-CA-C	-7.67	97.43	108.17
1	D	32	ASP	CA-CB-CG	7.67	120.27	112.60
1	B	227	LEU	CA-C-O	-7.67	112.42	120.55
1	B	351	LEU	CA-C-O	7.67	128.92	119.11
1	B	650	VAL	CA-CB-CG1	-7.67	97.37	110.40
1	C	49	HIS	N-CA-CB	7.67	124.97	112.63
1	D	296	ILE	CA-C-O	7.67	129.49	121.29
1	A	448	ILE	O-C-N	7.66	131.05	122.93
1	A	469	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	C	125	HIS	CA-CB-CG	-7.66	106.14	113.80
1	A	48	ASP	N-CA-CB	7.66	122.18	110.61
1	B	524	LYS	CA-C-O	-7.66	112.30	120.42
1	D	59	GLU	O-C-N	7.66	132.19	122.23
1	D	121	VAL	O-C-N	7.66	129.30	121.87
1	D	448	ILE	O-C-N	7.66	131.05	122.93
1	D	578	MET	O-C-N	7.66	132.44	123.17
1	E	448	ILE	O-C-N	7.66	131.05	122.93
1	F	59	GLU	O-C-N	7.66	132.19	122.23
1	A	234	GLU	CA-C-O	-7.66	112.43	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	489	ASN	CB-CA-C	7.66	121.93	109.07
1	E	351	LEU	CA-C-O	7.65	128.91	119.11
1	E	530	VAL	CA-CB-CG1	7.65	123.41	110.40
1	E	59	GLU	O-C-N	7.65	132.18	122.23
1	F	489	ASN	CB-CA-C	7.65	121.92	109.07
1	A	32	ASP	CA-CB-CG	7.65	120.25	112.60
1	C	650	VAL	CA-CB-CG1	-7.65	97.39	110.40
1	D	125	HIS	CA-CB-CG	-7.65	106.15	113.80
1	F	498	ALA	N-CA-C	7.65	123.55	113.30
1	B	489	ASN	CA-C-N	-7.65	112.75	123.08
1	B	489	ASN	C-N-CA	-7.65	112.75	123.08
1	B	489	ASN	CB-CA-C	7.65	121.92	109.07
1	F	448	ILE	O-C-N	7.65	131.04	122.93
1	A	59	GLU	O-C-N	7.65	132.17	122.23
1	C	489	ASN	CA-C-N	-7.65	112.76	123.08
1	C	489	ASN	C-N-CA	-7.65	112.76	123.08
1	A	121	VAL	O-C-N	7.64	129.28	121.87
1	A	489	ASN	CB-CA-C	7.64	121.91	109.07
1	B	469	ASN	OD1-CG-ND2	-7.64	114.95	122.60
1	C	48	ASP	N-CA-CB	7.64	122.15	110.61
1	D	213	LEU	N-CA-C	-7.64	98.12	110.20
1	A	125	HIS	CA-CB-CG	-7.64	106.16	113.80
1	B	125	HIS	CA-CB-CG	-7.64	106.16	113.80
1	F	234	GLU	CA-C-O	-7.64	112.45	120.55
1	E	121	VAL	O-C-N	7.64	129.28	121.87
1	B	48	ASP	N-CA-CB	7.64	122.14	110.61
1	E	48	ASP	N-CA-CB	7.64	122.14	110.61
1	A	489	ASN	CA-C-N	-7.63	112.77	123.08
1	A	489	ASN	C-N-CA	-7.63	112.77	123.08
1	C	35	GLU	N-CA-CB	-7.63	97.50	110.33
1	E	32	ASP	CA-CB-CG	7.63	120.23	112.60
1	E	489	ASN	CB-CA-C	7.63	121.89	109.07
1	F	227	LEU	CA-C-O	-7.63	112.46	120.55
1	A	213	LEU	N-CA-C	-7.63	98.14	110.20
1	C	489	ASN	CB-CA-C	7.63	121.89	109.07
1	F	213	LEU	N-CA-C	-7.63	98.14	110.20
1	F	469	ASN	OD1-CG-ND2	-7.63	114.97	122.60
1	F	530	VAL	CA-CB-CG1	7.63	123.38	110.40
1	B	213	LEU	N-CA-C	-7.63	98.14	110.20
1	C	498	ALA	N-CA-C	7.63	123.53	113.30
1	C	557	ALA	O-C-N	7.63	132.74	122.59
1	D	227	LEU	CA-C-O	-7.63	112.46	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	234	GLU	CA-C-O	-7.63	112.46	120.55
1	F	48	ASP	N-CA-CB	7.63	122.13	110.61
1	F	322	GLU	N-CA-CB	7.63	122.02	110.19
1	B	234	GLU	CA-C-O	-7.63	112.46	120.55
1	C	213	LEU	N-CA-C	-7.63	98.15	110.20
1	D	581	ASN	CA-CB-CG	-7.63	104.97	112.60
1	E	489	ASN	CA-C-N	-7.62	112.79	123.08
1	E	489	ASN	C-N-CA	-7.62	112.79	123.08
1	F	125	HIS	CA-CB-CG	-7.62	106.18	113.80
1	F	641	ASN	N-CA-C	7.62	121.05	112.97
1	D	35	GLU	N-CA-CB	-7.62	97.52	110.33
1	D	489	ASN	CA-C-N	-7.62	112.79	123.08
1	D	489	ASN	C-N-CA	-7.62	112.79	123.08
1	E	322	GLU	N-CA-CB	7.62	122.00	110.19
1	B	498	ALA	N-CA-C	7.62	123.51	113.30
1	B	581	ASN	CA-CB-CG	-7.62	104.98	112.60
1	E	18	LEU	N-CA-C	-7.62	104.89	112.97
1	E	524	LYS	CA-C-O	-7.62	112.34	120.42
1	F	121	VAL	O-C-N	7.62	129.26	121.87
1	A	498	ALA	N-CA-C	7.62	123.51	113.30
1	C	322	GLU	N-CA-CB	7.62	122.00	110.19
1	D	557	ALA	O-C-N	7.62	132.72	122.59
1	E	213	LEU	N-CA-C	-7.62	98.16	110.20
1	E	557	ALA	O-C-N	7.62	132.72	122.59
1	D	641	ASN	N-CA-C	7.62	121.04	112.97
1	A	227	LEU	CA-C-O	-7.62	112.48	120.55
1	A	322	GLU	N-CA-CB	7.62	121.99	110.19
1	F	557	ALA	O-C-N	7.62	132.72	122.59
1	D	181	VAL	CB-CA-C	7.61	123.78	111.29
1	D	322	GLU	N-CA-CB	7.61	121.99	110.19
1	F	581	ASN	CA-CB-CG	-7.61	104.99	112.60
1	E	498	ALA	N-CA-C	7.61	123.50	113.30
1	F	489	ASN	CA-C-N	-7.61	112.81	123.08
1	F	489	ASN	C-N-CA	-7.61	112.81	123.08
1	A	35	GLU	N-CA-CB	-7.61	97.55	110.33
1	C	227	LEU	CA-C-O	-7.61	112.48	120.55
1	A	557	ALA	O-C-N	7.61	132.71	122.59
1	A	581	ASN	CA-CB-CG	-7.61	104.99	112.60
1	B	18	LEU	N-CA-C	-7.61	104.91	112.97
1	E	491	ILE	CA-CB-CG2	-7.61	97.57	110.50
1	F	537	GLN	CB-CG-CD	-7.61	99.67	112.60
1	B	322	GLU	N-CA-CB	7.61	121.98	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	491	ILE	CA-CB-CG2	-7.61	97.57	110.50
1	B	537	GLN	CB-CG-CD	-7.61	99.67	112.60
1	C	537	GLN	CB-CG-CD	-7.61	99.67	112.60
1	F	535	SER	O-C-N	7.61	131.46	122.79
1	A	524	LYS	CA-C-O	-7.60	112.36	120.42
1	E	537	GLN	CB-CG-CD	-7.60	99.67	112.60
1	E	641	ASN	N-CA-C	7.60	121.03	112.97
1	A	181	VAL	CB-CA-C	7.60	123.75	111.29
1	A	537	GLN	CB-CG-CD	-7.60	99.68	112.60
1	B	32	ASP	CA-CB-CG	7.60	120.20	112.60
1	B	35	GLU	N-CA-CB	-7.60	97.56	110.33
1	B	362	ASN	N-CA-CB	-7.60	99.73	111.74
1	B	448	ILE	O-C-N	7.60	130.99	122.93
1	B	535	SER	O-C-N	7.60	131.45	122.79
1	C	448	ILE	O-C-N	7.60	130.99	122.93
1	D	580	PHE	O-C-N	-7.60	114.02	122.84
1	E	181	VAL	CB-CA-C	7.60	123.75	111.29
1	B	641	ASN	N-CA-C	7.60	121.02	112.97
1	D	491	ILE	CA-CB-CG2	-7.59	97.59	110.50
1	E	227	LEU	CA-C-O	-7.59	112.50	120.55
1	E	39	PRO	O-C-N	7.59	132.89	122.64
1	F	39	PRO	O-C-N	7.59	132.89	122.64
1	F	362	ASN	N-CA-CB	-7.59	99.74	111.74
1	A	18	LEU	N-CA-C	-7.59	104.92	112.97
1	A	491	ILE	CA-CB-CG2	-7.59	97.59	110.50
1	A	580	PHE	O-C-N	-7.59	114.03	122.84
1	B	94	LYS	N-CA-C	-7.59	101.90	112.45
1	D	537	GLN	CB-CG-CD	-7.59	99.70	112.60
1	E	535	SER	O-C-N	7.59	131.44	122.79
1	E	580	PHE	O-C-N	-7.59	114.03	122.84
1	F	35	GLU	N-CA-CB	-7.59	97.58	110.33
1	A	535	SER	O-C-N	7.59	131.44	122.79
1	A	641	ASN	N-CA-C	7.59	121.02	112.97
1	B	557	ALA	O-C-N	7.59	132.68	122.59
1	C	491	ILE	CA-CB-CG2	-7.59	97.60	110.50
1	D	498	ALA	N-CA-C	7.59	123.47	113.30
1	F	32	ASP	CA-CB-CG	7.59	120.19	112.60
1	C	580	PHE	O-C-N	-7.59	114.04	122.84
1	C	581	ASN	CA-CB-CG	-7.59	105.01	112.60
1	D	524	LYS	CA-C-O	-7.59	112.38	120.42
1	E	355	GLY	O-C-N	7.59	132.56	122.70
1	B	580	PHE	O-C-N	-7.58	114.04	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	35	GLU	N-CA-CB	-7.58	97.59	110.33
1	F	580	PHE	O-C-N	-7.58	114.04	122.84
1	A	362	ASN	N-CA-CB	-7.58	99.76	111.74
1	C	388	ASP	O-C-N	7.58	130.19	122.08
1	A	39	PRO	O-C-N	7.58	132.87	122.64
1	B	39	PRO	O-C-N	7.58	132.87	122.64
1	C	181	VAL	CB-CA-C	7.58	123.72	111.29
1	D	39	PRO	O-C-N	7.58	132.87	122.64
1	D	388	ASP	O-C-N	7.58	130.19	122.08
1	F	94	LYS	N-CA-C	-7.58	101.92	112.45
1	F	524	LYS	CA-C-O	-7.58	112.39	120.42
1	A	388	ASP	O-C-N	7.58	130.19	122.08
1	B	388	ASP	O-C-N	7.58	130.19	122.08
1	C	18	LEU	N-CA-C	-7.58	104.94	112.97
1	D	469	ASN	OD1-CG-ND2	-7.58	115.02	122.60
1	B	430	GLN	OE1-CD-NE2	7.57	130.17	122.60
1	E	193	HIS	CG-CD2-NE2	7.57	114.77	107.20
1	C	94	LYS	N-CA-C	-7.57	101.93	112.45
1	D	362	ASN	N-CA-CB	-7.57	99.78	111.74
1	B	181	VAL	CB-CA-C	7.57	123.70	111.29
1	B	289	LEU	O-C-N	7.57	131.03	122.32
1	F	18	LEU	N-CA-C	-7.57	104.95	112.97
1	F	181	VAL	CB-CA-C	7.57	123.70	111.29
1	C	32	ASP	CA-C-N	-7.57	110.88	120.56
1	C	32	ASP	C-N-CA	-7.57	110.88	120.56
1	C	362	ASN	N-CA-CB	-7.57	99.79	111.74
1	D	278	GLU	CA-CB-CG	-7.57	98.97	114.10
1	D	535	SER	O-C-N	7.57	131.41	122.79
1	F	278	GLU	CA-CB-CG	-7.56	98.97	114.10
1	A	32	ASP	CA-C-N	-7.56	110.88	120.56
1	A	32	ASP	C-N-CA	-7.56	110.88	120.56
1	A	94	LYS	N-CA-C	-7.56	101.94	112.45
1	C	278	GLU	CA-CB-CG	-7.56	98.98	114.10
1	D	32	ASP	CA-C-N	-7.56	110.88	120.56
1	D	32	ASP	C-N-CA	-7.56	110.88	120.56
1	F	491	ILE	CA-CB-CG2	-7.56	97.65	110.50
1	D	355	GLY	O-C-N	7.56	132.53	122.70
1	F	289	LEU	O-C-N	7.56	131.01	122.32
1	F	355	GLY	O-C-N	7.56	132.53	122.70
1	C	535	SER	O-C-N	7.56	131.41	122.79
1	D	18	LEU	N-CA-C	-7.56	104.96	112.97
1	E	278	GLU	CA-CB-CG	-7.56	98.99	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	362	ASN	N-CA-CB	-7.56	99.80	111.74
1	B	278	GLU	CA-CB-CG	-7.55	98.99	114.10
1	B	355	GLY	O-C-N	7.55	132.52	122.70
1	C	289	LEU	O-C-N	7.55	131.01	122.32
1	E	32	ASP	CA-C-N	-7.55	110.89	120.56
1	E	32	ASP	C-N-CA	-7.55	110.89	120.56
1	E	177	ARG	CB-CG-CD	-7.55	93.92	111.30
1	E	581	ASN	CA-CB-CG	-7.55	105.05	112.60
1	A	278	GLU	CA-CB-CG	-7.55	99.00	114.10
1	B	32	ASP	CA-C-N	-7.55	110.90	120.56
1	B	32	ASP	C-N-CA	-7.55	110.90	120.56
1	C	177	ARG	CB-CG-CD	-7.55	93.94	111.30
1	D	177	ARG	CB-CG-CD	-7.55	93.94	111.30
1	A	177	ARG	CB-CG-CD	-7.55	93.94	111.30
1	C	39	PRO	O-C-N	7.55	132.83	122.64
1	F	32	ASP	CA-C-N	-7.54	110.90	120.56
1	F	32	ASP	C-N-CA	-7.54	110.90	120.56
1	E	94	LYS	N-CA-C	-7.54	101.97	112.45
1	D	68	GLN	CA-C-O	-7.54	113.27	121.94
1	F	388	ASP	O-C-N	7.54	130.15	122.08
1	A	355	GLY	O-C-N	7.54	132.50	122.70
1	C	641	ASN	N-CA-C	7.54	120.96	112.97
1	D	352	GLY	CA-C-O	-7.54	107.45	120.57
1	F	177	ARG	CB-CG-CD	-7.54	93.96	111.30
1	B	139	GLN	CA-CB-CG	7.54	129.17	114.10
1	D	94	LYS	N-CA-C	-7.54	101.98	112.45
1	A	68	GLN	CA-C-O	-7.53	113.28	121.94
1	B	177	ARG	CB-CG-CD	-7.53	93.98	111.30
1	F	79	GLN	CG-CD-OE1	7.53	135.86	120.80
1	C	474	ARG	CB-CA-C	7.53	125.11	109.38
1	C	79	GLN	CG-CD-OE1	7.53	135.85	120.80
1	D	289	LEU	O-C-N	7.53	130.97	122.32
1	E	169	SER	N-CA-CB	-7.52	98.53	110.19
1	F	352	GLY	CA-C-O	-7.52	107.48	120.57
1	C	352	GLY	CA-C-O	-7.52	107.48	120.57
1	C	355	GLY	O-C-N	7.52	132.48	122.70
1	E	68	GLN	CA-C-O	-7.52	113.29	121.94
1	E	79	GLN	CG-CD-OE1	7.52	135.85	120.80
1	A	79	GLN	CG-CD-OE1	7.52	135.84	120.80
1	E	139	GLN	CA-CB-CG	7.52	129.14	114.10
1	A	289	LEU	O-C-N	7.52	130.97	122.32
1	B	60	LEU	CA-C-N	7.52	130.86	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	60	LEU	C-N-CA	7.52	130.86	120.63
1	B	68	GLN	CA-C-O	-7.52	113.29	121.94
1	E	388	ASP	O-C-N	7.52	130.13	122.08
1	F	193	HIS	CG-CD2-NE2	7.52	114.72	107.20
1	E	430	GLN	OE1-CD-NE2	7.52	130.12	122.60
1	F	68	GLN	CA-C-O	-7.52	113.30	121.94
1	A	193	HIS	CG-CD2-NE2	7.52	114.72	107.20
1	C	193	HIS	CG-CD2-NE2	7.52	114.72	107.20
1	B	474	ARG	CB-CA-C	7.51	125.09	109.38
1	C	430	GLN	OE1-CD-NE2	7.51	130.11	122.60
1	E	352	GLY	CA-C-O	-7.51	107.50	120.57
1	F	474	ARG	CB-CA-C	7.51	125.08	109.38
1	A	139	GLN	CA-CB-CG	7.51	129.12	114.10
1	B	77	THR	O-C-N	7.51	132.10	122.33
1	E	474	ARG	CB-CA-C	7.51	125.08	109.38
1	A	474	ARG	CB-CA-C	7.51	125.08	109.38
1	D	79	GLN	CG-CD-OE1	7.51	135.82	120.80
1	A	496	ASP	CA-C-N	-7.51	108.90	120.31
1	A	496	ASP	C-N-CA	-7.51	108.90	120.31
1	B	79	GLN	CG-CD-OE1	7.51	135.82	120.80
1	D	139	GLN	CA-CB-CG	7.51	129.12	114.10
1	F	139	GLN	CA-CB-CG	7.51	129.12	114.10
1	A	430	GLN	OE1-CD-NE2	7.51	130.11	122.60
1	A	77	THR	O-C-N	7.51	132.09	122.33
1	A	352	GLY	CA-C-O	-7.51	107.51	120.57
1	E	496	ASP	CA-C-N	-7.51	108.90	120.31
1	E	496	ASP	C-N-CA	-7.51	108.90	120.31
1	F	169	SER	N-CA-CB	-7.51	98.55	110.19
1	B	352	GLY	CA-C-O	-7.50	107.51	120.57
1	B	496	ASP	CA-C-N	-7.50	108.90	120.31
1	B	496	ASP	C-N-CA	-7.50	108.90	120.31
1	C	68	GLN	CA-C-O	-7.50	113.31	121.94
1	C	139	GLN	CA-CB-CG	7.50	129.11	114.10
1	E	77	THR	O-C-N	7.50	132.09	122.33
1	A	169	SER	N-CA-CB	-7.50	98.56	110.19
1	D	474	ARG	CB-CA-C	7.50	125.06	109.38
1	C	60	LEU	CA-C-N	7.50	130.83	120.63
1	C	60	LEU	C-N-CA	7.50	130.83	120.63
1	D	496	ASP	CA-C-N	-7.50	108.91	120.31
1	D	496	ASP	C-N-CA	-7.50	108.91	120.31
1	E	289	LEU	O-C-N	7.50	130.94	122.32
1	B	193	HIS	CG-CD2-NE2	7.50	114.70	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	83	ALA	CA-C-O	-7.49	112.61	120.55
1	F	77	THR	O-C-N	7.49	132.07	122.33
1	B	169	SER	N-CA-CB	-7.49	98.58	110.19
1	C	77	THR	O-C-N	7.49	132.07	122.33
1	D	77	THR	O-C-N	7.49	132.07	122.33
1	D	306	THR	OG1-CB-CG2	7.49	124.28	109.30
1	D	193	HIS	CG-CD2-NE2	7.49	114.69	107.20
1	E	104	ALA	O-C-N	7.49	132.55	122.59
1	A	60	LEU	CA-C-N	7.49	130.81	120.63
1	A	60	LEU	C-N-CA	7.49	130.81	120.63
1	B	83	ALA	CA-C-O	-7.49	112.62	120.55
1	D	430	GLN	OE1-CD-NE2	7.48	130.08	122.60
1	F	57	MET	CA-C-N	-7.48	110.13	120.38
1	F	57	MET	C-N-CA	-7.48	110.13	120.38
1	C	169	SER	N-CA-CB	-7.48	98.59	110.19
1	F	496	ASP	CA-C-N	-7.48	108.94	120.31
1	F	496	ASP	C-N-CA	-7.48	108.94	120.31
1	D	60	LEU	CA-C-N	7.48	130.80	120.63
1	D	60	LEU	C-N-CA	7.48	130.80	120.63
1	F	306	THR	OG1-CB-CG2	7.48	124.26	109.30
1	E	297	HIS	CB-CG-CD2	-7.48	121.48	131.20
1	D	169	SER	N-CA-CB	-7.48	98.60	110.19
1	A	306	THR	OG1-CB-CG2	7.47	124.25	109.30
1	B	104	ALA	O-C-N	7.47	132.53	122.59
1	A	104	ALA	O-C-N	7.47	132.53	122.59
1	F	430	GLN	OE1-CD-NE2	7.47	130.07	122.60
1	C	83	ALA	CA-C-O	-7.47	112.63	120.55
1	C	104	ALA	O-C-N	7.47	132.52	122.59
1	D	104	ALA	O-C-N	7.47	132.52	122.59
1	E	57	MET	CA-C-N	-7.47	110.15	120.38
1	E	57	MET	C-N-CA	-7.47	110.15	120.38
1	F	297	HIS	CB-CG-CD2	-7.47	121.49	131.20
1	C	306	THR	OG1-CB-CG2	7.46	124.23	109.30
1	E	60	LEU	CA-C-N	7.46	130.78	120.63
1	E	60	LEU	C-N-CA	7.46	130.78	120.63
1	A	83	ALA	CA-C-O	-7.46	112.64	120.55
1	E	306	THR	OG1-CB-CG2	7.46	124.22	109.30
1	F	60	LEU	CA-C-N	7.46	130.78	120.63
1	F	60	LEU	C-N-CA	7.46	130.78	120.63
1	A	57	MET	CA-C-N	-7.46	110.17	120.38
1	A	57	MET	C-N-CA	-7.46	110.17	120.38
1	C	57	MET	CA-C-N	-7.46	110.17	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	57	MET	C-N-CA	-7.46	110.17	120.38
1	C	270	VAL	N-CA-CB	-7.45	98.93	111.23
1	B	306	THR	OG1-CB-CG2	7.45	124.20	109.30
1	F	481	PHE	CA-CB-CG	-7.45	106.35	113.80
1	A	396	ASP	CA-CB-CG	7.45	120.05	112.60
1	B	481	PHE	CA-CB-CG	-7.45	106.35	113.80
1	E	396	ASP	CA-CB-CG	7.45	120.05	112.60
1	F	83	ALA	CA-C-O	-7.45	112.66	120.55
1	F	104	ALA	O-C-N	7.45	132.49	122.59
1	A	297	HIS	CB-CG-CD2	-7.44	121.52	131.20
1	B	103	ALA	CB-CA-C	7.44	125.23	110.42
1	D	6	GLY	N-CA-C	-7.44	95.54	113.18
1	C	481	PHE	CA-CB-CG	-7.44	106.36	113.80
1	D	57	MET	CA-C-N	-7.44	110.18	120.38
1	D	57	MET	C-N-CA	-7.44	110.18	120.38
1	D	297	HIS	CB-CG-CD2	-7.44	121.53	131.20
1	D	396	ASP	CA-CB-CG	7.44	120.04	112.60
1	C	6	GLY	N-CA-C	-7.44	95.55	113.18
1	D	32	ASP	N-CA-C	-7.44	103.47	112.54
1	A	6	GLY	N-CA-C	-7.43	95.56	113.18
1	B	57	MET	CA-C-N	-7.43	110.19	120.38
1	B	57	MET	C-N-CA	-7.43	110.19	120.38
1	E	270	VAL	N-CA-CB	-7.43	98.97	111.23
1	A	481	PHE	CA-CB-CG	-7.43	106.37	113.80
1	D	451	ARG	CB-CG-CD	7.43	128.39	111.30
1	E	451	ARG	CB-CG-CD	7.43	128.39	111.30
1	F	6	GLY	N-CA-C	-7.43	95.57	113.18
1	A	270	VAL	N-CA-CB	-7.43	98.97	111.23
1	B	396	ASP	CA-CB-CG	7.43	120.03	112.60
1	C	32	ASP	N-CA-C	-7.43	103.48	112.54
1	A	103	ALA	CB-CA-C	7.42	125.20	110.42
1	E	32	ASP	N-CA-C	-7.42	103.48	112.54
1	E	288	ASP	CA-CB-CG	-7.42	105.18	112.60
1	D	103	ALA	CB-CA-C	7.42	125.19	110.42
1	C	103	ALA	CB-CA-C	7.42	125.19	110.42
1	D	468	ASN	CA-C-O	-7.42	113.27	121.58
1	D	481	PHE	CA-CB-CG	-7.42	106.38	113.80
1	A	32	ASP	N-CA-C	-7.42	103.49	112.54
1	B	6	GLY	N-CA-C	-7.42	95.59	113.18
1	A	451	ARG	CB-CG-CD	7.42	128.36	111.30
1	D	270	VAL	N-CA-CB	-7.42	98.99	111.23
1	F	451	ARG	CB-CG-CD	7.42	128.36	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	297	HIS	CB-CG-CD2	-7.42	121.56	131.20
1	E	6	GLY	N-CA-C	-7.42	95.60	113.18
1	F	103	ALA	CB-CA-C	7.42	125.18	110.42
1	B	451	ARG	CB-CG-CD	7.41	128.35	111.30
1	F	270	VAL	N-CA-CB	-7.41	99.00	111.23
1	B	270	VAL	N-CA-CB	-7.41	99.00	111.23
1	C	451	ARG	CB-CG-CD	7.41	128.35	111.30
1	D	83	ALA	CA-C-O	-7.41	112.69	120.55
1	E	567	ARG	CD-NE-CZ	-7.41	114.03	124.40
1	F	293	GLU	CG-CD-OE2	7.41	135.44	118.40
1	E	103	ALA	CB-CA-C	7.41	125.17	110.42
1	B	32	ASP	N-CA-C	-7.41	103.51	112.54
1	C	361	PHE	O-C-N	7.40	131.46	122.35
1	D	483	CYS	CA-C-N	7.40	129.09	119.84
1	D	483	CYS	C-N-CA	7.40	129.09	119.84
1	C	288	ASP	CA-CB-CG	-7.40	105.20	112.60
1	E	78	ARG	CA-C-O	7.40	129.03	120.00
1	C	293	GLU	CG-CD-OE2	7.40	135.42	118.40
1	C	297	HIS	CB-CG-CD2	-7.40	121.58	131.20
1	F	78	ARG	CA-C-O	7.40	129.03	120.00
1	C	396	ASP	CA-CB-CG	7.40	120.00	112.60
1	D	293	GLU	CG-CD-OE2	7.40	135.41	118.40
1	F	288	ASP	CA-CB-CG	-7.40	105.20	112.60
1	A	293	GLU	CG-CD-OE2	7.40	135.41	118.40
1	F	289	LEU	CA-C-O	-7.40	111.61	120.56
1	F	32	ASP	N-CA-C	-7.39	103.52	112.54
1	F	361	PHE	O-C-N	7.39	131.44	122.35
1	A	468	ASN	CA-C-O	-7.39	113.30	121.58
1	C	289	LEU	CA-C-O	-7.39	111.62	120.56
1	F	468	ASN	CA-C-O	-7.39	113.30	121.58
1	B	289	LEU	CA-C-O	-7.39	111.62	120.56
1	B	567	ARG	CD-NE-CZ	-7.39	114.06	124.40
1	D	92	GLN	CG-CD-OE1	-7.39	106.02	120.80
1	D	288	ASP	CA-CB-CG	-7.39	105.21	112.60
1	A	288	ASP	CA-CB-CG	-7.39	105.21	112.60
1	D	376	ARG	O-C-N	7.39	131.11	122.17
1	E	481	PHE	CA-CB-CG	-7.39	106.41	113.80
1	A	361	PHE	O-C-N	7.39	131.44	122.35
1	B	288	ASP	CA-CB-CG	-7.39	105.21	112.60
1	D	431	TYR	N-CA-C	-7.39	98.51	109.81
1	E	465	THR	CA-C-N	-7.39	107.43	121.54
1	E	465	THR	C-N-CA	-7.39	107.43	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	92	GLN	CG-CD-OE1	-7.38	106.03	120.80
1	C	465	THR	CA-C-N	-7.38	107.44	121.54
1	C	465	THR	C-N-CA	-7.38	107.44	121.54
1	C	92	GLN	CG-CD-OE1	-7.38	106.03	120.80
1	E	293	GLU	CG-CD-OE2	7.38	135.38	118.40
1	A	431	TYR	N-CA-C	-7.38	98.52	109.81
1	C	567	ARG	CD-NE-CZ	-7.38	114.06	124.40
1	D	465	THR	CA-C-N	-7.38	107.44	121.54
1	D	465	THR	C-N-CA	-7.38	107.44	121.54
1	F	396	ASP	CA-CB-CG	7.38	119.98	112.60
1	F	431	TYR	N-CA-C	-7.38	98.52	109.81
1	F	567	ARG	CD-NE-CZ	-7.38	114.07	124.40
1	A	567	ARG	CD-NE-CZ	-7.38	114.07	124.40
1	F	92	GLN	CG-CD-OE1	-7.38	106.04	120.80
1	A	289	LEU	CA-C-O	-7.38	111.63	120.56
1	B	78	ARG	CA-C-O	7.38	129.00	120.00
1	B	431	TYR	N-CA-C	-7.38	98.52	109.81
1	C	78	ARG	CA-C-O	7.38	129.00	120.00
1	C	468	ASN	CA-C-O	-7.38	113.32	121.58
1	B	562	CYS	O-C-N	7.38	130.56	122.15
1	E	562	CYS	O-C-N	7.38	130.56	122.15
1	A	465	THR	CA-C-N	-7.37	107.45	121.54
1	A	465	THR	C-N-CA	-7.37	107.45	121.54
1	B	186	GLU	N-CA-CB	-7.37	99.16	110.44
1	B	468	ASN	CA-C-O	-7.37	113.32	121.58
1	E	468	ASN	CA-C-O	-7.37	113.32	121.58
1	B	36	ASN	CA-CB-CG	-7.37	105.23	112.60
1	B	483	CYS	CA-C-N	7.37	129.05	119.84
1	B	483	CYS	C-N-CA	7.37	129.05	119.84
1	C	186	GLU	N-CA-CB	-7.37	99.16	110.44
1	C	431	TYR	N-CA-C	-7.37	98.53	109.81
1	D	289	LEU	CA-C-O	-7.37	111.64	120.56
1	D	499	ARG	CA-C-O	7.37	128.43	120.10
1	F	499	ARG	CA-C-O	7.37	128.43	120.10
1	B	465	THR	CA-C-N	-7.37	107.47	121.54
1	B	465	THR	C-N-CA	-7.37	107.47	121.54
1	E	431	TYR	N-CA-C	-7.37	98.54	109.81
1	A	376	ARG	O-C-N	7.37	131.08	122.17
1	A	499	ARG	CA-C-O	7.37	128.43	120.10
1	C	11	GLN	CA-C-N	-7.37	110.59	120.54
1	C	11	GLN	C-N-CA	-7.37	110.59	120.54
1	A	78	ARG	CA-C-O	7.37	128.99	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	GLN	CG-CD-OE1	-7.37	106.07	120.80
1	B	293	GLU	CG-CD-OE2	7.37	135.34	118.40
1	B	555	LEU	CA-C-N	-7.37	110.12	121.02
1	B	555	LEU	C-N-CA	-7.37	110.12	121.02
1	D	67	GLU	CB-CA-C	-7.36	94.14	110.19
1	E	92	GLN	CG-CD-OE1	-7.36	106.07	120.80
1	F	465	THR	CA-C-N	-7.36	107.47	121.54
1	F	465	THR	C-N-CA	-7.36	107.47	121.54
1	D	310	GLY	CA-C-N	-7.36	110.97	121.50
1	D	310	GLY	C-N-CA	-7.36	110.97	121.50
1	B	361	PHE	O-C-N	7.36	131.40	122.35
1	A	483	CYS	CA-C-N	7.36	129.04	119.84
1	A	483	CYS	C-N-CA	7.36	129.04	119.84
1	D	361	PHE	O-C-N	7.36	131.40	122.35
1	D	631	PRO	CB-CA-C	-7.36	101.51	112.55
1	E	376	ARG	O-C-N	7.36	131.07	122.17
1	C	483	CYS	CA-C-N	7.36	129.03	119.84
1	C	483	CYS	C-N-CA	7.36	129.03	119.84
1	D	567	ARG	CD-NE-CZ	-7.36	114.10	124.40
1	F	186	GLU	N-CA-CB	-7.36	99.19	110.44
1	A	310	GLY	CA-C-N	-7.35	110.98	121.50
1	A	310	GLY	C-N-CA	-7.35	110.98	121.50
1	E	67	GLU	CB-CA-C	-7.35	94.16	110.19
1	E	310	GLY	CA-C-N	-7.35	110.99	121.50
1	E	310	GLY	C-N-CA	-7.35	110.99	121.50
1	E	483	CYS	CA-C-N	7.35	129.03	119.84
1	E	483	CYS	C-N-CA	7.35	129.03	119.84
1	F	562	CYS	O-C-N	7.35	130.53	122.15
1	A	186	GLU	N-CA-CB	-7.35	99.20	110.44
1	A	562	CYS	O-C-N	7.35	130.53	122.15
1	C	262	TYR	CA-C-O	-7.35	113.49	121.94
1	C	499	ARG	CA-C-O	7.35	128.41	120.10
1	D	78	ARG	CA-C-O	7.35	128.97	120.00
1	D	186	GLU	N-CA-CB	-7.35	99.19	110.44
1	F	483	CYS	CA-C-N	7.35	129.03	119.84
1	F	483	CYS	C-N-CA	7.35	129.03	119.84
1	E	186	GLU	N-CA-CB	-7.35	99.20	110.44
1	F	67	GLU	CB-CA-C	-7.35	94.17	110.19
1	F	376	ARG	O-C-N	7.35	131.06	122.17
1	D	242	PRO	CA-CB-CG	-7.34	90.55	104.50
1	A	36	ASN	CA-CB-CG	-7.34	105.26	112.60
1	C	310	GLY	CA-C-N	-7.34	111.00	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	310	GLY	C-N-CA	-7.34	111.00	121.50
1	E	289	LEU	CA-C-O	-7.34	111.68	120.56
1	A	11	GLN	CA-C-N	-7.34	110.63	120.54
1	A	11	GLN	C-N-CA	-7.34	110.63	120.54
1	B	499	ARG	CA-C-O	7.34	128.39	120.10
1	C	67	GLU	CB-CA-C	-7.34	94.19	110.19
1	D	555	LEU	CA-C-N	-7.34	110.16	121.02
1	D	555	LEU	C-N-CA	-7.34	110.16	121.02
1	E	584	VAL	N-CA-C	-7.34	97.04	107.75
1	F	11	GLN	CA-C-N	-7.34	110.63	120.54
1	F	11	GLN	C-N-CA	-7.34	110.63	120.54
1	C	463	LYS	CB-CA-C	7.34	121.70	110.62
1	E	631	PRO	CB-CA-C	-7.34	101.54	112.55
1	A	631	PRO	CB-CA-C	-7.34	101.54	112.55
1	B	376	ARG	O-C-N	7.34	131.05	122.17
1	A	67	GLU	CB-CA-C	-7.33	94.20	110.19
1	A	463	LYS	CB-CA-C	7.33	121.70	110.62
1	B	242	PRO	CA-CB-CG	-7.33	90.56	104.50
1	F	584	VAL	N-CA-C	-7.33	97.04	107.75
1	A	555	LEU	CA-C-N	-7.33	110.17	121.02
1	A	555	LEU	C-N-CA	-7.33	110.17	121.02
1	B	310	GLY	CA-C-N	-7.33	111.01	121.50
1	B	310	GLY	C-N-CA	-7.33	111.01	121.50
1	E	11	GLN	CA-C-N	-7.33	110.64	120.54
1	E	11	GLN	C-N-CA	-7.33	110.64	120.54
1	F	167	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	A	242	PRO	CA-CB-CG	-7.33	90.57	104.50
1	C	222	TRP	N-CA-C	7.33	119.91	111.11
1	C	562	CYS	O-C-N	7.33	130.51	122.15
1	E	361	PHE	O-C-N	7.33	131.37	122.35
1	E	463	LYS	CB-CA-C	7.33	121.69	110.62
1	B	463	LYS	CB-CA-C	7.33	121.69	110.62
1	D	584	VAL	N-CA-C	-7.33	97.05	107.75
1	E	451	ARG	CA-C-N	-7.33	110.48	122.57
1	E	451	ARG	C-N-CA	-7.33	110.48	122.57
1	F	36	ASN	CA-CB-CG	-7.33	105.27	112.60
1	B	67	GLU	CB-CA-C	-7.33	94.22	110.19
1	C	48	ASP	CA-C-N	-7.33	112.26	123.47
1	C	48	ASP	C-N-CA	-7.33	112.26	123.47
1	D	52	ALA	N-CA-C	-7.33	102.90	111.03
1	E	36	ASN	CA-CB-CG	-7.33	105.27	112.60
1	E	618	ASP	N-CA-C	-7.33	98.67	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	463	LYS	CB-CA-C	7.33	121.68	110.62
1	F	631	PRO	CB-CA-C	-7.33	101.56	112.55
1	A	48	ASP	CA-C-N	-7.32	112.26	123.47
1	A	48	ASP	C-N-CA	-7.32	112.26	123.47
1	A	584	VAL	N-CA-C	-7.32	97.06	107.75
1	B	11	GLN	CA-C-N	-7.32	110.65	120.54
1	B	11	GLN	C-N-CA	-7.32	110.65	120.54
1	D	36	ASN	CA-CB-CG	-7.32	105.28	112.60
1	D	48	ASP	CA-C-N	-7.32	112.27	123.47
1	D	48	ASP	C-N-CA	-7.32	112.27	123.47
1	E	222	TRP	N-CA-C	7.32	119.90	111.11
1	E	499	ARG	CA-C-O	7.32	128.37	120.10
1	E	555	LEU	CA-C-N	-7.32	110.18	121.02
1	E	555	LEU	C-N-CA	-7.32	110.18	121.02
1	F	555	LEU	CA-C-N	-7.32	110.18	121.02
1	F	555	LEU	C-N-CA	-7.32	110.18	121.02
1	D	262	TYR	CA-C-O	-7.32	113.52	121.94
1	D	562	CYS	O-C-N	7.32	130.50	122.15
1	E	242	PRO	CA-CB-CG	-7.32	90.59	104.50
1	F	310	GLY	CA-C-N	-7.32	111.03	121.50
1	F	310	GLY	C-N-CA	-7.32	111.03	121.50
1	C	451	ARG	CA-C-N	-7.32	110.49	122.57
1	C	451	ARG	C-N-CA	-7.32	110.49	122.57
1	C	631	PRO	CB-CA-C	-7.32	101.57	112.55
1	D	11	GLN	CA-C-N	-7.32	110.66	120.54
1	D	11	GLN	C-N-CA	-7.32	110.66	120.54
1	D	222	TRP	N-CA-C	7.32	119.89	111.11
1	D	463	LYS	CB-CA-C	7.32	121.67	110.62
1	B	48	ASP	CA-C-N	-7.32	112.28	123.47
1	B	48	ASP	C-N-CA	-7.32	112.28	123.47
1	B	584	VAL	N-CA-C	-7.32	97.07	107.75
1	C	36	ASN	CA-CB-CG	-7.32	105.28	112.60
1	E	489	ASN	CA-CB-CG	-7.32	105.28	112.60
1	C	584	VAL	N-CA-C	-7.31	97.07	107.75
1	B	618	ASP	N-CA-C	-7.31	98.69	110.32
1	C	242	PRO	CA-CB-CG	-7.31	90.61	104.50
1	C	555	LEU	CA-C-N	-7.31	110.20	121.02
1	C	555	LEU	C-N-CA	-7.31	110.20	121.02
1	F	262	TYR	CA-C-O	-7.31	113.53	121.94
1	E	434	ILE	O-C-N	7.31	131.49	121.84
1	F	48	ASP	CA-C-N	-7.31	112.29	123.47
1	F	48	ASP	C-N-CA	-7.31	112.29	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	225	HIS	N-CA-C	-7.31	103.34	111.82
1	B	631	PRO	CB-CA-C	-7.31	101.59	112.55
1	C	52	ALA	N-CA-C	-7.31	102.92	111.03
1	D	451	ARG	CA-C-N	-7.31	110.51	122.57
1	D	451	ARG	C-N-CA	-7.31	110.51	122.57
1	F	52	ALA	N-CA-C	-7.31	102.92	111.03
1	F	451	ARG	CA-C-N	-7.31	110.51	122.57
1	F	451	ARG	C-N-CA	-7.31	110.51	122.57
1	E	48	ASP	CA-C-N	-7.31	112.29	123.47
1	E	48	ASP	C-N-CA	-7.31	112.29	123.47
1	A	222	TRP	N-CA-C	7.30	119.88	111.11
1	A	618	ASP	N-CA-C	-7.30	98.71	110.32
1	B	451	ARG	CA-C-N	-7.30	110.52	122.57
1	B	451	ARG	C-N-CA	-7.30	110.52	122.57
1	D	618	ASP	N-CA-C	-7.30	98.71	110.32
1	A	262	TYR	CA-C-O	-7.30	113.54	121.94
1	B	167	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	B	262	TYR	CA-C-O	-7.30	113.54	121.94
1	D	377	ASP	O-C-N	7.30	128.58	121.28
1	E	80	ARG	CA-C-N	-7.30	110.38	120.38
1	E	80	ARG	C-N-CA	-7.30	110.38	120.38
1	F	242	PRO	CA-CB-CG	-7.30	90.62	104.50
1	F	333	TYR	O-C-N	-7.30	112.30	122.37
1	C	225	HIS	N-CA-C	-7.30	103.35	111.82
1	C	376	ARG	O-C-N	7.30	131.00	122.17
1	E	52	ALA	N-CA-C	-7.30	102.93	111.03
1	F	222	TRP	N-CA-C	7.30	119.87	111.11
1	F	618	ASP	N-CA-C	-7.30	98.71	110.32
1	A	225	HIS	N-CA-C	-7.30	103.36	111.82
1	C	618	ASP	N-CA-C	-7.30	98.72	110.32
1	A	451	ARG	CA-C-N	-7.29	110.53	122.57
1	A	451	ARG	C-N-CA	-7.29	110.53	122.57
1	E	333	TYR	O-C-N	-7.29	112.31	122.37
1	E	377	ASP	O-C-N	7.29	128.57	121.28
1	D	167	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	A	52	ALA	N-CA-C	-7.29	102.94	111.03
1	A	167	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	B	580	PHE	N-CA-C	-7.29	99.67	110.46
1	C	333	TYR	O-C-N	-7.29	112.31	122.37
1	D	434	ILE	O-C-N	7.29	131.46	121.84
1	C	278	GLU	O-C-N	7.29	131.48	123.10
1	A	333	TYR	O-C-N	-7.29	112.32	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	HIS	N-CA-C	-7.29	103.37	111.82
1	C	489	ASN	CA-CB-CG	-7.29	105.31	112.60
1	D	542	GLN	N-CA-CB	-7.29	98.99	110.28
1	E	107	ARG	CA-C-O	7.29	130.93	120.51
1	E	517	GLU	CG-CD-OE2	7.29	135.16	118.40
1	F	434	ILE	O-C-N	7.29	131.46	121.84
1	B	52	ALA	N-CA-C	-7.28	102.94	111.03
1	C	434	ILE	O-C-N	7.28	131.46	121.84
1	E	120	TYR	CB-CA-C	-7.28	99.44	110.88
1	F	80	ARG	CA-C-N	-7.28	110.40	120.38
1	F	80	ARG	C-N-CA	-7.28	110.40	120.38
1	E	225	HIS	N-CA-C	-7.28	103.37	111.82
1	A	517	GLU	CG-CD-OE2	7.28	135.15	118.40
1	B	222	TRP	N-CA-C	7.28	119.85	111.11
1	B	517	GLU	CG-CD-OE2	7.28	135.14	118.40
1	D	107	ARG	CA-C-O	7.28	130.92	120.51
1	E	262	TYR	CA-C-O	-7.28	113.57	121.94
1	D	225	HIS	N-CA-C	-7.28	103.38	111.82
1	F	517	GLU	CG-CD-OE2	7.28	135.14	118.40
1	F	580	PHE	N-CA-C	-7.28	99.69	110.46
1	A	489	ASN	CA-CB-CG	-7.28	105.32	112.60
1	B	489	ASN	CA-CB-CG	-7.28	105.32	112.60
1	B	542	GLN	N-CA-CB	-7.28	99.00	110.28
1	C	107	ARG	CA-C-O	7.28	130.92	120.51
1	A	377	ASP	O-C-N	7.28	128.56	121.28
1	A	434	ILE	O-C-N	7.28	131.44	121.84
1	A	542	GLN	N-CA-CB	-7.28	99.00	110.28
1	B	636	ILE	CB-CA-C	7.28	121.96	112.14
1	F	94	LYS	CB-CA-C	7.28	123.86	110.11
1	C	517	GLU	CG-CD-OE2	7.27	135.13	118.40
1	F	542	GLN	N-CA-CB	-7.27	99.01	110.28
1	B	94	LYS	CB-CA-C	7.27	123.85	110.11
1	B	333	TYR	O-C-N	-7.27	112.34	122.37
1	C	120	TYR	CB-CA-C	-7.27	99.47	110.88
1	D	489	ASN	CA-CB-CG	-7.27	105.33	112.60
1	D	580	PHE	N-CA-C	-7.27	99.70	110.46
1	F	47	ASN	N-CA-C	-7.27	104.50	113.15
1	D	333	TYR	O-C-N	-7.27	112.34	122.37
1	E	167	ASN	OD1-CG-ND2	-7.27	115.33	122.60
1	A	80	ARG	CA-C-N	-7.26	110.43	120.38
1	A	80	ARG	C-N-CA	-7.26	110.43	120.38
1	A	107	ARG	CA-C-O	7.26	130.90	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	580	PHE	N-CA-C	-7.26	99.71	110.46
1	C	580	PHE	N-CA-C	-7.26	99.71	110.46
1	D	94	LYS	CB-CA-C	7.26	123.84	110.11
1	F	382	ARG	N-CA-CB	-7.26	99.41	110.16
1	A	120	TYR	CB-CA-C	-7.26	99.48	110.88
1	B	278	GLU	O-C-N	7.26	131.45	123.10
1	B	80	ARG	CA-C-N	-7.26	110.43	120.38
1	B	80	ARG	C-N-CA	-7.26	110.43	120.38
1	C	167	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	D	80	ARG	CA-C-N	-7.26	110.44	120.38
1	D	80	ARG	C-N-CA	-7.26	110.44	120.38
1	A	636	ILE	CB-CA-C	7.26	121.94	112.14
1	C	47	ASN	N-CA-C	-7.26	104.51	113.15
1	A	94	LYS	CB-CA-C	7.26	123.83	110.11
1	A	278	GLU	O-C-N	7.26	131.44	123.10
1	C	94	LYS	CB-CA-C	7.26	123.83	110.11
1	D	517	GLU	CG-CD-OE2	7.26	135.09	118.40
1	E	94	LYS	CB-CA-C	7.26	123.82	110.11
1	F	120	TYR	CB-CA-C	-7.26	99.49	110.88
1	E	580	PHE	N-CA-C	-7.25	99.72	110.46
1	D	68	GLN	CG-CD-OE1	7.25	135.31	120.80
1	D	120	TYR	CB-CA-C	-7.25	99.49	110.88
1	E	382	ARG	N-CA-CB	-7.25	99.42	110.16
1	E	636	ILE	CB-CA-C	7.25	121.93	112.14
1	B	120	TYR	CB-CA-C	-7.25	99.50	110.88
1	E	68	GLN	CG-CD-OE1	7.25	135.30	120.80
1	F	239	TRP	CA-C-N	-7.25	110.12	122.67
1	F	239	TRP	C-N-CA	-7.25	110.12	122.67
1	F	278	GLU	O-C-N	7.25	131.44	123.10
1	D	278	GLU	O-C-N	7.25	131.44	123.10
1	F	489	ASN	CA-CB-CG	-7.25	105.35	112.60
1	C	68	GLN	CG-CD-OE1	7.25	135.29	120.80
1	F	416	VAL	CA-CB-CG1	7.25	122.72	110.40
1	C	542	GLN	N-CA-CB	-7.25	99.05	110.28
1	E	542	GLN	N-CA-CB	-7.25	99.05	110.28
1	A	47	ASN	N-CA-C	-7.25	104.53	113.15
1	C	80	ARG	CA-C-N	-7.25	110.45	120.38
1	C	80	ARG	C-N-CA	-7.25	110.45	120.38
1	C	636	ILE	CB-CA-C	7.24	121.92	112.14
1	E	239	TRP	CA-C-N	-7.24	110.14	122.67
1	E	239	TRP	C-N-CA	-7.24	110.14	122.67
1	F	636	ILE	CB-CA-C	7.24	121.92	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	ARG	CA-C-O	7.24	130.87	120.51
1	C	416	VAL	CA-CB-CG1	7.24	122.71	110.40
1	B	261	SER	O-C-N	7.24	132.15	123.24
1	A	68	GLN	CG-CD-OE1	7.24	135.28	120.80
1	A	239	TRP	CA-C-N	-7.24	110.15	122.67
1	A	239	TRP	C-N-CA	-7.24	110.15	122.67
1	B	68	GLN	CG-CD-OE1	7.24	135.28	120.80
1	F	272	PRO	CA-CB-CG	-7.24	90.75	104.50
1	A	382	ARG	N-CA-CB	-7.24	99.45	110.16
1	F	68	GLN	CG-CD-OE1	7.24	135.27	120.80
1	F	107	ARG	CA-C-O	7.24	130.86	120.51
1	D	239	TRP	CA-C-N	-7.23	110.16	122.67
1	D	239	TRP	C-N-CA	-7.23	110.16	122.67
1	D	47	ASN	N-CA-C	-7.23	104.54	113.15
1	E	143	HIS	CA-C-O	-7.23	110.48	119.38
1	B	143	HIS	CA-C-O	-7.23	110.49	119.38
1	C	245	GLU	CG-CD-OE2	7.23	135.03	118.40
1	C	382	ARG	N-CA-CB	-7.23	99.46	110.16
1	E	176	ASN	CA-C-O	-7.23	110.17	120.51
1	B	377	ASP	O-C-N	7.23	128.51	121.28
1	D	76	ASN	CB-CG-OD1	-7.23	106.34	120.80
1	B	434	ILE	O-C-N	7.23	131.38	121.84
1	C	361	PHE	CA-C-N	-7.23	112.22	122.63
1	C	361	PHE	C-N-CA	-7.23	112.22	122.63
1	D	143	HIS	CA-C-O	-7.23	110.49	119.38
1	D	272	PRO	CA-CB-CG	-7.23	90.77	104.50
1	D	636	ILE	CB-CA-C	7.23	121.89	112.14
1	A	143	HIS	CA-C-O	-7.22	110.49	119.38
1	A	176	ASN	CA-C-O	-7.22	110.18	120.51
1	A	361	PHE	CA-C-N	-7.22	112.23	122.63
1	A	361	PHE	C-N-CA	-7.22	112.23	122.63
1	B	47	ASN	N-CA-C	-7.22	104.55	113.15
1	B	272	PRO	CA-CB-CG	-7.22	90.77	104.50
1	B	416	VAL	CA-CB-CG1	7.22	122.68	110.40
1	D	171	THR	CA-CB-OG1	-7.22	98.76	109.60
1	E	245	GLU	CG-CD-OE2	7.22	135.01	118.40
1	A	245	GLU	CG-CD-OE2	7.22	135.01	118.40
1	C	239	TRP	CA-C-N	-7.22	110.17	122.67
1	C	239	TRP	C-N-CA	-7.22	110.17	122.67
1	C	369	GLU	CA-C-O	-7.22	108.80	120.65
1	D	295	ARG	CB-CA-C	7.22	122.78	110.79
1	C	377	ASP	O-C-N	7.22	128.50	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	176	ASN	CA-C-O	-7.22	110.19	120.51
1	F	143	HIS	CA-C-O	-7.22	110.50	119.38
1	F	377	ASP	O-C-N	7.22	128.50	121.28
1	A	416	VAL	CA-CB-CG1	7.22	122.67	110.40
1	E	278	GLU	O-C-N	7.22	131.40	123.10
1	B	171	THR	CA-CB-OG1	-7.22	98.78	109.60
1	B	239	TRP	CA-C-N	-7.22	110.19	122.67
1	B	239	TRP	C-N-CA	-7.22	110.19	122.67
1	F	171	THR	CA-CB-OG1	-7.22	98.78	109.60
1	C	261	SER	O-C-N	7.21	132.11	123.24
1	D	245	GLU	CG-CD-OE2	7.21	134.99	118.40
1	D	382	ARG	N-CA-CB	-7.21	99.48	110.16
1	E	361	PHE	CA-C-N	-7.21	112.24	122.63
1	E	361	PHE	C-N-CA	-7.21	112.24	122.63
1	F	361	PHE	CA-C-N	-7.21	112.24	122.63
1	F	361	PHE	C-N-CA	-7.21	112.24	122.63
1	A	261	SER	O-C-N	7.21	132.11	123.24
1	A	272	PRO	CA-CB-CG	-7.21	90.80	104.50
1	B	369	GLU	CA-C-O	-7.21	108.82	120.65
1	D	361	PHE	CA-C-N	-7.21	112.25	122.63
1	D	361	PHE	C-N-CA	-7.21	112.25	122.63
1	D	369	GLU	CA-C-O	-7.21	108.82	120.65
1	E	416	VAL	CA-CB-CG1	7.21	122.66	110.40
1	A	171	THR	CA-CB-OG1	-7.21	98.78	109.60
1	B	295	ARG	CB-CA-C	7.21	122.76	110.79
1	A	76	ASN	CB-CG-OD1	-7.21	106.38	120.80
1	C	272	PRO	CA-CB-CG	-7.21	90.81	104.50
1	D	632	ASP	CB-CA-C	7.21	121.67	110.14
1	E	171	THR	CA-CB-OG1	-7.21	98.79	109.60
1	B	245	GLU	CG-CD-OE2	7.21	134.97	118.40
1	B	382	ARG	N-CA-CB	-7.21	99.50	110.16
1	C	171	THR	CA-CB-OG1	-7.21	98.79	109.60
1	D	176	ASN	CA-C-O	-7.21	110.21	120.51
1	D	416	VAL	CA-CB-CG1	7.21	122.65	110.40
1	E	409	SER	N-CA-CB	-7.21	98.32	109.34
1	F	76	ASN	CB-CG-OD1	-7.21	106.39	120.80
1	F	245	GLU	CG-CD-OE2	7.20	134.97	118.40
1	C	176	ASN	CA-C-O	-7.20	110.21	120.51
1	C	30	LEU	N-CA-C	-7.20	102.62	111.33
1	C	76	ASN	CB-CG-OD1	-7.20	106.40	120.80
1	E	76	ASN	CB-CG-OD1	-7.20	106.40	120.80
1	D	397	SER	N-CA-CB	-7.20	99.43	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	261	SER	O-C-N	7.20	132.09	123.24
1	F	30	LEU	N-CA-C	-7.20	102.62	111.33
1	A	369	GLU	CA-C-O	-7.20	108.85	120.65
1	C	414	ASN	OD1-CG-ND2	7.20	129.80	122.60
1	E	272	PRO	CA-CB-CG	-7.20	90.83	104.50
1	B	632	ASP	CB-CA-C	7.19	121.65	110.14
1	F	76	ASN	N-CA-C	7.19	119.51	109.15
1	F	176	ASN	CA-C-O	-7.19	110.22	120.51
1	B	76	ASN	CB-CG-OD1	-7.19	106.42	120.80
1	B	361	PHE	CA-C-N	-7.19	112.27	122.63
1	B	361	PHE	C-N-CA	-7.19	112.27	122.63
1	A	632	ASP	CB-CA-C	7.19	121.64	110.14
1	B	417	ALA	N-CA-C	7.19	121.28	109.06
1	A	295	ARG	CB-CA-C	7.19	122.72	110.79
1	C	295	ARG	CB-CA-C	7.19	122.72	110.79
1	A	30	LEU	N-CA-C	-7.19	102.63	111.33
1	D	409	SER	N-CA-CB	-7.19	98.34	109.34
1	E	369	GLU	CA-C-O	-7.19	108.86	120.65
1	E	414	ASN	OD1-CG-ND2	7.19	129.79	122.60
1	E	632	ASP	CB-CA-C	7.19	121.64	110.14
1	C	143	HIS	CA-C-O	-7.19	110.54	119.38
1	E	47	ASN	N-CA-C	-7.19	104.60	113.15
1	E	398	PHE	O-C-N	7.19	129.58	121.53
1	A	417	ALA	N-CA-C	7.18	121.27	109.06
1	B	398	PHE	O-C-N	7.18	129.58	121.53
1	B	409	SER	N-CA-CB	-7.18	98.35	109.34
1	D	279	ASP	N-CA-C	-7.18	99.25	109.96
1	C	76	ASN	N-CA-C	7.18	119.49	109.15
1	E	316	ARG	NH1-CZ-NH2	-7.18	109.96	119.30
1	C	397	SER	N-CA-CB	-7.18	99.46	110.44
1	C	606	HIS	N-CA-C	7.18	131.10	111.00
1	C	632	ASP	CB-CA-C	7.18	121.63	110.14
1	D	261	SER	O-C-N	7.18	132.07	123.24
1	F	261	SER	O-C-N	7.18	132.07	123.24
1	F	417	ALA	N-CA-C	7.18	121.27	109.06
1	E	417	ALA	N-CA-C	7.18	121.26	109.06
1	F	632	ASP	CB-CA-C	7.18	121.62	110.14
1	A	376	ARG	CB-CA-C	-7.18	98.73	110.79
1	A	397	SER	N-CA-CB	-7.18	99.46	110.44
1	A	409	SER	N-CA-CB	-7.18	98.36	109.34
1	B	72	TYR	CA-C-N	-7.18	110.29	122.92
1	B	72	TYR	C-N-CA	-7.18	110.29	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	376	ARG	CB-CA-C	-7.18	98.73	110.79
1	A	72	TYR	CA-C-N	-7.17	110.29	122.92
1	A	72	TYR	C-N-CA	-7.17	110.29	122.92
1	C	417	ALA	N-CA-C	7.17	121.26	109.06
1	E	156	SER	N-CA-CB	7.17	120.89	110.20
1	B	606	HIS	N-CA-C	7.17	131.08	111.00
1	C	376	ARG	CB-CA-C	-7.17	98.74	110.79
1	D	72	TYR	CA-C-N	-7.17	110.30	122.92
1	D	72	TYR	C-N-CA	-7.17	110.30	122.92
1	E	295	ARG	CB-CA-C	7.17	122.69	110.79
1	F	409	SER	N-CA-CB	-7.17	98.37	109.34
1	B	216	LYS	N-CA-CB	7.17	120.84	109.51
1	C	573	SER	CA-CB-OG	-7.17	96.76	111.10
1	E	606	HIS	N-CA-C	7.17	131.08	111.00
1	B	76	ASN	N-CA-C	7.17	119.47	109.15
1	B	279	ASP	N-CA-C	-7.17	99.28	109.96
1	B	376	ARG	CB-CA-C	-7.17	98.75	110.79
1	C	232	ASP	CA-C-O	-7.17	112.89	120.63
1	E	376	ARG	CB-CA-C	-7.17	98.75	110.79
1	F	295	ARG	CB-CA-C	7.17	122.69	110.79
1	F	573	SER	CA-CB-OG	-7.17	96.76	111.10
1	A	232	ASP	CA-C-O	-7.17	112.89	120.63
1	A	279	ASP	N-CA-C	-7.17	99.28	109.96
1	A	606	HIS	N-CA-C	7.17	131.06	111.00
1	C	568	MET	CA-C-O	-7.17	110.61	119.28
1	E	30	LEU	N-CA-C	-7.17	102.66	111.33
1	E	279	ASP	N-CA-C	-7.17	99.28	109.96
1	A	398	PHE	O-C-N	7.17	129.56	121.53
1	B	170	PHE	O-C-N	7.16	132.12	122.59
1	C	409	SER	N-CA-CB	-7.16	98.38	109.34
1	E	72	TYR	CA-C-N	-7.16	110.31	122.92
1	E	72	TYR	C-N-CA	-7.16	110.31	122.92
1	F	156	SER	N-CA-CB	7.16	120.87	110.20
1	A	568	MET	CA-C-O	-7.16	110.61	119.28
1	B	397	SER	N-CA-CB	-7.16	99.48	110.44
1	B	568	MET	CA-C-O	-7.16	110.61	119.28
1	F	369	GLU	CA-C-O	-7.16	108.90	120.65
1	A	76	ASN	N-CA-C	7.16	119.46	109.15
1	B	156	SER	N-CA-CB	7.16	120.87	110.20
1	B	414	ASN	OD1-CG-ND2	7.16	129.76	122.60
1	D	376	ARG	CB-CA-C	-7.16	98.76	110.79
1	D	417	ALA	N-CA-C	7.16	121.23	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	573	SER	CA-CB-OG	-7.16	96.78	111.10
1	E	216	LYS	N-CA-CB	7.16	120.82	109.51
1	E	573	SER	CA-CB-OG	-7.16	96.78	111.10
1	A	573	SER	CA-CB-OG	-7.16	96.78	111.10
1	C	96	TRP	CB-CA-C	7.16	122.62	110.74
1	C	398	PHE	O-C-N	7.16	129.55	121.53
1	D	30	LEU	N-CA-C	-7.16	102.67	111.33
1	D	156	SER	N-CA-CB	7.16	120.87	110.20
1	D	216	LYS	N-CA-CB	7.16	120.82	109.51
1	F	606	HIS	N-CA-C	7.16	131.04	111.00
1	A	156	SER	N-CA-CB	7.16	120.86	110.20
1	E	232	ASP	CA-C-O	-7.16	112.90	120.63
1	F	170	PHE	O-C-N	7.16	132.11	122.59
1	A	316	ARG	NH1-CZ-NH2	-7.16	110.00	119.30
1	B	232	ASP	CA-C-O	-7.16	112.90	120.63
1	D	316	ARG	NH1-CZ-NH2	-7.16	110.00	119.30
1	F	72	TYR	CA-C-N	-7.16	110.33	122.92
1	F	72	TYR	C-N-CA	-7.16	110.33	122.92
1	D	76	ASN	N-CA-C	7.15	119.45	109.15
1	D	568	MET	CA-C-O	-7.15	110.62	119.28
1	A	216	LYS	N-CA-CB	7.15	120.81	109.51
1	C	72	TYR	CA-C-N	-7.15	110.33	122.92
1	C	72	TYR	C-N-CA	-7.15	110.33	122.92
1	D	398	PHE	O-C-N	7.15	129.54	121.53
1	D	414	ASN	OD1-CG-ND2	7.15	129.75	122.60
1	D	606	HIS	N-CA-C	7.15	131.03	111.00
1	E	71	TRP	CA-C-N	-7.15	109.48	121.64
1	E	71	TRP	C-N-CA	-7.15	109.48	121.64
1	F	96	TRP	CB-CA-C	7.15	122.61	110.74
1	C	279	ASP	N-CA-C	-7.15	99.31	109.96
1	C	305	ILE	CA-CB-CG1	-7.15	98.24	110.40
1	C	316	ARG	NH1-CZ-NH2	-7.15	110.00	119.30
1	D	170	PHE	O-C-N	7.15	132.10	122.59
1	E	397	SER	N-CA-CB	-7.15	99.50	110.44
1	F	397	SER	N-CA-CB	-7.15	99.50	110.44
1	A	96	TRP	CB-CA-C	7.15	122.61	110.74
1	B	316	ARG	NH1-CZ-NH2	-7.15	110.01	119.30
1	B	573	SER	CA-CB-OG	-7.15	96.80	111.10
1	D	96	TRP	CB-CA-C	7.15	122.61	110.74
1	E	76	ASN	N-CA-C	7.15	119.44	109.15
1	B	30	LEU	N-CA-C	-7.15	102.68	111.33
1	B	577	GLY	CA-C-N	-7.15	110.63	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	577	GLY	C-N-CA	-7.15	110.63	122.21
1	F	568	MET	CA-C-O	-7.15	110.63	119.28
1	A	170	PHE	O-C-N	7.14	132.09	122.59
1	A	414	ASN	OD1-CG-ND2	7.14	129.75	122.60
1	E	96	TRP	CB-CA-C	7.14	122.60	110.74
1	F	279	ASP	N-CA-C	-7.14	99.31	109.96
1	E	79	GLN	OE1-CD-NE2	7.14	129.74	122.60
1	F	216	LYS	N-CA-CB	7.14	120.80	109.51
1	F	367	VAL	CB-CA-C	7.14	122.48	112.05
1	F	398	PHE	O-C-N	7.14	129.53	121.53
1	D	71	TRP	CA-C-N	-7.14	109.47	121.89
1	D	71	TRP	C-N-CA	-7.14	109.47	121.89
1	F	577	GLY	CA-C-N	-7.14	110.64	122.21
1	F	577	GLY	C-N-CA	-7.14	110.64	122.21
1	B	79	GLN	OE1-CD-NE2	7.14	129.74	122.60
1	B	305	ILE	CA-CB-CG1	-7.14	98.26	110.40
1	D	232	ASP	CA-C-O	-7.14	112.92	120.63
1	D	305	ILE	CA-CB-CG1	-7.14	98.26	110.40
1	D	577	GLY	CA-C-N	-7.14	110.64	122.21
1	D	577	GLY	C-N-CA	-7.14	110.64	122.21
1	F	316	ARG	NH1-CZ-NH2	-7.14	110.02	119.30
1	E	305	ILE	CA-CB-CG1	-7.14	98.27	110.40
1	C	79	GLN	OE1-CD-NE2	7.13	129.73	122.60
1	E	577	GLY	CA-C-N	-7.13	110.65	122.21
1	E	577	GLY	C-N-CA	-7.13	110.65	122.21
1	B	96	TRP	CB-CA-C	7.13	122.58	110.74
1	C	577	GLY	CA-C-N	-7.13	110.66	122.21
1	C	577	GLY	C-N-CA	-7.13	110.66	122.21
1	F	232	ASP	CA-C-O	-7.13	112.93	120.63
1	A	305	ILE	CA-CB-CG1	-7.13	98.28	110.40
1	C	216	LYS	N-CA-CB	7.13	120.78	109.51
1	E	170	PHE	O-C-N	7.13	132.08	122.59
1	C	170	PHE	O-C-N	7.13	132.07	122.59
1	C	477	THR	CB-CA-C	7.13	122.57	110.81
1	A	71	TRP	CA-C-N	-7.13	109.49	121.89
1	A	71	TRP	C-N-CA	-7.13	109.49	121.89
1	B	71	TRP	CA-C-N	-7.13	109.49	121.89
1	B	71	TRP	C-N-CA	-7.13	109.49	121.89
1	F	305	ILE	CA-CB-CG1	-7.13	98.28	110.40
1	A	577	GLY	CA-C-N	-7.12	110.67	122.21
1	A	577	GLY	C-N-CA	-7.12	110.67	122.21
1	F	71	TRP	CA-C-N	-7.12	109.49	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	71	TRP	C-N-CA	-7.12	109.49	121.89
1	C	71	TRP	CA-C-N	-7.12	109.50	121.89
1	C	71	TRP	C-N-CA	-7.12	109.50	121.89
1	B	367	VAL	CB-CA-C	7.12	122.44	112.05
1	C	156	SER	N-CA-CB	7.12	120.80	110.20
1	E	568	MET	CA-C-O	-7.11	110.67	119.28
1	C	367	VAL	CB-CA-C	7.11	122.43	112.05
1	A	367	VAL	CB-CA-C	7.11	122.43	112.05
1	E	367	VAL	CB-CA-C	7.11	122.43	112.05
1	A	477	THR	CB-CA-C	7.11	122.54	110.81
1	F	414	ASN	OD1-CG-ND2	7.11	129.71	122.60
1	F	470	ASN	O-C-N	7.11	131.06	122.75
1	C	73	SER	CA-C-N	7.10	135.23	122.38
1	C	73	SER	C-N-CA	7.10	135.23	122.38
1	F	531	PRO	CA-C-O	-7.10	112.30	122.31
1	A	79	GLN	OE1-CD-NE2	7.10	129.70	122.60
1	D	443	ILE	CA-C-N	-7.10	110.35	123.05
1	D	443	ILE	C-N-CA	-7.10	110.35	123.05
1	E	596	HIS	CA-C-O	-7.10	108.73	120.80
1	B	121	VAL	N-CA-CB	-7.09	100.89	110.54
1	B	477	THR	CB-CA-C	7.09	122.52	110.81
1	D	367	VAL	CB-CA-C	7.09	122.41	112.05
1	A	73	SER	CA-C-N	7.09	135.22	122.38
1	A	73	SER	C-N-CA	7.09	135.22	122.38
1	A	443	ILE	CA-C-N	-7.09	110.36	123.05
1	A	443	ILE	C-N-CA	-7.09	110.36	123.05
1	B	344	HIS	CB-CG-ND1	-7.09	112.06	122.70
1	F	344	HIS	CB-CG-ND1	-7.09	112.06	122.70
1	A	121	VAL	N-CA-CB	-7.09	100.90	110.54
1	E	477	THR	CB-CA-C	7.09	122.51	110.81
1	E	510	GLN	CA-C-N	-7.09	109.94	122.07
1	E	510	GLN	C-N-CA	-7.09	109.94	122.07
1	F	403	HIS	N-CA-C	-7.09	103.16	111.03
1	F	443	ILE	CA-C-N	-7.09	110.36	123.05
1	F	443	ILE	C-N-CA	-7.09	110.36	123.05
1	C	443	ILE	CA-C-N	-7.09	110.36	123.05
1	C	443	ILE	C-N-CA	-7.09	110.36	123.05
1	D	79	GLN	OE1-CD-NE2	7.09	129.69	122.60
1	E	73	SER	CA-C-N	7.09	135.21	122.38
1	E	73	SER	C-N-CA	7.09	135.21	122.38
1	F	400	PRO	CA-C-N	-7.09	110.59	122.64
1	F	400	PRO	C-N-CA	-7.09	110.59	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	477	THR	CB-CA-C	7.09	122.50	110.81
1	C	344	HIS	CB-CG-ND1	-7.08	112.07	122.70
1	D	174	LYS	CA-C-O	7.08	128.94	121.15
1	D	596	HIS	CA-C-O	-7.08	108.76	120.80
1	F	73	SER	CA-C-N	7.08	135.20	122.38
1	F	73	SER	C-N-CA	7.08	135.20	122.38
1	B	73	SER	CA-C-N	7.08	135.20	122.38
1	B	73	SER	C-N-CA	7.08	135.20	122.38
1	A	596	HIS	CA-C-O	-7.08	108.76	120.80
1	E	443	ILE	CA-C-N	-7.08	110.38	123.05
1	E	443	ILE	C-N-CA	-7.08	110.38	123.05
1	F	79	GLN	OE1-CD-NE2	7.08	129.68	122.60
1	F	596	HIS	CA-C-O	-7.08	108.77	120.80
1	B	596	HIS	CA-C-O	-7.08	108.77	120.80
1	D	121	VAL	N-CA-CB	-7.08	100.92	110.54
1	D	477	THR	CB-CA-C	7.08	122.49	110.81
1	F	121	VAL	N-CA-CB	-7.08	100.92	110.54
1	C	596	HIS	CA-C-O	-7.07	108.77	120.80
1	D	531	PRO	CA-C-O	-7.07	112.34	122.31
1	E	218	GLU	O-C-N	7.07	130.21	122.15
1	A	403	HIS	N-CA-C	-7.07	103.18	111.03
1	E	250	ARG	CG-CD-NE	-7.07	96.44	112.00
1	D	470	ASN	O-C-N	7.07	131.02	122.75
1	D	510	GLN	CA-C-N	-7.07	109.98	122.07
1	D	510	GLN	C-N-CA	-7.07	109.98	122.07
1	A	470	ASN	O-C-N	7.07	131.02	122.75
1	A	531	PRO	CA-C-O	-7.07	112.34	122.31
1	B	443	ILE	CA-C-N	-7.07	110.40	123.05
1	B	443	ILE	C-N-CA	-7.07	110.40	123.05
1	D	400	PRO	CA-C-N	-7.07	110.62	122.64
1	D	400	PRO	C-N-CA	-7.07	110.62	122.64
1	A	510	GLN	CA-C-N	-7.07	109.99	122.07
1	A	510	GLN	C-N-CA	-7.07	109.99	122.07
1	B	475	LEU	CA-C-N	-7.07	111.28	122.73
1	B	475	LEU	C-N-CA	-7.07	111.28	122.73
1	C	121	VAL	N-CA-CB	-7.07	100.93	110.54
1	C	536	PHE	N-CA-CB	7.07	120.23	109.91
1	D	73	SER	CA-C-N	7.07	135.17	122.38
1	D	73	SER	C-N-CA	7.07	135.17	122.38
1	E	177	ARG	CA-C-O	7.07	130.61	120.51
1	E	531	PRO	CA-C-O	-7.07	112.35	122.31
1	A	177	ARG	CA-C-O	7.06	130.61	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	344	HIS	CB-CG-ND1	-7.06	112.11	122.70
1	A	400	PRO	CA-C-N	-7.06	110.63	122.64
1	A	400	PRO	C-N-CA	-7.06	110.63	122.64
1	E	121	VAL	N-CA-CB	-7.06	100.94	110.54
1	F	250	ARG	CG-CD-NE	-7.06	96.46	112.00
1	E	344	HIS	CB-CG-ND1	-7.06	112.11	122.70
1	E	403	HIS	N-CA-C	-7.06	103.19	111.03
1	B	531	PRO	CA-C-O	-7.06	112.36	122.31
1	C	317	GLN	OE1-CD-NE2	7.06	129.66	122.60
1	D	264	TYR	N-CA-C	-7.06	97.70	109.07
1	E	400	PRO	CA-C-N	-7.06	110.64	122.64
1	E	400	PRO	C-N-CA	-7.06	110.64	122.64
1	B	470	ASN	O-C-N	7.06	131.01	122.75
1	C	400	PRO	CA-C-N	-7.06	110.64	122.64
1	C	400	PRO	C-N-CA	-7.06	110.64	122.64
1	D	218	GLU	O-C-N	7.06	130.20	122.15
1	D	344	HIS	CB-CG-ND1	-7.06	112.11	122.70
1	E	174	LYS	CA-C-O	7.06	128.91	121.15
1	E	536	PHE	N-CA-CB	7.06	120.21	109.91
1	A	218	GLU	O-C-N	7.05	130.19	122.15
1	D	250	ARG	CG-CD-NE	-7.05	96.48	112.00
1	F	218	GLU	O-C-N	7.05	130.19	122.15
1	A	250	ARG	CG-CD-NE	-7.05	96.48	112.00
1	B	403	HIS	N-CA-C	-7.05	103.20	111.03
1	B	510	GLN	CA-C-N	-7.05	110.01	122.07
1	B	510	GLN	C-N-CA	-7.05	110.01	122.07
1	C	528	VAL	CA-C-O	-7.05	113.09	120.14
1	D	251	ILE	CA-C-O	-7.05	113.45	121.98
1	D	403	HIS	N-CA-C	-7.05	103.20	111.03
1	F	264	TYR	N-CA-C	-7.05	97.72	109.07
1	B	250	ARG	CG-CD-NE	-7.05	96.49	112.00
1	C	174	LYS	CA-C-O	7.05	128.90	121.15
1	C	403	HIS	N-CA-C	-7.05	103.20	111.03
1	D	24	PRO	N-CD-CG	-7.05	92.62	103.20
1	E	264	TYR	N-CA-C	-7.05	97.72	109.07
1	E	475	LEU	CA-C-N	-7.05	111.31	122.73
1	E	475	LEU	C-N-CA	-7.05	111.31	122.73
1	F	174	LYS	CA-C-O	7.05	128.90	121.15
1	C	95	GLU	N-CA-C	7.05	118.47	108.74
1	D	177	ARG	CA-C-O	7.05	130.59	120.51
1	E	470	ASN	O-C-N	7.05	131.00	122.75
1	F	510	GLN	CA-C-N	-7.05	110.02	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	510	GLN	C-N-CA	-7.05	110.02	122.07
1	B	400	PRO	CA-C-N	-7.05	110.66	122.64
1	B	400	PRO	C-N-CA	-7.05	110.66	122.64
1	B	536	PHE	N-CA-CB	7.05	120.20	109.91
1	C	195	VAL	CA-C-N	-7.05	111.03	120.54
1	C	195	VAL	C-N-CA	-7.05	111.03	120.54
1	C	510	GLN	CA-C-N	-7.05	110.02	122.07
1	C	510	GLN	C-N-CA	-7.05	110.02	122.07
1	E	24	PRO	N-CD-CG	-7.05	92.63	103.20
1	C	24	PRO	N-CD-CG	-7.04	92.63	103.20
1	A	251	ILE	CA-C-O	-7.04	113.46	121.98
1	B	177	ARG	CA-C-O	7.04	130.58	120.51
1	C	177	ARG	CA-C-O	7.04	130.58	120.51
1	C	218	GLU	O-C-N	7.04	130.18	122.15
1	F	195	VAL	CA-C-N	-7.04	111.03	120.54
1	F	195	VAL	C-N-CA	-7.04	111.03	120.54
1	A	24	PRO	N-CD-CG	-7.04	92.64	103.20
1	C	239	TRP	CB-CA-C	7.04	122.71	111.23
1	C	531	PRO	CA-C-O	-7.04	112.38	122.31
1	D	95	GLU	N-CA-C	7.04	118.46	108.74
1	D	475	LEU	CA-C-N	-7.04	111.32	122.73
1	D	475	LEU	C-N-CA	-7.04	111.32	122.73
1	A	195	VAL	CA-C-N	-7.04	111.04	120.54
1	A	195	VAL	C-N-CA	-7.04	111.04	120.54
1	A	264	TYR	N-CA-C	-7.04	97.74	109.07
1	A	475	LEU	CA-C-N	-7.04	111.33	122.73
1	A	475	LEU	C-N-CA	-7.04	111.33	122.73
1	B	317	GLN	OE1-CD-NE2	7.04	129.64	122.60
1	E	95	GLU	N-CA-C	7.04	118.45	108.74
1	F	177	ARG	CA-C-O	7.04	130.58	120.51
1	F	251	ILE	CA-C-O	-7.04	113.46	121.98
1	F	264	TYR	CB-CG-CD2	7.04	131.36	120.80
1	F	317	GLN	OE1-CD-NE2	7.04	129.64	122.60
1	B	218	GLU	O-C-N	7.04	130.17	122.15
1	D	520	GLU	CB-CG-CD	7.04	124.56	112.60
1	E	251	ILE	CA-C-O	-7.04	113.47	121.98
1	A	174	LYS	CA-C-O	7.04	128.89	121.15
1	C	250	ARG	CG-CD-NE	-7.04	96.52	112.00
1	D	387	MET	CB-CA-C	-7.04	98.72	110.68
1	F	316	ARG	N-CA-C	-7.04	100.90	110.68
1	A	95	GLU	N-CA-C	7.03	118.45	108.74
1	A	536	PHE	N-CA-CB	7.03	120.18	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	86	LEU	CB-CA-C	7.03	122.46	110.79
1	D	536	PHE	N-CA-CB	7.03	120.18	109.91
1	E	53	VAL	CB-CA-C	-7.03	102.88	111.88
1	E	528	VAL	CA-C-O	-7.03	113.11	120.14
1	B	24	PRO	N-CD-CG	-7.03	92.66	103.20
1	B	387	MET	CB-CA-C	-7.03	98.73	110.68
1	E	195	VAL	CA-C-N	-7.03	111.05	120.54
1	E	195	VAL	C-N-CA	-7.03	111.05	120.54
1	A	317	GLN	OE1-CD-NE2	7.03	129.63	122.60
1	A	528	VAL	CA-C-O	-7.03	113.11	120.14
1	C	475	LEU	CA-C-N	-7.03	111.34	122.73
1	C	475	LEU	C-N-CA	-7.03	111.34	122.73
1	D	438	ASP	OD1-CG-OD2	7.03	139.77	122.90
1	B	95	GLU	N-CA-C	7.03	118.44	108.74
1	B	264	TYR	N-CA-C	-7.03	97.76	109.07
1	C	264	TYR	N-CA-C	-7.03	97.76	109.07
1	C	470	ASN	O-C-N	7.03	130.97	122.75
1	C	524	LYS	CB-CA-C	7.03	122.00	110.90
1	E	387	MET	CB-CA-C	-7.03	98.73	110.68
1	F	95	GLU	N-CA-C	7.03	118.44	108.74
1	F	387	MET	CB-CA-C	-7.03	98.73	110.68
1	D	53	VAL	CB-CA-C	-7.03	102.89	111.88
1	D	528	VAL	CA-C-O	-7.03	113.11	120.14
1	F	348	HIS	N-CA-CB	7.03	120.40	110.07
1	A	387	MET	CB-CA-C	-7.02	98.74	110.68
1	E	239	TRP	CB-CA-C	7.02	122.68	111.23
1	D	492	THR	O-C-N	-7.02	113.25	122.59
1	E	348	HIS	N-CA-CB	7.02	120.39	110.07
1	F	528	VAL	CA-C-O	-7.02	113.12	120.14
1	C	251	ILE	CA-C-O	-7.02	113.48	121.98
1	D	510	GLN	CB-CA-C	-7.02	94.71	109.38
1	E	125	HIS	N-CA-C	7.02	121.97	113.41
1	E	520	GLU	CB-CG-CD	7.02	124.53	112.60
1	F	475	LEU	CA-C-N	-7.02	111.36	122.73
1	F	475	LEU	C-N-CA	-7.02	111.36	122.73
1	F	536	PHE	N-CA-CB	7.02	120.16	109.91
1	A	264	TYR	CB-CG-CD2	7.02	131.33	120.80
1	C	399	PRO	N-CA-C	-7.02	102.14	110.70
1	C	510	GLN	CB-CA-C	-7.02	94.72	109.38
1	D	86	LEU	CB-CA-C	7.02	122.44	110.79
1	D	264	TYR	CB-CG-CD2	7.02	131.33	120.80
1	A	125	HIS	N-CA-C	7.02	121.97	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	520	GLU	CB-CG-CD	7.02	124.53	112.60
1	B	316	ARG	N-CA-C	-7.02	100.93	110.68
1	B	510	GLN	CB-CA-C	-7.02	94.72	109.38
1	D	125	HIS	N-CA-C	7.02	121.97	113.41
1	A	239	TRP	CB-CA-C	7.01	122.67	111.23
1	A	316	ARG	N-CA-C	-7.01	100.93	110.68
1	B	53	VAL	CB-CA-C	-7.01	102.90	111.88
1	B	125	HIS	N-CA-C	7.01	121.97	113.41
1	B	247	HIS	CA-CB-CG	-7.01	106.79	113.80
1	C	316	ARG	N-CA-C	-7.01	100.93	110.68
1	C	542	GLN	CB-CG-CD	-7.01	100.67	112.60
1	E	86	LEU	CB-CA-C	7.01	122.44	110.79
1	F	24	PRO	N-CD-CG	-7.01	92.68	103.20
1	A	510	GLN	CB-CA-C	-7.01	94.72	109.38
1	B	251	ILE	CA-C-O	-7.01	113.49	121.98
1	E	134	LEU	CB-CA-C	7.01	118.76	108.87
1	F	632	ASP	CB-CG-OD1	-7.01	102.27	118.40
1	B	239	TRP	CB-CA-C	7.01	122.66	111.23
1	C	438	ASP	OD1-CG-OD2	7.01	139.73	122.90
1	D	195	VAL	CA-C-N	-7.01	111.07	120.54
1	D	195	VAL	C-N-CA	-7.01	111.07	120.54
1	D	348	HIS	N-CA-CB	7.01	120.38	110.07
1	E	510	GLN	CB-CA-C	-7.01	94.73	109.38
1	F	520	GLU	CB-CG-CD	7.01	124.52	112.60
1	A	53	VAL	CB-CA-C	-7.01	102.91	111.88
1	B	195	VAL	CA-C-N	-7.01	111.08	120.54
1	B	195	VAL	C-N-CA	-7.01	111.08	120.54
1	C	264	TYR	CB-CG-CD2	7.01	131.31	120.80
1	A	86	LEU	CB-CA-C	7.01	122.42	110.79
1	D	399	PRO	N-CA-C	-7.01	102.15	110.70
1	F	399	PRO	N-CA-C	-7.01	102.15	110.70
1	B	86	LEU	CB-CA-C	7.01	122.42	110.79
1	B	520	GLU	CB-CG-CD	7.01	124.51	112.60
1	B	542	GLN	CB-CG-CD	-7.01	100.69	112.60
1	C	125	HIS	N-CA-C	7.01	121.96	113.41
1	C	620	ARG	CG-CD-NE	-7.01	96.58	112.00
1	F	492	THR	O-C-N	-7.01	113.27	122.59
1	C	180	ARG	CG-CD-NE	7.00	127.41	112.00
1	F	125	HIS	N-CA-C	7.00	121.96	113.41
1	B	174	LYS	CA-C-O	7.00	128.85	121.15
1	B	264	TYR	CB-CG-CD2	7.00	131.31	120.80
1	B	399	PRO	N-CA-C	-7.00	102.16	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	387	MET	CB-CA-C	-7.00	98.78	110.68
1	D	317	GLN	OE1-CD-NE2	7.00	129.60	122.60
1	E	316	ARG	N-CA-C	-7.00	100.95	110.68
1	E	632	ASP	CB-CG-OD1	-7.00	102.29	118.40
1	A	438	ASP	OD1-CG-OD2	7.00	139.70	122.90
1	C	134	LEU	CB-CA-C	7.00	118.74	108.87
1	C	294	SER	CA-C-O	-7.00	111.46	120.00
1	D	247	HIS	CA-CB-CG	-7.00	106.80	113.80
1	E	264	TYR	CB-CG-CD2	7.00	131.30	120.80
1	A	399	PRO	N-CA-C	-7.00	102.16	110.70
1	C	520	GLU	CB-CG-CD	7.00	124.50	112.60
1	E	492	THR	O-C-N	-7.00	113.28	122.59
1	F	239	TRP	CB-CA-C	7.00	122.64	111.23
1	A	348	HIS	N-CA-CB	7.00	120.36	110.07
1	A	632	ASP	CB-CG-OD1	-7.00	102.30	118.40
1	F	53	VAL	CB-CA-C	-7.00	102.92	111.88
1	F	86	LEU	CB-CA-C	7.00	122.41	110.79
1	F	134	LEU	CB-CA-C	7.00	118.74	108.87
1	F	510	GLN	CB-CA-C	-7.00	94.75	109.38
1	B	528	VAL	CA-C-O	-7.00	113.14	120.14
1	D	294	SER	CA-C-O	-7.00	111.46	120.00
1	D	406	LEU	O-C-N	-7.00	112.81	122.46
1	D	620	ARG	CG-CD-NE	-7.00	96.61	112.00
1	E	620	ARG	CG-CD-NE	-7.00	96.61	112.00
1	E	230	ARG	O-C-N	7.00	129.37	122.09
1	E	542	GLN	CB-CG-CD	-7.00	100.71	112.60
1	B	620	ARG	CG-CD-NE	-6.99	96.61	112.00
1	D	134	LEU	CB-CA-C	6.99	118.73	108.87
1	D	146	THR	CB-CA-C	-6.99	97.68	109.50
1	D	180	ARG	CG-CD-NE	6.99	127.39	112.00
1	E	399	PRO	N-CA-C	-6.99	102.17	110.70
1	F	542	GLN	CB-CG-CD	-6.99	100.71	112.60
1	A	542	GLN	CB-CG-CD	-6.99	100.71	112.60
1	D	10	LYS	CB-CA-C	6.99	122.35	110.74
1	A	620	ARG	CG-CD-NE	-6.99	96.62	112.00
1	B	630	ILE	CA-C-N	6.99	126.47	118.85
1	B	630	ILE	C-N-CA	6.99	126.47	118.85
1	C	53	VAL	CB-CA-C	-6.99	102.93	111.88
1	F	438	ASP	OD1-CG-OD2	6.99	139.68	122.90
1	F	620	ARG	CG-CD-NE	-6.99	96.62	112.00
1	B	632	ASP	CB-CG-OD1	-6.99	102.33	118.40
1	D	542	GLN	CB-CG-CD	-6.99	100.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	180	ARG	CG-CD-NE	6.99	127.37	112.00
1	C	492	THR	O-C-N	-6.99	113.30	122.59
1	C	630	ILE	CA-C-N	6.99	126.47	118.85
1	C	630	ILE	C-N-CA	6.99	126.47	118.85
1	E	317	GLN	OE1-CD-NE2	6.99	129.59	122.60
1	F	10	LYS	CB-CA-C	6.99	122.34	110.74
1	A	294	SER	CA-C-O	-6.99	111.48	120.00
1	D	239	TRP	CB-CA-C	6.99	122.61	111.23
1	D	316	ARG	N-CA-C	-6.99	100.97	110.68
1	A	10	LYS	CB-CA-C	6.98	122.33	110.74
1	C	151	ILE	CA-C-N	-6.98	109.70	120.31
1	C	151	ILE	C-N-CA	-6.98	109.70	120.31
1	C	348	HIS	N-CA-CB	6.98	120.33	110.07
1	D	151	ILE	CA-C-N	-6.98	109.70	120.31
1	D	151	ILE	C-N-CA	-6.98	109.70	120.31
1	D	632	ASP	CB-CG-OD1	-6.98	102.34	118.40
1	E	10	LYS	CB-CA-C	6.98	122.33	110.74
1	E	348	HIS	N-CA-C	-6.98	102.23	111.24
1	E	438	ASP	OD1-CG-OD2	6.98	139.66	122.90
1	F	180	ARG	CG-CD-NE	6.98	127.36	112.00
1	A	406	LEU	O-C-N	-6.98	112.83	122.46
1	A	630	ILE	CA-C-N	6.98	126.46	118.85
1	A	630	ILE	C-N-CA	6.98	126.46	118.85
1	B	438	ASP	OD1-CG-OD2	6.98	139.66	122.90
1	C	632	ASP	CB-CG-OD1	-6.98	102.34	118.40
1	D	528	VAL	CA-C-N	-6.98	111.08	122.81
1	D	528	VAL	C-N-CA	-6.98	111.08	122.81
1	F	406	LEU	O-C-N	-6.98	112.83	122.46
1	B	294	SER	CA-C-O	-6.98	111.48	120.00
1	B	622	LEU	CB-CA-C	6.98	121.79	109.72
1	B	146	THR	CB-CA-C	-6.98	97.71	109.50
1	C	146	THR	CB-CA-C	-6.98	97.71	109.50
1	F	294	SER	CA-C-O	-6.98	111.49	120.00
1	F	630	ILE	CA-C-N	6.98	126.45	118.85
1	F	630	ILE	C-N-CA	6.98	126.45	118.85
1	B	151	ILE	CA-C-N	-6.98	109.71	120.31
1	B	151	ILE	C-N-CA	-6.98	109.71	120.31
1	B	348	HIS	N-CA-CB	6.98	120.32	110.07
1	E	146	THR	CB-CA-C	-6.98	97.71	109.50
1	A	492	THR	O-C-N	-6.97	113.31	122.59
1	B	48	ASP	N-CA-C	-6.97	103.95	113.30
1	C	471	ASP	N-CA-CB	6.97	120.37	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	623	GLY	N-CA-C	-6.97	105.24	115.63
1	C	42	ASP	N-CA-C	-6.97	95.95	110.80
1	A	134	LEU	CB-CA-C	6.97	118.70	108.87
1	A	151	ILE	CA-C-N	-6.97	109.71	120.31
1	A	151	ILE	C-N-CA	-6.97	109.71	120.31
1	B	492	THR	O-C-N	-6.97	113.32	122.59
1	A	622	LEU	CB-CA-C	6.97	121.78	109.72
1	B	10	LYS	CB-CA-C	6.97	122.31	110.74
1	B	134	LEU	CB-CA-C	6.97	118.70	108.87
1	B	180	ARG	CG-CD-NE	6.97	127.33	112.00
1	D	274	ASN	CB-CG-ND2	6.97	126.85	116.40
1	D	471	ASP	N-CA-CB	6.97	120.36	110.12
1	C	10	LYS	CB-CA-C	6.97	122.31	110.74
1	C	406	LEU	O-C-N	-6.97	112.84	122.46
1	E	180	ARG	CG-CD-NE	6.97	127.33	112.00
1	E	406	LEU	O-C-N	-6.97	112.84	122.46
1	A	471	ASP	N-CA-CB	6.97	120.36	110.12
1	A	528	VAL	CA-C-N	-6.97	111.11	122.81
1	A	528	VAL	C-N-CA	-6.97	111.11	122.81
1	F	528	VAL	CA-C-N	-6.97	111.11	122.81
1	F	528	VAL	C-N-CA	-6.97	111.11	122.81
1	A	247	HIS	CA-CB-CG	-6.96	106.84	113.80
1	C	622	LEU	CB-CA-C	6.96	121.77	109.72
1	E	528	VAL	CA-C-N	-6.96	111.11	122.81
1	E	528	VAL	C-N-CA	-6.96	111.11	122.81
1	E	630	ILE	CA-C-N	6.96	126.44	118.85
1	E	630	ILE	C-N-CA	6.96	126.44	118.85
1	F	42	ASP	N-CA-C	-6.96	95.97	110.80
1	F	622	LEU	CB-CA-C	6.96	121.77	109.72
1	B	42	ASP	N-CA-C	-6.96	95.97	110.80
1	B	230	ARG	O-C-N	6.96	129.33	122.09
1	A	42	ASP	N-CA-C	-6.96	95.97	110.80
1	A	146	THR	CB-CA-C	-6.96	97.73	109.50
1	B	528	VAL	CA-C-N	-6.96	111.12	122.81
1	B	528	VAL	C-N-CA	-6.96	111.12	122.81
1	C	348	HIS	N-CA-C	-6.96	102.26	111.24
1	E	151	ILE	CA-C-N	-6.96	109.73	120.31
1	E	151	ILE	C-N-CA	-6.96	109.73	120.31
1	E	622	LEU	CB-CA-C	6.96	121.76	109.72
1	B	348	HIS	N-CA-C	-6.96	102.26	111.24
1	B	406	LEU	O-C-N	-6.96	112.86	122.46
1	D	622	LEU	CB-CA-C	6.96	121.76	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	48	ASP	N-CA-C	-6.96	103.97	113.30
1	E	294	SER	CA-C-O	-6.96	111.51	120.00
1	C	496	ASP	CA-C-N	-6.96	108.85	120.68
1	C	496	ASP	C-N-CA	-6.96	108.85	120.68
1	F	151	ILE	CA-C-N	-6.96	109.74	120.31
1	F	151	ILE	C-N-CA	-6.96	109.74	120.31
1	B	471	ASP	N-CA-CB	6.96	120.34	110.12
1	D	42	ASP	N-CA-C	-6.95	95.99	110.80
1	D	48	ASP	N-CA-C	-6.95	103.98	113.30
1	E	471	ASP	N-CA-CB	6.95	120.34	110.12
1	C	100	ARG	CD-NE-CZ	-6.95	114.67	124.40
1	F	230	ARG	O-C-N	6.95	129.32	122.09
1	F	348	HIS	N-CA-C	-6.95	102.28	111.24
1	F	623	GLY	N-CA-C	-6.95	105.28	115.63
1	A	48	ASP	N-CA-C	-6.95	103.99	113.30
1	F	48	ASP	N-CA-C	-6.95	103.99	113.30
1	A	274	ASN	CB-CG-ND2	6.95	126.82	116.40
1	A	348	HIS	N-CA-C	-6.95	102.28	111.24
1	A	623	GLY	N-CA-C	-6.95	105.28	115.63
1	E	42	ASP	N-CA-C	-6.95	96.01	110.80
1	B	274	ASN	CB-CG-ND2	6.94	126.82	116.40
1	A	230	ARG	O-C-N	6.94	129.31	122.09
1	D	40	LEU	N-CA-C	6.94	121.06	112.59
1	E	274	ASN	CB-CG-ND2	6.94	126.81	116.40
1	C	247	HIS	CA-CB-CG	-6.94	106.86	113.80
1	C	274	ASN	CB-CG-ND2	6.94	126.81	116.40
1	D	230	ARG	O-C-N	6.94	129.31	122.09
1	D	623	GLY	N-CA-C	-6.94	105.29	115.63
1	E	55	THR	CA-CB-OG1	-6.94	99.19	109.60
1	F	247	HIS	CA-CB-CG	-6.94	106.86	113.80
1	F	274	ASN	CB-CG-ND2	6.94	126.81	116.40
1	E	333	TYR	CB-CA-C	6.94	122.50	110.01
1	F	141	THR	O-C-N	6.94	126.85	121.23
1	D	630	ILE	CA-C-N	6.94	126.41	118.85
1	D	630	ILE	C-N-CA	6.94	126.41	118.85
1	F	471	ASP	N-CA-CB	6.94	120.32	110.12
1	B	141	THR	O-C-N	6.93	126.85	121.23
1	C	48	ASP	N-CA-C	-6.93	104.01	113.30
1	E	141	THR	O-C-N	6.93	126.84	121.23
1	F	40	LEU	N-CA-C	6.93	121.05	112.59
1	B	100	ARG	CD-NE-CZ	-6.93	114.70	124.40
1	B	623	GLY	N-CA-C	-6.93	105.31	115.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	624	TYR	CG-CD2-CE2	6.93	131.59	121.20
1	F	100	ARG	CD-NE-CZ	-6.93	114.70	124.40
1	F	624	TYR	CG-CD2-CE2	6.93	131.60	121.20
1	A	55	THR	CA-CB-OG1	-6.93	99.21	109.60
1	C	230	ARG	O-C-N	6.93	129.29	122.09
1	D	348	HIS	N-CA-C	-6.93	102.31	111.24
1	F	55	THR	CA-CB-OG1	-6.93	99.21	109.60
1	A	100	ARG	CD-NE-CZ	-6.92	114.71	124.40
1	E	100	ARG	CD-NE-CZ	-6.92	114.71	124.40
1	C	333	TYR	CB-CA-C	6.92	122.47	110.01
1	C	528	VAL	CA-C-N	-6.92	111.18	122.81
1	C	528	VAL	C-N-CA	-6.92	111.18	122.81
1	E	247	HIS	CA-CB-CG	-6.92	106.88	113.80
1	A	40	LEU	N-CA-C	6.92	121.03	112.59
1	C	533	MET	CA-C-N	6.92	128.49	119.84
1	C	533	MET	C-N-CA	6.92	128.49	119.84
1	D	100	ARG	CD-NE-CZ	-6.92	114.71	124.40
1	B	439	SER	N-CA-C	-6.92	97.00	108.34
1	C	624	TYR	CG-CD2-CE2	6.92	131.57	121.20
1	C	55	THR	CA-CB-OG1	-6.91	99.23	109.60
1	D	624	TYR	CG-CD2-CE2	6.91	131.57	121.20
1	B	40	LEU	N-CA-C	6.91	121.02	112.59
1	D	333	TYR	CB-CA-C	6.91	122.45	110.01
1	B	55	THR	CA-CB-OG1	-6.91	99.23	109.60
1	B	124	ILE	O-C-N	6.91	128.68	121.91
1	D	500	TRP	O-C-N	6.91	132.00	122.46
1	A	333	TYR	CB-CA-C	6.91	122.44	110.01
1	A	624	TYR	CG-CD2-CE2	6.91	131.56	121.20
1	A	141	THR	O-C-N	6.91	126.82	121.23
1	B	624	TYR	CG-CD2-CE2	6.91	131.56	121.20
1	B	333	TYR	CB-CA-C	6.90	122.44	110.01
1	E	623	GLY	N-CA-C	-6.90	105.34	115.63
1	F	651	HIS	CA-C-N	-6.90	111.71	121.72
1	F	651	HIS	C-N-CA	-6.90	111.71	121.72
1	D	55	THR	CA-CB-OG1	-6.90	99.25	109.60
1	E	439	SER	N-CA-C	-6.90	97.02	108.34
1	A	78	ARG	CB-CG-CD	6.90	127.17	111.30
1	C	322	GLU	CA-C-N	-6.90	110.31	120.38
1	C	322	GLU	C-N-CA	-6.90	110.31	120.38
1	A	439	SER	N-CA-C	-6.90	97.03	108.34
1	C	78	ARG	CB-CG-CD	6.90	127.17	111.30
1	D	198	HIS	N-CA-CB	-6.90	98.83	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	61	ASN	CB-CA-C	6.89	121.64	110.95
1	D	322	GLU	CA-C-N	-6.89	110.31	120.38
1	D	322	GLU	C-N-CA	-6.89	110.31	120.38
1	D	439	SER	N-CA-C	-6.89	97.03	108.34
1	E	40	LEU	N-CA-C	6.89	121.00	112.59
1	B	651	HIS	CA-C-N	-6.89	111.73	121.72
1	B	651	HIS	C-N-CA	-6.89	111.73	121.72
1	D	82	GLU	CG-CD-OE2	6.89	134.25	118.40
1	B	78	ARG	CB-CG-CD	6.89	127.15	111.30
1	D	124	ILE	O-C-N	6.89	128.66	121.91
1	F	124	ILE	O-C-N	6.89	128.66	121.91
1	C	40	LEU	N-CA-C	6.89	121.00	112.59
1	C	82	GLU	CG-CD-OE2	6.89	134.25	118.40
1	C	124	ILE	O-C-N	6.89	128.66	121.91
1	D	651	HIS	CA-C-N	-6.89	111.73	121.72
1	D	651	HIS	C-N-CA	-6.89	111.73	121.72
1	E	274	ASN	CA-C-N	6.89	130.80	120.95
1	E	274	ASN	C-N-CA	6.89	130.80	120.95
1	D	78	ARG	CB-CG-CD	6.89	127.14	111.30
1	F	78	ARG	CB-CG-CD	6.89	127.14	111.30
1	F	500	TRP	O-C-N	6.89	131.96	122.46
1	B	274	ASN	CA-C-N	6.88	130.79	120.95
1	B	274	ASN	C-N-CA	6.88	130.79	120.95
1	F	428	GLU	OE1-CD-OE2	6.88	139.42	122.90
1	A	82	GLU	CG-CD-OE2	6.88	134.23	118.40
1	C	468	ASN	CB-CG-OD1	-6.88	107.03	120.80
1	F	468	ASN	CB-CG-OD1	-6.88	107.03	120.80
1	B	198	HIS	N-CA-CB	-6.88	98.86	110.49
1	C	141	THR	O-C-N	6.88	126.80	121.23
1	C	558	TYR	N-CA-CB	-6.88	101.56	111.54
1	F	82	GLU	CG-CD-OE2	6.88	134.23	118.40
1	F	333	TYR	CB-CA-C	6.88	122.40	110.01
1	A	651	HIS	CA-C-N	-6.88	111.74	121.72
1	A	651	HIS	C-N-CA	-6.88	111.74	121.72
1	B	575	PRO	N-CA-C	-6.88	104.62	114.18
1	C	651	HIS	CA-C-N	-6.88	111.74	121.72
1	C	651	HIS	C-N-CA	-6.88	111.74	121.72
1	A	468	ASN	CB-CG-OD1	-6.88	107.04	120.80
1	E	78	ARG	CB-CG-CD	6.88	127.12	111.30
1	E	322	GLU	CA-C-N	-6.88	110.34	120.38
1	E	322	GLU	C-N-CA	-6.88	110.34	120.38
1	A	533	MET	CA-C-N	6.88	128.44	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	533	MET	C-N-CA	6.88	128.44	119.84
1	B	82	GLU	CG-CD-OE2	6.88	134.22	118.40
1	B	322	GLU	CA-C-N	-6.88	110.34	120.38
1	B	322	GLU	C-N-CA	-6.88	110.34	120.38
1	C	198	HIS	N-CA-CB	-6.88	98.87	110.49
1	E	82	GLU	CG-CD-OE2	6.88	134.22	118.40
1	C	500	TRP	O-C-N	6.87	131.94	122.46
1	D	439	SER	CB-CA-C	-6.87	99.14	110.14
1	E	468	ASN	CB-CG-OD1	-6.87	107.05	120.80
1	E	575	PRO	N-CA-C	-6.87	104.63	114.18
1	F	558	TYR	N-CA-CB	-6.87	101.57	111.54
1	A	124	ILE	O-C-N	6.87	128.64	121.91
1	A	322	GLU	CA-C-N	-6.87	110.35	120.38
1	A	322	GLU	C-N-CA	-6.87	110.35	120.38
1	D	468	ASN	CB-CG-OD1	-6.87	107.06	120.80
1	A	428	GLU	OE1-CD-OE2	6.87	139.39	122.90
1	C	61	ASN	CB-CA-C	6.87	121.60	110.95
1	B	533	MET	CA-C-N	6.87	128.43	119.84
1	B	533	MET	C-N-CA	6.87	128.43	119.84
1	C	439	SER	N-CA-C	-6.87	97.08	108.34
1	E	651	HIS	CA-C-N	-6.87	111.76	121.72
1	E	651	HIS	C-N-CA	-6.87	111.76	121.72
1	F	146	THR	CB-CA-C	-6.87	97.76	109.51
1	A	61	ASN	CB-CA-C	6.87	121.59	110.95
1	B	272	PRO	CB-CG-CD	-6.87	84.12	106.10
1	D	274	ASN	CA-C-N	6.87	130.77	120.95
1	D	274	ASN	C-N-CA	6.87	130.77	120.95
1	E	533	MET	CA-C-N	6.87	128.42	119.84
1	E	533	MET	C-N-CA	6.87	128.42	119.84
1	F	322	GLU	CA-C-N	-6.87	110.36	120.38
1	F	322	GLU	C-N-CA	-6.87	110.36	120.38
1	A	198	HIS	N-CA-CB	-6.87	98.89	110.49
1	A	274	ASN	CA-C-N	6.86	130.77	120.95
1	A	274	ASN	C-N-CA	6.86	130.77	120.95
1	A	575	PRO	N-CA-C	-6.86	104.64	114.18
1	D	428	GLU	OE1-CD-OE2	6.86	139.37	122.90
1	D	558	TYR	N-CA-CB	-6.86	101.59	111.54
1	E	428	GLU	OE1-CD-OE2	6.86	139.37	122.90
1	F	575	PRO	N-CA-C	-6.86	104.64	114.18
1	A	439	SER	CB-CA-C	-6.86	99.16	110.14
1	B	558	TYR	N-CA-CB	-6.86	101.59	111.54
1	F	61	ASN	CB-CA-C	6.86	121.59	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	198	HIS	N-CA-CB	-6.86	98.89	110.49
1	A	558	TYR	N-CA-CB	-6.86	101.59	111.54
1	C	428	GLU	OE1-CD-OE2	6.86	139.37	122.90
1	F	272	PRO	CB-CG-CD	-6.86	84.15	106.10
1	E	272	PRO	CB-CG-CD	-6.86	84.15	106.10
1	A	272	PRO	CB-CG-CD	-6.86	84.16	106.10
1	B	428	GLU	OE1-CD-OE2	6.86	139.36	122.90
1	B	439	SER	CB-CA-C	-6.86	99.17	110.14
1	B	468	ASN	CB-CG-OD1	-6.86	107.08	120.80
1	C	272	PRO	CB-CG-CD	-6.86	84.16	106.10
1	D	272	PRO	CB-CG-CD	-6.86	84.16	106.10
1	D	533	MET	CA-C-N	6.86	128.41	119.84
1	D	533	MET	C-N-CA	6.86	128.41	119.84
1	F	274	ASN	CA-C-N	6.86	130.76	120.95
1	F	274	ASN	C-N-CA	6.86	130.76	120.95
1	F	533	MET	CA-C-N	6.86	128.41	119.84
1	F	533	MET	C-N-CA	6.86	128.41	119.84
1	A	500	TRP	O-C-N	6.85	131.92	122.46
1	E	77	THR	CA-CB-OG1	-6.85	99.32	109.60
1	B	500	TRP	O-C-N	6.85	131.92	122.46
1	D	61	ASN	CB-CA-C	6.85	121.57	110.95
1	D	575	PRO	N-CA-C	-6.85	104.65	114.18
1	E	61	ASN	CB-CA-C	6.85	121.57	110.95
1	E	124	ILE	O-C-N	6.85	128.62	121.91
1	E	198	HIS	CA-CB-CG	6.85	120.65	113.80
1	F	439	SER	N-CA-C	-6.85	97.10	108.34
1	E	147	ASN	CB-CA-C	-6.85	96.79	110.42
1	B	376	ARG	CA-C-N	6.85	129.85	120.67
1	B	376	ARG	C-N-CA	6.85	129.85	120.67
1	E	198	HIS	N-CA-CB	-6.85	98.92	110.49
1	E	213	LEU	CD1-CG-CD2	-6.85	95.74	110.80
1	B	147	ASN	CB-CA-C	-6.85	96.80	110.42
1	E	439	SER	CB-CA-C	-6.85	99.19	110.14
1	E	558	TYR	N-CA-CB	-6.85	101.61	111.54
1	F	20	LYS	CA-CB-CG	-6.85	100.41	114.10
1	B	395	THR	CA-C-N	6.84	134.77	122.38
1	B	395	THR	C-N-CA	6.84	134.77	122.38
1	D	179	GLN	CB-CG-CD	6.84	124.24	112.60
1	E	500	TRP	O-C-N	6.84	131.91	122.46
1	F	439	SER	CB-CA-C	-6.84	99.19	110.14
1	B	74	LEU	N-CA-C	-6.84	104.67	113.16
1	C	77	THR	CA-CB-OG1	-6.84	99.33	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	439	SER	CB-CA-C	-6.84	99.19	110.14
1	D	91	ASN	O-C-N	6.84	129.37	122.12
1	D	436	ALA	O-C-N	6.84	131.12	122.23
1	E	436	ALA	O-C-N	6.84	131.12	122.23
1	F	213	LEU	CD1-CG-CD2	-6.84	95.75	110.80
1	B	213	LEU	CD1-CG-CD2	-6.84	95.75	110.80
1	B	246	LEU	N-CA-CB	-6.84	99.73	110.06
1	D	12	GLN	OE1-CD-NE2	6.84	129.44	122.60
1	D	147	ASN	CB-CA-C	-6.84	96.81	110.42
1	E	20	LYS	CA-CB-CG	-6.84	100.42	114.10
1	E	246	LEU	N-CA-CB	-6.84	99.73	110.06
1	F	395	THR	CA-C-N	6.84	134.76	122.38
1	F	395	THR	C-N-CA	6.84	134.76	122.38
1	C	274	ASN	CA-C-N	6.84	130.73	120.95
1	C	274	ASN	C-N-CA	6.84	130.73	120.95
1	A	213	LEU	CD1-CG-CD2	-6.84	95.76	110.80
1	C	213	LEU	CD1-CG-CD2	-6.84	95.76	110.80
1	E	179	GLN	CB-CG-CD	6.84	124.22	112.60
1	F	179	GLN	CB-CG-CD	6.84	124.22	112.60
1	C	376	ARG	CA-C-N	6.83	129.83	120.67
1	C	376	ARG	C-N-CA	6.83	129.83	120.67
1	D	246	LEU	N-CA-CB	-6.83	99.74	110.06
1	F	198	HIS	CA-CB-CG	6.83	120.63	113.80
1	A	147	ASN	CB-CA-C	-6.83	96.83	110.42
1	A	246	LEU	N-CA-CB	-6.83	99.74	110.06
1	B	179	GLN	CB-CG-CD	6.83	124.21	112.60
1	D	213	LEU	CD1-CG-CD2	-6.83	95.77	110.80
1	A	436	ALA	O-C-N	6.83	131.11	122.23
1	C	436	ALA	O-C-N	6.83	131.11	122.23
1	C	575	PRO	N-CA-C	-6.83	104.69	114.18
1	F	147	ASN	CB-CA-C	-6.83	96.83	110.42
1	F	499	ARG	CD-NE-CZ	6.83	133.96	124.40
1	A	179	GLN	CB-CG-CD	6.83	124.21	112.60
1	C	246	LEU	N-CA-CB	-6.83	99.75	110.06
1	F	219	LEU	CA-C-O	-6.83	113.65	120.82
1	A	20	LYS	CA-CB-CG	-6.83	100.45	114.10
1	B	77	THR	CA-CB-OG1	-6.83	99.36	109.60
1	C	147	ASN	CB-CA-C	-6.82	96.84	110.42
1	D	20	LYS	CA-CB-CG	-6.82	100.45	114.10
1	D	141	THR	O-C-N	6.82	126.76	121.23
1	B	436	ALA	O-C-N	6.82	131.10	122.23
1	D	198	HIS	CA-CB-CG	6.82	120.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	91	ASN	O-C-N	6.82	129.35	122.12
1	A	77	THR	CA-CB-OG1	-6.82	99.37	109.60
1	C	20	LYS	CA-CB-CG	-6.82	100.46	114.10
1	C	91	ASN	O-C-N	6.82	129.35	122.12
1	C	328	ILE	O-C-N	-6.82	112.84	121.84
1	E	74	LEU	N-CA-C	-6.82	104.71	113.16
1	E	376	ARG	CA-C-N	6.82	129.80	120.67
1	E	376	ARG	C-N-CA	6.82	129.80	120.67
1	A	91	ASN	O-C-N	6.81	129.34	122.12
1	A	198	HIS	CA-CB-CG	6.81	120.61	113.80
1	B	20	LYS	CA-CB-CG	-6.81	100.47	114.10
1	C	455	LEU	CD1-CG-CD2	-6.81	95.81	110.80
1	C	520	GLU	O-C-N	6.81	132.09	123.23
1	B	219	LEU	CA-C-O	-6.81	113.67	120.82
1	B	397	SER	CA-C-N	-6.81	107.58	121.48
1	B	397	SER	C-N-CA	-6.81	107.58	121.48
1	F	74	LEU	N-CA-C	-6.81	104.71	113.16
1	A	74	LEU	N-CA-C	-6.81	104.71	113.16
1	B	520	GLU	O-C-N	6.81	132.08	123.23
1	C	198	HIS	CA-CB-CG	6.81	120.61	113.80
1	C	395	THR	CA-C-N	6.81	134.71	122.38
1	C	395	THR	C-N-CA	6.81	134.71	122.38
1	E	455	LEU	CD1-CG-CD2	-6.81	95.81	110.80
1	A	219	LEU	CA-C-O	-6.81	113.67	120.82
1	C	499	ARG	CD-NE-CZ	6.81	133.93	124.40
1	D	74	LEU	N-CA-C	-6.81	104.72	113.16
1	D	520	GLU	O-C-N	6.81	132.08	123.23
1	F	77	THR	CA-CB-OG1	-6.81	99.39	109.60
1	F	455	LEU	CD1-CG-CD2	-6.81	95.82	110.80
1	A	395	THR	CA-C-N	6.81	134.70	122.38
1	A	395	THR	C-N-CA	6.81	134.70	122.38
1	E	219	LEU	CA-C-O	-6.81	113.67	120.82
1	F	612	HIS	O-C-N	6.81	131.32	122.20
1	F	652	HIS	CA-C-N	-6.81	109.45	121.70
1	F	652	HIS	C-N-CA	-6.81	109.45	121.70
1	A	455	LEU	CD1-CG-CD2	-6.81	95.83	110.80
1	E	395	THR	CA-C-N	6.81	134.70	122.38
1	E	395	THR	C-N-CA	6.81	134.70	122.38
1	F	246	LEU	N-CA-CB	-6.81	99.78	110.06
1	B	212	HIS	CA-C-N	-6.80	111.69	121.42
1	B	212	HIS	C-N-CA	-6.80	111.69	121.42
1	F	397	SER	CA-C-N	-6.80	107.60	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	397	SER	C-N-CA	-6.80	107.60	121.48
1	F	436	ALA	O-C-N	6.80	131.08	122.23
1	B	455	LEU	CD1-CG-CD2	-6.80	95.83	110.80
1	B	612	HIS	O-C-N	6.80	131.32	122.20
1	D	652	HIS	CA-C-N	-6.80	109.45	121.70
1	D	652	HIS	C-N-CA	-6.80	109.45	121.70
1	F	376	ARG	CA-C-N	6.80	129.79	120.67
1	F	376	ARG	C-N-CA	6.80	129.79	120.67
1	A	12	GLN	OE1-CD-NE2	6.80	129.40	122.60
1	A	376	ARG	CA-C-N	6.80	129.78	120.67
1	A	376	ARG	C-N-CA	6.80	129.78	120.67
1	A	652	HIS	CA-C-N	-6.80	109.46	121.70
1	A	652	HIS	C-N-CA	-6.80	109.46	121.70
1	C	179	GLN	CB-CG-CD	6.80	124.16	112.60
1	C	237	SER	CA-CB-OG	-6.80	97.50	111.10
1	C	397	SER	CA-C-N	-6.80	107.61	121.48
1	C	397	SER	C-N-CA	-6.80	107.61	121.48
1	D	395	THR	CA-C-N	6.80	134.69	122.38
1	D	395	THR	C-N-CA	6.80	134.69	122.38
1	E	91	ASN	O-C-N	6.80	129.33	122.12
1	E	397	SER	CA-C-N	-6.80	107.61	121.48
1	E	397	SER	C-N-CA	-6.80	107.61	121.48
1	F	91	ASN	O-C-N	6.80	129.33	122.12
1	B	499	ARG	CD-NE-CZ	6.80	133.92	124.40
1	E	499	ARG	CD-NE-CZ	6.80	133.92	124.40
1	F	520	GLU	O-C-N	6.80	132.07	123.23
1	B	12	GLN	OE1-CD-NE2	6.80	129.40	122.60
1	D	126	SER	CA-C-N	6.80	129.72	120.54
1	D	126	SER	C-N-CA	6.80	129.72	120.54
1	C	219	LEU	CA-C-O	-6.80	113.68	120.82
1	E	212	HIS	CA-C-N	-6.80	111.70	121.42
1	E	212	HIS	C-N-CA	-6.80	111.70	121.42
1	E	520	GLU	O-C-N	6.80	132.06	123.23
1	A	499	ARG	CD-NE-CZ	6.79	133.91	124.40
1	D	455	LEU	CD1-CG-CD2	-6.79	95.86	110.80
1	E	652	HIS	CA-C-N	-6.79	109.47	121.70
1	E	652	HIS	C-N-CA	-6.79	109.47	121.70
1	C	12	GLN	OE1-CD-NE2	6.79	129.39	122.60
1	D	77	THR	CA-CB-OG1	-6.79	99.41	109.60
1	C	74	LEU	N-CA-C	-6.79	104.74	113.16
1	A	397	SER	CA-C-N	-6.79	107.63	121.48
1	A	397	SER	C-N-CA	-6.79	107.63	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	38	ASN	CA-CB-CG	-6.79	105.81	112.60
1	D	397	SER	CA-C-N	-6.79	107.63	121.48
1	D	397	SER	C-N-CA	-6.79	107.63	121.48
1	F	237	SER	CA-CB-OG	-6.79	97.53	111.10
1	A	328	ILE	O-C-N	-6.79	112.88	121.84
1	D	612	HIS	O-C-N	6.79	131.29	122.20
1	E	612	HIS	O-C-N	6.79	131.29	122.20
1	A	520	GLU	O-C-N	6.78	132.05	123.23
1	C	652	HIS	CA-C-N	-6.78	109.49	121.70
1	C	652	HIS	C-N-CA	-6.78	109.49	121.70
1	A	212	HIS	CA-C-N	-6.78	111.72	121.42
1	A	212	HIS	C-N-CA	-6.78	111.72	121.42
1	B	652	HIS	CA-C-N	-6.78	109.49	121.70
1	B	652	HIS	C-N-CA	-6.78	109.49	121.70
1	D	328	ILE	O-C-N	-6.78	112.89	121.84
1	B	328	ILE	O-C-N	-6.78	112.89	121.84
1	D	163	PRO	CA-C-O	-6.78	111.93	121.90
1	D	212	HIS	CA-C-N	-6.78	111.72	121.42
1	D	212	HIS	C-N-CA	-6.78	111.72	121.42
1	D	499	ARG	CD-NE-CZ	6.78	133.89	124.40
1	F	328	ILE	O-C-N	-6.78	112.89	121.84
1	A	237	SER	CA-CB-OG	-6.78	97.54	111.10
1	B	198	HIS	CA-CB-CG	6.78	120.58	113.80
1	D	376	ARG	CA-C-N	6.78	129.75	120.67
1	D	376	ARG	C-N-CA	6.78	129.75	120.67
1	F	12	GLN	OE1-CD-NE2	6.78	129.38	122.60
1	B	237	SER	CA-CB-OG	-6.78	97.55	111.10
1	B	643	LYS	CA-C-O	-6.77	112.21	120.54
1	D	237	SER	CA-CB-OG	-6.77	97.55	111.10
1	A	38	ASN	CA-CB-CG	-6.77	105.83	112.60
1	A	612	HIS	O-C-N	6.77	131.28	122.20
1	B	38	ASN	CA-CB-CG	-6.77	105.83	112.60
1	C	212	HIS	CA-C-N	-6.77	111.73	121.42
1	C	212	HIS	C-N-CA	-6.77	111.73	121.42
1	D	52	ALA	O-C-N	6.77	129.34	122.03
1	E	328	ILE	O-C-N	-6.77	112.90	121.84
1	C	163	PRO	CA-C-O	-6.77	111.95	121.90
1	F	52	ALA	O-C-N	6.77	129.34	122.03
1	F	212	HIS	CA-C-N	-6.77	111.74	121.42
1	F	212	HIS	C-N-CA	-6.77	111.74	121.42
1	A	126	SER	CA-C-N	6.77	129.68	120.54
1	A	126	SER	C-N-CA	6.77	129.68	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	38	ASN	CA-CB-CG	-6.77	105.83	112.60
1	E	237	SER	CA-CB-OG	-6.77	97.56	111.10
1	C	643	LYS	CA-C-O	-6.77	112.22	120.54
1	D	643	LYS	CA-C-O	-6.77	112.22	120.54
1	D	504	GLU	O-C-N	6.76	130.95	123.04
1	E	449	ASN	N-CA-C	6.76	120.01	109.52
1	F	38	ASN	CA-CB-CG	-6.76	105.84	112.60
1	F	378	PRO	CA-C-O	-6.76	109.27	119.55
1	D	219	LEU	CA-C-O	-6.76	113.72	120.82
1	A	449	ASN	N-CA-C	6.76	120.00	109.52
1	C	378	PRO	CA-C-O	-6.76	109.27	119.55
1	D	378	PRO	CA-C-O	-6.76	109.27	119.55
1	A	163	PRO	CA-C-O	-6.76	111.96	121.90
1	A	643	LYS	CA-C-O	-6.76	112.22	120.54
1	C	564	ILE	CB-CG1-CD1	-6.76	99.61	113.80
1	E	12	GLN	OE1-CD-NE2	6.76	129.36	122.60
1	E	52	ALA	O-C-N	6.76	129.33	122.03
1	E	163	PRO	CA-C-O	-6.76	111.96	121.90
1	C	126	SER	CA-C-N	6.76	129.66	120.54
1	C	126	SER	C-N-CA	6.76	129.66	120.54
1	E	126	SER	CA-C-N	6.76	129.66	120.54
1	E	126	SER	C-N-CA	6.76	129.66	120.54
1	E	181	VAL	O-C-N	-6.76	114.12	122.57
1	C	234	GLU	O-C-N	6.75	129.28	122.12
1	F	126	SER	CA-C-N	6.75	129.66	120.54
1	F	126	SER	C-N-CA	6.75	129.66	120.54
1	F	564	ILE	CB-CG1-CD1	-6.75	99.61	113.80
1	B	126	SER	CA-C-N	6.75	129.66	120.54
1	B	126	SER	C-N-CA	6.75	129.66	120.54
1	C	181	VAL	O-C-N	-6.75	114.13	122.57
1	E	564	ILE	CB-CG1-CD1	-6.75	99.62	113.80
1	B	163	PRO	CA-C-O	-6.75	111.97	121.90
1	B	378	PRO	CA-C-O	-6.75	109.29	119.55
1	E	451	ARG	NE-CZ-NH1	-6.75	114.75	121.50
1	A	378	PRO	CA-C-O	-6.75	109.29	119.55
1	F	163	PRO	CA-C-O	-6.75	111.98	121.90
1	E	643	LYS	CA-C-O	-6.75	112.24	120.54
1	F	224	HIS	N-CA-CB	-6.75	99.40	110.40
1	A	150	VAL	O-C-N	6.75	128.68	121.87
1	D	149	GLU	O-C-N	6.75	130.33	122.17
1	D	393	LYS	CB-CA-C	-6.75	98.15	110.63
1	D	564	ILE	CB-CG1-CD1	-6.75	99.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	150	VAL	O-C-N	6.75	128.68	121.87
1	F	643	LYS	CA-C-O	-6.75	112.24	120.54
1	C	393	LYS	CB-CA-C	-6.74	98.15	110.63
1	D	181	VAL	O-C-N	-6.74	114.14	122.57
1	F	504	GLU	O-C-N	6.74	130.93	123.04
1	B	504	GLU	O-C-N	6.74	130.93	123.04
1	A	564	ILE	CB-CG1-CD1	-6.74	99.64	113.80
1	B	449	ASN	N-CA-C	6.74	119.97	109.52
1	C	451	ARG	NE-CZ-NH1	-6.74	114.76	121.50
1	D	449	ASN	N-CA-C	6.74	119.97	109.52
1	F	150	VAL	O-C-N	6.74	128.68	121.87
1	A	52	ALA	O-C-N	6.74	129.31	122.03
1	A	504	GLU	O-C-N	6.74	130.93	123.04
1	B	150	VAL	O-C-N	6.74	128.68	121.87
1	C	449	ASN	N-CA-C	6.74	119.97	109.52
1	F	110	MET	N-CA-C	-6.74	99.70	110.14
1	F	181	VAL	O-C-N	-6.74	114.15	122.57
1	F	449	ASN	N-CA-C	6.74	119.96	109.52
1	A	181	VAL	O-C-N	-6.74	114.15	122.57
1	D	150	VAL	O-C-N	6.74	128.67	121.87
1	E	110	MET	N-CA-C	-6.74	99.70	110.14
1	E	378	PRO	CA-C-O	-6.74	109.31	119.55
1	F	300	ILE	CA-C-N	-6.74	110.07	120.31
1	F	300	ILE	C-N-CA	-6.74	110.07	120.31
1	F	393	LYS	CB-CA-C	-6.74	98.17	110.63
1	B	393	LYS	CB-CA-C	-6.73	98.17	110.63
1	E	234	GLU	O-C-N	6.73	129.26	122.12
1	A	393	LYS	CB-CA-C	-6.73	98.17	110.63
1	D	409	SER	CA-C-N	-6.73	108.22	121.41
1	D	409	SER	C-N-CA	-6.73	108.22	121.41
1	B	564	ILE	CB-CG1-CD1	-6.73	99.67	113.80
1	B	622	LEU	N-CA-CB	-6.73	100.00	110.57
1	C	504	GLU	O-C-N	6.73	130.91	123.04
1	E	38	ASN	CA-CB-CG	-6.73	105.87	112.60
1	A	234	GLU	O-C-N	6.73	129.25	122.12
1	C	612	HIS	O-C-N	6.73	131.21	122.20
1	B	409	SER	CA-C-N	-6.72	108.23	121.41
1	B	409	SER	C-N-CA	-6.72	108.23	121.41
1	C	150	VAL	O-C-N	6.72	128.66	121.87
1	E	409	SER	CA-C-N	-6.72	108.23	121.41
1	E	409	SER	C-N-CA	-6.72	108.23	121.41
1	A	409	SER	CA-C-N	-6.72	108.23	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	409	SER	C-N-CA	-6.72	108.23	121.41
1	B	424	THR	O-C-N	6.72	131.97	123.23
1	D	224	HIS	N-CA-CB	-6.72	99.44	110.40
1	D	424	THR	O-C-N	6.72	131.97	123.23
1	A	224	HIS	N-CA-CB	-6.72	99.44	110.40
1	C	300	ILE	CA-C-N	-6.72	110.09	120.31
1	C	300	ILE	C-N-CA	-6.72	110.09	120.31
1	A	110	MET	N-CA-C	-6.72	99.72	110.14
1	C	52	ALA	O-C-N	6.72	129.29	122.03
1	E	300	ILE	CA-C-N	-6.72	110.10	120.31
1	E	300	ILE	C-N-CA	-6.72	110.10	120.31
1	E	393	LYS	CB-CA-C	-6.72	98.20	110.63
1	E	424	THR	O-C-N	6.72	131.97	123.23
1	E	622	LEU	N-CA-CB	-6.72	100.02	110.57
1	F	149	GLU	O-C-N	6.72	130.30	122.17
1	F	409	SER	CA-C-N	-6.72	108.24	121.41
1	F	409	SER	C-N-CA	-6.72	108.24	121.41
1	B	181	VAL	O-C-N	-6.72	114.17	122.57
1	C	135	PRO	CB-CA-C	-6.72	102.73	110.92
1	A	451	ARG	NE-CZ-NH1	-6.71	114.79	121.50
1	C	117	TYR	CA-C-O	-6.71	113.77	120.82
1	E	504	GLU	O-C-N	6.71	130.90	123.04
1	F	117	TYR	CA-C-O	-6.71	113.77	120.82
1	C	224	HIS	N-CA-CB	-6.71	99.46	110.40
1	D	110	MET	N-CA-C	-6.71	99.74	110.14
1	D	297	HIS	CB-CA-C	-6.71	97.07	110.42
1	A	622	LEU	N-CA-CB	-6.71	100.04	110.57
1	B	224	HIS	N-CA-CB	-6.71	99.47	110.40
1	B	234	GLU	O-C-N	6.71	129.23	122.12
1	C	297	HIS	CB-CA-C	-6.71	97.07	110.42
1	E	224	HIS	N-CA-CB	-6.71	99.46	110.40
1	E	297	HIS	CB-CA-C	-6.71	97.07	110.42
1	A	297	HIS	CB-CA-C	-6.70	97.08	110.42
1	A	424	THR	O-C-N	6.70	131.94	123.23
1	C	424	THR	O-C-N	6.70	131.95	123.23
1	C	622	LEU	N-CA-CB	-6.70	100.05	110.57
1	C	348	HIS	CA-C-O	-6.70	113.76	120.80
1	D	234	GLU	O-C-N	6.70	129.22	122.12
1	D	622	LEU	N-CA-CB	-6.70	100.05	110.57
1	A	300	ILE	CA-C-N	-6.70	110.12	120.31
1	A	300	ILE	C-N-CA	-6.70	110.12	120.31
1	C	409	SER	CA-C-N	-6.70	108.28	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	409	SER	C-N-CA	-6.70	108.28	121.41
1	A	117	TYR	CA-C-O	-6.70	113.79	120.82
1	B	110	MET	N-CA-C	-6.70	99.76	110.14
1	B	297	HIS	CB-CA-C	-6.70	97.09	110.42
1	E	117	TYR	CA-C-O	-6.70	113.79	120.82
1	E	149	GLU	O-C-N	6.70	130.27	122.17
1	F	625	PRO	N-CD-CG	-6.70	95.76	103.80
1	D	117	TYR	CA-C-O	-6.70	113.79	120.82
1	E	135	PRO	CB-CA-C	-6.69	102.75	110.92
1	B	135	PRO	CB-CA-C	-6.69	102.75	110.92
1	C	245	GLU	N-CA-CB	-6.69	99.50	110.41
1	F	297	HIS	CB-CA-C	-6.69	97.10	110.42
1	B	300	ILE	CA-C-N	-6.69	110.14	120.31
1	B	300	ILE	C-N-CA	-6.69	110.14	120.31
1	C	110	MET	N-CA-C	-6.69	99.77	110.14
1	D	300	ILE	CA-C-N	-6.69	110.14	120.31
1	D	300	ILE	C-N-CA	-6.69	110.14	120.31
1	F	622	LEU	N-CA-CB	-6.69	100.07	110.57
1	B	348	HIS	CA-C-O	-6.69	113.78	120.80
1	A	149	GLU	O-C-N	6.69	130.26	122.17
1	F	234	GLU	O-C-N	6.69	129.21	122.12
1	D	245	GLU	N-CA-CB	-6.69	99.51	110.41
1	A	135	PRO	CB-CA-C	-6.68	102.77	110.92
1	D	153	LYS	CA-CB-CG	-6.68	100.73	114.10
1	F	135	PRO	CB-CA-C	-6.68	102.77	110.92
1	A	245	GLU	N-CA-CB	-6.68	99.52	110.41
1	E	1	ASP	CA-C-N	6.68	133.68	122.79
1	E	1	ASP	C-N-CA	6.68	133.68	122.79
1	C	1	ASP	CA-C-N	6.68	133.68	122.79
1	C	1	ASP	C-N-CA	6.68	133.68	122.79
1	E	132	ILE	O-C-N	6.68	129.72	122.57
1	E	245	GLU	N-CA-CB	-6.68	99.52	110.41
1	E	348	HIS	CA-C-O	-6.68	113.79	120.80
1	A	1	ASP	CA-C-N	6.68	133.67	122.79
1	A	1	ASP	C-N-CA	6.68	133.67	122.79
1	B	1	ASP	CA-C-N	6.68	133.67	122.79
1	B	1	ASP	C-N-CA	6.68	133.67	122.79
1	B	149	GLU	O-C-N	6.68	130.25	122.17
1	B	451	ARG	NE-CZ-NH1	-6.68	114.82	121.50
1	D	487	ASP	CA-C-N	-6.68	116.38	126.86
1	D	487	ASP	C-N-CA	-6.68	116.38	126.86
1	E	153	LYS	CA-CB-CG	-6.68	100.75	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	301	ASP	CA-CB-CG	-6.68	105.92	112.60
1	F	1	ASP	CA-C-N	6.68	133.67	122.79
1	F	1	ASP	C-N-CA	6.68	133.67	122.79
1	A	153	LYS	CA-CB-CG	-6.67	100.75	114.10
1	B	52	ALA	O-C-N	6.67	129.24	122.03
1	E	217	GLY	CA-C-O	-6.67	108.96	120.57
1	E	487	ASP	CA-C-N	-6.67	116.38	126.86
1	E	487	ASP	C-N-CA	-6.67	116.38	126.86
1	D	451	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	C	153	LYS	CA-CB-CG	-6.67	100.76	114.10
1	D	353	ARG	CA-C-O	6.67	127.50	119.43
1	F	153	LYS	CA-CB-CG	-6.67	100.75	114.10
1	F	245	GLU	N-CA-CB	-6.67	99.53	110.41
1	C	487	ASP	CA-C-N	-6.67	116.39	126.86
1	C	487	ASP	C-N-CA	-6.67	116.39	126.86
1	A	625	PRO	N-CD-CG	-6.67	95.80	103.80
1	B	245	GLU	N-CA-CB	-6.67	99.54	110.41
1	C	625	PRO	N-CD-CG	-6.67	95.80	103.80
1	D	135	PRO	CB-CA-C	-6.67	102.78	110.92
1	F	217	GLY	CA-C-O	-6.67	108.97	120.57
1	A	348	HIS	CA-C-O	-6.67	113.80	120.80
1	A	487	ASP	CA-C-N	-6.67	116.39	126.86
1	A	487	ASP	C-N-CA	-6.67	116.39	126.86
1	B	487	ASP	CA-C-N	-6.67	116.39	126.86
1	B	487	ASP	C-N-CA	-6.67	116.39	126.86
1	C	149	GLU	O-C-N	6.67	130.24	122.17
1	D	1	ASP	CA-C-N	6.67	133.65	122.79
1	D	1	ASP	C-N-CA	6.67	133.65	122.79
1	A	301	ASP	CA-CB-CG	-6.66	105.94	112.60
1	B	117	TYR	CA-C-O	-6.66	113.82	120.82
1	D	625	PRO	N-CD-CG	-6.66	95.80	103.80
1	F	487	ASP	CA-C-N	-6.66	116.40	126.86
1	F	487	ASP	C-N-CA	-6.66	116.40	126.86
1	B	153	LYS	CA-CB-CG	-6.66	100.78	114.10
1	D	217	GLY	CA-C-O	-6.66	108.98	120.57
1	A	217	GLY	CA-C-O	-6.66	108.98	120.57
1	C	580	PHE	CA-C-N	6.66	132.37	123.05
1	C	580	PHE	C-N-CA	6.66	132.37	123.05
1	D	348	HIS	CA-C-O	-6.66	113.81	120.80
1	D	567	ARG	NE-CZ-NH1	-6.66	114.84	121.50
1	D	580	PHE	CA-C-N	6.66	132.37	123.05
1	D	580	PHE	C-N-CA	6.66	132.37	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	451	ARG	NE-CZ-NH1	-6.66	114.84	121.50
1	F	424	THR	O-C-N	6.66	131.88	123.23
1	F	301	ASP	CA-CB-CG	-6.66	105.94	112.60
1	C	217	GLY	CA-C-O	-6.65	108.99	120.57
1	D	301	ASP	CA-CB-CG	-6.65	105.95	112.60
1	C	301	ASP	CA-CB-CG	-6.65	105.95	112.60
1	E	625	PRO	N-CD-CG	-6.65	95.82	103.80
1	D	331	SER	CA-C-N	-6.64	111.14	122.56
1	D	331	SER	C-N-CA	-6.64	111.14	122.56
1	E	481	PHE	N-CA-CB	-6.64	99.58	110.41
1	D	481	PHE	N-CA-CB	-6.64	99.58	110.41
1	E	353	ARG	CA-C-O	6.64	127.47	119.43
1	B	217	GLY	CA-C-O	-6.64	109.02	120.57
1	B	481	PHE	N-CA-CB	-6.64	99.59	110.41
1	B	554	ASP	N-CA-CB	6.64	124.05	110.64
1	B	580	PHE	CA-C-N	6.64	132.34	123.05
1	B	580	PHE	C-N-CA	6.64	132.34	123.05
1	B	625	PRO	N-CD-CG	-6.64	95.83	103.80
1	E	272	PRO	CA-C-N	-6.64	108.86	121.54
1	E	272	PRO	C-N-CA	-6.64	108.86	121.54
1	F	567	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	C	344	HIS	CA-CB-CG	-6.64	107.16	113.80
1	E	554	ASP	N-CA-CB	6.64	124.05	110.64
1	E	580	PHE	CA-C-N	6.64	132.34	123.05
1	E	580	PHE	C-N-CA	6.64	132.34	123.05
1	A	481	PHE	N-CA-CB	-6.64	99.59	110.41
1	B	301	ASP	CA-CB-CG	-6.64	105.96	112.60
1	F	348	HIS	CA-C-O	-6.64	113.83	120.80
1	C	481	PHE	N-CA-CB	-6.63	99.60	110.41
1	C	554	ASP	N-CA-CB	6.63	124.04	110.64
1	F	385	LYS	N-CA-C	-6.63	103.97	111.14
1	A	554	ASP	N-CA-CB	6.63	124.03	110.64
1	C	549	GLY	CA-C-N	-6.63	108.41	121.41
1	C	549	GLY	C-N-CA	-6.63	108.41	121.41
1	C	567	ARG	NE-CZ-NH1	-6.63	114.87	121.50
1	F	481	PHE	N-CA-CB	-6.63	99.60	110.41
1	A	580	PHE	CA-C-N	6.63	132.33	123.05
1	A	580	PHE	C-N-CA	6.63	132.33	123.05
1	E	549	GLY	CA-C-N	-6.63	108.42	121.41
1	E	549	GLY	C-N-CA	-6.63	108.42	121.41
1	B	567	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	C	336	ASN	CA-CB-CG	-6.62	105.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	554	ASP	N-CA-CB	6.62	124.02	110.64
1	F	549	GLY	CA-C-N	-6.62	108.43	121.41
1	F	549	GLY	C-N-CA	-6.62	108.43	121.41
1	B	344	HIS	CA-CB-CG	-6.62	107.18	113.80
1	D	290	GLU	CG-CD-OE2	6.62	133.62	118.40
1	A	331	SER	CA-C-N	-6.62	111.18	122.56
1	A	331	SER	C-N-CA	-6.62	111.18	122.56
1	A	567	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	C	290	GLU	CG-CD-OE2	6.62	133.62	118.40
1	C	385	LYS	N-CA-C	-6.62	104.00	111.14
1	D	142	PRO	CA-C-N	-6.62	109.67	120.72
1	D	142	PRO	C-N-CA	-6.62	109.67	120.72
1	D	385	LYS	N-CA-C	-6.62	104.00	111.14
1	F	344	HIS	CA-CB-CG	-6.62	107.18	113.80
1	E	107	ARG	CD-NE-CZ	-6.61	115.14	124.40
1	A	353	ARG	CA-C-O	6.61	127.43	119.43
1	A	549	GLY	CA-C-N	-6.61	108.45	121.41
1	A	549	GLY	C-N-CA	-6.61	108.45	121.41
1	A	132	ILE	O-C-N	6.61	129.64	122.57
1	A	385	LYS	N-CA-C	-6.61	104.00	111.14
1	C	272	PRO	CA-C-N	-6.61	108.92	121.54
1	C	272	PRO	C-N-CA	-6.61	108.92	121.54
1	C	353	ARG	CA-C-O	6.61	127.43	119.43
1	B	290	GLU	CG-CD-OE2	6.61	133.60	118.40
1	B	353	ARG	CA-C-O	6.61	127.42	119.43
1	B	385	LYS	N-CA-C	-6.61	104.00	111.14
1	C	335	SER	N-CA-C	-6.61	103.27	112.45
1	F	331	SER	CA-C-N	-6.61	111.20	122.56
1	F	331	SER	C-N-CA	-6.61	111.20	122.56
1	F	580	PHE	CA-C-N	6.61	132.30	123.05
1	F	580	PHE	C-N-CA	6.61	132.30	123.05
1	D	549	GLY	CA-C-N	-6.61	108.47	121.41
1	D	549	GLY	C-N-CA	-6.61	108.47	121.41
1	F	112	GLU	CA-CB-CG	-6.61	100.89	114.10
1	F	290	GLU	CG-CD-OE2	6.61	133.59	118.40
1	F	595	GLY	CA-C-N	-6.61	109.81	121.70
1	F	595	GLY	C-N-CA	-6.61	109.81	121.70
1	A	290	GLU	CG-CD-OE2	6.60	133.59	118.40
1	B	549	GLY	CA-C-N	-6.60	108.47	121.41
1	B	549	GLY	C-N-CA	-6.60	108.47	121.41
1	B	636	ILE	CB-CG1-CD1	-6.60	99.93	113.80
1	E	344	HIS	CA-CB-CG	-6.60	107.20	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	595	GLY	CA-C-N	-6.60	109.81	121.70
1	E	595	GLY	C-N-CA	-6.60	109.81	121.70
1	A	344	HIS	CA-CB-CG	-6.60	107.20	113.80
1	A	595	GLY	CA-C-N	-6.60	109.81	121.70
1	A	595	GLY	C-N-CA	-6.60	109.81	121.70
1	C	112	GLU	CA-CB-CG	-6.60	100.89	114.10
1	C	373	THR	CA-C-O	6.60	126.25	118.79
1	C	595	GLY	CA-C-N	-6.60	109.81	121.70
1	C	595	GLY	C-N-CA	-6.60	109.81	121.70
1	D	287	HIS	CA-CB-CG	-6.60	107.20	113.80
1	D	595	GLY	CA-C-N	-6.60	109.81	121.70
1	D	595	GLY	C-N-CA	-6.60	109.81	121.70
1	E	142	PRO	CA-C-N	-6.60	109.69	120.72
1	E	142	PRO	C-N-CA	-6.60	109.69	120.72
1	A	272	PRO	CA-C-N	-6.60	108.93	121.54
1	A	272	PRO	C-N-CA	-6.60	108.93	121.54
1	B	335	SER	N-CA-C	-6.60	103.28	112.45
1	C	142	PRO	CA-C-N	-6.60	109.70	120.72
1	C	142	PRO	C-N-CA	-6.60	109.70	120.72
1	C	525	ASP	CA-C-O	-6.60	109.07	119.23
1	D	112	GLU	CA-CB-CG	-6.60	100.90	114.10
1	F	263	LYS	N-CA-CB	6.60	119.77	110.07
1	D	336	ASN	CA-CB-CG	-6.60	106.00	112.60
1	D	554	ASP	N-CA-CB	6.60	123.97	110.64
1	E	331	SER	CA-C-N	-6.60	111.21	122.56
1	E	331	SER	C-N-CA	-6.60	111.21	122.56
1	A	112	GLU	CA-CB-CG	-6.60	100.91	114.10
1	B	430	GLN	O-C-N	-6.60	115.31	123.36
1	C	132	ILE	O-C-N	6.60	129.63	122.57
1	F	353	ARG	CA-C-O	6.60	127.41	119.43
1	C	75	PHE	N-CA-C	-6.59	105.23	113.28
1	D	272	PRO	CA-C-N	-6.59	108.95	121.54
1	D	272	PRO	C-N-CA	-6.59	108.95	121.54
1	E	112	GLU	CA-CB-CG	-6.59	100.91	114.10
1	A	636	ILE	CB-CG1-CD1	-6.59	99.96	113.80
1	B	112	GLU	CA-CB-CG	-6.59	100.91	114.10
1	C	636	ILE	CB-CG1-CD1	-6.59	99.95	113.80
1	F	272	PRO	CA-C-N	-6.59	108.95	121.54
1	F	272	PRO	C-N-CA	-6.59	108.95	121.54
1	B	336	ASN	CA-CB-CG	-6.59	106.01	112.60
1	D	75	PHE	N-CA-C	-6.59	105.24	113.28
1	D	344	HIS	CA-CB-CG	-6.59	107.21	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	107	ARG	CD-NE-CZ	-6.59	115.17	124.40
1	B	331	SER	CA-C-N	-6.59	111.23	122.56
1	B	331	SER	C-N-CA	-6.59	111.23	122.56
1	C	331	SER	CA-C-N	-6.59	111.22	122.56
1	C	331	SER	C-N-CA	-6.59	111.22	122.56
1	D	107	ARG	CD-NE-CZ	-6.59	115.17	124.40
1	E	259	LEU	N-CA-CB	-6.59	102.46	112.28
1	F	75	PHE	N-CA-C	-6.59	105.24	113.28
1	A	107	ARG	CD-NE-CZ	-6.59	115.18	124.40
1	D	132	ILE	O-C-N	6.59	129.62	122.57
1	E	141	THR	CA-C-O	-6.59	114.03	121.28
1	E	335	SER	N-CA-C	-6.59	103.30	112.45
1	F	259	LEU	N-CA-CB	-6.59	102.47	112.28
1	F	636	ILE	CB-CG1-CD1	-6.59	99.97	113.80
1	A	142	PRO	CA-C-N	-6.58	109.72	120.72
1	A	142	PRO	C-N-CA	-6.58	109.72	120.72
1	C	107	ARG	CD-NE-CZ	-6.58	115.18	124.40
1	E	265	GLY	O-C-N	-6.58	114.14	122.70
1	C	402	THR	CA-CB-CG2	6.58	121.69	110.50
1	D	263	LYS	N-CA-CB	6.58	119.75	110.07
1	E	430	GLN	O-C-N	-6.58	115.33	123.36
1	F	31	LYS	CB-CG-CD	-6.58	96.16	111.30
1	A	525	ASP	CA-C-O	-6.58	109.09	119.23
1	E	263	LYS	N-CA-CB	6.58	119.74	110.07
1	F	142	PRO	CA-C-N	-6.58	109.73	120.72
1	F	142	PRO	C-N-CA	-6.58	109.73	120.72
1	F	287	HIS	CA-CB-CG	-6.58	107.22	113.80
1	F	336	ASN	CA-CB-CG	-6.58	106.02	112.60
1	A	336	ASN	CA-CB-CG	-6.58	106.02	112.60
1	B	272	PRO	CA-C-N	-6.58	108.97	121.54
1	B	272	PRO	C-N-CA	-6.58	108.97	121.54
1	D	31	LYS	CB-CG-CD	-6.58	96.17	111.30
1	D	525	ASP	CA-C-O	-6.58	109.10	119.23
1	E	75	PHE	N-CA-C	-6.58	105.25	113.28
1	E	385	LYS	N-CA-C	-6.58	104.03	111.14
1	E	636	ILE	CB-CG1-CD1	-6.58	99.98	113.80
1	B	107	ARG	CD-NE-CZ	-6.58	115.19	124.40
1	B	263	LYS	N-CA-CB	6.58	119.74	110.07
1	B	595	GLY	CA-C-N	-6.58	109.86	121.70
1	B	595	GLY	C-N-CA	-6.58	109.86	121.70
1	C	287	HIS	CA-CB-CG	-6.58	107.22	113.80
1	D	265	GLY	O-C-N	-6.58	114.15	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	210	GLY	N-CA-C	6.58	128.77	113.18
1	E	290	GLU	CG-CD-OE2	6.58	133.53	118.40
1	F	231	PHE	CA-CB-CG	6.58	120.38	113.80
1	F	373	THR	CA-C-O	6.58	126.22	118.79
1	F	525	ASP	CA-C-O	-6.58	109.10	119.23
1	B	1	ASP	CA-C-O	6.58	131.98	120.80
1	B	141	THR	CA-C-O	-6.58	114.05	121.28
1	C	430	GLN	O-C-N	-6.58	115.34	123.36
1	D	335	SER	N-CA-C	-6.58	103.31	112.45
1	D	547	VAL	O-C-N	6.58	134.40	121.91
1	E	210	GLY	N-CA-C	6.58	128.77	113.18
1	F	132	ILE	O-C-N	6.58	129.61	122.57
1	A	287	HIS	CA-CB-CG	-6.57	107.23	113.80
1	A	335	SER	N-CA-C	-6.57	103.31	112.45
1	B	31	LYS	CB-CG-CD	-6.57	96.18	111.30
1	D	210	GLY	N-CA-C	6.57	128.76	113.18
1	F	430	GLN	O-C-N	-6.57	115.34	123.36
1	B	259	LEU	N-CA-CB	-6.57	102.49	112.28
1	C	69	ARG	NE-CZ-NH1	-6.57	114.93	121.50
1	C	265	GLY	O-C-N	-6.57	114.16	122.70
1	A	263	LYS	N-CA-CB	6.57	119.73	110.07
1	A	265	GLY	O-C-N	-6.57	114.16	122.70
1	E	525	ASP	CA-C-O	-6.57	109.11	119.23
1	A	75	PHE	N-CA-C	-6.57	105.27	113.28
1	A	210	GLY	N-CA-C	6.57	128.75	113.18
1	B	547	VAL	O-C-N	6.57	134.39	121.91
1	C	263	LYS	N-CA-CB	6.57	119.73	110.07
1	D	373	THR	CA-C-O	6.57	126.21	118.79
1	D	636	ILE	CB-CG1-CD1	-6.57	100.01	113.80
1	E	31	LYS	CB-CG-CD	-6.57	96.19	111.30
1	A	31	LYS	CB-CG-CD	-6.57	96.20	111.30
1	A	259	LEU	N-CA-CB	-6.57	102.50	112.28
1	B	132	ILE	O-C-N	6.57	129.59	122.57
1	C	259	LEU	N-CA-CB	-6.57	102.50	112.28
1	E	336	ASN	CA-CB-CG	-6.57	106.03	112.60
1	A	430	GLN	O-C-N	-6.56	115.35	123.36
1	D	338	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	E	1	ASP	CA-C-O	6.56	131.96	120.80
1	D	430	GLN	O-C-N	-6.56	115.36	123.36
1	E	607	ALA	CB-CA-C	6.56	121.65	111.02
1	F	141	THR	CA-C-O	-6.56	114.06	121.28
1	F	335	SER	N-CA-C	-6.56	103.33	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	607	ALA	CB-CA-C	6.56	121.65	111.02
1	F	1	ASP	CA-C-O	6.56	131.95	120.80
1	C	31	LYS	CB-CG-CD	-6.56	96.22	111.30
1	C	81	LYS	O-C-N	-6.56	115.17	122.12
1	D	231	PHE	CA-CB-CG	6.56	120.36	113.80
1	E	567	ARG	NE-CZ-NH1	-6.56	114.94	121.50
1	A	141	THR	CA-C-O	-6.56	114.07	121.28
1	A	547	VAL	O-C-N	6.56	134.37	121.91
1	B	287	HIS	CA-CB-CG	-6.56	107.24	113.80
1	C	141	THR	CA-C-O	-6.56	114.07	121.28
1	C	230	ARG	CD-NE-CZ	-6.56	115.22	124.40
1	C	231	PHE	CA-CB-CG	6.56	120.36	113.80
1	B	142	PRO	CA-C-N	-6.56	109.77	120.72
1	B	142	PRO	C-N-CA	-6.56	109.77	120.72
1	A	373	THR	CA-C-O	6.55	126.20	118.79
1	E	402	THR	CA-CB-CG2	6.55	121.64	110.50
1	A	402	THR	CA-CB-CG2	6.55	121.64	110.50
1	B	276	HIS	CE1-NE2-CD2	-6.55	102.45	109.00
1	F	265	GLY	O-C-N	-6.55	114.18	122.70
1	F	402	THR	CA-CB-CG2	6.55	121.64	110.50
1	B	75	PHE	N-CA-C	-6.55	105.29	113.28
1	B	81	LYS	O-C-N	-6.55	115.18	122.12
1	B	210	GLY	N-CA-C	6.55	128.70	113.18
1	B	265	GLY	O-C-N	-6.55	114.19	122.70
1	D	402	THR	CA-CB-CG2	6.55	121.63	110.50
1	A	607	ALA	CB-CA-C	6.55	121.63	111.02
1	C	210	GLY	N-CA-C	6.55	128.69	113.18
1	D	552	ASP	CA-CB-CG	6.55	119.15	112.60
1	D	607	ALA	CB-CA-C	6.55	121.63	111.02
1	E	201	PHE	CA-CB-CG	-6.55	107.25	113.80
1	F	524	LYS	CB-CA-C	6.55	121.98	110.85
1	F	552	ASP	CA-CB-CG	6.55	119.15	112.60
1	B	525	ASP	CA-C-O	-6.54	109.15	119.23
1	C	276	HIS	CE1-NE2-CD2	-6.54	102.45	109.00
1	A	1	ASP	CA-C-O	6.54	131.92	120.80
1	C	552	ASP	CA-CB-CG	6.54	119.14	112.60
1	D	76	ASN	CA-C-N	-6.54	110.10	120.63
1	D	76	ASN	C-N-CA	-6.54	110.10	120.63
1	E	547	VAL	O-C-N	6.54	134.34	121.91
1	F	201	PHE	CA-CB-CG	-6.54	107.26	113.80
1	F	607	ALA	CB-CA-C	6.54	121.62	111.02
1	B	402	THR	CA-CB-CG2	6.54	121.62	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	201	PHE	CA-CB-CG	-6.54	107.26	113.80
1	D	259	LEU	N-CA-CB	-6.54	102.53	112.28
1	E	373	THR	CA-C-O	6.54	126.18	118.79
1	F	84	LEU	N-CA-C	-6.54	105.28	113.20
1	A	338	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	B	552	ASP	CA-CB-CG	6.54	119.14	112.60
1	E	69	ARG	NE-CZ-NH1	-6.54	114.96	121.50
1	F	468	ASN	CB-CG-ND2	6.54	126.21	116.40
1	D	149	GLU	CA-C-N	-6.54	110.14	120.47
1	D	149	GLU	C-N-CA	-6.54	110.14	120.47
1	D	276	HIS	CE1-NE2-CD2	-6.54	102.46	109.00
1	E	149	GLU	CA-C-N	-6.54	110.14	120.47
1	E	149	GLU	C-N-CA	-6.54	110.14	120.47
1	E	287	HIS	CA-CB-CG	-6.54	107.26	113.80
1	F	338	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	A	201	PHE	CA-CB-CG	-6.54	107.26	113.80
1	E	524	LYS	CB-CA-C	6.54	121.96	110.85
1	F	385	LYS	CA-CB-CG	-6.54	101.03	114.10
1	B	231	PHE	CA-CB-CG	6.54	120.33	113.80
1	C	1	ASP	CA-C-O	6.54	131.91	120.80
1	C	547	VAL	O-C-N	6.54	134.33	121.91
1	F	69	ARG	NE-CZ-NH1	-6.54	114.97	121.50
1	F	149	GLU	CA-C-N	-6.54	110.14	120.47
1	F	149	GLU	C-N-CA	-6.54	110.14	120.47
1	B	373	THR	CA-C-O	6.53	126.17	118.79
1	B	524	LYS	CA-CB-CG	-6.53	101.03	114.10
1	D	223	VAL	O-C-N	6.53	128.21	121.87
1	F	547	VAL	O-C-N	6.53	134.32	121.91
1	A	524	LYS	CB-CA-C	6.53	121.95	110.85
1	B	149	GLU	CA-C-N	-6.53	110.15	120.47
1	B	149	GLU	C-N-CA	-6.53	110.15	120.47
1	B	385	LYS	CA-CB-CG	-6.53	101.04	114.10
1	B	607	ALA	CB-CA-C	6.53	121.60	111.02
1	D	385	LYS	CA-CB-CG	-6.53	101.04	114.10
1	E	276	HIS	CE1-NE2-CD2	-6.53	102.47	109.00
1	D	69	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	E	139	GLN	CA-C-O	-6.53	112.03	119.41
1	A	552	ASP	CA-CB-CG	6.53	119.13	112.60
1	B	69	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	A	385	LYS	CA-CB-CG	-6.53	101.05	114.10
1	E	385	LYS	CA-CB-CG	-6.52	101.05	114.10
1	F	119	LEU	CB-CG-CD2	-6.52	91.13	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	ARG	NE-CZ-NH1	-6.52	114.98	121.50
1	A	231	PHE	CA-CB-CG	6.52	120.32	113.80
1	A	276	HIS	CE1-NE2-CD2	-6.52	102.48	109.00
1	A	524	LYS	CA-CB-CG	-6.52	101.06	114.10
1	B	653	LEU	N-CA-CB	-6.52	99.42	110.50
1	C	338	GLN	OE1-CD-NE2	-6.52	116.08	122.60
1	D	1	ASP	CA-C-O	6.52	131.88	120.80
1	D	201	PHE	CA-CB-CG	-6.52	107.28	113.80
1	E	230	ARG	CD-NE-CZ	-6.52	115.27	124.40
1	E	524	LYS	CA-CB-CG	-6.52	101.06	114.10
1	F	451	ARG	CD-NE-CZ	-6.52	115.27	124.40
1	F	653	LEU	N-CA-CB	-6.52	99.42	110.50
1	A	149	GLU	CA-C-N	-6.52	110.17	120.47
1	A	149	GLU	C-N-CA	-6.52	110.17	120.47
1	C	376	ARG	CB-CG-CD	6.52	126.29	111.30
1	D	141	THR	CA-C-O	-6.52	114.11	121.28
1	D	524	LYS	CA-CB-CG	-6.52	101.07	114.10
1	D	653	LEU	N-CA-CB	-6.52	99.42	110.50
1	E	81	LYS	O-C-N	-6.52	115.21	122.12
1	E	231	PHE	CA-CB-CG	6.52	120.32	113.80
1	B	338	GLN	OE1-CD-NE2	-6.52	116.08	122.60
1	E	552	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	119	LEU	CB-CG-CD2	-6.51	91.16	110.70
1	B	119	LEU	CB-CG-CD2	-6.51	91.16	110.70
1	C	385	LYS	CA-CB-CG	-6.51	101.07	114.10
1	D	546	ALA	N-CA-CB	6.51	121.73	110.98
1	E	548	ASN	N-CA-C	-6.51	96.45	108.24
1	F	546	ALA	N-CA-CB	6.51	121.73	110.98
1	A	81	LYS	O-C-N	-6.51	115.22	122.12
1	A	548	ASN	N-CA-C	-6.51	96.45	108.24
1	D	119	LEU	CB-CG-CD2	-6.51	91.16	110.70
1	F	430	GLN	N-CA-CB	-6.51	99.87	110.81
1	A	230	ARG	CD-NE-CZ	-6.51	115.28	124.40
1	A	653	LEU	N-CA-CB	-6.51	99.43	110.50
1	B	548	ASN	N-CA-C	-6.51	96.45	108.24
1	C	149	GLU	CA-C-N	-6.51	110.18	120.47
1	C	149	GLU	C-N-CA	-6.51	110.18	120.47
1	D	214	ASP	CB-CA-C	-6.51	97.46	110.42
1	B	84	LEU	N-CA-C	-6.51	105.32	113.20
1	B	376	ARG	CB-CG-CD	6.51	126.27	111.30
1	C	119	LEU	CB-CG-CD2	-6.51	91.17	110.70
1	D	275	ILE	CB-CG1-CD1	-6.51	100.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	119	LEU	CB-CG-CD2	-6.51	91.17	110.70
1	F	548	ASN	N-CA-C	-6.51	96.46	108.24
1	A	376	ARG	CB-CG-CD	6.51	126.27	111.30
1	A	546	ALA	N-CA-CB	6.51	121.72	110.98
1	B	214	ASP	CB-CA-C	-6.51	97.47	110.42
1	D	548	ASN	N-CA-C	-6.51	96.46	108.24
1	B	275	ILE	CB-CG1-CD1	-6.51	100.14	113.80
1	B	524	LYS	CB-CA-C	6.51	121.91	110.85
1	B	546	ALA	N-CA-CB	6.51	121.72	110.98
1	C	653	LEU	N-CA-CB	-6.51	99.44	110.50
1	D	230	ARG	CD-NE-CZ	-6.51	115.29	124.40
1	E	275	ILE	CB-CG1-CD1	-6.51	100.14	113.80
1	C	524	LYS	CA-CB-CG	-6.50	101.09	114.10
1	D	524	LYS	CB-CA-C	6.50	121.91	110.85
1	A	76	ASN	CA-C-N	-6.50	110.16	120.63
1	A	76	ASN	C-N-CA	-6.50	110.16	120.63
1	A	84	LEU	N-CA-C	-6.50	105.33	113.20
1	A	468	ASN	CB-CG-ND2	6.50	126.16	116.40
1	B	201	PHE	CA-CB-CG	-6.50	107.30	113.80
1	D	81	LYS	O-C-N	-6.50	115.23	122.12
1	F	524	LYS	CA-CB-CG	-6.50	101.09	114.10
1	A	275	ILE	CB-CG1-CD1	-6.50	100.15	113.80
1	C	548	ASN	N-CA-C	-6.50	96.47	108.24
1	D	547	VAL	CA-CB-CG2	6.50	121.45	110.40
1	E	547	VAL	CA-CB-CG2	6.50	121.45	110.40
1	C	546	ALA	N-CA-CB	6.50	121.70	110.98
1	B	430	GLN	N-CA-CB	-6.50	99.89	110.81
1	C	430	GLN	N-CA-CB	-6.50	99.89	110.81
1	D	376	ARG	CB-CG-CD	6.50	126.25	111.30
1	E	376	ARG	CB-CG-CD	6.50	126.25	111.30
1	F	230	ARG	CD-NE-CZ	-6.50	115.30	124.40
1	F	275	ILE	CB-CG1-CD1	-6.50	100.15	113.80
1	F	276	HIS	CE1-NE2-CD2	-6.50	102.50	109.00
1	A	214	ASP	CB-CA-C	-6.50	97.49	110.42
1	A	430	GLN	N-CA-CB	-6.50	99.89	110.81
1	D	468	ASN	CB-CG-ND2	6.50	126.15	116.40
1	E	653	LEU	N-CA-CB	-6.50	99.46	110.50
1	F	376	ARG	CB-CG-CD	6.50	126.24	111.30
1	B	230	ARG	CD-NE-CZ	-6.50	115.31	124.40
1	B	547	VAL	CA-CB-CG2	6.50	121.44	110.40
1	E	335	SER	CA-C-N	-6.50	113.24	123.24
1	E	335	SER	C-N-CA	-6.50	113.24	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	546	ALA	N-CA-CB	6.50	121.70	110.98
1	B	27	TYR	N-CA-CB	-6.49	100.37	110.11
1	B	76	ASN	CA-C-N	-6.49	110.17	120.63
1	B	76	ASN	C-N-CA	-6.49	110.17	120.63
1	C	232	ASP	O-C-N	6.49	129.00	122.12
1	C	275	ILE	CB-CG1-CD1	-6.49	100.16	113.80
1	C	451	ARG	CD-NE-CZ	-6.49	115.31	124.40
1	C	547	VAL	CA-CB-CG2	6.49	121.44	110.40
1	D	232	ASP	O-C-N	6.49	129.00	122.12
1	E	76	ASN	CA-C-N	-6.49	110.18	120.63
1	E	76	ASN	C-N-CA	-6.49	110.18	120.63
1	F	214	ASP	CB-CA-C	-6.49	97.50	110.42
1	B	513	PRO	CA-C-N	-6.49	111.88	122.65
1	B	513	PRO	C-N-CA	-6.49	111.88	122.65
1	E	430	GLN	N-CA-CB	-6.49	99.91	110.81
1	F	81	LYS	O-C-N	-6.49	115.24	122.12
1	A	451	ARG	CD-NE-CZ	-6.49	115.31	124.40
1	B	13	ASP	CA-CB-CG	-6.49	106.11	112.60
1	D	84	LEU	N-CA-C	-6.49	105.35	113.20
1	F	13	ASP	CA-CB-CG	-6.49	106.11	112.60
1	F	335	SER	CA-C-N	-6.49	113.25	123.24
1	F	335	SER	C-N-CA	-6.49	113.25	123.24
1	D	513	PRO	CA-C-N	-6.49	111.88	122.65
1	D	513	PRO	C-N-CA	-6.49	111.88	122.65
1	E	223	VAL	O-C-N	6.49	128.16	121.87
1	E	338	GLN	OE1-CD-NE2	-6.49	116.11	122.60
1	A	547	VAL	CA-CB-CG2	6.49	121.42	110.40
1	B	451	ARG	CD-NE-CZ	-6.49	115.32	124.40
1	C	139	GLN	CA-C-O	-6.49	112.08	119.41
1	B	571	PRO	O-C-N	-6.48	114.82	122.86
1	C	393	LYS	CA-C-O	-6.48	112.77	120.10
1	C	468	ASN	CB-CG-ND2	6.48	126.13	116.40
1	D	581	ASN	CB-CG-ND2	-6.48	106.67	116.40
1	F	27	TYR	N-CA-CB	-6.48	100.38	110.11
1	B	467	SER	CB-CA-C	-6.48	99.17	109.80
1	C	76	ASN	CA-C-N	-6.48	110.19	120.63
1	C	76	ASN	C-N-CA	-6.48	110.19	120.63
1	C	84	LEU	N-CA-C	-6.48	105.36	113.20
1	A	513	PRO	CA-C-N	-6.48	111.89	122.65
1	A	513	PRO	C-N-CA	-6.48	111.89	122.65
1	B	527	SER	O-C-N	6.48	131.61	122.41
1	C	513	PRO	CA-C-N	-6.48	111.89	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	513	PRO	C-N-CA	-6.48	111.89	122.65
1	D	467	SER	CB-CA-C	-6.48	99.17	109.80
1	E	232	ASP	O-C-N	6.48	128.99	122.12
1	A	232	ASP	O-C-N	6.48	128.99	122.12
1	C	214	ASP	CB-CA-C	-6.48	97.53	110.42
1	D	430	GLN	N-CA-CB	-6.48	99.92	110.81
1	E	84	LEU	N-CA-C	-6.48	105.36	113.20
1	A	139	GLN	CA-C-O	-6.48	112.09	119.41
1	A	146	THR	OG1-CB-CG2	6.48	122.25	109.30
1	B	468	ASN	CB-CG-ND2	6.48	126.12	116.40
1	D	146	THR	OG1-CB-CG2	6.48	122.25	109.30
1	E	13	ASP	CA-CB-CG	-6.48	106.12	112.60
1	A	335	SER	CA-C-N	-6.47	113.27	123.24
1	A	335	SER	C-N-CA	-6.47	113.27	123.24
1	B	11	GLN	OE1-CD-NE2	6.47	129.07	122.60
1	C	581	ASN	CB-CG-ND2	-6.47	106.69	116.40
1	D	139	GLN	CA-C-O	-6.47	112.09	119.41
1	D	404	ASP	CA-CB-CG	-6.47	106.13	112.60
1	D	451	ARG	CD-NE-CZ	-6.47	115.33	124.40
1	E	214	ASP	CB-CA-C	-6.47	97.54	110.42
1	F	185	GLY	CA-C-O	6.47	127.42	120.30
1	C	467	SER	CB-CA-C	-6.47	99.19	109.80
1	E	513	PRO	CA-C-N	-6.47	111.91	122.65
1	E	513	PRO	C-N-CA	-6.47	111.91	122.65
1	F	190	MET	CB-CG-SD	-6.47	93.28	112.70
1	F	513	PRO	CA-C-N	-6.47	111.91	122.65
1	F	513	PRO	C-N-CA	-6.47	111.91	122.65
1	D	571	PRO	O-C-N	-6.47	114.84	122.86
1	A	467	SER	CB-CA-C	-6.47	99.19	109.80
1	A	581	ASN	CB-CG-ND2	-6.47	106.69	116.40
1	B	91	ASN	CA-C-N	-6.47	112.21	122.95
1	B	91	ASN	C-N-CA	-6.47	112.21	122.95
1	B	223	VAL	O-C-N	6.47	128.15	121.87
1	F	146	THR	OG1-CB-CG2	6.47	122.24	109.30
1	A	223	VAL	O-C-N	6.47	128.14	121.87
1	B	335	SER	CA-C-N	-6.47	113.28	123.24
1	B	335	SER	C-N-CA	-6.47	113.28	123.24
1	C	471	ASP	CA-CB-CG	6.47	119.07	112.60
1	E	27	TYR	N-CA-CB	-6.47	100.41	110.11
1	E	468	ASN	CB-CG-ND2	6.47	126.10	116.40
1	E	532	ASP	OD1-CG-OD2	-6.47	107.38	122.90
1	E	649	ILE	CA-C-N	-6.47	114.14	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	649	ILE	C-N-CA	-6.47	114.14	123.06
1	C	27	TYR	N-CA-CB	-6.46	100.41	110.11
1	D	649	ILE	CA-C-N	-6.46	114.14	123.06
1	D	649	ILE	C-N-CA	-6.46	114.14	123.06
1	E	527	SER	O-C-N	6.46	131.59	122.41
1	F	76	ASN	CA-C-N	-6.46	110.22	120.63
1	F	76	ASN	C-N-CA	-6.46	110.22	120.63
1	B	139	GLN	CA-C-O	-6.46	112.11	119.41
1	D	393	LYS	CA-C-O	-6.46	112.80	120.10
1	E	11	GLN	OE1-CD-NE2	6.46	129.06	122.60
1	E	146	THR	OG1-CB-CG2	6.46	122.23	109.30
1	F	571	PRO	O-C-N	-6.46	114.84	122.86
1	A	27	TYR	N-CA-CB	-6.46	100.42	110.11
1	B	146	THR	OG1-CB-CG2	6.46	122.22	109.30
1	B	581	ASN	CB-CG-ND2	-6.46	106.71	116.40
1	C	335	SER	CA-C-N	-6.46	113.29	123.24
1	C	335	SER	C-N-CA	-6.46	113.29	123.24
1	C	532	ASP	OD1-CG-OD2	-6.46	107.39	122.90
1	D	27	TYR	N-CA-CB	-6.46	100.42	110.11
1	E	190	MET	CB-CG-SD	-6.46	93.31	112.70
1	E	467	SER	CB-CA-C	-6.46	99.20	109.80
1	F	581	ASN	CB-CG-ND2	-6.46	106.71	116.40
1	A	13	ASP	CA-CB-CG	-6.46	106.14	112.60
1	A	527	SER	O-C-N	6.46	131.58	122.41
1	E	64	ARG	CA-C-O	-6.46	112.30	119.34
1	F	223	VAL	O-C-N	6.46	128.14	121.87
1	A	649	ILE	CA-C-N	-6.46	114.15	123.06
1	A	649	ILE	C-N-CA	-6.46	114.15	123.06
1	B	190	MET	CB-CG-SD	-6.46	93.32	112.70
1	C	404	ASP	CA-CB-CG	-6.46	106.14	112.60
1	D	13	ASP	CA-CB-CG	-6.46	106.14	112.60
1	D	91	ASN	CA-C-N	-6.46	112.23	122.95
1	D	91	ASN	C-N-CA	-6.46	112.23	122.95
1	D	185	GLY	CA-C-O	6.46	127.40	120.30
1	E	581	ASN	CB-CG-ND2	-6.46	106.71	116.40
1	F	547	VAL	CA-CB-CG2	6.46	121.38	110.40
1	A	190	MET	CB-CG-SD	-6.46	93.33	112.70
1	A	532	ASP	OD1-CG-OD2	-6.46	107.41	122.90
1	B	532	ASP	OD1-CG-OD2	-6.46	107.40	122.90
1	B	584	VAL	O-C-N	-6.46	116.36	123.20
1	C	91	ASN	CA-C-N	-6.46	112.23	122.95
1	C	91	ASN	C-N-CA	-6.46	112.23	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	571	PRO	O-C-N	-6.46	114.85	122.86
1	D	190	MET	CB-CG-SD	-6.46	93.33	112.70
1	D	335	SER	CA-C-N	-6.46	113.30	123.24
1	D	335	SER	C-N-CA	-6.46	113.30	123.24
1	E	98	CYS	CB-CA-C	6.46	123.55	110.38
1	E	451	ARG	CD-NE-CZ	-6.46	115.36	124.40
1	F	532	ASP	OD1-CG-OD2	-6.46	107.41	122.90
1	F	467	SER	CB-CA-C	-6.46	99.21	109.80
1	A	64	ARG	CA-C-O	-6.45	112.31	119.34
1	A	185	GLY	CA-C-O	6.45	127.40	120.30
1	A	571	PRO	O-C-N	-6.45	114.86	122.86
1	B	404	ASP	CA-CB-CG	-6.45	106.15	112.60
1	C	190	MET	CB-CG-SD	-6.45	93.34	112.70
1	E	106	PHE	CA-CB-CG	-6.45	107.35	113.80
1	E	471	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	43	THR	CA-CB-OG1	-6.45	99.92	109.60
1	C	146	THR	OG1-CB-CG2	6.45	122.20	109.30
1	C	284	ALA	O-C-N	6.45	131.17	122.59
1	C	353	ARG	CD-NE-CZ	6.45	133.43	124.40
1	C	469	ASN	CB-CA-C	6.45	123.80	110.31
1	C	64	ARG	CA-C-O	-6.45	112.31	119.34
1	D	532	ASP	OD1-CG-OD2	-6.45	107.42	122.90
1	F	139	GLN	CA-C-O	-6.45	112.12	119.41
1	F	232	ASP	O-C-N	6.45	128.96	122.12
1	F	314	ASP	CB-CG-OD2	6.45	133.23	118.40
1	F	527	SER	O-C-N	6.45	131.57	122.41
1	A	91	ASN	CA-C-N	-6.45	112.25	122.95
1	A	91	ASN	C-N-CA	-6.45	112.25	122.95
1	C	310	GLY	CA-C-O	-6.45	112.71	118.77
1	D	64	ARG	CA-C-O	-6.45	112.31	119.34
1	E	38	ASN	CA-C-O	6.45	127.69	120.34
1	E	91	ASN	CA-C-N	-6.45	112.25	122.95
1	E	91	ASN	C-N-CA	-6.45	112.25	122.95
1	E	334	SER	CA-CB-OG	-6.45	98.20	111.10
1	B	232	ASP	O-C-N	6.45	128.95	122.12
1	C	314	ASP	CB-CG-OD2	6.45	133.23	118.40
1	C	527	SER	O-C-N	6.45	131.56	122.41
1	D	284	ALA	O-C-N	6.45	131.16	122.59
1	A	284	ALA	O-C-N	6.45	131.16	122.59
1	B	64	ARG	CA-C-O	-6.45	112.31	119.34
1	B	471	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	649	ILE	CA-C-N	-6.45	114.17	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	649	ILE	C-N-CA	-6.45	114.17	123.06
1	C	334	SER	CA-CB-OG	-6.45	98.21	111.10
1	D	78	ARG	CD-NE-CZ	-6.45	115.38	124.40
1	D	314	ASP	CB-CG-OD2	6.45	133.22	118.40
1	E	185	GLY	CA-C-O	6.45	127.39	120.30
1	E	571	PRO	O-C-N	-6.45	114.87	122.86
1	F	43	THR	CA-CB-OG1	-6.45	99.93	109.60
1	B	78	ARG	CD-NE-CZ	-6.44	115.38	124.40
1	F	404	ASP	CA-CB-CG	-6.44	106.16	112.60
1	F	649	ILE	CA-C-N	-6.44	114.17	123.06
1	F	649	ILE	C-N-CA	-6.44	114.17	123.06
1	A	43	THR	CA-CB-OG1	-6.44	99.94	109.60
1	A	78	ARG	CD-NE-CZ	-6.44	115.38	124.40
1	B	106	PHE	CA-CB-CG	-6.44	107.36	113.80
1	B	506	ASP	O-C-N	6.44	131.16	122.59
1	C	185	GLY	CA-C-O	6.44	127.39	120.30
1	C	277	PHE	N-CA-C	6.44	119.56	109.96
1	C	614	GLU	CA-C-O	-6.44	111.30	120.51
1	A	11	GLN	OE1-CD-NE2	6.44	129.04	122.60
1	A	404	ASP	CA-CB-CG	-6.44	106.16	112.60
1	B	432	SER	CA-CB-OG	-6.44	98.22	111.10
1	F	471	ASP	CA-CB-CG	6.44	119.04	112.60
1	C	89	VAL	N-CA-C	-6.44	95.95	109.34
1	D	499	ARG	NH1-CZ-NH2	-6.44	110.93	119.30
1	A	314	ASP	CB-CG-OD2	6.44	133.21	118.40
1	B	393	LYS	CA-C-O	-6.44	112.83	120.10
1	D	370	HIS	CE1-NE2-CD2	-6.44	102.56	109.00
1	F	89	VAL	N-CA-C	-6.44	95.95	109.34
1	C	98	CYS	CB-CA-C	6.44	123.51	110.38
1	D	632	ASP	N-CA-C	-6.44	97.78	108.34
1	A	334	SER	CA-CB-OG	-6.43	98.23	111.10
1	B	185	GLY	CA-C-O	6.43	127.38	120.30
1	B	314	ASP	CB-CG-OD2	6.43	133.20	118.40
1	C	11	GLN	OE1-CD-NE2	6.43	129.03	122.60
1	C	223	VAL	O-C-N	6.43	128.11	121.87
1	D	43	THR	CA-CB-OG1	-6.43	99.95	109.60
1	D	471	ASP	CA-CB-CG	6.43	119.03	112.60
1	E	78	ARG	CD-NE-CZ	-6.43	115.39	124.40
1	E	89	VAL	N-CA-C	-6.43	95.96	109.34
1	F	64	ARG	CA-C-O	-6.43	112.33	119.34
1	F	91	ASN	CA-C-N	-6.43	112.27	122.95
1	F	91	ASN	C-N-CA	-6.43	112.27	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	PHE	CA-CB-CG	-6.43	107.37	113.80
1	A	432	SER	CA-CB-OG	-6.43	98.23	111.10
1	A	471	ASP	CA-CB-CG	6.43	119.03	112.60
1	D	106	PHE	CA-CB-CG	-6.43	107.37	113.80
1	D	432	SER	CA-CB-OG	-6.43	98.24	111.10
1	D	584	VAL	O-C-N	-6.43	116.38	123.20
1	F	78	ARG	CD-NE-CZ	-6.43	115.39	124.40
1	F	284	ALA	O-C-N	6.43	131.15	122.59
1	A	89	VAL	N-CA-C	-6.43	95.96	109.34
1	A	469	ASN	CB-CA-C	6.43	123.75	110.31
1	B	186	GLU	N-CA-C	6.43	121.13	113.16
1	C	13	ASP	CA-CB-CG	-6.43	106.17	112.60
1	C	649	ILE	CA-C-N	-6.43	114.19	123.06
1	C	649	ILE	C-N-CA	-6.43	114.19	123.06
1	E	469	ASN	CB-CA-C	6.43	123.75	110.31
1	E	584	VAL	O-C-N	-6.43	116.38	123.20
1	F	334	SER	CA-CB-OG	-6.43	98.24	111.10
1	F	432	SER	CA-CB-OG	-6.43	98.24	111.10
1	A	98	CYS	CB-CA-C	6.43	123.50	110.38
1	A	393	LYS	CA-C-O	-6.43	112.83	120.10
1	B	89	VAL	N-CA-C	-6.43	95.97	109.34
1	C	432	SER	CA-CB-OG	-6.43	98.24	111.10
1	D	11	GLN	OE1-CD-NE2	6.43	129.03	122.60
1	D	334	SER	CA-CB-OG	-6.43	98.25	111.10
1	E	432	SER	CA-CB-OG	-6.43	98.24	111.10
1	B	43	THR	CA-CB-OG1	-6.43	99.96	109.60
1	F	11	GLN	OE1-CD-NE2	6.43	129.03	122.60
1	A	584	VAL	O-C-N	-6.42	116.39	123.20
1	B	108	GLU	CA-C-O	-6.42	110.89	119.11
1	D	310	GLY	CA-C-O	-6.42	112.73	118.77
1	D	353	ARG	CD-NE-CZ	6.42	133.39	124.40
1	E	314	ASP	CB-CG-OD2	6.42	133.17	118.40
1	F	506	ASP	O-C-N	6.42	131.13	122.59
1	B	334	SER	CA-CB-OG	-6.42	98.26	111.10
1	B	632	ASP	N-CA-C	-6.42	97.81	108.34
1	C	38	ASN	CA-C-O	6.42	127.66	120.34
1	C	78	ARG	CD-NE-CZ	-6.42	115.41	124.40
1	D	454	ARG	CA-CB-CG	6.42	126.94	114.10
1	E	43	THR	CA-CB-OG1	-6.42	99.97	109.60
1	E	632	ASP	N-CA-C	-6.42	97.81	108.34
1	B	17	LEU	CB-CG-CD2	-6.42	91.44	110.70
1	C	186	GLU	N-CA-C	6.42	121.12	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	348	HIS	CE1-NE2-CD2	-6.42	102.58	109.00
1	B	284	ALA	O-C-N	6.42	131.13	122.59
1	C	108	GLU	CA-C-O	-6.42	110.89	119.11
1	C	499	ARG	NH1-CZ-NH2	-6.42	110.95	119.30
1	C	585	ALA	CA-C-N	-6.42	114.56	123.10
1	C	585	ALA	C-N-CA	-6.42	114.56	123.10
1	C	632	ASP	N-CA-C	-6.42	97.81	108.34
1	D	98	CYS	CB-CA-C	6.42	123.47	110.38
1	D	527	SER	O-C-N	6.42	131.52	122.41
1	D	585	ALA	CA-C-N	-6.42	114.56	123.10
1	D	585	ALA	C-N-CA	-6.42	114.56	123.10
1	F	17	LEU	CB-CG-CD2	-6.42	91.44	110.70
1	B	98	CYS	CB-CA-C	6.42	123.47	110.38
1	C	17	LEU	CB-CG-CD2	-6.42	91.45	110.70
1	E	120	TYR	N-CA-C	6.42	117.94	111.07
1	E	353	ARG	CD-NE-CZ	6.42	133.38	124.40
1	E	404	ASP	CA-CB-CG	-6.42	106.18	112.60
1	F	38	ASN	CA-C-O	6.42	127.66	120.34
1	F	98	CYS	CB-CA-C	6.42	123.47	110.38
1	A	353	ARG	CD-NE-CZ	6.42	133.38	124.40
1	A	614	GLU	CA-C-O	-6.42	111.34	120.51
1	C	584	VAL	O-C-N	-6.42	116.40	123.20
1	E	17	LEU	CB-CG-CD2	-6.42	91.46	110.70
1	A	506	ASP	O-C-N	6.41	131.12	122.59
1	A	632	ASP	N-CA-C	-6.41	97.82	108.34
1	B	614	GLU	CA-C-O	-6.41	111.34	120.51
1	C	106	PHE	CA-CB-CG	-6.41	107.39	113.80
1	E	393	LYS	CA-C-O	-6.41	112.85	120.10
1	F	469	ASN	CB-CA-C	6.41	123.72	110.31
1	B	469	ASN	CB-CA-C	6.41	123.71	110.31
1	B	585	ALA	CA-C-N	-6.41	114.57	123.10
1	B	585	ALA	C-N-CA	-6.41	114.57	123.10
1	D	17	LEU	CB-CG-CD2	-6.41	91.46	110.70
1	F	353	ARG	CD-NE-CZ	6.41	133.38	124.40
1	A	17	LEU	CB-CG-CD2	-6.41	91.47	110.70
1	B	350	MET	CG-SD-CE	-6.41	86.80	100.90
1	E	186	GLU	N-CA-C	6.41	121.11	113.16
1	F	108	GLU	CA-C-O	-6.41	110.91	119.11
1	A	38	ASN	CA-C-O	6.41	127.64	120.34
1	B	499	ARG	NH1-CZ-NH2	-6.41	110.97	119.30
1	A	108	GLU	CA-C-O	-6.41	110.91	119.11
1	A	499	ARG	NH1-CZ-NH2	-6.41	110.97	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	7	ASN	N-CA-C	-6.41	97.15	110.80
1	B	348	HIS	CE1-NE2-CD2	-6.41	102.59	109.00
1	D	89	VAL	N-CA-C	-6.41	96.01	109.34
1	D	469	ASN	CB-CA-C	6.41	123.70	110.31
1	D	614	GLU	CA-C-O	-6.41	111.35	120.51
1	A	7	ASN	N-CA-C	-6.41	97.16	110.80
1	A	454	ARG	CA-CB-CG	6.41	126.91	114.10
1	C	350	MET	CG-SD-CE	-6.41	86.81	100.90
1	E	506	ASP	O-C-N	6.41	131.11	122.59
1	F	7	ASN	N-CA-C	-6.41	97.16	110.80
1	F	632	ASP	N-CA-C	-6.41	97.84	108.34
1	A	277	PHE	N-CA-C	6.40	119.50	109.96
1	B	353	ARG	CD-NE-CZ	6.40	133.37	124.40
1	B	454	ARG	CA-CB-CG	6.40	126.91	114.10
1	F	614	GLU	CA-C-O	-6.40	111.35	120.51
1	A	350	MET	CG-SD-CE	-6.40	86.81	100.90
1	C	7	ASN	N-CA-C	-6.40	97.16	110.80
1	C	30	LEU	CB-CA-C	6.40	121.56	110.68
1	C	454	ARG	CA-CB-CG	6.40	126.90	114.10
1	D	444	GLU	N-CA-CB	6.40	120.24	110.70
1	E	454	ARG	CA-CB-CG	6.40	126.90	114.10
1	A	370	HIS	CE1-NE2-CD2	-6.40	102.60	109.00
1	F	30	LEU	CB-CA-C	6.40	121.56	110.68
1	F	106	PHE	CA-CB-CG	-6.40	107.40	113.80
1	F	393	LYS	CA-C-O	-6.40	112.87	120.10
1	F	370	HIS	CE1-NE2-CD2	-6.40	102.60	109.00
1	A	585	ALA	CA-C-N	-6.40	114.59	123.10
1	A	585	ALA	C-N-CA	-6.40	114.59	123.10
1	D	7	ASN	N-CA-C	-6.40	97.17	110.80
1	D	506	ASP	O-C-N	6.40	131.10	122.59
1	E	7	ASN	N-CA-C	-6.40	97.17	110.80
1	E	284	ALA	O-C-N	6.40	131.10	122.59
1	E	350	MET	CG-SD-CE	-6.40	86.82	100.90
1	D	186	GLU	N-CA-C	6.40	121.09	113.16
1	B	444	GLU	N-CA-CB	6.39	120.23	110.70
1	E	277	PHE	N-CA-C	6.39	119.49	109.96
1	E	593	THR	CA-C-O	-6.39	111.36	120.51
1	E	614	GLU	CA-C-O	-6.39	111.37	120.51
1	F	350	MET	CG-SD-CE	-6.39	86.83	100.90
1	A	348	HIS	CE1-NE2-CD2	-6.39	102.61	109.00
1	B	497	GLU	O-C-N	6.39	130.13	122.27
1	B	536	PHE	CB-CA-C	-6.39	101.12	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	551	HIS	CG-CD2-NE2	6.39	113.59	107.20
1	E	585	ALA	CA-C-N	-6.39	114.60	123.10
1	E	585	ALA	C-N-CA	-6.39	114.60	123.10
1	F	558	TYR	N-CA-C	6.39	120.38	111.56
1	B	38	ASN	CA-C-O	6.39	127.63	120.34
1	D	350	MET	CG-SD-CE	-6.39	86.84	100.90
1	B	370	HIS	CE1-NE2-CD2	-6.39	102.61	109.00
1	D	108	GLU	CA-C-O	-6.39	110.93	119.11
1	F	584	VAL	O-C-N	-6.39	116.43	123.20
1	A	310	GLY	CA-C-O	-6.39	112.77	118.77
1	C	348	HIS	CE1-NE2-CD2	-6.39	102.61	109.00
1	C	558	TYR	N-CA-C	6.39	120.38	111.56
1	A	186	GLU	N-CA-C	6.39	121.08	113.16
1	B	167	ASN	CB-CA-C	6.39	120.27	109.80
1	E	30	LEU	CB-CA-C	6.39	121.54	110.68
1	F	277	PHE	N-CA-C	6.39	119.47	109.96
1	B	558	TYR	N-CA-C	6.38	120.37	111.56
1	E	499	ARG	NH1-CZ-NH2	-6.38	111.00	119.30
1	F	149	GLU	CA-C-O	-6.38	113.72	120.55
1	F	454	ARG	CA-CB-CG	6.38	126.87	114.10
1	F	497	GLU	O-C-N	6.38	130.12	122.27
1	D	408	PHE	CB-CA-C	-6.38	102.38	111.76
1	D	593	THR	CA-C-O	-6.38	111.38	120.51
1	E	108	GLU	CA-C-O	-6.38	110.94	119.11
1	D	167	ASN	CB-CA-C	6.38	120.27	109.80
1	D	277	PHE	N-CA-C	6.38	119.47	109.96
1	E	558	TYR	N-CA-C	6.38	120.37	111.56
1	D	149	GLU	CA-C-O	-6.38	113.72	120.55
1	F	214	ASP	N-CA-C	6.38	124.39	110.80
1	A	30	LEU	CB-CA-C	6.38	121.52	110.68
1	D	497	GLU	O-C-N	6.38	130.12	122.27
1	E	310	GLY	CA-C-O	-6.38	112.77	118.77
1	F	167	ASN	CB-CA-C	6.38	120.26	109.80
1	D	30	LEU	CB-CA-C	6.38	121.52	110.68
1	F	499	ARG	NH1-CZ-NH2	-6.38	111.01	119.30
1	B	120	TYR	N-CA-C	6.38	117.89	111.07
1	E	348	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
1	F	348	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
1	C	296	ILE	CB-CA-C	-6.37	103.84	111.81
1	C	394	HIS	O-C-N	6.37	131.65	122.28
1	F	444	GLU	N-CA-CB	6.37	120.20	110.70
1	A	444	GLU	N-CA-CB	6.37	120.19	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	497	GLU	O-C-N	6.37	130.11	122.27
1	D	296	ILE	CB-CA-C	-6.37	103.84	111.81
1	D	551	HIS	CG-CD2-NE2	6.37	113.57	107.20
1	E	408	PHE	CB-CA-C	-6.37	102.39	111.76
1	F	186	GLU	N-CA-C	6.37	121.06	113.16
1	F	215	ARG	CB-CG-CD	6.37	125.96	111.30
1	F	585	ALA	CA-C-N	-6.37	114.62	123.10
1	F	585	ALA	C-N-CA	-6.37	114.62	123.10
1	B	310	GLY	CA-C-O	-6.37	112.78	118.77
1	B	593	THR	CA-C-O	-6.37	111.40	120.51
1	D	558	TYR	N-CA-C	6.37	120.35	111.56
1	E	394	HIS	O-C-N	6.37	131.64	122.28
1	A	167	ASN	CB-CA-C	6.37	120.25	109.80
1	A	593	THR	CA-C-O	-6.37	111.40	120.51
1	B	30	LEU	CB-CA-C	6.37	121.51	110.68
1	B	199	MET	O-C-N	6.37	131.06	122.59
1	F	593	THR	CA-C-O	-6.37	111.40	120.51
1	A	408	PHE	CB-CA-C	-6.37	102.40	111.76
1	A	558	TYR	N-CA-C	6.37	120.34	111.56
1	C	197	TRP	N-CA-CB	6.37	120.16	109.78
1	C	214	ASP	N-CA-C	6.37	124.36	110.80
1	D	199	MET	O-C-N	6.37	131.06	122.59
1	A	149	GLU	CA-C-O	-6.36	113.74	120.55
1	C	506	ASP	O-C-N	6.36	131.05	122.59
1	E	370	HIS	CE1-NE2-CD2	-6.36	102.64	109.00
1	F	120	TYR	N-CA-C	6.36	117.88	111.07
1	C	444	GLU	N-CA-CB	6.36	120.18	110.70
1	A	199	MET	O-C-N	6.36	131.05	122.59
1	C	149	GLU	CA-C-O	-6.36	113.74	120.55
1	C	167	ASN	CB-CA-C	6.36	120.23	109.80
1	C	408	PHE	CB-CA-C	-6.36	102.41	111.76
1	D	38	ASN	CA-C-O	6.36	127.59	120.34
1	E	67	GLU	N-CA-C	6.36	118.23	110.41
1	E	473	GLU	CA-C-O	6.36	129.61	120.51
1	F	310	GLY	CA-C-O	-6.36	112.79	118.77
1	F	371	PHE	CG-CD2-CE2	6.36	131.51	120.70
1	F	176	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	B	277	PHE	N-CA-C	6.36	119.43	109.96
1	C	112	GLU	CB-CA-C	-6.36	100.23	110.79
1	D	536	PHE	CB-CA-C	-6.36	101.17	110.96
1	E	444	GLU	N-CA-CB	6.36	120.17	110.70
1	A	197	TRP	N-CA-CB	6.36	120.14	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ASP	N-CA-C	6.36	124.34	110.80
1	A	215	ARG	CB-CG-CD	6.36	125.92	111.30
1	E	197	TRP	N-CA-CB	6.36	120.14	109.78
1	F	408	PHE	CB-CA-C	-6.36	102.42	111.76
1	C	473	GLU	CA-C-O	6.35	129.60	120.51
1	E	149	GLU	CA-C-O	-6.35	113.75	120.55
1	A	296	ILE	CB-CA-C	-6.35	103.87	111.81
1	C	139	GLN	N-CA-CB	6.35	119.75	110.47
1	C	215	ARG	CB-CG-CD	6.35	125.91	111.30
1	E	167	ASN	CB-CA-C	6.35	120.22	109.80
1	F	67	GLU	N-CA-C	6.35	118.22	110.41
1	F	139	GLN	N-CA-CB	6.35	119.74	110.47
1	A	473	GLU	CA-C-O	6.35	129.59	120.51
1	D	120	TYR	N-CA-C	6.35	117.86	111.07
1	F	112	GLU	CB-CA-C	-6.35	100.25	110.79
1	F	197	TRP	N-CA-CB	6.35	120.13	109.78
1	A	112	GLU	CB-CA-C	-6.35	100.25	110.79
1	A	536	PHE	CB-CA-C	-6.35	101.18	110.96
1	F	199	MET	O-C-N	6.35	131.03	122.59
1	D	394	HIS	O-C-N	6.35	131.61	122.28
1	E	215	ARG	CB-CG-CD	6.35	125.90	111.30
1	A	120	TYR	N-CA-C	6.34	117.86	111.07
1	B	176	ASN	OD1-CG-ND2	-6.34	116.25	122.60
1	B	296	ILE	CB-CA-C	-6.34	103.88	111.81
1	B	408	PHE	CB-CA-C	-6.34	102.43	111.76
1	D	197	TRP	N-CA-CB	6.34	120.12	109.78
1	D	214	ASP	N-CA-C	6.34	124.31	110.80
1	D	215	ARG	CB-CG-CD	6.34	125.89	111.30
1	D	473	GLU	CA-C-O	6.34	129.58	120.51
1	D	521	ARG	O-C-N	6.34	130.59	123.48
1	E	199	MET	O-C-N	6.34	131.03	122.59
1	E	214	ASP	N-CA-C	6.34	124.31	110.80
1	E	371	PHE	CG-CD2-CE2	6.34	131.49	120.70
1	B	215	ARG	CB-CG-CD	6.34	125.89	111.30
1	B	521	ARG	O-C-N	6.34	130.58	123.48
1	E	112	GLU	CB-CA-C	-6.34	100.26	110.79
1	E	536	PHE	CB-CA-C	-6.34	101.19	110.96
1	B	197	TRP	N-CA-CB	6.34	120.12	109.78
1	B	214	ASP	N-CA-C	6.34	124.31	110.80
1	B	394	HIS	O-C-N	6.34	131.60	122.28
1	E	206	GLU	CA-CB-CG	-6.34	101.42	114.10
1	F	551	HIS	CG-CD2-NE2	6.34	113.54	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	394	HIS	O-C-N	6.34	131.60	122.28
1	C	199	MET	O-C-N	6.34	131.02	122.59
1	C	536	PHE	CB-CA-C	-6.34	101.20	110.96
1	D	112	GLU	CB-CA-C	-6.34	100.27	110.79
1	E	551	HIS	CG-CD2-NE2	6.34	113.54	107.20
1	A	206	GLU	CA-CB-CG	-6.34	101.42	114.10
1	B	473	GLU	CA-C-O	6.34	129.57	120.51
1	C	593	THR	CA-C-O	-6.34	111.45	120.51
1	A	139	GLN	N-CA-CB	6.34	119.72	110.47
1	C	370	HIS	CE1-NE2-CD2	-6.34	102.66	109.00
1	D	139	GLN	N-CA-CB	6.34	119.72	110.47
1	D	206	GLU	CA-CB-CG	-6.34	101.43	114.10
1	F	296	ILE	CB-CA-C	-6.34	103.89	111.81
1	B	112	GLU	CB-CA-C	-6.33	100.27	110.79
1	C	206	GLU	CA-CB-CG	-6.33	101.43	114.10
1	E	497	GLU	O-C-N	6.33	130.06	122.27
1	F	536	PHE	CB-CA-C	-6.33	101.20	110.96
1	B	139	GLN	N-CA-CB	6.33	119.72	110.47
1	D	176	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	E	139	GLN	N-CA-CB	6.33	119.72	110.47
1	E	296	ILE	CB-CA-C	-6.33	103.89	111.81
1	A	176	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	B	149	GLU	CA-C-O	-6.33	113.78	120.55
1	C	371	PHE	CG-CD2-CE2	6.33	131.46	120.70
1	C	521	ARG	O-C-N	6.33	130.57	123.48
1	C	176	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	F	394	HIS	O-C-N	6.33	131.58	122.28
1	C	67	GLU	N-CA-C	6.33	118.19	110.41
1	E	616	TYR	N-CA-CB	-6.33	98.69	109.57
1	B	206	GLU	CA-CB-CG	-6.33	101.45	114.10
1	C	120	TYR	N-CA-C	6.33	117.84	111.07
1	F	206	GLU	CA-CB-CG	-6.33	101.45	114.10
1	A	371	PHE	CG-CD2-CE2	6.32	131.45	120.70
1	A	521	ARG	O-C-N	6.32	130.56	123.48
1	A	551	HIS	CG-CD2-NE2	6.32	113.52	107.20
1	E	23	GLU	CA-C-N	6.32	127.74	119.84
1	E	23	GLU	C-N-CA	6.32	127.74	119.84
1	E	247	HIS	ND1-CG-CD2	6.32	112.42	106.10
1	B	207	ASP	CB-CA-C	6.32	122.05	110.36
1	A	67	GLU	N-CA-C	6.31	118.18	110.41
1	C	551	HIS	CG-CD2-NE2	6.31	113.51	107.20
1	F	473	GLU	CA-C-O	6.31	129.54	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	ASP	CB-CA-C	6.31	122.03	110.36
1	B	371	PHE	CG-CD2-CE2	6.31	131.43	120.70
1	B	616	TYR	N-CA-CB	-6.31	98.72	109.57
1	C	207	ASP	CB-CA-C	6.31	122.03	110.36
1	C	23	GLU	CA-C-N	6.31	127.73	119.84
1	C	23	GLU	C-N-CA	6.31	127.73	119.84
1	D	441	GLU	CA-CB-CG	-6.31	101.49	114.10
1	F	441	GLU	CA-CB-CG	-6.31	101.49	114.10
1	D	399	PRO	N-CA-CB	-6.31	96.96	103.08
1	B	382	ARG	N-CA-C	-6.30	104.49	111.36
1	C	382	ARG	N-CA-C	-6.30	104.49	111.36
1	C	589	GLY	CA-C-N	-6.30	110.19	120.72
1	C	589	GLY	C-N-CA	-6.30	110.19	120.72
1	E	176	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	E	441	GLU	CA-CB-CG	-6.30	101.49	114.10
1	A	616	TYR	N-CA-CB	-6.30	98.73	109.57
1	B	441	GLU	CA-CB-CG	-6.30	101.50	114.10
1	D	23	GLU	CA-C-N	6.30	127.72	119.84
1	D	23	GLU	C-N-CA	6.30	127.72	119.84
1	D	207	ASP	CB-CA-C	6.30	122.02	110.36
1	D	371	PHE	CG-CD2-CE2	6.30	131.41	120.70
1	E	589	GLY	CA-C-N	-6.30	110.20	120.72
1	E	589	GLY	C-N-CA	-6.30	110.20	120.72
1	A	23	GLU	CA-C-N	6.30	127.72	119.84
1	A	23	GLU	C-N-CA	6.30	127.72	119.84
1	A	441	GLU	CA-CB-CG	-6.30	101.50	114.10
1	B	589	GLY	CA-C-N	-6.30	110.20	120.72
1	B	589	GLY	C-N-CA	-6.30	110.20	120.72
1	F	616	TYR	N-CA-CB	-6.30	98.74	109.57
1	A	382	ARG	N-CA-C	-6.30	104.50	111.36
1	D	636	ILE	CA-CB-CG2	6.30	121.20	110.50
1	F	333	TYR	N-CA-CB	-6.30	100.81	110.44
1	A	333	TYR	N-CA-CB	-6.29	100.81	110.44
1	D	67	GLU	N-CA-C	6.29	118.15	110.41
1	D	333	TYR	N-CA-CB	-6.29	100.81	110.44
1	F	518	THR	N-CA-CB	6.29	122.82	111.36
1	C	111	ASN	N-CA-C	6.29	118.84	110.53
1	C	186	GLU	OE1-CD-OE2	6.29	138.01	122.90
1	C	636	ILE	CA-CB-CG2	6.29	121.20	110.50
1	E	207	ASP	CB-CA-C	6.29	122.00	110.36
1	E	521	ARG	O-C-N	6.29	130.53	123.48
1	F	207	ASP	CB-CA-C	6.29	122.00	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	589	GLY	CA-C-N	-6.29	110.21	120.72
1	A	589	GLY	C-N-CA	-6.29	110.21	120.72
1	B	67	GLU	N-CA-C	6.29	118.15	110.41
1	B	333	TYR	N-CA-CB	-6.29	100.81	110.44
1	C	333	TYR	N-CA-CB	-6.29	100.81	110.44
1	D	186	GLU	OE1-CD-OE2	6.29	138.00	122.90
1	D	518	THR	N-CA-CB	6.29	122.81	111.36
1	F	589	GLY	CA-C-N	-6.29	110.22	120.72
1	F	589	GLY	C-N-CA	-6.29	110.22	120.72
1	C	399	PRO	N-CA-CB	-6.29	96.98	103.08
1	F	23	GLU	CA-C-N	6.29	127.70	119.84
1	F	23	GLU	C-N-CA	6.29	127.70	119.84
1	D	589	GLY	CA-C-N	-6.29	110.22	120.72
1	D	589	GLY	C-N-CA	-6.29	110.22	120.72
1	D	616	TYR	N-CA-CB	-6.29	98.76	109.57
1	B	111	ASN	N-CA-C	6.29	118.83	110.53
1	A	636	ILE	CA-CB-CG2	6.28	121.18	110.50
1	B	23	GLU	CA-C-N	6.28	127.69	119.84
1	B	23	GLU	C-N-CA	6.28	127.69	119.84
1	C	441	GLU	CA-CB-CG	-6.28	101.53	114.10
1	D	382	ARG	N-CA-C	-6.28	104.51	111.36
1	D	446	VAL	N-CA-C	-6.28	99.42	108.53
1	E	636	ILE	CA-CB-CG2	6.28	121.18	110.50
1	F	186	GLU	OE1-CD-OE2	6.28	137.98	122.90
1	F	521	ARG	O-C-N	6.28	130.52	123.48
1	A	186	GLU	OE1-CD-OE2	6.28	137.98	122.90
1	C	616	TYR	N-CA-CB	-6.28	98.76	109.57
1	E	205	TRP	N-CA-C	6.28	119.38	109.96
1	E	399	PRO	N-CA-CB	-6.28	96.99	103.08
1	B	199	MET	CA-CB-CG	6.28	126.66	114.10
1	F	111	ASN	N-CA-C	6.28	118.82	110.53
1	D	113	GLY	O-C-N	6.28	130.86	122.70
1	F	529	THR	N-CA-C	6.28	119.77	109.85
1	B	483	CYS	CA-CB-SG	-6.28	99.96	114.40
1	B	636	ILE	CA-CB-CG2	6.28	121.17	110.50
1	C	456	ASN	CA-C-O	6.28	128.01	121.10
1	D	111	ASN	N-CA-C	6.28	118.82	110.53
1	D	205	TRP	N-CA-C	6.28	119.38	109.96
1	E	333	TYR	N-CA-CB	-6.28	100.83	110.44
1	E	483	CYS	CA-CB-SG	-6.28	99.96	114.40
1	A	205	TRP	N-CA-C	6.28	119.37	109.96
1	B	205	TRP	N-CA-C	6.28	119.37	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	227	LEU	CA-C-N	-6.28	111.24	120.28
1	D	227	LEU	C-N-CA	-6.28	111.24	120.28
1	E	518	THR	N-CA-CB	6.28	122.78	111.36
1	F	483	CYS	CA-CB-SG	-6.28	99.97	114.40
1	A	483	CYS	CA-CB-SG	-6.27	99.97	114.40
1	B	186	GLU	OE1-CD-OE2	6.27	137.96	122.90
1	D	199	MET	CA-CB-CG	6.27	126.65	114.10
1	A	399	PRO	N-CA-CB	-6.27	97.00	103.08
1	B	298	GLU	OE1-CD-OE2	6.27	137.95	122.90
1	D	483	CYS	CA-CB-SG	-6.27	99.97	114.40
1	E	111	ASN	N-CA-C	6.27	118.81	110.53
1	F	636	ILE	CA-CB-CG2	6.27	121.16	110.50
1	B	247	HIS	ND1-CG-CD2	6.27	112.37	106.10
1	B	250	ARG	NE-CZ-NH2	-6.27	113.56	119.20
1	C	529	THR	N-CA-C	6.27	119.75	109.85
1	E	382	ARG	N-CA-C	-6.27	104.53	111.36
1	A	247	HIS	ND1-CG-CD2	6.27	112.37	106.10
1	A	518	THR	N-CA-CB	6.27	122.77	111.36
1	C	518	THR	N-CA-CB	6.27	122.77	111.36
1	D	181	VAL	CA-CB-CG2	6.27	121.05	110.40
1	F	205	TRP	N-CA-C	6.27	119.36	109.96
1	F	399	PRO	N-CA-CB	-6.27	97.00	103.08
1	B	113	GLY	O-C-N	6.26	130.84	122.70
1	C	483	CYS	CA-CB-SG	-6.26	99.99	114.40
1	D	298	GLU	OE1-CD-OE2	6.26	137.94	122.90
1	D	585	ALA	CB-CA-C	6.26	121.17	109.71
1	E	186	GLU	OE1-CD-OE2	6.26	137.93	122.90
1	E	495	LEU	N-CA-CB	6.26	121.54	112.08
1	F	247	HIS	ND1-CG-CD2	6.26	112.36	106.10
1	F	382	ARG	N-CA-C	-6.26	104.53	111.36
1	D	529	THR	N-CA-C	6.26	119.75	109.85
1	A	111	ASN	N-CA-C	6.26	118.80	110.53
1	A	199	MET	CA-CB-CG	6.26	126.62	114.10
1	C	305	ILE	CB-CG1-CD1	-6.26	100.65	113.80
1	E	298	GLU	OE1-CD-OE2	6.26	137.93	122.90
1	F	245	GLU	N-CA-C	-6.26	100.36	110.32
1	F	298	GLU	OE1-CD-OE2	6.26	137.93	122.90
1	C	41	GLY	CA-C-O	-6.26	109.68	120.57
1	C	205	TRP	N-CA-C	6.26	119.35	109.96
1	D	41	GLY	CA-C-O	-6.26	109.68	120.57
1	D	561	SER	CA-C-O	6.26	129.46	120.51
1	E	113	GLY	O-C-N	6.26	130.84	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	392	LYS	CA-CB-CG	6.26	126.62	114.10
1	A	298	GLU	OE1-CD-OE2	6.26	137.92	122.90
1	B	41	GLY	CA-C-O	-6.26	109.68	120.57
1	C	245	GLU	N-CA-C	-6.26	100.37	110.32
1	F	495	LEU	N-CA-CB	6.26	121.53	112.08
1	A	446	VAL	N-CA-C	-6.26	99.46	108.53
1	A	529	THR	N-CA-C	6.26	119.73	109.85
1	C	198	HIS	CE1-NE2-CD2	-6.26	102.74	109.00
1	F	585	ALA	CB-CA-C	6.26	121.16	109.71
1	B	446	VAL	N-CA-C	-6.25	99.46	108.53
1	A	41	GLY	CA-C-O	-6.25	109.69	120.57
1	B	426	PHE	N-CA-C	6.25	120.26	107.69
1	C	298	GLU	OE1-CD-OE2	6.25	137.91	122.90
1	E	41	GLY	CA-C-O	-6.25	109.69	120.57
1	F	199	MET	CA-CB-CG	6.25	126.61	114.10
1	A	245	GLU	N-CA-C	-6.25	100.38	110.32
1	D	102	ASN	OD1-CG-ND2	6.25	128.85	122.60
1	F	41	GLY	CA-C-O	-6.25	109.69	120.57
1	A	495	LEU	N-CA-CB	6.25	121.52	112.08
1	A	585	ALA	CB-CA-C	6.25	121.15	109.71
1	D	495	LEU	N-CA-CB	6.25	121.52	112.08
1	A	426	PHE	N-CA-C	6.25	120.25	107.69
1	B	245	GLU	N-CA-C	-6.25	100.39	110.32
1	B	529	THR	N-CA-C	6.25	119.72	109.85
1	C	446	VAL	N-CA-C	-6.25	99.47	108.53
1	D	250	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	D	426	PHE	N-CA-C	6.25	120.25	107.69
1	E	199	MET	CA-CB-CG	6.25	126.60	114.10
1	E	426	PHE	N-CA-C	6.25	120.25	107.69
1	E	527	SER	CA-C-N	-6.25	114.51	122.26
1	E	527	SER	C-N-CA	-6.25	114.51	122.26
1	C	250	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	E	529	THR	N-CA-C	6.25	119.72	109.85
1	F	227	LEU	CA-C-N	-6.25	111.28	120.28
1	F	227	LEU	C-N-CA	-6.25	111.28	120.28
1	F	426	PHE	N-CA-C	6.25	120.25	107.69
1	B	392	LYS	CA-CB-CG	6.25	126.59	114.10
1	A	250	ARG	NE-CZ-NH2	-6.24	113.58	119.20
1	A	456	ASN	CA-C-O	6.24	127.97	121.10
1	B	518	THR	N-CA-CB	6.24	122.72	111.36
1	D	247	HIS	ND1-CG-CD2	6.24	112.34	106.10
1	D	456	ASN	CA-C-O	6.24	127.97	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	227	LEU	CA-C-N	-6.24	111.29	120.28
1	E	227	LEU	C-N-CA	-6.24	111.29	120.28
1	E	585	ALA	CB-CA-C	6.24	121.14	109.71
1	A	198	HIS	CE1-NE2-CD2	-6.24	102.76	109.00
1	C	199	MET	CA-CB-CG	6.24	126.58	114.10
1	E	245	GLU	N-CA-C	-6.24	100.39	110.32
1	E	392	LYS	CA-CB-CG	6.24	126.58	114.10
1	A	113	GLY	O-C-N	6.24	130.81	122.70
1	A	227	LEU	CA-C-N	-6.24	111.29	120.28
1	A	227	LEU	C-N-CA	-6.24	111.29	120.28
1	B	305	ILE	CB-CG1-CD1	-6.24	100.69	113.80
1	C	426	PHE	N-CA-C	6.24	120.23	107.69
1	B	399	PRO	N-CA-CB	-6.24	97.03	103.08
1	F	113	GLY	O-C-N	6.24	130.81	122.70
1	D	593	THR	N-CA-CB	-6.24	99.95	110.49
1	F	593	THR	N-CA-CB	-6.24	99.95	110.49
1	E	102	ASN	OD1-CG-ND2	6.24	128.84	122.60
1	E	250	ARG	NE-CZ-NH2	-6.24	113.59	119.20
1	E	450	ALA	CB-CA-C	6.24	121.28	109.37
1	E	446	VAL	N-CA-C	-6.23	99.49	108.53
1	A	561	SER	CA-C-O	6.23	129.42	120.51
1	D	245	GLU	N-CA-C	-6.23	100.41	110.32
1	A	181	VAL	CA-CB-CG2	6.23	120.99	110.40
1	A	305	ILE	CB-CG1-CD1	-6.23	100.71	113.80
1	A	392	LYS	CA-CB-CG	6.23	126.56	114.10
1	B	102	ASN	OD1-CG-ND2	6.23	128.83	122.60
1	B	198	HIS	CE1-NE2-CD2	-6.23	102.77	109.00
1	B	476	ALA	O-C-N	-6.23	115.67	123.27
1	B	495	LEU	N-CA-CB	6.23	121.49	112.08
1	B	585	ALA	CB-CA-C	6.23	121.11	109.71
1	D	305	ILE	CB-CG1-CD1	-6.23	100.72	113.80
1	E	561	SER	CA-C-O	6.23	129.42	120.51
1	F	250	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	F	446	VAL	N-CA-C	-6.23	99.50	108.53
1	F	450	ALA	CB-CA-C	6.23	121.27	109.37
1	D	358	HIS	CB-CA-C	6.23	121.22	110.01
1	E	305	ILE	CB-CG1-CD1	-6.23	100.72	113.80
1	E	352	GLY	O-C-N	6.23	130.79	122.70
1	F	102	ASN	OD1-CG-ND2	6.23	128.83	122.60
1	E	191	ASN	CB-CG-ND2	6.23	125.74	116.40
1	F	305	ILE	CB-CG1-CD1	-6.23	100.72	113.80
1	C	247	HIS	ND1-CG-CD2	6.22	112.32	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	561	SER	CA-C-O	6.22	129.41	120.51
1	D	276	HIS	CA-C-O	-6.22	113.64	120.43
1	B	227	LEU	CA-C-N	-6.22	111.32	120.28
1	B	227	LEU	C-N-CA	-6.22	111.32	120.28
1	B	527	SER	CA-C-N	-6.22	114.54	122.26
1	B	527	SER	C-N-CA	-6.22	114.54	122.26
1	E	456	ASN	CA-C-O	6.22	127.94	121.10
1	F	181	VAL	CA-CB-CG2	6.22	120.98	110.40
1	F	620	ARG	N-CA-C	-6.22	100.99	110.01
1	C	495	LEU	N-CA-CB	6.22	121.47	112.08
1	A	527	SER	CA-C-N	-6.22	114.55	122.26
1	A	527	SER	C-N-CA	-6.22	114.55	122.26
1	A	593	THR	N-CA-CB	-6.22	99.98	110.49
1	B	456	ASN	CA-C-O	6.22	127.94	121.10
1	C	181	VAL	CA-CB-CG2	6.22	120.97	110.40
1	E	503	ILE	N-CA-CB	-6.22	99.70	111.21
1	A	102	ASN	OD1-CG-ND2	6.22	128.82	122.60
1	B	391	PHE	CA-C-N	-6.22	110.66	120.60
1	B	391	PHE	C-N-CA	-6.22	110.66	120.60
1	C	392	LYS	CA-CB-CG	6.22	126.53	114.10
1	E	181	VAL	CA-CB-CG2	6.22	120.97	110.40
1	C	227	LEU	CA-C-N	-6.21	111.33	120.28
1	C	227	LEU	C-N-CA	-6.21	111.33	120.28
1	C	585	ALA	CB-CA-C	6.21	121.08	109.71
1	D	191	ASN	CB-CG-ND2	6.21	125.72	116.40
1	E	276	HIS	CA-C-O	-6.21	113.66	120.43
1	F	191	ASN	CB-CG-ND2	6.21	125.72	116.40
1	F	561	SER	CA-C-O	6.21	129.40	120.51
1	A	35	GLU	CA-C-O	6.21	128.82	120.13
1	A	358	HIS	CB-CA-C	6.21	121.19	110.01
1	A	450	ALA	CB-CA-C	6.21	121.23	109.37
1	A	620	ARG	N-CA-C	-6.21	101.00	110.01
1	B	358	HIS	CB-CA-C	6.21	121.19	110.01
1	C	391	PHE	CA-C-N	-6.21	110.66	120.60
1	C	391	PHE	C-N-CA	-6.21	110.66	120.60
1	C	593	THR	N-CA-CB	-6.21	99.99	110.49
1	C	620	ARG	N-CA-C	-6.21	101.00	110.01
1	D	35	GLU	CA-C-O	6.21	128.83	120.13
1	D	620	ARG	N-CA-C	-6.21	101.00	110.01
1	E	35	GLU	CA-C-O	6.21	128.82	120.13
1	A	191	ASN	CB-CG-ND2	6.21	125.72	116.40
1	B	389	ASN	CA-C-N	6.21	129.68	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	389	ASN	C-N-CA	6.21	129.68	122.35
1	D	476	ALA	O-C-N	-6.21	115.69	123.27
1	F	407	GLU	CB-CG-CD	6.21	123.16	112.60
1	F	476	ALA	O-C-N	-6.21	115.69	123.27
1	B	276	HIS	CA-C-O	-6.21	113.66	120.43
1	B	620	ARG	N-CA-C	-6.21	101.01	110.01
1	C	450	ALA	CB-CA-C	6.21	121.23	109.37
1	C	527	SER	CA-C-N	-6.21	114.56	122.26
1	C	527	SER	C-N-CA	-6.21	114.56	122.26
1	F	391	PHE	CA-C-N	-6.21	110.67	120.60
1	F	391	PHE	C-N-CA	-6.21	110.67	120.60
1	B	450	ALA	CB-CA-C	6.21	121.22	109.37
1	B	593	THR	N-CA-CB	-6.21	100.00	110.49
1	C	481	PHE	CA-C-O	-6.21	113.91	121.36
1	D	115	PHE	CA-C-N	-6.21	112.59	120.60
1	D	115	PHE	C-N-CA	-6.21	112.59	120.60
1	D	538	SER	CA-CB-OG	-6.21	98.69	111.10
1	F	115	PHE	CA-C-N	-6.21	112.59	120.60
1	F	115	PHE	C-N-CA	-6.21	112.59	120.60
1	F	481	PHE	CA-C-O	-6.21	113.91	121.36
1	F	503	ILE	N-CA-CB	-6.21	99.73	111.21
1	B	191	ASN	CB-CG-ND2	6.21	125.71	116.40
1	D	391	PHE	CA-C-N	-6.21	110.67	120.60
1	D	391	PHE	C-N-CA	-6.21	110.67	120.60
1	F	352	GLY	O-C-N	6.21	130.77	122.70
1	F	456	ASN	CA-C-O	6.21	127.92	121.10
1	A	352	GLY	O-C-N	6.20	130.76	122.70
1	A	503	ILE	N-CA-CB	-6.20	99.73	111.21
1	B	181	VAL	CA-CB-CG2	6.20	120.94	110.40
1	C	113	GLY	O-C-N	6.20	130.76	122.70
1	E	358	HIS	CB-CA-C	6.20	121.18	110.01
1	E	620	ARG	N-CA-C	-6.20	101.01	110.01
1	F	358	HIS	CB-CA-C	6.20	121.18	110.01
1	B	35	GLU	CA-C-O	6.20	128.81	120.13
1	C	411	MET	CB-CA-C	-6.20	98.08	110.42
1	D	557	ALA	N-CA-C	-6.20	97.59	110.80
1	F	35	GLU	CA-C-O	6.20	128.81	120.13
1	A	391	PHE	CA-C-N	-6.20	110.68	120.60
1	A	391	PHE	C-N-CA	-6.20	110.68	120.60
1	A	411	MET	CB-CA-C	-6.20	98.08	110.42
1	A	557	ALA	N-CA-C	-6.20	97.59	110.80
1	B	411	MET	CB-CA-C	-6.20	98.08	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	407	GLU	CB-CG-CD	6.20	123.14	112.60
1	D	198	HIS	CE1-NE2-CD2	-6.20	102.80	109.00
1	D	392	LYS	CA-CB-CG	6.20	126.50	114.10
1	D	527	SER	CA-C-N	-6.20	114.57	122.26
1	D	527	SER	C-N-CA	-6.20	114.57	122.26
1	F	411	MET	CB-CA-C	-6.20	98.08	110.42
1	B	503	ILE	N-CA-CB	-6.20	99.74	111.21
1	D	285	HIS	CA-C-N	-6.20	109.63	120.29
1	D	285	HIS	C-N-CA	-6.20	109.63	120.29
1	D	411	MET	CB-CA-C	-6.20	98.09	110.42
1	E	391	PHE	CA-C-N	-6.20	110.68	120.60
1	E	391	PHE	C-N-CA	-6.20	110.68	120.60
1	E	411	MET	CB-CA-C	-6.20	98.09	110.42
1	C	557	ALA	N-CA-C	-6.20	97.60	110.80
1	A	407	GLU	CB-CG-CD	6.20	123.13	112.60
1	A	538	SER	CA-CB-OG	-6.20	98.71	111.10
1	B	538	SER	CA-CB-OG	-6.20	98.71	111.10
1	C	115	PHE	CA-C-N	-6.20	112.61	120.60
1	C	115	PHE	C-N-CA	-6.20	112.61	120.60
1	C	494	THR	CA-CB-OG1	-6.20	100.31	109.60
1	C	538	SER	CA-CB-OG	-6.20	98.71	111.10
1	D	352	GLY	O-C-N	6.20	130.75	122.70
1	D	407	GLU	CB-CG-CD	6.20	123.13	112.60
1	F	557	ALA	N-CA-C	-6.20	97.60	110.80
1	A	542	GLN	N-CA-C	6.19	119.00	111.82
1	A	276	HIS	CA-C-O	-6.19	113.68	120.43
1	A	389	ASN	CA-C-N	6.19	129.66	122.35
1	A	389	ASN	C-N-CA	6.19	129.66	122.35
1	B	161	GLN	N-CA-CB	-6.19	102.89	112.30
1	C	191	ASN	CB-CG-ND2	6.19	125.69	116.40
1	E	476	ALA	O-C-N	-6.19	115.72	123.27
1	E	542	GLN	N-CA-C	6.19	119.00	111.82
1	E	593	THR	N-CA-CB	-6.19	100.03	110.49
1	A	115	PHE	CA-C-N	-6.19	112.61	120.60
1	A	115	PHE	C-N-CA	-6.19	112.61	120.60
1	A	396	ASP	CA-C-N	-6.19	111.18	122.38
1	A	396	ASP	C-N-CA	-6.19	111.18	122.38
1	B	352	GLY	O-C-N	6.19	130.75	122.70
1	B	407	GLU	CB-CG-CD	6.19	123.12	112.60
1	C	358	HIS	CB-CA-C	6.19	121.15	110.01
1	C	594	GLU	CA-CB-CG	6.19	126.48	114.10
1	D	396	ASP	CA-C-N	-6.19	111.17	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	396	ASP	C-N-CA	-6.19	111.17	122.38
1	D	503	ILE	N-CA-CB	-6.19	99.76	111.21
1	E	115	PHE	CA-C-N	-6.19	112.61	120.60
1	E	115	PHE	C-N-CA	-6.19	112.61	120.60
1	E	538	SER	CA-CB-OG	-6.19	98.72	111.10
1	F	198	HIS	CE1-NE2-CD2	-6.19	102.81	109.00
1	C	396	ASP	CA-C-N	-6.19	111.18	122.38
1	C	396	ASP	C-N-CA	-6.19	111.18	122.38
1	D	450	ALA	CB-CA-C	6.19	121.19	109.37
1	C	102	ASN	OD1-CG-ND2	6.19	128.79	122.60
1	C	352	GLY	O-C-N	6.19	130.74	122.70
1	F	594	GLU	CA-CB-CG	6.19	126.47	114.10
1	B	557	ALA	N-CA-C	-6.19	97.62	110.80
1	F	538	SER	CA-CB-OG	-6.19	98.73	111.10
1	A	476	ALA	O-C-N	-6.18	115.73	123.27
1	B	542	GLN	N-CA-C	6.18	118.99	111.82
1	D	542	GLN	N-CA-C	6.18	119.00	111.82
1	D	594	GLU	CA-CB-CG	6.18	126.47	114.10
1	E	396	ASP	CA-C-N	-6.18	111.19	122.38
1	E	396	ASP	C-N-CA	-6.18	111.19	122.38
1	E	557	ALA	N-CA-C	-6.18	97.63	110.80
1	B	238	ASN	CA-C-O	-6.18	113.07	120.55
1	B	396	ASP	CA-C-N	-6.18	111.19	122.38
1	B	396	ASP	C-N-CA	-6.18	111.19	122.38
1	E	161	GLN	N-CA-CB	-6.18	102.90	112.30
1	E	494	THR	CA-CB-OG1	-6.18	100.33	109.60
1	B	637	ASP	N-CA-C	6.18	120.29	112.87
1	C	389	ASN	CA-C-N	6.18	129.64	122.35
1	C	389	ASN	C-N-CA	6.18	129.64	122.35
1	C	476	ALA	O-C-N	-6.18	115.73	123.27
1	B	115	PHE	CA-C-N	-6.18	112.63	120.60
1	B	115	PHE	C-N-CA	-6.18	112.63	120.60
1	B	561	SER	CA-C-O	6.18	129.35	120.51
1	C	503	ILE	N-CA-CB	-6.18	99.78	111.21
1	D	494	THR	CA-CB-OG1	-6.18	100.33	109.60
1	E	198	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
1	E	238	ASN	CA-C-O	-6.18	113.07	120.55
1	E	594	GLU	CA-CB-CG	6.18	126.46	114.10
1	F	527	SER	CA-C-N	-6.18	114.60	122.26
1	F	527	SER	C-N-CA	-6.18	114.60	122.26
1	B	494	THR	CA-CB-OG1	-6.18	100.34	109.60
1	C	161	GLN	N-CA-CB	-6.18	102.91	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	285	HIS	N-CA-CB	-6.18	100.96	110.04
1	E	389	ASN	CA-C-N	6.18	129.64	122.35
1	E	389	ASN	C-N-CA	6.18	129.64	122.35
1	D	161	GLN	N-CA-CB	-6.17	102.92	112.30
1	F	542	GLN	N-CA-C	6.17	118.98	111.82
1	A	481	PHE	CA-C-O	-6.17	113.95	121.36
1	A	594	GLU	CA-CB-CG	6.17	126.44	114.10
1	C	276	HIS	CA-C-O	-6.17	113.70	120.43
1	D	389	ASN	CA-C-N	6.17	129.63	122.35
1	D	389	ASN	C-N-CA	6.17	129.63	122.35
1	F	389	ASN	CA-C-N	6.17	129.63	122.35
1	F	389	ASN	C-N-CA	6.17	129.63	122.35
1	F	396	ASP	CA-C-N	-6.17	111.21	122.38
1	F	396	ASP	C-N-CA	-6.17	111.21	122.38
1	A	494	THR	CA-CB-OG1	-6.17	100.34	109.60
1	D	285	HIS	N-CA-CB	-6.17	100.97	110.04
1	A	161	GLN	N-CA-CB	-6.17	102.92	112.30
1	A	238	ASN	CA-C-O	-6.17	113.08	120.55
1	B	481	PHE	CA-C-O	-6.17	113.96	121.36
1	F	285	HIS	CA-C-N	-6.17	109.68	120.29
1	F	285	HIS	C-N-CA	-6.17	109.68	120.29
1	A	285	HIS	CA-C-N	-6.17	109.69	120.29
1	A	285	HIS	C-N-CA	-6.17	109.69	120.29
1	B	285	HIS	N-CA-CB	-6.17	100.97	110.04
1	B	594	GLU	CA-CB-CG	6.17	126.43	114.10
1	C	238	ASN	CA-C-O	-6.17	113.09	120.55
1	E	407	GLU	CB-CG-CD	6.17	123.08	112.60
1	F	276	HIS	CA-C-O	-6.17	113.71	120.43
1	F	161	GLN	N-CA-CB	-6.17	102.93	112.30
1	B	564	ILE	O-C-N	-6.16	114.07	121.10
1	E	285	HIS	CA-C-N	-6.16	109.69	120.29
1	E	285	HIS	C-N-CA	-6.16	109.69	120.29
1	F	285	HIS	N-CA-CB	-6.16	100.98	110.04
1	C	35	GLU	CA-C-O	6.16	128.76	120.13
1	F	494	THR	CA-CB-OG1	-6.16	100.36	109.60
1	A	285	HIS	N-CA-CB	-6.16	100.98	110.04
1	D	238	ASN	CA-C-O	-6.16	113.10	120.55
1	E	453	HIS	CA-C-O	-6.16	114.13	120.54
1	C	542	GLN	N-CA-C	6.16	118.97	111.82
1	B	285	HIS	CA-C-N	-6.16	109.70	120.29
1	B	285	HIS	C-N-CA	-6.16	109.70	120.29
1	E	481	PHE	CA-C-O	-6.16	113.97	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	222	TRP	CA-C-N	-6.16	112.03	120.46
1	B	222	TRP	C-N-CA	-6.16	112.03	120.46
1	C	285	HIS	CA-C-N	-6.15	109.70	120.29
1	C	285	HIS	C-N-CA	-6.15	109.70	120.29
1	A	564	ILE	O-C-N	-6.15	114.09	121.10
1	B	458	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	D	222	TRP	CA-C-N	-6.15	112.03	120.46
1	D	222	TRP	C-N-CA	-6.15	112.03	120.46
1	D	481	PHE	CA-C-O	-6.15	113.98	121.36
1	F	272	PRO	N-CD-CG	-6.15	93.98	103.20
1	F	564	ILE	O-C-N	-6.15	114.09	121.10
1	B	27	TYR	CA-C-O	6.15	124.69	119.71
1	C	453	HIS	CA-C-O	-6.15	114.15	120.54
1	C	564	ILE	O-C-N	-6.15	114.09	121.10
1	F	238	ASN	CA-C-O	-6.14	113.12	120.55
1	F	545	ASN	CA-C-N	-6.14	112.91	122.37
1	F	545	ASN	C-N-CA	-6.14	112.91	122.37
1	C	222	TRP	CA-C-N	-6.14	112.04	120.46
1	C	222	TRP	C-N-CA	-6.14	112.04	120.46
1	C	285	HIS	N-CA-CB	-6.14	101.01	110.04
1	E	222	TRP	CA-C-N	-6.14	112.05	120.46
1	E	222	TRP	C-N-CA	-6.14	112.05	120.46
1	E	564	ILE	O-C-N	-6.14	114.10	121.10
1	F	637	ASP	N-CA-C	6.14	120.24	112.87
1	D	545	ASN	CA-C-N	-6.14	112.92	122.37
1	D	545	ASN	C-N-CA	-6.14	112.92	122.37
1	C	47	ASN	CB-CA-C	-6.14	99.01	110.36
1	C	545	ASN	CA-C-N	-6.14	112.92	122.37
1	C	545	ASN	C-N-CA	-6.14	112.92	122.37
1	E	27	TYR	CA-C-O	6.14	124.68	119.71
1	E	637	ASP	N-CA-C	6.14	120.23	112.87
1	F	565	PRO	CB-CA-C	-6.14	103.91	111.64
1	E	328	ILE	CA-C-O	-6.13	114.15	120.71
1	F	336	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	A	222	TRP	CA-C-N	-6.13	112.06	120.46
1	A	222	TRP	C-N-CA	-6.13	112.06	120.46
1	A	545	ASN	CA-C-N	-6.13	112.93	122.37
1	A	545	ASN	C-N-CA	-6.13	112.93	122.37
1	C	27	TYR	CA-C-O	6.13	124.68	119.71
1	D	272	PRO	N-CD-CG	-6.13	94.00	103.20
1	D	637	ASP	N-CA-C	6.13	120.23	112.87
1	A	637	ASP	N-CA-C	6.13	120.23	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	491	ILE	N-CA-C	6.13	122.09	109.34
1	D	328	ILE	CA-C-O	-6.13	114.15	120.71
1	E	374	ALA	CA-C-N	-6.13	109.83	121.54
1	E	374	ALA	C-N-CA	-6.13	109.83	121.54
1	C	539	LEU	CA-C-O	-6.13	111.09	119.12
1	F	47	ASN	CB-CA-C	-6.13	99.02	110.36
1	B	583	TYR	O-C-N	6.13	130.52	123.29
1	C	458	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	F	583	TYR	O-C-N	6.13	130.52	123.29
1	B	565	PRO	CB-CA-C	-6.12	103.92	111.64
1	A	272	PRO	N-CD-CG	-6.12	94.02	103.20
1	B	47	ASN	CB-CA-C	-6.12	99.03	110.36
1	C	336	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	E	565	PRO	CB-CA-C	-6.12	103.92	111.64
1	E	336	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	D	47	ASN	CB-CA-C	-6.12	99.04	110.36
1	D	134	LEU	N-CA-CB	-6.12	102.03	110.29
1	B	502	CYS	CB-CA-C	-6.12	99.19	109.53
1	B	36	ASN	N-CA-C	6.12	118.92	111.82
1	A	27	TYR	CA-C-O	6.12	124.66	119.71
1	A	565	PRO	CB-CA-C	-6.12	103.94	111.64
1	B	545	ASN	CA-C-N	-6.12	112.95	122.37
1	B	545	ASN	C-N-CA	-6.12	112.95	122.37
1	C	374	ALA	CA-C-N	-6.12	109.86	121.54
1	C	374	ALA	C-N-CA	-6.12	109.86	121.54
1	C	557	ALA	CA-C-N	-6.12	111.37	122.50
1	C	557	ALA	C-N-CA	-6.12	111.37	122.50
1	A	328	ILE	CA-C-O	-6.11	114.17	120.71
1	D	574	LYS	CB-CA-C	6.11	118.26	108.91
1	A	47	ASN	CB-CA-C	-6.11	99.05	110.36
1	D	336	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	E	272	PRO	N-CD-CG	-6.11	94.03	103.20
1	F	474	ARG	N-CA-CB	-6.11	100.25	111.37
1	B	328	ILE	CA-C-O	-6.11	114.17	120.71
1	C	272	PRO	N-CD-CG	-6.11	94.03	103.20
1	C	561	SER	CB-CA-C	6.11	122.58	110.42
1	D	539	LEU	CA-C-O	-6.11	111.11	119.12
1	D	564	ILE	O-C-N	-6.11	114.14	121.10
1	E	47	ASN	CB-CA-C	-6.11	99.06	110.36
1	A	502	CYS	CB-CA-C	-6.11	99.21	109.53
1	A	336	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	B	336	ASN	OD1-CG-ND2	-6.11	116.49	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	545	ASN	CA-C-N	-6.11	112.97	122.37
1	E	545	ASN	C-N-CA	-6.11	112.97	122.37
1	B	272	PRO	N-CD-CG	-6.11	94.04	103.20
1	C	565	PRO	CB-CA-C	-6.11	103.95	111.64
1	D	374	ALA	CA-C-N	-6.11	109.88	121.54
1	D	374	ALA	C-N-CA	-6.11	109.88	121.54
1	F	328	ILE	CA-C-O	-6.11	114.18	120.71
1	A	491	ILE	N-CA-C	6.10	122.03	109.34
1	B	539	LEU	CA-C-O	-6.10	111.13	119.12
1	C	491	ILE	N-CA-C	6.10	122.03	109.34
1	D	583	TYR	O-C-N	6.10	130.49	123.29
1	F	374	ALA	CA-C-N	-6.10	109.88	121.54
1	F	374	ALA	C-N-CA	-6.10	109.88	121.54
1	B	561	SER	CB-CA-C	6.10	122.56	110.42
1	A	374	ALA	CA-C-N	-6.10	109.89	121.54
1	A	374	ALA	C-N-CA	-6.10	109.89	121.54
1	A	583	TYR	O-C-N	6.10	130.49	123.29
1	A	474	ARG	N-CA-CB	-6.10	100.27	111.37
1	A	624	TYR	CB-CG-CD1	6.10	129.95	120.80
1	C	637	ASP	N-CA-C	6.10	120.19	112.87
1	E	36	ASN	N-CA-C	6.10	118.89	111.82
1	E	491	ILE	N-CA-C	6.10	122.02	109.34
1	A	557	ALA	CA-C-N	-6.10	111.41	122.50
1	A	557	ALA	C-N-CA	-6.10	111.41	122.50
1	B	473	GLU	CB-CG-CD	6.10	122.96	112.60
1	C	583	TYR	O-C-N	6.10	130.48	123.29
1	E	561	SER	CB-CA-C	6.10	122.55	110.42
1	A	453	HIS	CA-C-O	-6.09	114.20	120.54
1	A	458	ASN	OD1-CG-ND2	-6.09	116.50	122.60
1	B	374	ALA	CA-C-N	-6.09	109.90	121.54
1	B	374	ALA	C-N-CA	-6.09	109.90	121.54
1	B	378	PRO	O-C-N	6.09	130.08	122.22
1	C	36	ASN	N-CA-C	6.09	118.89	111.82
1	C	328	ILE	CA-C-O	-6.09	114.19	120.71
1	D	557	ALA	CA-C-N	-6.09	111.41	122.50
1	D	557	ALA	C-N-CA	-6.09	111.41	122.50
1	F	458	ASN	OD1-CG-ND2	-6.09	116.50	122.60
1	C	474	ARG	N-CA-CB	-6.09	100.28	111.37
1	F	222	TRP	CA-C-N	-6.09	112.11	120.46
1	F	222	TRP	C-N-CA	-6.09	112.11	120.46
1	C	54	GLU	CB-CG-CD	-6.09	102.25	112.60
1	D	36	ASN	N-CA-C	6.09	118.89	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	134	LEU	N-CA-CB	-6.09	102.07	110.29
1	E	502	CYS	CB-CA-C	-6.09	99.24	109.53
1	E	557	ALA	CA-C-N	-6.09	111.41	122.50
1	E	557	ALA	C-N-CA	-6.09	111.41	122.50
1	E	624	TYR	CB-CG-CD1	6.09	129.94	120.80
1	F	473	GLU	CB-CG-CD	6.09	122.96	112.60
1	C	502	CYS	CB-CA-C	-6.09	99.24	109.53
1	D	33	ILE	N-CA-CB	-6.09	102.78	110.57
1	D	502	CYS	CB-CA-C	-6.09	99.24	109.53
1	E	474	ARG	N-CA-CB	-6.09	100.29	111.37
1	A	539	LEU	CA-C-O	-6.09	111.14	119.12
1	C	624	TYR	CB-CG-CD1	6.09	129.93	120.80
1	D	491	ILE	N-CA-C	6.09	122.00	109.34
1	D	565	PRO	CB-CA-C	-6.09	103.97	111.64
1	E	288	ASP	CB-CG-OD2	-6.09	104.40	118.40
1	F	491	ILE	N-CA-C	6.09	122.00	109.34
1	F	624	TYR	CB-CG-CD1	6.09	129.93	120.80
1	A	561	SER	CB-CA-C	6.08	122.53	110.42
1	B	134	LEU	N-CA-CB	-6.08	102.08	110.29
1	B	557	ALA	CA-C-N	-6.08	111.42	122.50
1	B	557	ALA	C-N-CA	-6.08	111.42	122.50
1	F	453	HIS	CA-C-O	-6.08	114.21	120.54
1	F	502	CYS	CB-CA-C	-6.08	99.25	109.53
1	F	561	SER	CB-CA-C	6.08	122.53	110.42
1	A	36	ASN	N-CA-C	6.08	118.88	111.82
1	A	134	LEU	N-CA-CB	-6.08	102.08	110.29
1	B	474	ARG	N-CA-CB	-6.08	100.30	111.37
1	B	624	TYR	CB-CG-CD1	6.08	129.93	120.80
1	D	561	SER	CB-CA-C	6.08	122.53	110.42
1	E	211	TYR	CB-CA-C	6.08	124.44	111.91
1	F	557	ALA	CA-C-N	-6.08	111.43	122.50
1	F	557	ALA	C-N-CA	-6.08	111.43	122.50
1	B	507	LYS	CB-CA-C	-6.08	101.83	110.34
1	D	220	PHE	CG-CD1-CE1	6.08	131.04	120.70
1	D	458	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	D	624	TYR	CB-CG-CD1	6.08	129.92	120.80
1	D	629	ARG	N-CA-C	-6.08	101.67	110.24
1	F	27	TYR	CA-C-O	6.08	124.64	119.71
1	C	108	GLU	CB-CA-C	6.08	122.05	109.95
1	C	288	ASP	CB-CG-OD2	-6.08	104.42	118.40
1	A	473	GLU	CB-CG-CD	6.08	122.93	112.60
1	D	149	GLU	CG-CD-OE1	6.08	132.38	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	473	GLU	CB-CG-CD	6.08	122.93	112.60
1	D	474	ARG	N-CA-CB	-6.08	100.31	111.37
1	F	211	TYR	CB-CA-C	6.08	124.43	111.91
1	D	19	ASP	CA-C-O	-6.08	114.01	121.67
1	F	264	TYR	CB-CA-C	6.08	120.23	109.72
1	B	149	GLU	CG-CD-OE1	6.08	132.38	118.40
1	E	629	ARG	N-CA-C	-6.08	101.67	110.24
1	F	236	LEU	O-C-N	6.08	128.65	122.09
1	A	378	PRO	O-C-N	6.07	130.05	122.22
1	A	574	LYS	CB-CA-C	6.07	118.20	108.91
1	C	220	PHE	CG-CD1-CE1	6.07	131.03	120.70
1	C	269	PRO	CA-C-N	-6.07	111.04	121.97
1	C	269	PRO	C-N-CA	-6.07	111.04	121.97
1	C	507	LYS	CB-CA-C	-6.07	101.84	110.34
1	D	264	TYR	CB-CA-C	6.07	120.23	109.72
1	B	428	GLU	CB-CG-CD	-6.07	102.28	112.60
1	D	378	PRO	O-C-N	6.07	130.05	122.22
1	E	458	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	F	288	ASP	CB-CG-OD2	-6.07	104.43	118.40
1	F	539	LEU	CA-C-O	-6.07	111.17	119.12
1	A	264	TYR	CB-CA-C	6.07	120.22	109.72
1	B	453	HIS	CA-C-O	-6.07	114.23	120.54
1	C	254	GLU	CB-CG-CD	6.07	122.92	112.60
1	D	108	GLU	CB-CA-C	6.07	122.03	109.95
1	D	211	TYR	CB-CA-C	6.07	124.42	111.91
1	D	254	GLU	CB-CG-CD	6.07	122.92	112.60
1	E	108	GLU	CB-CA-C	6.07	122.03	109.95
1	E	264	TYR	CB-CA-C	6.07	120.22	109.72
1	F	220	PHE	CG-CD1-CE1	6.07	131.02	120.70
1	F	254	GLU	CB-CG-CD	6.07	122.92	112.60
1	F	269	PRO	CA-C-N	-6.07	111.04	121.97
1	F	269	PRO	C-N-CA	-6.07	111.04	121.97
1	B	54	GLU	CB-CG-CD	-6.07	102.28	112.60
1	F	378	PRO	O-C-N	6.07	130.05	122.22
1	A	149	GLU	CG-CD-OE1	6.07	132.36	118.40
1	A	211	TYR	CB-CA-C	6.07	124.41	111.91
1	A	288	ASP	CB-CG-OD2	-6.07	104.45	118.40
1	B	629	ARG	N-CA-C	-6.07	101.68	110.24
1	C	473	GLU	CB-CG-CD	6.07	122.92	112.60
1	C	574	LYS	CB-CA-C	6.07	118.19	108.91
1	D	453	HIS	CA-C-O	-6.07	114.23	120.54
1	E	242	PRO	CA-C-O	-6.07	109.56	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	583	TYR	O-C-N	6.07	130.45	123.29
1	F	629	ARG	N-CA-C	-6.07	101.68	110.24
1	B	242	PRO	CA-C-O	-6.07	109.56	120.60
1	C	33	ILE	N-CA-CB	-6.07	102.81	110.57
1	C	211	TYR	CB-CA-C	6.07	124.41	111.91
1	C	242	PRO	CA-C-O	-6.07	109.56	120.60
1	D	27	TYR	CA-C-O	6.07	124.62	119.71
1	E	149	GLU	CG-CD-OE1	6.07	132.35	118.40
1	F	36	ASN	N-CA-C	6.07	118.86	111.82
1	F	54	GLU	CB-CG-CD	-6.07	102.29	112.60
1	F	134	LEU	N-CA-CB	-6.07	102.10	110.29
1	B	574	LYS	CB-CA-C	6.06	118.19	108.91
1	F	434	ILE	CA-C-N	-6.06	107.33	121.52
1	F	434	ILE	C-N-CA	-6.06	107.33	121.52
1	A	242	PRO	CA-C-O	-6.06	109.57	120.60
1	A	629	ARG	N-CA-C	-6.06	101.69	110.24
1	B	368	MET	CA-C-O	6.06	126.39	119.18
1	C	134	LEU	N-CA-CB	-6.06	102.11	110.29
1	C	378	PRO	O-C-N	6.06	130.04	122.22
1	D	288	ASP	CB-CG-OD2	-6.06	104.46	118.40
1	D	507	LYS	CB-CA-C	-6.06	101.85	110.34
1	E	33	ILE	N-CA-CB	-6.06	102.81	110.57
1	E	439	SER	N-CA-CB	-6.06	101.25	110.77
1	F	33	ILE	N-CA-CB	-6.06	102.81	110.57
1	F	574	LYS	CB-CA-C	6.06	118.19	108.91
1	F	648	LYS	N-CA-CB	6.06	120.78	110.71
1	A	54	GLU	CB-CG-CD	-6.06	102.30	112.60
1	A	507	LYS	CB-CA-C	-6.06	101.86	110.34
1	E	648	LYS	N-CA-CB	6.06	120.77	110.71
1	A	220	PHE	CG-CD1-CE1	6.06	131.00	120.70
1	A	244	ASP	OD1-CG-OD2	-6.06	108.36	122.90
1	A	269	PRO	CA-C-N	-6.06	111.06	121.97
1	A	269	PRO	C-N-CA	-6.06	111.06	121.97
1	B	211	TYR	CB-CA-C	6.06	124.39	111.91
1	C	149	GLU	CG-CD-OE1	6.06	132.34	118.40
1	C	244	ASP	OD1-CG-OD2	-6.06	108.36	122.90
1	C	629	ARG	N-CA-C	-6.06	101.70	110.24
1	D	242	PRO	CA-C-O	-6.06	109.57	120.60
1	F	309	ASP	O-C-N	6.06	130.76	122.46
1	F	484	PRO	CB-CA-C	-6.06	101.56	111.56
1	F	507	LYS	CB-CA-C	-6.06	101.86	110.34
1	A	33	ILE	N-CA-CB	-6.06	102.82	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	GLU	CB-CA-C	6.06	122.01	109.95
1	A	254	GLU	CB-CG-CD	6.06	122.90	112.60
1	B	648	LYS	N-CA-CB	6.06	120.77	110.71
1	D	368	MET	CA-C-O	6.06	126.39	119.18
1	D	642	ILE	CB-CA-C	6.06	121.19	110.71
1	E	54	GLU	CB-CG-CD	-6.06	102.30	112.60
1	E	236	LEU	O-C-N	6.06	128.63	122.09
1	E	539	LEU	CA-C-O	-6.06	111.19	119.12
1	E	574	LYS	CB-CA-C	6.06	118.18	108.91
1	E	642	ILE	CB-CA-C	6.06	121.19	110.71
1	F	244	ASP	OD1-CG-OD2	-6.06	108.36	122.90
1	C	643	LYS	CB-CG-CD	6.06	125.23	111.30
1	D	196	THR	O-C-N	6.06	128.39	122.09
1	D	244	ASP	OD1-CG-OD2	-6.06	108.37	122.90
1	A	434	ILE	CA-C-N	-6.05	107.35	121.52
1	A	434	ILE	C-N-CA	-6.05	107.35	121.52
1	B	244	ASP	OD1-CG-OD2	-6.05	108.37	122.90
1	B	264	TYR	CB-CA-C	6.05	120.19	109.72
1	C	264	TYR	CB-CA-C	6.05	120.19	109.72
1	C	484	PRO	CB-CA-C	-6.05	101.57	111.56
1	C	642	ILE	CB-CA-C	6.05	121.18	110.71
1	D	434	ILE	CA-C-N	-6.05	107.35	121.52
1	D	434	ILE	C-N-CA	-6.05	107.35	121.52
1	E	507	LYS	CB-CA-C	-6.05	101.87	110.34
1	A	484	PRO	CB-CA-C	-6.05	101.58	111.56
1	D	54	GLU	CB-CG-CD	-6.05	102.31	112.60
1	E	434	ILE	CA-C-N	-6.05	107.36	121.52
1	E	434	ILE	C-N-CA	-6.05	107.36	121.52
1	F	149	GLU	CG-CD-OE1	6.05	132.32	118.40
1	F	289	LEU	N-CA-C	-6.05	102.30	111.56
1	A	643	LYS	CB-CG-CD	6.05	125.21	111.30
1	B	220	PHE	CG-CD1-CE1	6.05	130.99	120.70
1	B	643	LYS	CB-CG-CD	6.05	125.21	111.30
1	D	428	GLU	CB-CG-CD	-6.05	102.32	112.60
1	E	196	THR	O-C-N	6.05	128.38	122.09
1	F	643	LYS	CB-CG-CD	6.05	125.21	111.30
1	A	648	LYS	N-CA-CB	6.05	120.75	110.71
1	B	642	ILE	CB-CA-C	6.05	121.17	110.71
1	F	268	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	236	LEU	O-C-N	6.05	128.62	122.09
1	A	428	GLU	CB-CG-CD	-6.05	102.32	112.60
1	B	236	LEU	O-C-N	6.05	128.62	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	269	PRO	CA-C-N	-6.05	111.09	121.97
1	B	269	PRO	C-N-CA	-6.05	111.09	121.97
1	C	404	ASP	CA-C-O	6.05	126.74	119.61
1	C	434	ILE	CA-C-N	-6.05	107.37	121.52
1	C	434	ILE	C-N-CA	-6.05	107.37	121.52
1	D	268	PHE	CA-CB-CG	6.05	119.85	113.80
1	D	269	PRO	CA-C-N	-6.05	111.09	121.97
1	D	269	PRO	C-N-CA	-6.05	111.09	121.97
1	E	254	GLU	CB-CG-CD	6.05	122.88	112.60
1	E	643	LYS	CB-CG-CD	6.05	125.21	111.30
1	F	242	PRO	CA-C-O	-6.05	109.60	120.60
1	B	649	ILE	CA-C-O	-6.04	113.60	120.67
1	C	526	SER	CA-CB-OG	-6.04	99.01	111.10
1	E	244	ASP	OD1-CG-OD2	-6.04	108.39	122.90
1	B	196	THR	O-C-N	6.04	128.38	122.09
1	A	196	THR	O-C-N	6.04	128.37	122.09
1	B	288	ASP	CB-CG-OD2	-6.04	104.50	118.40
1	C	368	MET	CA-C-O	6.04	126.37	119.18
1	C	648	LYS	N-CA-CB	6.04	120.74	110.71
1	C	651	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	D	526	SER	CA-CB-OG	-6.04	99.02	111.10
1	E	428	GLU	CB-CG-CD	-6.04	102.33	112.60
1	E	473	GLU	CB-CG-CD	6.04	122.87	112.60
1	C	19	ASP	CA-C-O	-6.04	114.06	121.67
1	E	268	PHE	CA-CB-CG	6.04	119.84	113.80
1	E	526	SER	CA-CB-OG	-6.04	99.02	111.10
1	F	108	GLU	CB-CA-C	6.04	121.97	109.95
1	A	642	ILE	CB-CA-C	6.04	121.15	110.71
1	D	643	LYS	CB-CG-CD	6.04	125.19	111.30
1	F	526	SER	CA-CB-OG	-6.04	99.03	111.10
1	A	268	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	368	MET	CA-C-O	6.04	126.36	119.18
1	B	33	ILE	N-CA-CB	-6.04	102.84	110.57
1	B	289	LEU	N-CA-C	-6.04	102.33	111.56
1	C	649	ILE	CA-C-O	-6.04	113.61	120.67
1	D	289	LEU	N-CA-C	-6.04	102.33	111.56
1	D	404	ASP	CA-C-O	6.04	126.73	119.61
1	D	439	SER	N-CA-CB	-6.04	101.30	110.77
1	F	404	ASP	CA-C-O	6.04	126.73	119.61
1	F	428	GLU	CB-CG-CD	-6.04	102.34	112.60
1	F	642	ILE	CB-CA-C	6.04	121.15	110.71
1	A	289	LEU	N-CA-C	-6.03	102.33	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	281	ASP	N-CA-CB	6.03	118.92	109.69
1	B	434	ILE	CA-C-N	-6.03	107.40	121.52
1	B	434	ILE	C-N-CA	-6.03	107.40	121.52
1	E	269	PRO	CA-C-N	-6.03	111.11	121.97
1	E	269	PRO	C-N-CA	-6.03	111.11	121.97
1	E	378	PRO	O-C-N	6.03	130.00	122.22
1	E	484	PRO	CB-CA-C	-6.03	101.60	111.56
1	B	484	PRO	CB-CA-C	-6.03	101.61	111.56
1	D	484	PRO	CB-CA-C	-6.03	101.61	111.56
1	F	196	THR	O-C-N	6.03	128.36	122.09
1	A	391	PHE	N-CA-C	-6.03	104.63	111.14
1	A	526	SER	CA-CB-OG	-6.03	99.04	111.10
1	B	254	GLU	CB-CG-CD	6.03	122.85	112.60
1	B	268	PHE	CA-CB-CG	6.03	119.83	113.80
1	E	136	PRO	O-C-N	6.03	129.84	123.03
1	F	450	ALA	CA-C-N	-6.03	114.49	122.99
1	F	450	ALA	C-N-CA	-6.03	114.49	122.99
1	F	649	ILE	CA-C-O	-6.03	113.61	120.67
1	A	649	ILE	CA-C-O	-6.03	113.62	120.67
1	B	108	GLU	CB-CA-C	6.03	121.95	109.95
1	B	198	HIS	O-C-N	-6.03	114.57	122.59
1	B	19	ASP	CA-C-O	-6.03	114.08	121.67
1	C	450	ALA	CA-C-N	-6.03	114.49	122.99
1	C	450	ALA	C-N-CA	-6.03	114.49	122.99
1	A	439	SER	N-CA-CB	-6.03	101.31	110.77
1	E	228	THR	N-CA-C	6.03	118.64	111.71
1	F	281	ASP	N-CA-CB	6.03	118.91	109.69
1	D	648	LYS	N-CA-CB	6.02	120.71	110.71
1	A	404	ASP	CA-C-O	6.02	126.72	119.61
1	B	404	ASP	CA-C-O	6.02	126.72	119.61
1	E	309	ASP	O-C-N	6.02	130.71	122.46
1	C	375	THR	OG1-CB-CG2	6.02	121.34	109.30
1	D	651	HIS	CB-CG-CD2	-6.02	123.37	131.20
1	E	289	LEU	N-CA-C	-6.02	102.35	111.56
1	F	508	PHE	O-C-N	6.02	130.13	123.33
1	B	309	ASP	O-C-N	6.02	130.71	122.46
1	B	375	THR	OG1-CB-CG2	6.02	121.34	109.30
1	B	526	SER	CA-CB-OG	-6.02	99.06	111.10
1	C	428	GLU	CB-CG-CD	-6.02	102.37	112.60
1	D	391	PHE	N-CA-C	-6.02	104.64	111.14
1	F	642	ILE	O-C-N	6.02	129.73	123.05
1	A	19	ASP	CA-C-O	-6.02	114.09	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	375	THR	OG1-CB-CG2	6.02	121.34	109.30
1	A	450	ALA	CA-C-N	-6.02	114.51	122.99
1	A	450	ALA	C-N-CA	-6.02	114.51	122.99
1	B	439	SER	N-CA-CB	-6.02	101.32	110.77
1	D	375	THR	OG1-CB-CG2	6.02	121.33	109.30
1	F	228	THR	N-CA-C	6.02	118.63	111.71
1	C	236	LEU	O-C-N	6.02	128.59	122.09
1	D	649	ILE	CA-C-O	-6.02	113.63	120.67
1	A	309	ASP	O-C-N	6.01	130.70	122.46
1	A	651	HIS	CB-CG-CD2	-6.01	123.38	131.20
1	E	651	HIS	CB-CG-CD2	-6.01	123.38	131.20
1	A	136	PRO	O-C-N	6.01	129.82	123.03
1	B	450	ALA	CA-C-N	-6.01	114.51	122.99
1	B	450	ALA	C-N-CA	-6.01	114.51	122.99
1	C	268	PHE	CA-CB-CG	6.01	119.81	113.80
1	C	309	ASP	O-C-N	6.01	130.70	122.46
1	E	281	ASP	N-CA-CB	6.01	118.89	109.69
1	F	375	THR	OG1-CB-CG2	6.01	121.33	109.30
1	C	127	LYS	CB-CA-C	6.01	120.43	110.81
1	C	198	HIS	O-C-N	-6.01	114.59	122.59
1	C	391	PHE	N-CA-C	-6.01	104.65	111.14
1	C	439	SER	N-CA-CB	-6.01	101.33	110.77
1	D	236	LEU	O-C-N	6.01	128.58	122.09
1	E	215	ARG	O-C-N	6.01	130.25	122.19
1	F	322	GLU	N-CA-C	-6.01	103.38	112.04
1	F	368	MET	CA-C-O	6.01	126.33	119.18
1	F	391	PHE	N-CA-C	-6.01	104.65	111.14
1	C	485	ILE	CA-C-O	-6.01	113.27	120.78
1	E	357	PRO	CA-CB-CG	-6.01	93.08	104.50
1	E	404	ASP	CA-C-O	6.01	126.70	119.61
1	F	439	SER	N-CA-CB	-6.01	101.33	110.77
1	A	281	ASP	N-CA-CB	6.01	118.88	109.69
1	C	289	LEU	N-CA-C	-6.01	102.37	111.56
1	D	309	ASP	O-C-N	6.01	130.69	122.46
1	E	220	PHE	CG-CD1-CE1	6.01	130.91	120.70
1	B	391	PHE	N-CA-C	-6.01	104.65	111.14
1	B	608	GLN	CA-C-O	-6.01	111.72	120.13
1	D	281	ASP	N-CA-CB	6.01	118.88	109.69
1	E	375	THR	OG1-CB-CG2	6.01	121.31	109.30
1	E	391	PHE	N-CA-C	-6.01	104.65	111.14
1	C	136	PRO	O-C-N	6.00	129.81	123.03
1	A	228	THR	N-CA-C	6.00	118.61	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ARG	O-C-N	6.00	130.24	122.19
1	C	228	THR	N-CA-C	6.00	118.61	111.71
1	D	450	ALA	CA-C-N	-6.00	114.53	122.99
1	D	450	ALA	C-N-CA	-6.00	114.53	122.99
1	F	215	ARG	O-C-N	6.00	130.23	122.19
1	F	291	ILE	CA-C-O	-6.00	114.81	121.17
1	A	127	LYS	CB-CA-C	6.00	120.41	110.81
1	B	136	PRO	O-C-N	6.00	129.81	123.03
1	C	357	PRO	CA-CB-CG	-6.00	93.10	104.50
1	D	127	LYS	CB-CA-C	6.00	120.41	110.81
1	D	136	PRO	O-C-N	6.00	129.81	123.03
1	F	80	ARG	N-CA-C	-6.00	104.66	111.14
1	B	431	TYR	CB-CA-C	6.00	121.52	110.24
1	B	579	GLU	N-CA-C	-6.00	98.74	108.52
1	D	228	THR	N-CA-C	6.00	118.61	111.71
1	D	259	LEU	CA-C-N	6.00	132.53	122.87
1	D	259	LEU	C-N-CA	6.00	132.53	122.87
1	F	651	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	A	431	TYR	CB-CA-C	6.00	121.51	110.24
1	B	228	THR	N-CA-C	6.00	118.61	111.71
1	C	80	ARG	N-CA-C	-6.00	104.67	111.14
1	C	608	GLN	CA-C-O	-6.00	111.73	120.13
1	E	368	MET	CA-C-O	6.00	126.32	119.18
1	E	450	ALA	CA-C-N	-6.00	114.53	122.99
1	E	450	ALA	C-N-CA	-6.00	114.53	122.99
1	F	136	PRO	O-C-N	6.00	129.81	123.03
1	C	215	ARG	O-C-N	6.00	130.22	122.19
1	B	322	GLU	N-CA-C	-5.99	103.41	112.04
1	B	551	HIS	CA-C-N	-5.99	110.09	121.54
1	B	551	HIS	C-N-CA	-5.99	110.09	121.54
1	D	431	TYR	CB-CA-C	5.99	121.51	110.24
1	E	127	LYS	CB-CA-C	5.99	120.40	110.81
1	F	485	ILE	CA-C-O	-5.99	113.29	120.78
1	F	608	GLN	CA-C-O	-5.99	111.74	120.13
1	B	259	LEU	CA-C-N	5.99	132.51	122.87
1	B	259	LEU	C-N-CA	5.99	132.51	122.87
1	B	651	HIS	CB-CG-CD2	-5.99	123.41	131.20
1	D	551	HIS	CA-C-N	-5.99	110.10	121.54
1	D	551	HIS	C-N-CA	-5.99	110.10	121.54
1	E	649	ILE	CA-C-O	-5.99	113.66	120.67
1	A	198	HIS	O-C-N	-5.99	114.62	122.59
1	A	485	ILE	CA-C-O	-5.99	113.30	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	127	LYS	CB-CA-C	5.99	120.39	110.81
1	F	127	LYS	CB-CA-C	5.99	120.39	110.81
1	F	551	HIS	CA-C-N	-5.99	110.10	121.54
1	F	551	HIS	C-N-CA	-5.99	110.10	121.54
1	A	357	PRO	CA-CB-CG	-5.99	93.13	104.50
1	C	431	TYR	CB-CA-C	5.99	121.49	110.24
1	D	633	GLU	CB-CG-CD	5.99	122.77	112.60
1	E	19	ASP	CA-C-O	-5.99	114.13	121.67
1	E	198	HIS	O-C-N	-5.99	114.63	122.59
1	E	485	ILE	CA-C-O	-5.99	113.30	120.78
1	E	633	GLU	CB-CG-CD	5.99	122.78	112.60
1	F	259	LEU	CA-C-N	5.99	132.51	122.87
1	F	259	LEU	C-N-CA	5.99	132.51	122.87
1	F	357	PRO	CA-CB-CG	-5.99	93.13	104.50
1	F	431	TYR	CB-CA-C	5.99	121.49	110.24
1	A	608	GLN	CA-C-O	-5.98	111.75	120.13
1	C	281	ASP	N-CA-CB	5.98	118.85	109.69
1	A	215	ARG	O-C-N	5.98	130.21	122.19
1	B	357	PRO	CA-CB-CG	-5.98	93.13	104.50
1	D	357	PRO	CA-CB-CG	-5.98	93.13	104.50
1	D	579	GLU	N-CA-C	-5.98	98.77	108.52
1	A	322	GLU	N-CA-C	-5.98	103.43	112.04
1	B	485	ILE	CA-C-O	-5.98	113.31	120.78
1	D	215	ARG	O-C-N	5.98	130.20	122.19
1	E	226	GLN	CG-CD-NE2	-5.98	107.43	116.40
1	E	465	THR	CA-CB-OG1	5.98	118.57	109.60
1	A	465	THR	CA-CB-OG1	5.98	118.56	109.60
1	C	226	GLN	CG-CD-NE2	-5.98	107.43	116.40
1	C	465	THR	CA-CB-OG1	5.98	118.57	109.60
1	D	465	THR	CA-CB-OG1	5.98	118.57	109.60
1	F	579	GLU	N-CA-C	-5.98	98.78	108.52
1	E	431	TYR	CB-CA-C	5.98	121.47	110.24
1	A	508	PHE	O-C-N	5.97	130.08	123.33
1	E	322	GLU	N-CA-C	-5.97	103.44	112.04
1	F	465	THR	CA-CB-OG1	5.97	118.56	109.60
1	A	551	HIS	CA-C-N	-5.97	110.13	121.54
1	A	551	HIS	C-N-CA	-5.97	110.13	121.54
1	A	579	GLU	N-CA-C	-5.97	98.78	108.52
1	C	196	THR	O-C-N	5.97	128.30	122.09
1	C	551	HIS	CA-C-N	-5.97	110.13	121.54
1	C	551	HIS	C-N-CA	-5.97	110.13	121.54
1	C	633	GLU	CB-CG-CD	5.97	122.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	608	GLN	CA-C-O	-5.97	111.77	120.13
1	B	80	ARG	N-CA-C	-5.97	104.69	111.14
1	B	642	ILE	O-C-N	5.97	129.68	123.05
1	C	322	GLU	N-CA-C	-5.97	103.44	112.04
1	A	226	GLN	CG-CD-NE2	-5.97	107.45	116.40
1	A	633	GLU	CB-CG-CD	5.97	122.75	112.60
1	D	198	HIS	O-C-N	-5.97	114.65	122.59
1	D	485	ILE	CA-C-O	-5.97	113.32	120.78
1	E	508	PHE	O-C-N	5.97	130.08	123.33
1	B	32	ASP	CB-CA-C	5.97	122.78	110.31
1	C	276	HIS	ND1-CE1-NE2	5.97	114.37	108.40
1	C	579	GLU	N-CA-C	-5.97	98.79	108.52
1	D	322	GLU	N-CA-C	-5.97	103.45	112.04
1	D	477	THR	CA-CB-OG1	-5.97	100.65	109.60
1	E	80	ARG	N-CA-C	-5.97	104.70	111.14
1	E	113	GLY	CA-C-N	-5.97	112.69	120.44
1	E	113	GLY	C-N-CA	-5.97	112.69	120.44
1	E	579	GLU	N-CA-C	-5.97	98.79	108.52
1	F	640	SER	O-C-N	5.97	129.61	122.27
1	A	80	ARG	N-CA-C	-5.96	104.70	111.14
1	B	226	GLN	CG-CD-NE2	-5.96	107.45	116.40
1	D	226	GLN	CG-CD-NE2	-5.96	107.45	116.40
1	D	608	GLN	CA-C-O	-5.96	111.78	120.13
1	F	633	GLU	CB-CG-CD	5.96	122.74	112.60
1	D	113	GLY	CA-C-N	-5.96	112.69	120.44
1	D	113	GLY	C-N-CA	-5.96	112.69	120.44
1	A	259	LEU	CA-C-N	5.96	132.47	122.87
1	A	259	LEU	C-N-CA	5.96	132.47	122.87
1	A	642	ILE	O-C-N	5.96	129.67	123.05
1	B	447	GLU	O-C-N	5.96	130.08	122.93
1	D	276	HIS	ND1-CE1-NE2	5.96	114.36	108.40
1	E	477	THR	CA-CB-OG1	-5.96	100.66	109.60
1	F	477	THR	CA-CB-OG1	-5.96	100.66	109.60
1	E	551	HIS	CA-C-N	-5.96	110.16	121.54
1	E	551	HIS	C-N-CA	-5.96	110.16	121.54
1	F	113	GLY	CA-C-N	-5.96	112.69	120.44
1	F	113	GLY	C-N-CA	-5.96	112.69	120.44
1	B	477	THR	CA-CB-OG1	-5.96	100.67	109.60
1	B	633	GLU	CB-CG-CD	5.96	122.72	112.60
1	E	213	LEU	CA-C-N	5.96	132.92	121.54
1	E	213	LEU	C-N-CA	5.96	132.92	121.54
1	F	32	ASP	CB-CA-C	5.96	122.76	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	508	PHE	O-C-N	5.96	130.06	123.33
1	E	221	PHE	O-C-N	5.96	130.51	122.59
1	E	276	HIS	ND1-CE1-NE2	5.96	114.36	108.40
1	D	80	ARG	N-CA-C	-5.95	104.71	111.14
1	F	198	HIS	O-C-N	-5.95	114.67	122.59
1	F	226	GLN	CG-CD-NE2	-5.95	107.47	116.40
1	F	276	HIS	ND1-CE1-NE2	5.95	114.35	108.40
1	B	113	GLY	CA-C-N	-5.95	112.70	120.44
1	B	113	GLY	C-N-CA	-5.95	112.70	120.44
1	B	276	HIS	ND1-CE1-NE2	5.95	114.35	108.40
1	E	342	SER	CB-CA-C	-5.95	102.20	112.44
1	A	276	HIS	ND1-CE1-NE2	5.95	114.35	108.40
1	B	465	THR	CA-CB-OG1	5.95	118.52	109.60
1	C	642	ILE	O-C-N	5.95	129.65	123.05
1	D	642	ILE	O-C-N	5.95	129.65	123.05
1	E	406	LEU	CA-C-N	5.95	130.72	121.26
1	E	406	LEU	C-N-CA	5.95	130.72	121.26
1	F	19	ASP	CA-C-O	-5.95	114.17	121.67
1	E	32	ASP	CB-CA-C	5.95	122.74	110.31
1	A	213	LEU	CA-C-N	5.94	132.89	121.54
1	A	213	LEU	C-N-CA	5.94	132.89	121.54
1	A	291	ILE	CA-C-O	-5.94	114.87	121.17
1	A	406	LEU	CA-C-N	5.94	130.71	121.26
1	A	406	LEU	C-N-CA	5.94	130.71	121.26
1	B	342	SER	CB-CA-C	-5.94	102.22	112.44
1	C	518	THR	O-C-N	5.94	130.17	123.28
1	D	406	LEU	CA-C-O	5.94	126.68	119.31
1	E	447	GLU	O-C-N	5.94	130.06	122.93
1	A	32	ASP	CB-CA-C	5.94	122.72	110.31
1	A	113	GLY	CA-C-N	-5.94	112.72	120.44
1	A	113	GLY	C-N-CA	-5.94	112.72	120.44
1	A	477	THR	CA-CB-OG1	-5.94	100.69	109.60
1	C	32	ASP	CB-CA-C	5.94	122.73	110.31
1	C	291	ILE	CA-C-O	-5.94	114.87	121.17
1	A	640	SER	O-C-N	5.94	129.57	122.27
1	B	213	LEU	N-CA-CB	-5.94	101.10	110.06
1	C	259	LEU	CA-C-N	5.94	132.43	122.87
1	C	259	LEU	C-N-CA	5.94	132.43	122.87
1	E	259	LEU	CA-C-N	5.94	132.43	122.87
1	E	259	LEU	C-N-CA	5.94	132.43	122.87
1	E	291	ILE	CA-C-O	-5.94	114.88	121.17
1	C	406	LEU	CA-C-N	5.93	130.70	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	406	LEU	C-N-CA	5.93	130.70	121.26
1	D	213	LEU	CA-C-N	5.93	132.87	121.54
1	D	213	LEU	C-N-CA	5.93	132.87	121.54
1	E	213	LEU	N-CA-CB	-5.93	101.10	110.06
1	E	487	ASP	N-CA-CB	-5.93	101.38	110.16
1	F	447	GLU	O-C-N	5.93	130.05	122.93
1	D	517	GLU	CA-CB-CG	5.93	125.97	114.10
1	D	518	THR	O-C-N	5.93	130.16	123.28
1	F	213	LEU	N-CA-CB	-5.93	101.10	110.06
1	A	447	GLU	O-C-N	5.93	130.05	122.93
1	B	640	SER	O-C-N	5.93	129.56	122.27
1	A	221	PHE	O-C-N	5.93	130.48	122.59
1	B	221	PHE	O-C-N	5.93	130.48	122.59
1	D	406	LEU	CA-C-N	5.93	130.69	121.26
1	D	406	LEU	C-N-CA	5.93	130.69	121.26
1	E	627	GLU	CA-C-N	-5.93	112.85	122.81
1	E	627	GLU	C-N-CA	-5.93	112.85	122.81
1	F	518	THR	O-C-N	5.93	130.16	123.28
1	C	508	PHE	O-C-N	5.93	130.03	123.33
1	D	213	LEU	N-CA-CB	-5.93	101.11	110.06
1	F	386	TYR	CA-C-N	-5.93	112.26	120.38
1	F	386	TYR	C-N-CA	-5.93	112.26	120.38
1	A	487	ASP	N-CA-CB	-5.93	101.39	110.16
1	B	406	LEU	CA-C-N	5.93	130.68	121.26
1	B	406	LEU	C-N-CA	5.93	130.68	121.26
1	E	496	ASP	O-C-N	5.93	130.47	122.59
1	E	642	ILE	O-C-N	5.93	129.63	123.05
1	F	342	SER	CB-CA-C	-5.93	102.25	112.44
1	A	213	LEU	N-CA-CB	-5.92	101.11	110.06
1	B	213	LEU	CA-C-N	5.92	132.85	121.54
1	B	213	LEU	C-N-CA	5.92	132.85	121.54
1	C	496	ASP	O-C-N	5.92	130.47	122.59
1	D	32	ASP	CB-CA-C	5.92	122.69	110.31
1	B	103	ALA	O-C-N	-5.92	114.71	122.59
1	C	213	LEU	CA-C-N	5.92	132.85	121.54
1	C	213	LEU	C-N-CA	5.92	132.85	121.54
1	C	342	SER	CB-CA-C	-5.92	102.25	112.44
1	C	429	PHE	N-CA-CB	-5.92	100.59	111.37
1	F	572	LYS	O-C-N	5.92	128.49	122.09
1	A	342	SER	CB-CA-C	-5.92	102.25	112.44
1	C	447	GLU	O-C-N	5.92	130.04	122.93
1	C	477	THR	CA-CB-OG1	-5.92	100.72	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	342	SER	CB-CA-C	-5.92	102.26	112.44
1	F	213	LEU	CA-C-N	5.92	132.85	121.54
1	F	213	LEU	C-N-CA	5.92	132.85	121.54
1	E	397	SER	CA-C-O	5.92	126.44	119.28
1	A	429	PHE	N-CA-CB	-5.92	100.60	111.37
1	A	501	PHE	O-C-N	5.92	130.53	122.37
1	F	429	PHE	N-CA-CB	-5.92	100.60	111.37
1	F	548	ASN	O-C-N	5.92	129.24	122.55
1	A	548	ASN	O-C-N	5.91	129.23	122.55
1	B	178	GLU	CB-CA-C	-5.91	98.65	110.42
1	B	429	PHE	N-CA-CB	-5.91	100.61	111.37
1	B	508	PHE	O-C-N	5.91	130.01	123.33
1	B	630	ILE	CA-CB-CG1	5.91	120.45	110.40
1	D	178	GLU	CB-CA-C	-5.91	98.65	110.42
1	F	178	GLU	CB-CA-C	-5.91	98.65	110.42
1	F	627	GLU	CA-C-N	-5.91	112.88	122.81
1	F	627	GLU	C-N-CA	-5.91	112.88	122.81
1	B	397	SER	CA-C-O	5.91	126.43	119.28
1	C	548	ASN	O-C-N	5.91	129.23	122.55
1	A	178	GLU	CB-CA-C	-5.91	98.66	110.42
1	B	9	GLN	CA-C-N	-5.91	111.95	120.82
1	B	9	GLN	C-N-CA	-5.91	111.95	120.82
1	B	487	ASP	N-CA-CB	-5.91	101.41	110.16
1	C	113	GLY	CA-C-N	-5.91	112.76	120.44
1	C	113	GLY	C-N-CA	-5.91	112.76	120.44
1	C	630	ILE	CA-CB-CG1	5.91	120.45	110.40
1	D	291	ILE	CA-C-O	-5.91	114.91	121.17
1	D	501	PHE	O-C-N	5.91	130.53	122.37
1	E	107	ARG	CG-CD-NE	-5.91	99.00	112.00
1	E	518	THR	O-C-N	5.91	130.14	123.28
1	E	576	GLU	CG-CD-OE1	-5.91	104.81	118.40
1	F	9	GLN	CA-C-N	-5.91	111.95	120.82
1	F	9	GLN	C-N-CA	-5.91	111.95	120.82
1	F	487	ASP	N-CA-CB	-5.91	101.41	110.16
1	B	291	ILE	CA-C-O	-5.91	114.91	121.17
1	C	517	GLU	CA-CB-CG	5.91	125.92	114.10
1	D	399	PRO	O-C-N	5.91	128.43	121.46
1	F	406	LEU	CA-C-N	5.91	130.65	121.26
1	F	406	LEU	C-N-CA	5.91	130.65	121.26
1	F	517	GLU	CA-CB-CG	5.91	125.92	114.10
1	A	518	THR	O-C-N	5.91	130.13	123.28
1	B	399	PRO	O-C-N	5.91	128.43	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	397	SER	CA-C-O	5.91	126.43	119.28
1	C	576	GLU	CG-CD-OE1	-5.91	104.81	118.40
1	E	640	SER	O-C-N	5.91	129.53	122.27
1	B	548	ASN	O-C-N	5.91	129.22	122.55
1	B	627	GLU	CA-C-N	-5.91	112.89	122.81
1	B	627	GLU	C-N-CA	-5.91	112.89	122.81
1	D	429	PHE	N-CA-CB	-5.91	100.62	111.37
1	E	178	GLU	CB-CA-C	-5.91	98.67	110.42
1	E	501	PHE	O-C-N	5.91	130.52	122.37
1	B	107	ARG	CG-CD-NE	-5.90	99.01	112.00
1	C	640	SER	O-C-N	5.90	129.53	122.27
1	D	9	GLN	CA-C-N	-5.90	111.96	120.82
1	D	9	GLN	C-N-CA	-5.90	111.96	120.82
1	D	576	GLU	CG-CD-OE1	-5.90	104.82	118.40
1	D	630	ILE	CA-CB-CG1	5.90	120.44	110.40
1	E	517	GLU	CA-CB-CG	5.90	125.91	114.10
1	F	221	PHE	O-C-N	5.90	130.44	122.59
1	A	517	GLU	CA-CB-CG	5.90	125.91	114.10
1	D	487	ASP	N-CA-CB	-5.90	101.42	110.16
1	E	406	LEU	CA-C-O	5.90	126.63	119.31
1	F	15	ASN	CB-CG-OD1	-5.90	109.00	120.80
1	A	627	GLU	CA-C-N	-5.90	112.90	122.81
1	A	627	GLU	C-N-CA	-5.90	112.90	122.81
1	A	630	ILE	CA-CB-CG1	5.90	120.43	110.40
1	C	107	ARG	CG-CD-NE	-5.90	99.02	112.00
1	C	213	LEU	N-CA-CB	-5.90	101.15	110.06
1	C	501	PHE	O-C-N	5.90	130.51	122.37
1	D	386	TYR	CA-C-N	-5.90	112.30	120.38
1	D	386	TYR	C-N-CA	-5.90	112.30	120.38
1	F	406	LEU	CA-C-O	5.90	126.63	119.31
1	C	221	PHE	O-C-N	5.90	130.44	122.59
1	D	89	VAL	CA-CB-CG1	5.90	120.43	110.40
1	A	107	ARG	CG-CD-NE	-5.90	99.02	112.00
1	A	496	ASP	O-C-N	5.90	130.43	122.59
1	A	576	GLU	CG-CD-OE1	-5.90	104.84	118.40
1	C	103	ALA	O-C-N	-5.90	114.75	122.59
1	D	447	GLU	O-C-N	5.90	130.01	122.93
1	E	101	SER	O-C-N	5.90	128.39	122.08
1	E	429	PHE	N-CA-CB	-5.90	100.64	111.37
1	E	630	ILE	CA-CB-CG1	5.90	120.42	110.40
1	A	406	LEU	CA-C-O	5.90	126.62	119.31
1	B	517	GLU	CA-CB-CG	5.90	125.89	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	501	PHE	O-C-N	5.90	130.51	122.37
1	F	576	GLU	CG-CD-OE1	-5.90	104.84	118.40
1	C	627	GLU	CA-C-N	-5.89	112.91	122.81
1	C	627	GLU	C-N-CA	-5.89	112.91	122.81
1	D	101	SER	O-C-N	5.89	128.39	122.08
1	D	103	ALA	O-C-N	-5.89	114.75	122.59
1	D	221	PHE	O-C-N	5.89	130.43	122.59
1	D	619	ASN	CA-CB-CG	-5.89	106.71	112.60
1	D	627	GLU	CA-C-N	-5.89	112.91	122.81
1	D	627	GLU	C-N-CA	-5.89	112.91	122.81
1	A	101	SER	O-C-N	5.89	128.38	122.08
1	A	397	SER	CA-C-O	5.89	126.41	119.28
1	C	635	VAL	O-C-N	5.89	132.62	121.84
1	D	413	VAL	CA-C-O	-5.89	114.32	121.04
1	E	386	TYR	CA-C-N	-5.89	112.31	120.38
1	E	386	TYR	C-N-CA	-5.89	112.31	120.38
1	F	107	ARG	CG-CD-NE	-5.89	99.03	112.00
1	A	9	GLN	CA-C-N	-5.89	111.98	120.82
1	A	9	GLN	C-N-CA	-5.89	111.98	120.82
1	C	487	ASP	N-CA-CB	-5.89	101.44	110.16
1	F	103	ALA	O-C-N	-5.89	114.75	122.59
1	A	386	TYR	CA-C-N	-5.89	112.31	120.38
1	A	386	TYR	C-N-CA	-5.89	112.31	120.38
1	B	15	ASN	CB-CG-OD1	-5.89	109.02	120.80
1	C	406	LEU	CA-C-O	5.89	126.61	119.31
1	E	15	ASN	CB-CG-OD1	-5.89	109.02	120.80
1	F	630	ILE	CA-CB-CG1	5.89	120.41	110.40
1	C	9	GLN	CA-C-N	-5.89	111.99	120.82
1	C	9	GLN	C-N-CA	-5.89	111.99	120.82
1	C	178	GLU	CB-CA-C	-5.89	98.70	110.42
1	E	635	VAL	O-C-N	5.89	132.61	121.84
1	F	496	ASP	O-C-N	5.89	130.42	122.59
1	A	103	ALA	O-C-N	-5.89	114.76	122.59
1	C	386	TYR	CA-C-N	-5.89	112.32	120.38
1	C	386	TYR	C-N-CA	-5.89	112.32	120.38
1	C	413	VAL	CA-C-O	-5.89	114.33	121.04
1	D	640	SER	O-C-N	5.89	129.51	122.27
1	E	89	VAL	CA-CB-CG1	5.89	120.41	110.40
1	B	101	SER	O-C-N	5.88	128.38	122.08
1	B	492	THR	CA-CB-OG1	-5.88	100.77	109.60
1	B	501	PHE	O-C-N	5.88	130.49	122.37
1	C	89	VAL	CA-CB-CG1	5.88	120.40	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	9	GLN	CA-C-N	-5.88	111.99	120.82
1	E	9	GLN	C-N-CA	-5.88	111.99	120.82
1	E	626	LEU	CA-C-O	5.88	126.45	119.56
1	A	89	VAL	CA-CB-CG1	5.88	120.40	110.40
1	B	576	GLU	CG-CD-OE1	-5.88	104.87	118.40
1	D	15	ASN	CB-CG-OD1	-5.88	109.04	120.80
1	D	496	ASP	O-C-N	5.88	130.41	122.59
1	D	193	HIS	CB-CG-ND1	5.88	131.52	122.70
1	A	15	ASN	CB-CG-OD1	-5.88	109.04	120.80
1	D	107	ARG	CG-CD-NE	-5.88	99.07	112.00
1	D	296	ILE	N-CA-C	5.88	116.00	110.30
1	B	496	ASP	O-C-N	5.88	130.41	122.59
1	D	397	SER	CA-C-O	5.88	126.39	119.28
1	F	89	VAL	CA-CB-CG1	5.88	120.39	110.40
1	C	15	ASN	CB-CG-OD1	-5.88	109.05	120.80
1	E	296	ILE	N-CA-C	5.88	116.00	110.30
1	E	435	ASN	CB-CA-C	5.88	121.67	110.27
1	F	397	SER	CA-C-O	5.88	126.39	119.28
1	A	413	VAL	CA-C-O	-5.87	114.34	121.04
1	A	626	LEU	CA-C-O	5.87	126.43	119.56
1	D	548	ASN	O-C-N	5.87	129.19	122.55
1	B	89	VAL	CA-CB-CG1	5.87	120.38	110.40
1	E	572	LYS	O-C-N	5.87	128.43	122.09
1	F	101	SER	O-C-N	5.87	128.36	122.08
1	F	619	ASN	CA-CB-CG	-5.87	106.73	112.60
1	B	406	LEU	CA-C-O	5.87	126.59	119.31
1	C	114	GLU	CB-CA-C	5.87	120.09	110.88
1	A	254	GLU	N-CA-CB	-5.87	101.81	110.49
1	A	572	LYS	O-C-N	5.87	128.43	122.09
1	A	619	ASN	CA-CB-CG	-5.87	106.73	112.60
1	C	435	ASN	CB-CA-C	5.87	121.65	110.27
1	A	399	PRO	O-C-N	5.87	128.38	121.46
1	A	635	VAL	O-C-N	5.87	132.57	121.84
1	B	254	GLU	N-CA-CB	-5.87	101.81	110.49
1	C	399	PRO	O-C-N	5.87	128.38	121.46
1	B	386	TYR	CA-C-N	-5.86	112.35	120.38
1	B	386	TYR	C-N-CA	-5.86	112.35	120.38
1	B	435	ASN	CB-CA-C	5.86	121.64	110.27
1	B	518	THR	O-C-N	5.86	130.08	123.28
1	B	619	ASN	CA-CB-CG	-5.86	106.74	112.60
1	E	413	VAL	CA-C-O	-5.86	114.36	121.04
1	E	548	ASN	O-C-N	5.86	129.18	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	413	VAL	CA-C-O	-5.86	114.36	121.04
1	E	103	ALA	O-C-N	-5.86	114.79	122.59
1	E	110	MET	CB-CG-SD	-5.86	95.11	112.70
1	C	572	LYS	O-C-N	5.86	128.42	122.09
1	C	619	ASN	CA-CB-CG	-5.86	106.74	112.60
1	D	492	THR	CA-CB-OG1	-5.86	100.81	109.60
1	F	626	LEU	CA-C-O	5.86	126.42	119.56
1	A	435	ASN	CB-CA-C	5.86	121.64	110.27
1	A	492	THR	CA-CB-OG1	-5.86	100.81	109.60
1	E	432	SER	O-C-N	-5.86	116.54	123.22
1	C	626	LEU	CA-C-O	5.86	126.41	119.56
1	D	110	MET	CB-CG-SD	-5.86	95.13	112.70
1	D	114	GLU	CB-CA-C	5.86	120.08	110.88
1	D	435	ASN	CB-CA-C	5.86	121.63	110.27
1	F	110	MET	CB-CG-SD	-5.86	95.12	112.70
1	C	492	THR	CA-CB-OG1	-5.86	100.82	109.60
1	E	399	PRO	O-C-N	5.86	128.37	121.46
1	A	114	GLU	CB-CA-C	5.85	120.07	110.88
1	C	101	SER	O-C-N	5.85	128.34	122.08
1	D	573	SER	CB-CA-C	-5.85	108.16	115.89
1	E	492	THR	CA-CB-OG1	-5.85	100.82	109.60
1	F	492	THR	CA-CB-OG1	-5.85	100.82	109.60
1	F	573	SER	CB-CA-C	-5.85	108.16	115.89
1	A	110	MET	CB-CG-SD	-5.85	95.14	112.70
1	D	254	GLU	N-CA-CB	-5.85	101.83	110.49
1	D	626	LEU	CA-C-O	5.85	126.41	119.56
1	F	260	THR	O-C-N	5.85	130.53	123.16
1	B	573	SER	CB-CA-C	-5.85	108.17	115.89
1	E	619	ASN	CA-CB-CG	-5.85	106.75	112.60
1	B	413	VAL	CA-C-O	-5.85	114.37	121.04
1	F	254	GLU	N-CA-CB	-5.85	101.83	110.49
1	B	110	MET	CB-CG-SD	-5.85	95.16	112.70
1	B	193	HIS	CB-CG-ND1	5.85	131.47	122.70
1	D	572	LYS	O-C-N	5.85	128.40	122.09
1	B	114	GLU	CB-CA-C	5.84	120.06	110.88
1	E	114	GLU	CB-CA-C	5.84	120.05	110.88
1	F	432	SER	O-C-N	-5.84	116.56	123.22
1	C	110	MET	CB-CG-SD	-5.84	95.17	112.70
1	A	193	HIS	CB-CG-ND1	5.84	131.46	122.70
1	A	296	ILE	N-CA-C	5.84	115.97	110.30
1	A	432	SER	O-C-N	-5.84	116.56	123.22
1	C	476	ALA	N-CA-C	5.84	118.99	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	635	VAL	O-C-N	5.84	132.53	121.84
1	F	114	GLU	CB-CA-C	5.84	120.05	110.88
1	C	254	GLU	N-CA-CB	-5.84	101.85	110.49
1	C	432	SER	O-C-N	-5.84	116.56	123.22
1	D	238	ASN	O-C-N	5.84	129.67	122.20
1	D	260	THR	O-C-N	5.84	130.52	123.16
1	E	254	GLU	N-CA-CB	-5.84	101.85	110.49
1	F	193	HIS	CB-CG-ND1	5.84	131.46	122.70
1	B	432	SER	O-C-N	-5.84	116.56	123.22
1	C	193	HIS	CB-CG-ND1	5.84	131.46	122.70
1	F	435	ASN	CB-CA-C	5.84	121.59	110.27
1	D	248	TRP	N-CA-CB	5.84	119.91	110.40
1	E	40	LEU	CB-CA-C	5.83	120.42	111.02
1	B	238	ASN	O-C-N	5.83	129.67	122.20
1	B	626	LEU	CA-C-O	5.83	126.39	119.56
1	C	260	THR	O-C-N	5.83	130.51	123.16
1	A	573	SER	CB-CA-C	-5.83	108.19	115.89
1	C	296	ILE	N-CA-C	5.83	115.96	110.30
1	E	22	TYR	N-CA-C	-5.83	106.40	112.93
1	C	248	TRP	N-CA-CB	5.83	119.90	110.40
1	E	193	HIS	CB-CG-ND1	5.83	131.44	122.70
1	A	40	LEU	CB-CA-C	5.83	120.40	111.02
1	D	432	SER	O-C-N	-5.83	116.58	123.22
1	E	47	ASN	CA-C-N	-5.83	113.46	122.49
1	E	47	ASN	C-N-CA	-5.83	113.46	122.49
1	E	238	ASN	O-C-N	5.83	129.66	122.20
1	D	374	ALA	CA-C-O	-5.83	112.91	119.79
1	B	58	LYS	CA-CB-CG	-5.83	102.45	114.10
1	B	572	LYS	O-C-N	5.83	128.38	122.09
1	D	58	LYS	CA-CB-CG	-5.83	102.45	114.10
1	A	238	ASN	O-C-N	5.82	129.65	122.20
1	B	260	THR	O-C-N	5.82	130.50	123.16
1	D	361	PHE	CA-C-O	5.82	125.46	119.05
1	D	476	ALA	N-CA-C	5.82	118.96	109.24
1	F	399	PRO	O-C-N	5.82	128.33	121.46
1	A	260	THR	O-C-N	5.82	130.50	123.16
1	A	58	LYS	CA-CB-CG	-5.82	102.46	114.10
1	D	40	LEU	CB-CA-C	5.82	120.39	111.02
1	D	47	ASN	CA-C-N	-5.82	113.47	122.49
1	D	47	ASN	C-N-CA	-5.82	113.47	122.49
1	F	244	ASP	CB-CG-OD1	5.82	131.79	118.40
1	A	248	TRP	N-CA-CB	5.82	119.89	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	47	ASN	CA-C-N	-5.82	113.47	122.49
1	F	47	ASN	C-N-CA	-5.82	113.47	122.49
1	B	248	TRP	N-CA-CB	5.82	119.88	110.40
1	C	40	LEU	CB-CA-C	5.82	120.39	111.02
1	C	58	LYS	CA-CB-CG	-5.82	102.46	114.10
1	E	361	PHE	CA-C-O	5.82	125.45	119.05
1	E	476	ALA	N-CA-C	5.82	118.95	109.24
1	F	224	HIS	CB-CA-C	5.82	122.15	109.99
1	B	47	ASN	CA-C-N	-5.82	113.47	122.49
1	B	47	ASN	C-N-CA	-5.82	113.47	122.49
1	B	425	PHE	N-CA-C	5.82	115.96	108.34
1	C	244	ASP	CB-CG-OD1	5.82	131.78	118.40
1	D	487	ASP	CB-CA-C	-5.82	100.97	110.85
1	E	58	LYS	CA-CB-CG	-5.82	102.47	114.10
1	E	487	ASP	CB-CA-C	-5.82	100.97	110.85
1	F	238	ASN	O-C-N	5.82	129.64	122.20
1	A	244	ASP	CB-CG-OD1	5.81	131.77	118.40
1	C	238	ASN	O-C-N	5.81	129.64	122.20
1	C	487	ASP	CB-CA-C	-5.81	100.97	110.85
1	F	248	TRP	N-CA-CB	5.81	119.88	110.40
1	A	476	ALA	N-CA-C	5.81	118.95	109.24
1	C	573	SER	CB-CA-C	-5.81	108.22	115.89
1	C	575	PRO	O-C-N	-5.81	114.30	122.38
1	E	260	THR	O-C-N	5.81	130.48	123.16
1	F	40	LEU	CB-CA-C	5.81	120.38	111.02
1	E	248	TRP	N-CA-CB	5.81	119.87	110.40
1	B	575	PRO	O-C-N	-5.81	114.31	122.38
1	C	374	ALA	CA-C-O	-5.81	112.94	119.79
1	F	425	PHE	N-CA-C	5.81	115.95	108.34
1	A	425	PHE	N-CA-C	5.80	115.94	108.34
1	A	575	PRO	O-C-N	-5.80	114.31	122.38
1	B	244	ASP	CB-CG-OD1	5.80	131.75	118.40
1	B	296	ILE	N-CA-C	5.80	115.93	110.30
1	B	361	PHE	CA-C-O	5.80	125.44	119.05
1	D	224	HIS	CB-CA-C	5.80	122.12	109.99
1	F	487	ASP	CB-CA-C	-5.80	100.98	110.85
1	A	487	ASP	CB-CA-C	-5.80	100.99	110.85
1	B	249	ASP	CA-CB-CG	-5.80	106.80	112.60
1	C	47	ASN	CA-C-N	-5.80	113.50	122.49
1	C	47	ASN	C-N-CA	-5.80	113.50	122.49
1	C	497	GLU	O-C-N	5.80	130.10	122.33
1	D	244	ASP	CB-CG-OD1	5.80	131.75	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	462	TYR	CA-C-N	-5.80	114.62	122.86
1	D	462	TYR	C-N-CA	-5.80	114.62	122.86
1	F	361	PHE	CA-C-O	5.80	125.43	119.05
1	D	463	LYS	N-CA-C	-5.80	97.70	108.02
1	E	224	HIS	CB-CA-C	5.80	122.11	109.99
1	E	244	ASP	CB-CG-OD1	5.80	131.74	118.40
1	E	573	SER	CB-CA-C	-5.80	108.24	115.89
1	F	58	LYS	CA-CB-CG	-5.80	102.50	114.10
1	F	249	ASP	CA-CB-CG	-5.80	106.80	112.60
1	A	47	ASN	CA-C-N	-5.80	113.50	122.49
1	A	47	ASN	C-N-CA	-5.80	113.50	122.49
1	B	487	ASP	CB-CA-C	-5.80	100.99	110.85
1	A	609	CYS	CA-C-O	-5.80	113.98	121.11
1	B	40	LEU	CB-CA-C	5.80	120.35	111.02
1	B	296	ILE	N-CA-CB	5.80	116.94	110.62
1	C	224	HIS	CB-CA-C	5.80	122.10	109.99
1	D	425	PHE	N-CA-C	5.80	115.93	108.34
1	F	551	HIS	O-C-N	5.80	129.90	123.52
1	E	425	PHE	N-CA-C	5.79	115.93	108.34
1	F	293	GLU	OE1-CD-OE2	-5.79	108.99	122.90
1	A	224	HIS	CB-CA-C	5.79	122.10	109.99
1	C	551	HIS	O-C-N	5.79	129.89	123.52
1	B	476	ALA	N-CA-C	5.79	118.91	109.24
1	E	375	THR	CA-CB-OG1	-5.79	100.91	109.60
1	F	375	THR	CA-CB-OG1	-5.79	100.91	109.60
1	F	609	CYS	CA-C-O	-5.79	113.99	121.11
1	A	375	THR	CA-CB-OG1	-5.79	100.92	109.60
1	F	374	ALA	CA-C-O	-5.79	112.96	119.79
1	D	375	THR	CA-CB-OG1	-5.79	100.92	109.60
1	F	462	TYR	CA-C-N	-5.79	114.64	122.86
1	F	462	TYR	C-N-CA	-5.79	114.64	122.86
1	B	375	THR	CA-CB-OG1	-5.79	100.92	109.60
1	C	609	CYS	CA-C-O	-5.79	113.99	121.11
1	D	293	GLU	OE1-CD-OE2	-5.79	109.01	122.90
1	F	296	ILE	N-CA-CB	5.79	116.93	110.62
1	F	575	PRO	O-C-N	-5.79	114.34	122.38
1	A	22	TYR	N-CA-C	-5.78	106.45	112.93
1	B	164	GLY	N-CA-C	5.78	128.42	111.71
1	B	463	LYS	N-CA-C	-5.78	97.73	108.02
1	C	375	THR	CA-CB-OG1	-5.78	100.92	109.60
1	E	495	LEU	N-CA-C	-5.78	104.27	111.90
1	F	463	LYS	N-CA-C	-5.78	97.72	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	476	ALA	N-CA-C	5.78	118.90	109.24
1	E	463	LYS	N-CA-C	-5.78	97.73	108.02
1	A	374	ALA	CA-C-O	-5.78	112.97	119.79
1	B	224	HIS	CB-CA-C	5.78	122.07	109.99
1	D	22	TYR	N-CA-C	-5.78	106.45	112.93
1	E	609	CYS	CA-C-O	-5.78	114.00	121.11
1	B	609	CYS	CA-C-O	-5.78	114.00	121.11
1	C	293	GLU	OE1-CD-OE2	-5.78	109.03	122.90
1	D	296	ILE	N-CA-CB	5.78	116.92	110.62
1	E	164	GLY	N-CA-C	5.78	128.41	111.71
1	A	293	GLU	OE1-CD-OE2	-5.78	109.03	122.90
1	C	341	GLY	O-C-N	5.78	130.21	122.70
1	D	164	GLY	N-CA-C	5.78	128.41	111.71
1	D	575	PRO	O-C-N	-5.78	114.35	122.38
1	E	575	PRO	O-C-N	-5.78	114.35	122.38
1	A	463	LYS	N-CA-C	-5.78	97.74	108.02
1	B	181	VAL	N-CA-CB	-5.78	101.70	111.23
1	B	551	HIS	O-C-N	5.78	129.87	123.52
1	C	22	TYR	N-CA-C	-5.78	106.46	112.93
1	D	641	ASN	N-CA-CB	-5.78	102.45	110.65
1	A	495	LEU	N-CA-C	-5.77	104.28	111.90
1	C	462	TYR	CA-C-N	-5.77	114.66	122.86
1	C	462	TYR	C-N-CA	-5.77	114.66	122.86
1	E	296	ILE	N-CA-CB	5.77	116.91	110.62
1	E	341	GLY	O-C-N	5.77	130.21	122.70
1	C	296	ILE	N-CA-CB	5.77	116.91	110.62
1	C	463	LYS	N-CA-C	-5.77	97.74	108.02
1	D	495	LEU	N-CA-C	-5.77	104.28	111.90
1	F	315	ILE	CB-CA-C	-5.77	101.82	111.29
1	F	341	GLY	O-C-N	5.77	130.21	122.70
1	A	462	TYR	CA-C-N	-5.77	114.67	122.86
1	A	462	TYR	C-N-CA	-5.77	114.67	122.86
1	A	641	ASN	N-CA-CB	-5.77	102.46	110.65
1	D	609	CYS	CA-C-O	-5.77	114.01	121.11
1	E	31	LYS	N-CA-C	5.77	118.79	111.69
1	F	296	ILE	N-CA-C	5.77	115.90	110.30
1	A	361	PHE	CA-C-O	5.77	125.40	119.05
1	B	462	TYR	CA-C-N	-5.77	114.67	122.86
1	B	462	TYR	C-N-CA	-5.77	114.67	122.86
1	E	551	HIS	O-C-N	5.77	129.87	123.52
1	F	22	TYR	N-CA-C	-5.77	106.47	112.93
1	B	22	TYR	N-CA-C	-5.77	106.47	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	249	ASP	CA-CB-CG	-5.77	106.83	112.60
1	E	374	ALA	CA-C-O	-5.77	112.99	119.79
1	F	164	GLY	N-CA-C	5.77	128.37	111.71
1	C	181	VAL	N-CA-CB	-5.76	101.72	111.23
1	C	425	PHE	N-CA-C	5.76	115.89	108.34
1	E	429	PHE	O-C-N	5.76	130.33	123.24
1	F	57	MET	CB-CA-C	5.76	120.48	110.68
1	F	181	VAL	N-CA-CB	-5.76	101.72	111.23
1	F	429	PHE	O-C-N	5.76	130.33	123.24
1	F	641	ASN	N-CA-CB	-5.76	102.46	110.65
1	A	164	GLY	N-CA-C	5.76	128.36	111.71
1	A	181	VAL	N-CA-CB	-5.76	101.72	111.23
1	C	495	LEU	N-CA-C	-5.76	104.29	111.90
1	A	296	ILE	N-CA-CB	5.76	116.90	110.62
1	E	112	GLU	OE1-CD-OE2	5.76	136.73	122.90
1	E	641	ASN	N-CA-CB	-5.76	102.47	110.65
1	F	269	PRO	O-C-N	5.76	129.88	122.91
1	F	445	ASP	N-CA-C	5.76	118.06	109.59
1	C	641	ASN	N-CA-CB	-5.76	102.47	110.65
1	D	315	ILE	CB-CA-C	-5.76	101.84	111.29
1	E	293	GLU	OE1-CD-OE2	-5.76	109.08	122.90
1	F	495	LEU	N-CA-C	-5.76	104.30	111.90
1	C	164	GLY	N-CA-C	5.76	128.35	111.71
1	D	429	PHE	O-C-N	5.76	130.32	123.24
1	A	315	ILE	CB-CA-C	-5.76	101.85	111.29
1	B	269	PRO	O-C-N	5.76	129.88	122.91
1	B	445	ASP	N-CA-C	5.76	118.05	109.59
1	B	495	LEU	N-CA-C	-5.76	104.30	111.90
1	D	112	GLU	OE1-CD-OE2	5.76	136.72	122.90
1	E	181	VAL	N-CA-CB	-5.76	101.73	111.23
1	A	112	GLU	OE1-CD-OE2	5.75	136.71	122.90
1	A	341	GLY	O-C-N	5.75	130.18	122.70
1	A	249	ASP	CA-CB-CG	-5.75	106.85	112.60
1	A	551	HIS	O-C-N	5.75	129.85	123.52
1	D	249	ASP	CA-CB-CG	-5.75	106.85	112.60
1	B	57	MET	CB-CA-C	5.75	120.46	110.68
1	B	641	ASN	N-CA-CB	-5.75	102.48	110.65
1	C	226	GLN	CA-C-N	-5.75	112.57	120.28
1	C	226	GLN	C-N-CA	-5.75	112.57	120.28
1	D	181	VAL	N-CA-CB	-5.75	101.74	111.23
1	E	57	MET	CB-CA-C	5.75	120.46	110.68
1	A	57	MET	CB-CA-C	5.75	120.46	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	293	GLU	OE1-CD-OE2	-5.75	109.10	122.90
1	D	551	HIS	O-C-N	5.75	129.84	123.52
1	A	70	HIS	CA-C-N	-5.75	111.15	122.02
1	A	70	HIS	C-N-CA	-5.75	111.15	122.02
1	B	31	LYS	N-CA-C	5.75	118.76	111.69
1	B	315	ILE	CB-CA-C	-5.75	101.86	111.29
1	C	315	ILE	CB-CA-C	-5.75	101.86	111.29
1	C	370	HIS	CA-C-N	-5.75	111.57	120.31
1	C	370	HIS	C-N-CA	-5.75	111.57	120.31
1	E	70	HIS	CA-C-N	-5.75	111.16	122.02
1	E	70	HIS	C-N-CA	-5.75	111.16	122.02
1	E	266	GLY	CA-C-N	-5.75	111.85	121.39
1	E	266	GLY	C-N-CA	-5.75	111.85	121.39
1	F	112	GLU	OE1-CD-OE2	5.75	136.70	122.90
1	A	445	ASP	N-CA-C	5.75	118.04	109.59
1	C	85	MET	O-C-N	5.75	130.03	122.33
1	C	269	PRO	O-C-N	5.75	129.86	122.91
1	D	269	PRO	O-C-N	5.75	129.86	122.91
1	E	315	ILE	CB-CA-C	-5.75	101.86	111.29
1	E	462	TYR	CA-C-N	-5.75	114.70	122.86
1	E	462	TYR	C-N-CA	-5.75	114.70	122.86
1	A	429	PHE	O-C-N	5.75	130.31	123.24
1	C	57	MET	CB-CA-C	5.74	120.44	110.68
1	C	266	GLY	CA-C-N	-5.74	111.86	121.39
1	C	266	GLY	C-N-CA	-5.74	111.86	121.39
1	D	70	HIS	CA-C-N	-5.74	111.16	122.02
1	D	70	HIS	C-N-CA	-5.74	111.16	122.02
1	E	226	GLN	CA-C-N	-5.74	112.58	120.28
1	E	226	GLN	C-N-CA	-5.74	112.58	120.28
1	D	458	ASN	N-CA-CB	-5.74	100.84	110.83
1	A	269	PRO	O-C-N	5.74	129.86	122.91
1	B	70	HIS	CA-C-N	-5.74	111.17	122.02
1	B	70	HIS	C-N-CA	-5.74	111.17	122.02
1	C	70	HIS	CA-C-N	-5.74	111.17	122.02
1	C	70	HIS	C-N-CA	-5.74	111.17	122.02
1	F	227	LEU	N-CA-CB	5.74	118.56	110.12
1	C	249	ASP	CA-CB-CG	-5.74	106.86	112.60
1	E	445	ASP	N-CA-C	5.74	118.03	109.59
1	F	70	HIS	CA-C-N	-5.74	111.17	122.02
1	F	70	HIS	C-N-CA	-5.74	111.17	122.02
1	C	361	PHE	CA-C-O	5.74	125.36	119.05
1	A	266	GLY	CA-C-N	-5.74	111.87	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	GLY	C-N-CA	-5.74	111.87	121.39
1	F	31	LYS	N-CA-C	5.74	118.74	111.69
1	B	112	GLU	OE1-CD-OE2	5.73	136.66	122.90
1	C	31	LYS	N-CA-C	5.73	118.74	111.69
1	C	445	ASP	N-CA-C	5.73	118.02	109.59
1	A	227	LEU	N-CA-CB	5.73	118.55	110.12
1	A	458	ASN	N-CA-CB	-5.73	100.86	110.83
1	C	227	LEU	N-CA-CB	5.73	118.55	110.12
1	C	330	SER	CA-C-O	-5.73	112.31	120.51
1	F	458	ASN	N-CA-CB	-5.73	100.86	110.83
1	A	31	LYS	N-CA-C	5.73	118.74	111.69
1	B	341	GLY	O-C-N	5.73	130.15	122.70
1	B	383	LEU	N-CA-C	-5.73	105.17	111.82
1	C	458	ASN	N-CA-CB	-5.73	100.86	110.83
1	D	341	GLY	O-C-N	5.73	130.15	122.70
1	D	445	ASP	N-CA-C	5.73	118.01	109.59
1	D	330	SER	CA-C-O	-5.73	112.32	120.51
1	B	85	MET	O-C-N	5.73	130.01	122.33
1	B	266	GLY	CA-C-N	-5.73	111.88	121.39
1	B	266	GLY	C-N-CA	-5.73	111.88	121.39
1	B	297	HIS	CG-ND1-CE1	-5.73	99.56	109.30
1	B	374	ALA	CA-C-O	-5.73	113.03	119.79
1	B	527	SER	CA-C-O	-5.73	112.36	119.18
1	D	92	GLN	N-CA-C	5.73	120.04	112.25
1	D	226	GLN	CA-C-N	-5.73	112.60	120.28
1	D	226	GLN	C-N-CA	-5.73	112.60	120.28
1	E	109	ARG	CA-CB-CG	-5.73	102.64	114.10
1	F	620	ARG	CB-CA-C	5.73	119.81	109.61
1	C	109	ARG	CA-CB-CG	-5.73	102.65	114.10
1	B	130	ASP	OD1-CG-OD2	5.72	136.64	122.90
1	C	112	GLU	OE1-CD-OE2	5.72	136.64	122.90
1	A	370	HIS	CA-C-N	-5.72	111.61	120.31
1	A	370	HIS	C-N-CA	-5.72	111.61	120.31
1	B	429	PHE	O-C-N	5.72	130.28	123.24
1	D	266	GLY	CA-C-N	-5.72	111.89	121.39
1	D	266	GLY	C-N-CA	-5.72	111.89	121.39
1	E	458	ASN	N-CA-CB	-5.72	100.87	110.83
1	E	620	ARG	CB-CA-C	5.72	119.80	109.61
1	A	109	ARG	CA-CB-CG	-5.72	102.66	114.10
1	B	227	LEU	N-CA-CB	5.72	118.53	110.12
1	E	130	ASP	OD1-CG-OD2	5.72	136.63	122.90
1	E	527	SER	CA-C-O	-5.72	112.37	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	109	ARG	CA-CB-CG	-5.72	102.66	114.10
1	F	370	HIS	CA-C-N	-5.72	111.61	120.31
1	F	370	HIS	C-N-CA	-5.72	111.61	120.31
1	A	85	MET	O-C-N	5.72	130.00	122.33
1	D	85	MET	O-C-N	5.72	129.99	122.33
1	D	620	ARG	CB-CA-C	5.72	119.79	109.61
1	E	370	HIS	CA-C-N	-5.72	111.62	120.31
1	E	370	HIS	C-N-CA	-5.72	111.62	120.31
1	A	226	GLN	CA-C-N	-5.72	112.62	120.28
1	A	226	GLN	C-N-CA	-5.72	112.62	120.28
1	A	620	ARG	CB-CA-C	5.72	119.79	109.61
1	D	109	ARG	CA-CB-CG	-5.72	102.67	114.10
1	D	370	HIS	CA-C-N	-5.72	111.62	120.31
1	D	370	HIS	C-N-CA	-5.72	111.62	120.31
1	F	266	GLY	CA-C-N	-5.71	111.91	121.39
1	F	266	GLY	C-N-CA	-5.71	111.91	121.39
1	C	429	PHE	O-C-N	5.71	130.27	123.24
1	D	57	MET	CB-CA-C	5.71	120.39	110.68
1	A	130	ASP	OD1-CG-OD2	5.71	136.61	122.90
1	A	330	SER	CA-C-O	-5.71	112.34	120.51
1	B	226	GLN	CA-C-N	-5.71	112.63	120.28
1	B	226	GLN	C-N-CA	-5.71	112.63	120.28
1	D	227	LEU	N-CA-CB	5.71	118.52	110.12
1	F	85	MET	O-C-N	5.71	129.99	122.33
1	F	527	SER	CA-C-O	-5.71	112.38	119.18
1	F	560	ARG	NH1-CZ-NH2	5.71	126.73	119.30
1	B	370	HIS	CA-C-N	-5.71	111.63	120.31
1	B	370	HIS	C-N-CA	-5.71	111.63	120.31
1	B	458	ASN	N-CA-CB	-5.71	100.89	110.83
1	F	130	ASP	OD1-CG-OD2	5.71	136.60	122.90
1	B	109	ARG	CA-CB-CG	-5.71	102.68	114.10
1	B	330	SER	CA-C-O	-5.71	112.35	120.51
1	C	383	LEU	N-CA-C	-5.71	105.20	111.82
1	E	383	LEU	N-CA-C	-5.71	105.20	111.82
1	D	383	LEU	N-CA-C	-5.71	105.20	111.82
1	B	92	GLN	N-CA-C	5.71	120.01	112.25
1	C	527	SER	CA-C-O	-5.71	112.39	119.18
1	E	227	LEU	N-CA-CB	5.71	118.51	110.12
1	A	527	SER	CA-C-O	-5.70	112.39	119.18
1	E	85	MET	O-C-N	5.70	129.97	122.33
1	E	92	GLN	N-CA-C	5.70	120.01	112.25
1	B	560	ARG	NH1-CZ-NH2	5.70	126.71	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	GLN	N-CA-C	5.70	120.00	112.25
1	C	211	TYR	CA-C-N	-5.70	113.96	122.74
1	C	211	TYR	C-N-CA	-5.70	113.96	122.74
1	B	97	TYR	O-C-N	-5.70	115.01	122.59
1	D	130	ASP	OD1-CG-OD2	5.70	136.57	122.90
1	D	297	HIS	CG-ND1-CE1	-5.70	99.61	109.30
1	C	620	ARG	CB-CA-C	5.70	119.75	109.61
1	D	73	SER	N-CA-C	-5.70	101.31	110.14
1	F	226	GLN	CA-C-N	-5.70	112.64	120.28
1	F	226	GLN	C-N-CA	-5.70	112.64	120.28
1	A	297	HIS	CG-ND1-CE1	-5.70	99.62	109.30
1	B	620	ARG	CB-CA-C	5.70	119.75	109.61
1	C	56	LEU	O-C-N	5.70	129.06	122.17
1	C	614	GLU	O-C-N	5.70	130.16	122.59
1	D	69	ARG	N-CA-CB	-5.70	102.65	111.65
1	E	206	GLU	OE1-CD-OE2	5.70	136.57	122.90
1	E	269	PRO	O-C-N	5.70	129.80	122.91
1	E	297	HIS	CG-ND1-CE1	-5.70	99.62	109.30
1	F	623	GLY	CA-C-N	5.70	128.97	120.83
1	F	623	GLY	C-N-CA	5.70	128.97	120.83
1	D	97	TYR	O-C-N	-5.69	115.02	122.59
1	A	383	LEU	N-CA-C	-5.69	105.22	111.82
1	B	105	TYR	CA-CB-CG	-5.69	103.65	113.90
1	E	56	LEU	O-C-N	5.69	129.06	122.17
1	E	97	TYR	O-C-N	-5.69	115.02	122.59
1	F	330	SER	CA-C-O	-5.69	112.37	120.51
1	D	31	LYS	N-CA-C	5.69	118.69	111.69
1	D	432	SER	CA-C-O	5.69	126.45	120.36
1	F	92	GLN	N-CA-C	5.69	119.99	112.25
1	F	105	TYR	CA-CB-CG	-5.69	103.66	113.90
1	F	297	HIS	CG-ND1-CE1	-5.69	99.63	109.30
1	C	130	ASP	OD1-CG-OD2	5.69	136.55	122.90
1	C	206	GLU	OE1-CD-OE2	5.69	136.55	122.90
1	E	158	LYS	O-C-N	-5.69	116.17	122.09
1	C	73	SER	N-CA-C	-5.69	101.32	110.14
1	D	105	TYR	CA-CB-CG	-5.69	103.66	113.90
1	F	383	LEU	N-CA-C	-5.69	105.22	111.82
1	A	206	GLU	OE1-CD-OE2	5.69	136.55	122.90
1	A	560	ARG	NH1-CZ-NH2	5.69	126.69	119.30
1	A	623	GLY	CA-C-N	5.69	128.96	120.83
1	A	623	GLY	C-N-CA	5.69	128.96	120.83
1	B	56	LEU	O-C-N	5.68	129.05	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	297	HIS	CG-ND1-CE1	-5.68	99.64	109.30
1	D	614	GLU	O-C-N	5.68	130.15	122.59
1	E	560	ARG	NH1-CZ-NH2	5.68	126.69	119.30
1	A	105	TYR	CA-CB-CG	-5.68	103.67	113.90
1	B	608	GLN	N-CA-CB	5.68	119.88	110.33
1	C	92	GLN	N-CA-C	5.68	119.98	112.25
1	D	220	PHE	CA-C-O	-5.68	114.85	120.82
1	E	396	ASP	CA-C-O	5.68	126.16	119.28
1	E	399	PRO	CA-C-N	5.68	126.47	120.11
1	E	399	PRO	C-N-CA	5.68	126.47	120.11
1	F	206	GLU	OE1-CD-OE2	5.68	136.54	122.90
1	C	608	GLN	N-CA-CB	5.68	119.87	110.33
1	E	391	PHE	CZ-CE2-CD2	-5.68	109.78	120.00
1	F	73	SER	N-CA-C	-5.68	101.33	110.14
1	A	73	SER	N-CA-C	-5.68	101.33	110.14
1	A	158	LYS	O-C-N	-5.68	116.19	122.09
1	B	69	ARG	N-CA-CB	-5.68	102.68	111.65
1	B	345	ASN	N-CA-C	-5.68	104.78	110.97
1	B	587	THR	CA-C-N	5.68	131.43	122.34
1	B	587	THR	C-N-CA	5.68	131.43	122.34
1	B	73	SER	N-CA-C	-5.68	101.34	110.14
1	C	105	TYR	CA-CB-CG	-5.68	103.68	113.90
1	E	330	SER	CA-C-O	-5.68	112.39	120.51
1	E	587	THR	CA-C-N	5.68	131.42	122.34
1	E	587	THR	C-N-CA	5.68	131.42	122.34
1	E	614	GLU	O-C-N	5.68	130.14	122.59
1	F	69	ARG	N-CA-CB	-5.68	102.68	111.65
1	F	608	GLN	N-CA-CB	5.68	119.87	110.33
1	A	608	GLN	N-CA-CB	5.67	119.86	110.33
1	B	391	PHE	CZ-CE2-CD2	-5.67	109.79	120.00
1	C	158	LYS	O-C-N	-5.67	116.19	122.09
1	C	623	GLY	CA-C-N	5.67	128.94	120.83
1	C	623	GLY	C-N-CA	5.67	128.94	120.83
1	D	158	LYS	O-C-N	-5.67	116.19	122.09
1	D	608	GLN	N-CA-CB	5.67	119.86	110.33
1	E	73	SER	N-CA-C	-5.67	101.34	110.14
1	F	537	GLN	CG-CD-NE2	-5.67	107.89	116.40
1	D	165	THR	OG1-CB-CG2	5.67	120.64	109.30
1	B	614	GLU	O-C-N	5.67	130.13	122.59
1	C	391	PHE	CZ-CE2-CD2	-5.67	109.79	120.00
1	E	211	TYR	CA-C-N	-5.67	114.01	122.74
1	E	211	TYR	C-N-CA	-5.67	114.01	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	239	TRP	CA-C-O	5.67	125.85	119.78
1	E	608	GLN	N-CA-CB	5.67	119.86	110.33
1	F	396	ASP	CA-C-O	5.67	126.14	119.28
1	A	97	TYR	O-C-N	-5.67	115.05	122.59
1	E	105	TYR	CA-CB-CG	-5.67	103.69	113.90
1	F	432	SER	CA-C-O	5.67	126.43	120.36
1	A	396	ASP	CA-C-O	5.67	126.14	119.28
1	A	614	GLU	O-C-N	5.67	130.13	122.59
1	B	2	ALA	N-CA-C	-5.67	103.88	111.87
1	B	206	GLU	OE1-CD-OE2	5.67	136.51	122.90
1	D	206	GLU	OE1-CD-OE2	5.67	136.51	122.90
1	D	239	TRP	CA-C-O	5.67	125.84	119.78
1	F	169	SER	CA-CB-OG	5.67	122.44	111.10
1	A	391	PHE	CZ-CE2-CD2	-5.67	109.80	120.00
1	B	417	ALA	CA-C-O	5.67	127.40	120.60
1	B	623	GLY	CA-C-N	5.67	128.93	120.83
1	B	623	GLY	C-N-CA	5.67	128.93	120.83
1	C	97	TYR	O-C-N	-5.67	115.05	122.59
1	D	527	SER	CA-C-O	-5.67	112.44	119.18
1	F	345	ASN	N-CA-C	-5.67	104.79	110.97
1	A	69	ARG	N-CA-CB	-5.67	102.70	111.65
1	A	399	PRO	CA-C-N	5.67	126.45	120.11
1	A	399	PRO	C-N-CA	5.67	126.45	120.11
1	A	211	TYR	CA-C-N	-5.66	114.02	122.74
1	A	211	TYR	C-N-CA	-5.66	114.02	122.74
1	C	2	ALA	N-CA-C	-5.66	103.89	111.87
1	C	432	SER	CA-C-O	5.66	126.42	120.36
1	D	623	GLY	CA-C-N	5.66	128.93	120.83
1	D	623	GLY	C-N-CA	5.66	128.93	120.83
1	E	432	SER	CA-C-O	5.66	126.42	120.36
1	F	111	ASN	O-C-N	-5.66	116.33	122.79
1	B	608	GLN	N-CA-C	-5.66	105.15	112.68
1	D	454	ARG	CA-C-N	5.66	130.44	120.87
1	D	454	ARG	C-N-CA	5.66	130.44	120.87
1	A	56	LEU	O-C-N	5.66	129.02	122.17
1	A	345	ASN	N-CA-C	-5.66	104.80	110.97
1	B	111	ASN	O-C-N	-5.66	116.34	122.79
1	B	454	ARG	CA-C-N	5.66	130.44	120.87
1	B	454	ARG	C-N-CA	5.66	130.44	120.87
1	D	345	ASN	N-CA-C	-5.66	104.80	110.97
1	E	169	SER	CA-CB-OG	5.66	122.42	111.10
1	E	454	ARG	CA-C-N	5.66	130.44	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	454	ARG	C-N-CA	5.66	130.44	120.87
1	E	623	GLY	CA-C-N	5.66	128.93	120.83
1	E	623	GLY	C-N-CA	5.66	128.93	120.83
1	F	399	PRO	CA-C-N	5.66	126.45	120.11
1	F	399	PRO	C-N-CA	5.66	126.45	120.11
1	B	165	THR	OG1-CB-CG2	5.66	120.62	109.30
1	C	165	THR	OG1-CB-CG2	5.66	120.62	109.30
1	D	560	ARG	NH1-CZ-NH2	5.66	126.66	119.30
1	F	158	LYS	O-C-N	-5.66	116.21	122.09
1	A	432	SER	CA-C-O	5.66	126.41	120.36
1	B	211	TYR	CA-C-N	-5.66	114.03	122.74
1	B	211	TYR	C-N-CA	-5.66	114.03	122.74
1	C	417	ALA	CA-C-O	5.66	127.39	120.60
1	C	587	THR	CA-C-N	5.66	131.39	122.34
1	C	587	THR	C-N-CA	5.66	131.39	122.34
1	D	391	PHE	CZ-CE2-CD2	-5.66	109.82	120.00
1	D	399	PRO	CA-C-N	5.66	126.44	120.11
1	D	399	PRO	C-N-CA	5.66	126.44	120.11
1	E	375	THR	N-CA-CB	-5.66	100.93	110.49
1	F	56	LEU	O-C-N	5.66	129.01	122.17
1	A	2	ALA	N-CA-C	-5.66	103.89	111.87
1	C	80	ARG	CA-CB-CG	-5.66	102.79	114.10
1	C	560	ARG	NH1-CZ-NH2	5.66	126.65	119.30
1	D	56	LEU	O-C-N	5.66	129.01	122.17
1	D	587	THR	CA-C-N	5.66	131.39	122.34
1	D	587	THR	C-N-CA	5.66	131.39	122.34
1	E	547	VAL	N-CA-C	-5.66	105.58	111.58
1	F	165	THR	OG1-CB-CG2	5.66	120.61	109.30
1	A	165	THR	OG1-CB-CG2	5.65	120.61	109.30
1	A	537	GLN	CG-CD-NE2	-5.65	107.92	116.40
1	E	69	ARG	N-CA-CB	-5.65	102.72	111.65
1	B	20	LYS	CB-CG-CD	5.65	124.30	111.30
1	B	537	GLN	CG-CD-NE2	-5.65	107.92	116.40
1	C	69	ARG	N-CA-CB	-5.65	102.72	111.65
1	F	80	ARG	CA-CB-CG	-5.65	102.79	114.10
1	F	239	TRP	CA-C-O	5.65	125.83	119.78
1	A	169	SER	CA-CB-OG	5.65	122.40	111.10
1	A	239	TRP	CA-C-O	5.65	125.83	119.78
1	A	547	VAL	N-CA-C	-5.65	105.59	111.58
1	A	587	THR	CA-C-N	5.65	131.38	122.34
1	A	587	THR	C-N-CA	5.65	131.38	122.34
1	C	239	TRP	CA-C-O	5.65	125.83	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	375	THR	N-CA-CB	-5.65	100.94	110.49
1	D	396	ASP	CA-C-O	5.65	126.12	119.28
1	F	119	LEU	CB-CA-C	5.65	120.17	110.79
1	F	375	THR	N-CA-CB	-5.65	100.94	110.49
1	F	614	GLU	O-C-N	5.65	130.10	122.59
1	A	136	PRO	CA-C-N	-5.65	112.35	120.82
1	A	136	PRO	C-N-CA	-5.65	112.35	120.82
1	B	432	SER	CA-C-O	5.65	126.40	120.36
1	D	119	LEU	CB-CA-C	5.65	120.17	110.79
1	E	111	ASN	O-C-N	-5.65	116.35	122.79
1	A	417	ALA	CA-C-O	5.65	127.38	120.60
1	A	454	ARG	CA-C-N	5.65	130.42	120.87
1	A	454	ARG	C-N-CA	5.65	130.42	120.87
1	C	119	LEU	CB-CA-C	5.65	120.17	110.79
1	C	136	PRO	CA-C-N	-5.65	112.35	120.82
1	C	136	PRO	C-N-CA	-5.65	112.35	120.82
1	C	399	PRO	CA-C-N	5.65	126.43	120.11
1	C	399	PRO	C-N-CA	5.65	126.43	120.11
1	D	172	GLY	CA-C-N	5.65	131.30	122.26
1	D	172	GLY	C-N-CA	5.65	131.30	122.26
1	F	97	TYR	O-C-N	-5.65	115.08	122.59
1	F	587	THR	CA-C-N	5.65	131.38	122.34
1	F	587	THR	C-N-CA	5.65	131.38	122.34
1	A	80	ARG	CA-CB-CG	-5.65	102.81	114.10
1	E	165	THR	OG1-CB-CG2	5.65	120.59	109.30
1	E	172	GLY	CA-C-N	5.65	131.29	122.26
1	E	172	GLY	C-N-CA	5.65	131.29	122.26
1	A	537	GLN	OE1-CD-NE2	5.64	128.24	122.60
1	C	323	LEU	CD1-CG-CD2	-5.64	98.38	110.80
1	D	2	ALA	N-CA-C	-5.64	103.91	111.87
1	D	136	PRO	CA-C-N	-5.64	112.35	120.82
1	D	136	PRO	C-N-CA	-5.64	112.35	120.82
1	D	417	ALA	CA-C-O	5.64	127.37	120.60
1	D	547	VAL	N-CA-C	-5.64	105.60	111.58
1	E	136	PRO	CA-C-N	-5.64	112.35	120.82
1	E	136	PRO	C-N-CA	-5.64	112.35	120.82
1	F	417	ALA	CA-C-O	5.64	127.37	120.60
1	F	537	GLN	OE1-CD-NE2	5.64	128.24	122.60
1	C	645	VAL	CA-C-N	-5.64	113.25	121.71
1	C	645	VAL	C-N-CA	-5.64	113.25	121.71
1	E	220	PHE	CA-C-O	-5.64	114.90	120.82
1	E	645	VAL	CA-C-N	-5.64	113.25	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	645	VAL	C-N-CA	-5.64	113.25	121.71
1	A	20	LYS	CB-CG-CD	5.64	124.28	111.30
1	A	375	THR	N-CA-CB	-5.64	100.96	110.49
1	F	172	GLY	CA-C-N	5.64	131.29	122.26
1	F	172	GLY	C-N-CA	5.64	131.29	122.26
1	F	633	GLU	CA-C-O	5.64	126.32	119.38
1	B	169	SER	CA-CB-OG	5.64	122.38	111.10
1	B	406	LEU	N-CA-CB	-5.64	101.21	110.40
1	C	537	GLN	CG-CD-NE2	-5.64	107.94	116.40
1	D	20	LYS	CB-CG-CD	5.64	124.27	111.30
1	F	211	TYR	CA-C-N	-5.64	114.06	122.74
1	F	211	TYR	C-N-CA	-5.64	114.06	122.74
1	F	391	PHE	CZ-CE2-CD2	-5.64	109.85	120.00
1	C	20	LYS	CB-CG-CD	5.64	124.27	111.30
1	F	264	TYR	CB-CG-CD1	-5.64	112.34	120.80
1	A	119	LEU	CB-CA-C	5.64	120.15	110.79
1	B	220	PHE	CA-C-O	-5.64	114.90	120.82
1	D	80	ARG	CA-CB-CG	-5.64	102.83	114.10
1	D	211	TYR	CA-C-N	-5.64	114.06	122.74
1	D	211	TYR	C-N-CA	-5.64	114.06	122.74
1	D	375	THR	N-CA-CB	-5.64	100.97	110.49
1	F	2	ALA	N-CA-C	-5.64	103.92	111.87
1	F	136	PRO	CA-C-N	-5.64	112.37	120.82
1	F	136	PRO	C-N-CA	-5.64	112.37	120.82
1	F	608	GLN	N-CA-C	-5.64	105.18	112.68
1	B	172	GLY	CA-C-N	5.63	131.27	122.26
1	B	172	GLY	C-N-CA	5.63	131.27	122.26
1	B	537	GLN	OE1-CD-NE2	5.63	128.23	122.60
1	C	169	SER	CA-CB-OG	5.63	122.37	111.10
1	C	396	ASP	CA-C-O	5.63	126.10	119.28
1	C	584	VAL	CA-C-O	5.63	126.25	120.39
1	D	312	THR	CA-C-N	5.63	130.44	123.12
1	D	312	THR	C-N-CA	5.63	130.44	123.12
1	D	537	GLN	CG-CD-NE2	-5.63	107.95	116.40
1	E	80	ARG	CA-CB-CG	-5.63	102.83	114.10
1	F	323	LEU	CD1-CG-CD2	-5.63	98.41	110.80
1	A	608	GLN	N-CA-C	-5.63	105.19	112.68
1	B	119	LEU	CB-CA-C	5.63	120.14	110.79
1	B	239	TRP	CA-C-O	5.63	125.81	119.78
1	C	454	ARG	CA-C-N	5.63	130.39	120.87
1	C	454	ARG	C-N-CA	5.63	130.39	120.87
1	D	452	VAL	CA-C-N	-5.63	115.52	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	452	VAL	C-N-CA	-5.63	115.52	122.84
1	A	111	ASN	O-C-N	-5.63	116.37	122.79
1	B	399	PRO	CA-C-N	5.63	126.42	120.11
1	B	399	PRO	C-N-CA	5.63	126.42	120.11
1	B	633	GLU	CA-C-O	5.63	126.31	119.38
1	C	345	ASN	N-CA-C	-5.63	104.83	110.97
1	D	584	VAL	CA-C-O	5.63	126.25	120.39
1	E	20	LYS	CB-CG-CD	5.63	124.25	111.30
1	D	111	ASN	O-C-N	-5.63	116.37	122.79
1	B	158	LYS	O-C-N	-5.63	116.24	122.09
1	D	242	PRO	N-CD-CG	-5.63	94.76	103.20
1	D	323	LEU	CD1-CG-CD2	-5.63	98.42	110.80
1	E	345	ASN	N-CA-C	-5.63	104.83	110.97
1	A	172	GLY	CA-C-N	5.63	131.26	122.26
1	A	172	GLY	C-N-CA	5.63	131.26	122.26
1	A	406	LEU	N-CA-CB	-5.63	101.23	110.40
1	B	80	ARG	CA-CB-CG	-5.63	102.85	114.10
1	F	20	LYS	CB-CG-CD	5.63	124.24	111.30
1	F	642	ILE	CA-CB-CG2	5.63	120.07	110.50
1	B	375	THR	N-CA-CB	-5.62	100.98	110.49
1	E	2	ALA	N-CA-C	-5.62	103.94	111.87
1	A	323	LEU	CD1-CG-CD2	-5.62	98.43	110.80
1	C	406	LEU	N-CA-CB	-5.62	101.23	110.40
1	D	169	SER	CA-CB-OG	5.62	122.35	111.10
1	D	608	GLN	N-CA-C	-5.62	105.20	112.68
1	E	406	LEU	N-CA-CB	-5.62	101.23	110.40
1	F	406	LEU	N-CA-CB	-5.62	101.23	110.40
1	A	645	VAL	CA-C-N	-5.62	113.28	121.71
1	A	645	VAL	C-N-CA	-5.62	113.28	121.71
1	B	642	ILE	CA-CB-CG2	5.62	120.06	110.50
1	C	547	VAL	N-CA-C	-5.62	105.62	111.58
1	E	417	ALA	CA-C-O	5.62	127.34	120.60
1	E	452	VAL	CA-C-N	-5.62	115.53	122.84
1	E	452	VAL	C-N-CA	-5.62	115.53	122.84
1	F	454	ARG	CA-C-N	5.62	130.37	120.87
1	F	454	ARG	C-N-CA	5.62	130.37	120.87
1	B	323	LEU	CD1-CG-CD2	-5.62	98.44	110.80
1	E	355	GLY	CA-C-O	-5.62	110.79	120.57
1	E	537	GLN	CG-CD-NE2	-5.62	107.97	116.40
1	A	220	PHE	CA-C-O	-5.62	114.92	120.82
1	C	220	PHE	CA-C-O	-5.62	114.92	120.82
1	D	264	TYR	CB-CG-CD1	-5.62	112.37	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	396	ASP	CA-C-O	5.62	126.08	119.28
1	D	435	ASN	OD1-CG-ND2	5.62	128.22	122.60
1	F	452	VAL	CA-C-N	-5.62	115.54	122.84
1	F	452	VAL	C-N-CA	-5.62	115.54	122.84
1	B	452	VAL	CA-C-N	-5.62	115.54	122.84
1	B	452	VAL	C-N-CA	-5.62	115.54	122.84
1	D	406	LEU	N-CA-CB	-5.62	101.25	110.40
1	E	119	LEU	CB-CA-C	5.62	120.11	110.79
1	F	225	HIS	ND1-CG-CD2	5.62	111.72	106.10
1	F	645	VAL	CA-C-N	-5.62	113.29	121.71
1	F	645	VAL	C-N-CA	-5.62	113.29	121.71
1	A	642	ILE	CA-CB-CG2	5.61	120.04	110.50
1	C	242	PRO	N-CD-CG	-5.61	94.78	103.20
1	C	307	ASP	CA-CB-CG	-5.61	106.99	112.60
1	E	537	GLN	OE1-CD-NE2	5.61	128.21	122.60
1	F	220	PHE	CA-C-O	-5.61	114.93	120.82
1	B	136	PRO	CA-C-N	-5.61	112.40	120.82
1	B	136	PRO	C-N-CA	-5.61	112.40	120.82
1	A	242	PRO	N-CD-CG	-5.61	94.78	103.20
1	B	307	ASP	CA-CB-CG	-5.61	106.99	112.60
1	B	645	VAL	CA-C-N	-5.61	113.30	121.71
1	B	645	VAL	C-N-CA	-5.61	113.30	121.71
1	C	111	ASN	O-C-N	-5.61	116.39	122.79
1	E	323	LEU	CD1-CG-CD2	-5.61	98.45	110.80
1	E	584	VAL	CA-C-O	5.61	126.22	120.39
1	F	547	VAL	N-CA-C	-5.61	105.63	111.58
1	B	458	ASN	CA-C-N	-5.61	112.57	120.82
1	B	458	ASN	C-N-CA	-5.61	112.57	120.82
1	E	332	LYS	CG-CD-CE	-5.61	98.40	111.30
1	B	411	MET	N-CA-CB	-5.61	101.01	110.49
1	B	355	GLY	CA-C-O	-5.61	110.81	120.57
1	C	91	ASN	N-CA-C	5.61	117.39	111.28
1	D	20	LYS	CG-CD-CE	-5.61	98.41	111.30
1	F	411	MET	N-CA-CB	-5.61	101.02	110.49
1	D	537	GLN	OE1-CD-NE2	5.60	128.20	122.60
1	D	633	GLU	CA-C-O	5.60	126.27	119.38
1	E	608	GLN	N-CA-C	-5.60	105.23	112.68
1	A	264	TYR	CB-CG-CD1	-5.60	112.40	120.80
1	B	547	VAL	N-CA-C	-5.60	105.64	111.58
1	C	355	GLY	CA-C-O	-5.60	110.82	120.57
1	C	537	GLN	OE1-CD-NE2	5.60	128.20	122.60
1	C	608	GLN	N-CA-C	-5.60	105.23	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	411	MET	N-CA-CB	-5.60	101.02	110.49
1	E	307	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	584	VAL	CA-C-O	5.60	126.22	120.39
1	B	584	VAL	CA-C-O	5.60	126.22	120.39
1	C	584	VAL	CA-C-N	-5.60	115.09	122.99
1	C	584	VAL	C-N-CA	-5.60	115.09	122.99
1	C	642	ILE	CA-CB-CG2	5.60	120.02	110.50
1	F	635	VAL	O-C-N	5.60	132.55	121.91
1	A	633	GLU	CA-C-O	5.60	126.27	119.38
1	B	242	PRO	N-CD-CG	-5.60	94.80	103.20
1	D	458	ASN	CA-C-N	-5.60	112.59	120.82
1	D	458	ASN	C-N-CA	-5.60	112.59	120.82
1	E	264	TYR	CB-CG-CD1	-5.60	112.40	120.80
1	E	458	ASN	CA-C-N	-5.60	112.59	120.82
1	E	458	ASN	C-N-CA	-5.60	112.59	120.82
1	E	642	ILE	CA-CB-CG2	5.60	120.02	110.50
1	A	355	GLY	CA-C-O	-5.60	110.83	120.57
1	C	332	LYS	CG-CD-CE	-5.60	98.43	111.30
1	D	225	HIS	ND1-CG-CD2	5.60	111.70	106.10
1	D	307	ASP	CA-CB-CG	-5.60	107.00	112.60
1	D	642	ILE	CA-CB-CG2	5.60	120.02	110.50
1	F	91	ASN	N-CA-C	5.60	117.38	111.28
1	A	307	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	312	THR	CA-C-N	5.60	130.39	123.12
1	A	312	THR	C-N-CA	5.60	130.39	123.12
1	C	20	LYS	CG-CD-CE	-5.60	98.43	111.30
1	A	225	HIS	ND1-CG-CD2	5.59	111.69	106.10
1	A	452	VAL	CA-C-N	-5.59	115.57	122.84
1	A	452	VAL	C-N-CA	-5.59	115.57	122.84
1	B	20	LYS	CG-CD-CE	-5.59	98.43	111.30
1	D	355	GLY	CA-C-O	-5.59	110.84	120.57
1	F	332	LYS	CG-CD-CE	-5.59	98.43	111.30
1	B	264	TYR	CB-CG-CD1	-5.59	112.41	120.80
1	E	318	PRO	N-CD-CG	-5.59	94.81	103.20
1	F	242	PRO	N-CD-CG	-5.59	94.81	103.20
1	F	307	ASP	CA-CB-CG	-5.59	107.01	112.60
1	A	332	LYS	CG-CD-CE	-5.59	98.44	111.30
1	B	340	TYR	CB-CG-CD2	5.59	129.19	120.80
1	A	20	LYS	CG-CD-CE	-5.59	98.44	111.30
1	A	458	ASN	CA-C-N	-5.59	112.61	120.82
1	A	458	ASN	C-N-CA	-5.59	112.61	120.82
1	E	242	PRO	N-CD-CG	-5.59	94.82	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	20	LYS	CG-CD-CE	-5.59	98.45	111.30
1	A	91	ASN	N-CA-C	5.59	117.37	111.28
1	A	411	MET	N-CA-CB	-5.59	101.05	110.49
1	C	172	GLY	CA-C-N	5.59	131.20	122.26
1	C	172	GLY	C-N-CA	5.59	131.20	122.26
1	E	91	ASN	N-CA-C	5.59	117.37	111.28
1	E	411	MET	N-CA-CB	-5.59	101.05	110.49
1	C	340	TYR	CB-CG-CD2	5.58	129.18	120.80
1	D	91	ASN	N-CA-C	5.58	117.37	111.28
1	E	369	GLU	N-CA-C	-5.58	104.65	112.25
1	F	355	GLY	CA-C-O	-5.58	110.85	120.57
1	F	584	VAL	CA-C-O	5.58	126.20	120.39
1	B	91	ASN	N-CA-C	5.58	117.36	111.28
1	B	225	HIS	ND1-CG-CD2	5.58	111.68	106.10
1	B	308	SER	CA-CB-OG	-5.58	99.93	111.10
1	B	635	VAL	O-C-N	5.58	132.52	121.91
1	C	154	ALA	CA-C-O	-5.58	113.20	119.79
1	D	170	PHE	N-CA-C	-5.58	98.91	110.80
1	C	264	TYR	CB-CG-CD1	-5.58	112.43	120.80
1	D	645	VAL	CA-C-N	-5.58	113.34	121.71
1	D	645	VAL	C-N-CA	-5.58	113.34	121.71
1	F	312	THR	CA-C-N	5.58	130.37	123.12
1	F	312	THR	C-N-CA	5.58	130.37	123.12
1	C	11	GLN	CA-C-O	-5.58	114.93	120.90
1	D	332	LYS	CG-CD-CE	-5.58	98.47	111.30
1	A	369	GLU	N-CA-C	-5.58	104.67	112.25
1	B	369	GLU	N-CA-C	-5.58	104.67	112.25
1	F	584	VAL	CA-C-N	-5.58	115.13	122.99
1	F	584	VAL	C-N-CA	-5.58	115.13	122.99
1	B	51	ALA	O-C-N	5.57	129.12	122.27
1	B	244	ASP	O-C-N	-5.57	115.95	122.81
1	B	312	THR	CA-C-N	5.57	130.37	123.12
1	B	312	THR	C-N-CA	5.57	130.37	123.12
1	B	332	LYS	CG-CD-CE	-5.57	98.48	111.30
1	C	444	GLU	CB-CG-CD	-5.57	103.13	112.60
1	C	170	PHE	N-CA-C	-5.57	98.93	110.80
1	E	147	ASN	CA-C-O	-5.57	112.54	120.51
1	E	312	THR	CA-C-N	5.57	130.36	123.12
1	E	312	THR	C-N-CA	5.57	130.36	123.12
1	E	340	TYR	CB-CG-CD2	5.57	129.16	120.80
1	A	154	ALA	CA-C-O	-5.57	113.22	119.79
1	A	170	PHE	N-CA-C	-5.57	98.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	154	ALA	CA-C-O	-5.57	113.22	119.79
1	B	435	ASN	OD1-CG-ND2	5.57	128.17	122.60
1	C	51	ALA	O-C-N	5.57	129.12	122.27
1	C	244	ASP	O-C-N	-5.57	115.96	122.81
1	E	20	LYS	CG-CD-CE	-5.57	98.49	111.30
1	E	154	ALA	CA-C-O	-5.57	113.22	119.79
1	E	584	VAL	CA-C-N	-5.57	115.14	122.99
1	E	584	VAL	C-N-CA	-5.57	115.14	122.99
1	F	340	TYR	CB-CG-CD2	5.57	129.16	120.80
1	A	340	TYR	CB-CG-CD2	5.57	129.15	120.80
1	C	452	VAL	CA-C-N	-5.57	115.60	122.84
1	C	452	VAL	C-N-CA	-5.57	115.60	122.84
1	E	225	HIS	ND1-CG-CD2	5.57	111.67	106.10
1	C	308	SER	CA-CB-OG	-5.57	99.97	111.10
1	E	170	PHE	N-CA-C	-5.57	98.94	110.80
1	E	556	SER	CA-CB-OG	-5.57	99.97	111.10
1	F	369	GLU	N-CA-C	-5.57	104.68	112.25
1	A	318	PRO	N-CD-CG	-5.57	94.85	103.20
1	C	225	HIS	ND1-CG-CD2	5.57	111.67	106.10
1	C	369	GLU	N-CA-C	-5.57	104.68	112.25
1	C	633	GLU	CA-C-O	5.57	126.23	119.38
1	F	170	PHE	N-CA-C	-5.57	98.95	110.80
1	A	308	SER	CA-CB-OG	-5.56	99.97	111.10
1	B	318	PRO	N-CD-CG	-5.56	94.85	103.20
1	C	312	THR	CA-C-N	5.56	130.35	123.12
1	C	312	THR	C-N-CA	5.56	130.35	123.12
1	C	318	PRO	N-CD-CG	-5.56	94.86	103.20
1	C	435	ASN	OD1-CG-ND2	5.56	128.16	122.60
1	C	458	ASN	CA-C-N	-5.56	112.64	120.82
1	C	458	ASN	C-N-CA	-5.56	112.64	120.82
1	F	318	PRO	N-CD-CG	-5.56	94.86	103.20
1	D	308	SER	CA-CB-OG	-5.56	99.98	111.10
1	C	212	HIS	O-C-N	5.56	129.81	123.31
1	F	308	SER	CA-CB-OG	-5.56	99.98	111.10
1	F	650	VAL	CA-C-O	5.56	127.17	120.67
1	A	11	GLN	CA-C-O	-5.56	114.95	120.90
1	A	435	ASN	OD1-CG-ND2	5.56	128.16	122.60
1	A	444	GLU	CB-CG-CD	-5.56	103.15	112.60
1	D	244	ASP	O-C-N	-5.56	115.97	122.81
1	B	170	PHE	N-CA-C	-5.55	98.97	110.80
1	B	444	GLU	CB-CG-CD	-5.55	103.16	112.60
1	B	556	SER	CA-CB-OG	-5.55	99.99	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	147	ASN	CA-C-O	-5.55	112.57	120.51
1	D	154	ALA	CA-C-O	-5.55	113.23	119.79
1	D	340	TYR	CB-CG-CD2	5.55	129.13	120.80
1	D	584	VAL	CA-C-N	-5.55	115.16	122.99
1	D	584	VAL	C-N-CA	-5.55	115.16	122.99
1	F	375	THR	CB-CA-C	5.55	121.47	110.42
1	F	458	ASN	CA-C-N	-5.55	112.66	120.82
1	F	458	ASN	C-N-CA	-5.55	112.66	120.82
1	A	584	VAL	CA-C-N	-5.55	115.16	122.99
1	A	584	VAL	C-N-CA	-5.55	115.16	122.99
1	D	369	GLU	N-CA-C	-5.55	104.70	112.25
1	E	444	GLU	CB-CG-CD	-5.55	103.16	112.60
1	C	411	MET	N-CA-CB	-5.55	101.11	110.49
1	E	212	HIS	O-C-N	5.55	129.81	123.31
1	A	556	SER	CA-CB-OG	-5.55	100.00	111.10
1	B	212	HIS	O-C-N	5.55	129.80	123.31
1	D	444	GLU	CB-CG-CD	-5.55	103.17	112.60
1	D	499	ARG	CB-CG-CD	5.55	124.06	111.30
1	E	308	SER	CA-CB-OG	-5.55	100.00	111.10
1	F	154	ALA	CA-C-O	-5.55	113.24	119.79
1	B	147	ASN	CA-C-O	-5.55	112.58	120.51
1	E	650	VAL	CA-C-O	5.55	127.16	120.67
1	F	444	GLU	CB-CG-CD	-5.55	103.17	112.60
1	A	147	ASN	CA-C-O	-5.54	112.58	120.51
1	C	582	LEU	O-C-N	-5.54	117.01	123.27
1	E	499	ARG	CB-CG-CD	5.54	124.05	111.30
1	F	435	ASN	OD1-CG-ND2	5.54	128.14	122.60
1	A	375	THR	CB-CA-C	5.54	121.45	110.42
1	D	212	HIS	O-C-N	5.54	129.79	123.31
1	D	318	PRO	N-CD-CG	-5.54	94.89	103.20
1	D	650	VAL	CA-C-O	5.54	127.15	120.67
1	E	11	GLN	CA-C-O	-5.54	114.97	120.90
1	E	244	ASP	O-C-N	-5.54	116.00	122.81
1	F	147	ASN	CA-C-O	-5.54	112.59	120.51
1	A	51	ALA	O-C-N	5.54	129.08	122.27
1	B	11	GLN	CA-C-O	-5.54	114.97	120.90
1	B	318	PRO	CA-C-O	-5.54	111.13	119.55
1	B	584	VAL	CA-C-N	-5.54	115.18	122.99
1	B	584	VAL	C-N-CA	-5.54	115.18	122.99
1	B	375	THR	CB-CA-C	5.54	121.44	110.42
1	C	375	THR	CB-CA-C	5.54	121.43	110.42
1	D	556	SER	CA-CB-OG	-5.54	100.03	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	254	GLU	CG-CD-OE1	-5.53	105.67	118.40
1	E	633	GLU	CA-C-O	5.53	126.19	119.38
1	F	556	SER	CA-CB-OG	-5.53	100.03	111.10
1	A	212	HIS	O-C-N	5.53	129.78	123.31
1	F	51	ALA	O-C-N	5.53	129.07	122.27
1	A	499	ARG	CB-CG-CD	5.53	124.02	111.30
1	B	650	VAL	CA-C-O	5.53	127.14	120.67
1	C	254	GLU	CG-CD-OE1	-5.53	105.68	118.40
1	C	650	VAL	CA-C-O	5.53	127.14	120.67
1	D	375	THR	CB-CA-C	5.53	121.43	110.42
1	E	357	PRO	N-CA-CB	5.53	109.06	103.25
1	A	650	VAL	CA-C-O	5.53	127.14	120.67
1	F	161	GLN	OE1-CD-NE2	5.53	128.13	122.60
1	C	556	SER	CA-CB-OG	-5.53	100.04	111.10
1	D	582	LEU	O-C-N	-5.53	117.02	123.27
1	E	51	ALA	O-C-N	5.53	129.07	122.27
1	E	582	LEU	O-C-N	-5.53	117.02	123.27
1	B	493	LEU	O-C-N	5.53	129.45	122.65
1	B	499	ARG	CB-CG-CD	5.53	124.01	111.30
1	C	499	ARG	CB-CG-CD	5.53	124.01	111.30
1	D	451	ARG	CA-CB-CG	5.53	125.15	114.10
1	E	375	THR	CB-CA-C	5.53	121.41	110.42
1	E	405	ASN	N-CA-C	5.53	117.16	111.03
1	E	434	ILE	N-CA-C	5.53	117.02	111.00
1	E	451	ARG	CA-CB-CG	5.53	125.15	114.10
1	A	318	PRO	CA-C-O	-5.52	111.15	119.55
1	B	254	GLU	CG-CD-OE1	-5.52	105.69	118.40
1	B	314	ASP	OD1-CG-OD2	-5.52	109.64	122.90
1	F	254	GLU	CG-CD-OE1	-5.52	105.69	118.40
1	F	499	ARG	CB-CG-CD	5.52	124.00	111.30
1	A	254	GLU	CG-CD-OE1	-5.52	105.70	118.40
1	A	451	ARG	CA-CB-CG	5.52	125.14	114.10
1	A	582	LEU	O-C-N	-5.52	117.03	123.27
1	C	301	ASP	N-CA-C	5.52	118.23	111.82
1	D	11	GLN	CA-C-O	-5.52	114.99	120.90
1	E	301	ASP	N-CA-C	5.52	118.22	111.82
1	F	451	ARG	CA-CB-CG	5.52	125.14	114.10
1	A	244	ASP	O-C-N	-5.52	116.02	122.81
1	D	301	ASP	N-CA-C	5.52	118.22	111.82
1	F	212	HIS	O-C-N	5.52	129.77	123.31
1	A	517	GLU	N-CA-C	-5.52	101.28	109.94
1	B	517	GLU	N-CA-C	-5.52	101.27	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	147	ASN	CA-C-O	-5.52	112.62	120.51
1	C	161	GLN	OE1-CD-NE2	5.52	128.12	122.60
1	C	314	ASP	OD1-CG-OD2	-5.52	109.66	122.90
1	D	434	ILE	N-CA-C	5.52	117.01	111.00
1	E	342	SER	N-CA-C	5.52	119.67	109.24
1	F	11	GLN	CA-C-O	-5.52	115.00	120.90
1	A	314	ASP	OD1-CG-OD2	-5.52	109.66	122.90
1	E	435	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	B	451	ARG	CA-CB-CG	5.51	125.13	114.10
1	E	609	CYS	CA-CB-SG	-5.51	101.72	114.40
1	A	301	ASP	N-CA-C	5.51	118.22	111.82
1	E	314	ASP	OD1-CG-OD2	-5.51	109.67	122.90
1	F	314	ASP	OD1-CG-OD2	-5.51	109.67	122.90
1	C	493	LEU	O-C-N	5.51	129.43	122.65
1	D	51	ALA	O-C-N	5.51	129.05	122.27
1	D	221	PHE	N-CA-CB	5.51	119.80	110.49
1	D	517	GLU	N-CA-C	-5.51	101.29	109.94
1	F	221	PHE	N-CA-CB	5.51	119.80	110.49
1	F	244	ASP	O-C-N	-5.51	116.03	122.81
1	F	439	SER	CA-C-N	-5.51	110.61	121.41
1	F	439	SER	C-N-CA	-5.51	110.61	121.41
1	F	532	ASP	N-CA-CB	5.51	118.24	110.36
1	B	357	PRO	N-CA-CB	5.51	109.03	103.25
1	D	318	PRO	CA-C-O	-5.51	111.17	119.55
1	D	439	SER	CA-C-N	-5.51	110.61	121.41
1	D	439	SER	C-N-CA	-5.51	110.61	121.41
1	E	254	GLU	CG-CD-OE1	-5.51	105.73	118.40
1	A	342	SER	N-CA-C	5.51	119.65	109.24
1	C	466	MET	N-CA-C	5.51	122.53	110.80
1	F	357	PRO	N-CA-CB	5.51	109.03	103.25
1	B	342	SER	N-CA-C	5.51	119.65	109.24
1	B	439	SER	CA-C-N	-5.51	110.62	121.41
1	B	439	SER	C-N-CA	-5.51	110.62	121.41
1	C	451	ARG	CA-CB-CG	5.51	125.11	114.10
1	C	517	GLU	N-CA-C	-5.51	101.29	109.94
1	F	609	CYS	CA-CB-SG	-5.51	101.73	114.40
1	D	314	ASP	OD1-CG-OD2	-5.50	109.69	122.90
1	D	342	SER	N-CA-C	5.50	119.64	109.24
1	D	493	LEU	O-C-N	5.50	129.42	122.65
1	A	439	SER	CA-C-N	-5.50	110.62	121.41
1	A	439	SER	C-N-CA	-5.50	110.62	121.41
1	B	301	ASP	N-CA-C	5.50	118.20	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	405	ASN	N-CA-C	5.50	117.14	111.03
1	D	609	CYS	CA-CB-SG	-5.50	101.74	114.40
1	F	329	GLU	O-C-N	5.50	129.71	122.33
1	F	517	GLU	N-CA-C	-5.50	101.30	109.94
1	A	532	ASP	N-CA-CB	5.50	118.23	110.36
1	B	532	ASP	N-CA-CB	5.50	118.23	110.36
1	C	439	SER	CA-C-N	-5.50	110.63	121.41
1	C	439	SER	C-N-CA	-5.50	110.63	121.41
1	D	33	ILE	CA-CB-CG2	-5.50	101.15	110.50
1	F	301	ASP	N-CA-C	5.50	118.20	111.82
1	C	62	ASP	CB-CG-OD2	5.50	131.05	118.40
1	F	16	HIS	O-C-N	5.50	128.42	122.15
1	A	609	CYS	CA-CB-SG	-5.50	101.75	114.40
1	C	303	GLY	CA-C-N	-5.50	113.96	122.59
1	C	303	GLY	C-N-CA	-5.50	113.96	122.59
1	C	609	CYS	CA-CB-SG	-5.50	101.75	114.40
1	D	532	ASP	N-CA-CB	5.50	118.22	110.36
1	F	318	PRO	CA-C-O	-5.50	111.19	119.55
1	F	466	MET	N-CA-C	5.50	122.51	110.80
1	A	221	PHE	N-CA-CB	5.50	119.78	110.49
1	A	357	PRO	N-CA-CB	5.50	109.02	103.25
1	A	466	MET	N-CA-C	5.50	122.51	110.80
1	C	318	PRO	CA-C-O	-5.50	111.19	119.55
1	C	342	SER	N-CA-C	5.50	119.63	109.24
1	D	16	HIS	O-C-N	5.50	128.42	122.15
1	D	561	SER	N-CA-CB	-5.50	101.20	110.49
1	E	318	PRO	CA-C-O	-5.50	111.19	119.55
1	A	434	ILE	N-CA-C	5.49	116.99	111.00
1	B	111	ASN	CB-CG-ND2	-5.49	108.16	116.40
1	B	578	MET	CA-C-N	-5.49	115.36	123.05
1	B	578	MET	C-N-CA	-5.49	115.36	123.05
1	D	466	MET	N-CA-C	5.49	122.50	110.80
1	E	61	ASN	CB-CG-OD1	-5.49	109.81	120.80
1	A	16	HIS	O-C-N	5.49	128.41	122.15
1	C	357	PRO	N-CA-CB	5.49	109.02	103.25
1	F	342	SER	N-CA-C	5.49	119.62	109.24
1	A	61	ASN	CB-CG-OD1	-5.49	109.82	120.80
1	B	466	MET	N-CA-C	5.49	122.50	110.80
1	B	609	CYS	CA-CB-SG	-5.49	101.77	114.40
1	C	221	PHE	N-CA-CB	5.49	119.77	110.49
1	C	347	ALA	N-CA-C	-5.49	105.39	111.71
1	C	532	ASP	N-CA-CB	5.49	118.21	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	61	ASN	CB-CG-OD1	-5.49	109.82	120.80
1	B	16	HIS	O-C-N	5.49	128.41	122.15
1	D	405	ASN	N-CA-C	5.49	117.12	111.03
1	E	62	ASP	CB-CG-OD2	5.49	131.02	118.40
1	E	466	MET	N-CA-C	5.49	122.49	110.80
1	E	517	GLU	N-CA-C	-5.49	101.32	109.94
1	E	532	ASP	N-CA-CB	5.49	118.21	110.36
1	F	434	ILE	N-CA-C	5.49	116.98	111.00
1	B	381	PHE	CZ-CE2-CD2	-5.49	110.12	120.00
1	B	405	ASN	N-CA-C	5.49	117.12	111.03
1	E	33	ILE	CA-CB-CG2	-5.49	101.17	110.50
1	A	405	ASN	N-CA-C	5.49	117.12	111.03
1	C	111	ASN	CB-CG-ND2	-5.49	108.17	116.40
1	E	303	GLY	CA-C-N	-5.49	113.98	122.59
1	E	303	GLY	C-N-CA	-5.49	113.98	122.59
1	F	62	ASP	CB-CG-OD2	5.49	131.02	118.40
1	F	493	LEU	O-C-N	5.49	129.40	122.65
1	C	561	SER	N-CA-CB	-5.48	101.22	110.49
1	D	161	GLN	OE1-CD-NE2	5.48	128.08	122.60
1	D	415	GLY	CA-C-O	5.48	127.46	121.48
1	E	16	HIS	O-C-N	5.48	128.40	122.15
1	E	329	GLU	O-C-N	5.48	129.68	122.33
1	E	561	SER	N-CA-CB	-5.48	101.22	110.49
1	F	405	ASN	N-CA-C	5.48	117.12	111.03
1	A	62	ASP	CB-CG-OD2	5.48	131.00	118.40
1	A	493	LEU	O-C-N	5.48	129.39	122.65
1	A	561	SER	N-CA-CB	-5.48	101.23	110.49
1	B	582	LEU	O-C-N	-5.48	117.08	123.27
1	F	561	SER	N-CA-CB	-5.48	101.23	110.49
1	A	33	ILE	CA-CB-CG2	-5.48	101.19	110.50
1	A	329	GLU	O-C-N	5.48	129.67	122.33
1	B	303	GLY	CA-C-N	-5.48	113.99	122.59
1	B	303	GLY	C-N-CA	-5.48	113.99	122.59
1	A	303	GLY	CA-C-N	-5.48	113.99	122.59
1	A	303	GLY	C-N-CA	-5.48	113.99	122.59
1	B	329	GLU	O-C-N	5.48	129.67	122.33
1	D	61	ASN	CB-CG-OD1	-5.48	109.84	120.80
1	D	357	PRO	N-CA-CB	5.48	109.00	103.25
1	E	221	PHE	N-CA-CB	5.48	119.75	110.49
1	F	582	LEU	O-C-N	-5.48	117.08	123.27
1	C	61	ASN	CB-CG-OD1	-5.48	109.85	120.80
1	F	33	ILE	CA-CB-CG2	-5.48	101.19	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	GLN	OE1-CD-NE2	5.47	128.07	122.60
1	E	111	ASN	CB-CG-ND2	-5.47	108.19	116.40
1	E	439	SER	CA-C-N	-5.47	110.68	121.41
1	E	439	SER	C-N-CA	-5.47	110.68	121.41
1	F	425	PHE	CA-CB-CG	-5.47	108.33	113.80
1	C	16	HIS	O-C-N	5.47	128.39	122.15
1	C	33	ILE	CA-CB-CG2	-5.47	101.20	110.50
1	B	221	PHE	N-CA-CB	5.47	119.73	110.49
1	B	434	ILE	N-CA-C	5.47	116.96	111.00
1	C	47	ASN	CA-CB-CG	-5.47	107.13	112.60
1	E	493	LEU	O-C-N	5.47	129.38	122.65
1	C	522	SER	N-CA-CB	-5.47	101.37	110.23
1	D	62	ASP	CB-CG-OD2	5.47	130.98	118.40
1	D	522	SER	N-CA-CB	-5.47	101.37	110.23
1	A	111	ASN	CB-CG-ND2	-5.47	108.20	116.40
1	B	62	ASP	CB-CG-OD2	5.47	130.97	118.40
1	E	347	ALA	N-CA-C	-5.47	105.42	111.71
1	B	33	ILE	CA-CB-CG2	-5.46	101.21	110.50
1	F	303	GLY	CA-C-N	-5.46	114.01	122.59
1	F	303	GLY	C-N-CA	-5.46	114.01	122.59
1	F	415	GLY	CA-C-O	5.46	127.44	121.48
1	E	415	GLY	CA-C-O	5.46	127.43	121.48
1	F	578	MET	CA-C-N	-5.46	115.40	123.05
1	F	578	MET	C-N-CA	-5.46	115.40	123.05
1	A	381	PHE	CZ-CE2-CD2	-5.46	110.17	120.00
1	B	61	ASN	CB-CG-OD1	-5.46	109.88	120.80
1	B	142	PRO	N-CD-CG	-5.46	95.01	103.20
1	B	347	ALA	N-CA-C	-5.46	105.43	111.71
1	C	142	PRO	N-CD-CG	-5.46	95.01	103.20
1	E	628	ARG	CD-NE-CZ	-5.46	116.75	124.40
1	F	102	ASN	CA-C-N	-5.46	111.11	121.54
1	F	102	ASN	C-N-CA	-5.46	111.11	121.54
1	C	349	VAL	N-CA-CB	5.46	117.30	110.47
1	D	303	GLY	CA-C-N	-5.46	114.02	122.59
1	D	303	GLY	C-N-CA	-5.46	114.02	122.59
1	B	161	GLN	OE1-CD-NE2	5.46	128.06	122.60
1	D	111	ASN	CB-CG-ND2	-5.46	108.21	116.40
1	B	551	HIS	CE1-NE2-CD2	-5.46	103.54	109.00
1	D	142	PRO	N-CD-CG	-5.46	95.02	103.20
1	D	381	PHE	CZ-CE2-CD2	-5.46	110.18	120.00
1	E	381	PHE	CZ-CE2-CD2	-5.46	110.18	120.00
1	E	578	MET	CA-C-N	-5.46	115.41	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	578	MET	C-N-CA	-5.46	115.41	123.05
1	A	102	ASN	CA-C-N	-5.46	111.12	121.54
1	A	102	ASN	C-N-CA	-5.46	111.12	121.54
1	C	102	ASN	CA-C-N	-5.46	111.12	121.54
1	C	102	ASN	C-N-CA	-5.46	111.12	121.54
1	D	86	LEU	CD1-CG-CD2	-5.46	98.80	110.80
1	E	86	LEU	CD1-CG-CD2	-5.46	98.80	110.80
1	E	391	PHE	CE1-CZ-CE2	5.46	129.82	120.00
1	F	111	ASN	CB-CG-ND2	-5.46	108.22	116.40
1	F	190	MET	CG-SD-CE	-5.46	88.90	100.90
1	A	347	ALA	N-CA-C	-5.45	105.44	111.71
1	B	561	SER	N-CA-CB	-5.45	101.27	110.49
1	C	381	PHE	CZ-CE2-CD2	-5.45	110.18	120.00
1	D	190	MET	CG-SD-CE	-5.45	88.90	100.90
1	A	578	MET	CA-C-N	-5.45	115.42	123.05
1	A	578	MET	C-N-CA	-5.45	115.42	123.05
1	B	124	ILE	CA-CB-CG2	5.45	119.77	110.50
1	B	190	MET	CG-SD-CE	-5.45	88.91	100.90
1	C	86	LEU	CD1-CG-CD2	-5.45	98.81	110.80
1	C	190	MET	CG-SD-CE	-5.45	88.91	100.90
1	D	329	GLU	O-C-N	5.45	129.64	122.33
1	B	415	GLY	CA-C-O	5.45	127.42	121.48
1	C	434	ILE	N-CA-C	5.45	116.94	111.00
1	E	190	MET	CG-SD-CE	-5.45	88.91	100.90
1	F	38	ASN	CB-CA-C	5.45	118.53	111.01
1	F	347	ALA	N-CA-C	-5.45	105.44	111.71
1	A	190	MET	CG-SD-CE	-5.45	88.91	100.90
1	A	415	GLY	CA-C-O	5.45	127.42	121.48
1	E	469	ASN	CA-CB-CG	-5.45	107.15	112.60
1	D	539	LEU	O-C-N	5.45	130.45	122.39
1	A	86	LEU	CD1-CG-CD2	-5.45	98.82	110.80
1	A	142	PRO	N-CD-CG	-5.45	95.03	103.20
1	C	329	GLU	O-C-N	5.45	129.63	122.33
1	D	533	MET	N-CA-CB	5.45	117.61	109.88
1	E	197	TRP	O-C-N	5.45	128.37	122.11
1	A	425	PHE	CA-CB-CG	-5.44	108.36	113.80
1	F	52	ALA	CA-C-N	-5.44	113.58	120.60
1	F	52	ALA	C-N-CA	-5.44	113.58	120.60
1	B	10	LYS	CB-CG-CD	5.44	123.82	111.30
1	B	102	ASN	CA-C-N	-5.44	111.14	121.54
1	B	102	ASN	C-N-CA	-5.44	111.14	121.54
1	E	392	LYS	CG-CD-CE	5.44	123.82	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	392	LYS	CG-CD-CE	5.44	123.82	111.30
1	C	279	ASP	CB-CG-OD2	-5.44	105.89	118.40
1	E	425	PHE	CA-CB-CG	-5.44	108.36	113.80
1	E	611	VAL	CA-CB-CG1	5.44	119.65	110.40
1	F	86	LEU	CD1-CG-CD2	-5.44	98.83	110.80
1	F	124	ILE	CA-CB-CG2	5.44	119.75	110.50
1	F	142	PRO	N-CD-CG	-5.44	95.04	103.20
1	B	38	ASN	CB-CA-C	5.44	118.52	111.01
1	B	279	ASP	CB-CG-OD2	-5.44	105.89	118.40
1	B	469	ASN	CA-CB-CG	-5.44	107.16	112.60
1	B	522	SER	N-CA-CB	-5.44	101.42	110.23
1	D	38	ASN	CB-CA-C	5.44	118.52	111.01
1	E	52	ALA	CA-C-N	-5.44	113.58	120.60
1	E	52	ALA	C-N-CA	-5.44	113.58	120.60
1	B	86	LEU	CD1-CG-CD2	-5.44	98.84	110.80
1	C	124	ILE	CA-CB-CG2	5.44	119.74	110.50
1	C	539	LEU	O-C-N	5.44	130.44	122.39
1	D	10	LYS	CB-CG-CD	5.44	123.81	111.30
1	D	102	ASN	CA-C-N	-5.44	111.16	121.54
1	D	102	ASN	C-N-CA	-5.44	111.16	121.54
1	E	124	ILE	CA-CB-CG2	5.44	119.75	110.50
1	F	47	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	522	SER	N-CA-CB	-5.44	101.42	110.23
1	C	391	PHE	CE1-CZ-CE2	5.44	129.78	120.00
1	D	279	ASP	CB-CG-OD2	-5.44	105.90	118.40
1	D	392	LYS	CG-CD-CE	5.44	123.80	111.30
1	D	425	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	124	ILE	CA-CB-CG2	5.43	119.74	110.50
1	C	578	MET	CA-C-N	-5.43	115.44	123.05
1	C	578	MET	C-N-CA	-5.43	115.44	123.05
1	D	628	ARG	CD-NE-CZ	-5.43	116.79	124.40
1	E	142	PRO	N-CD-CG	-5.43	95.05	103.20
1	F	370	HIS	O-C-N	5.43	129.68	123.48
1	A	10	LYS	CB-CG-CD	5.43	123.79	111.30
1	B	425	PHE	CA-CB-CG	-5.43	108.37	113.80
1	C	141	THR	CA-CB-OG1	5.43	117.75	109.60
1	D	578	MET	CA-C-N	-5.43	115.44	123.05
1	D	578	MET	C-N-CA	-5.43	115.44	123.05
1	F	141	THR	CA-CB-OG1	5.43	117.75	109.60
1	F	381	PHE	CZ-CE2-CD2	-5.43	110.22	120.00
1	F	522	SER	N-CA-CB	-5.43	101.43	110.23
1	E	161	GLN	OE1-CD-NE2	5.43	128.03	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	10	LYS	CB-CG-CD	5.43	123.79	111.30
1	A	38	ASN	CB-CA-C	5.43	118.50	111.01
1	B	47	ASN	CA-CB-CG	-5.43	107.17	112.60
1	D	124	ILE	CA-CB-CG2	5.43	119.73	110.50
1	E	509	PHE	CA-C-N	5.43	131.09	122.62
1	E	509	PHE	C-N-CA	5.43	131.09	122.62
1	F	197	TRP	O-C-N	5.43	128.35	122.11
1	A	141	THR	CA-CB-OG1	5.43	117.74	109.60
1	A	391	PHE	CE1-CZ-CE2	5.43	129.77	120.00
1	C	628	ARG	CD-NE-CZ	-5.43	116.80	124.40
1	D	141	THR	CA-CB-OG1	5.43	117.74	109.60
1	D	469	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	52	ALA	CA-C-N	-5.43	113.60	120.60
1	A	52	ALA	C-N-CA	-5.43	113.60	120.60
1	A	628	ARG	CD-NE-CZ	-5.43	116.80	124.40
1	D	197	TRP	O-C-N	5.43	128.35	122.11
1	E	141	THR	CA-CB-OG1	5.43	117.74	109.60
1	E	279	ASP	CB-CG-OD2	-5.43	105.92	118.40
1	E	363	LEU	N-CA-CB	-5.43	103.45	109.74
1	F	217	GLY	O-C-N	5.43	129.75	122.70
1	A	279	ASP	CB-CG-OD2	-5.42	105.92	118.40
1	A	392	LYS	CG-CD-CE	5.42	123.78	111.30
1	B	392	LYS	CG-CD-CE	5.42	123.78	111.30
1	D	253	ARG	CD-NE-CZ	-5.42	116.81	124.40
1	E	10	LYS	CB-CG-CD	5.42	123.78	111.30
1	E	102	ASN	CA-C-N	-5.42	111.18	121.54
1	E	102	ASN	C-N-CA	-5.42	111.18	121.54
1	E	522	SER	N-CA-CB	-5.42	101.44	110.23
1	F	391	PHE	CE1-CZ-CE2	5.42	129.76	120.00
1	A	509	PHE	CA-C-N	5.42	131.08	122.62
1	A	509	PHE	C-N-CA	5.42	131.08	122.62
1	B	391	PHE	CE1-CZ-CE2	5.42	129.76	120.00
1	C	253	ARG	CD-NE-CZ	-5.42	116.81	124.40
1	C	392	LYS	CG-CD-CE	5.42	123.77	111.30
1	C	415	GLY	CA-C-O	5.42	127.39	121.48
1	C	425	PHE	CA-CB-CG	-5.42	108.38	113.80
1	E	35	GLU	CB-CG-CD	-5.42	103.38	112.60
1	F	533	MET	N-CA-CB	5.42	117.58	109.88
1	C	10	LYS	CB-CG-CD	5.42	123.77	111.30
1	D	220	PHE	CD1-CE1-CZ	-5.42	110.25	120.00
1	D	349	VAL	N-CA-CB	5.42	117.24	110.47
1	E	217	GLY	O-C-N	5.42	129.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	414	ASN	CA-C-O	-5.42	114.00	120.56
1	F	611	VAL	CA-CB-CG1	5.42	119.61	110.40
1	A	47	ASN	CA-CB-CG	-5.42	107.18	112.60
1	A	611	VAL	CA-CB-CG1	5.42	119.61	110.40
1	D	347	ALA	N-CA-C	-5.42	105.48	111.71
1	D	576	GLU	OE1-CD-OE2	5.42	135.90	122.90
1	E	450	ALA	N-CA-CB	-5.42	101.41	110.83
1	E	576	GLU	OE1-CD-OE2	5.42	135.90	122.90
1	F	469	ASN	CA-CB-CG	-5.42	107.18	112.60
1	C	191	ASN	CA-CB-CG	5.42	118.02	112.60
1	C	220	PHE	CD1-CE1-CZ	-5.42	110.25	120.00
1	D	651	HIS	N-CA-C	5.42	117.57	107.99
1	A	197	TRP	O-C-N	5.41	128.34	122.11
1	A	253	ARG	CD-NE-CZ	-5.41	116.82	124.40
1	C	38	ASN	CB-CA-C	5.41	118.48	111.01
1	F	35	GLU	CB-CG-CD	-5.41	103.40	112.60
1	A	35	GLU	CB-CG-CD	-5.41	103.40	112.60
1	B	509	PHE	CA-C-N	5.41	131.06	122.62
1	B	509	PHE	C-N-CA	5.41	131.06	122.62
1	D	391	PHE	CE1-CZ-CE2	5.41	129.74	120.00
1	A	349	VAL	N-CA-CB	5.41	117.23	110.47
1	A	363	LEU	N-CA-CB	-5.41	103.46	109.74
1	A	539	LEU	O-C-N	5.41	130.40	122.39
1	B	35	GLU	CB-CG-CD	-5.41	103.40	112.60
1	C	509	PHE	CA-C-N	5.41	131.06	122.62
1	C	509	PHE	C-N-CA	5.41	131.06	122.62
1	C	576	GLU	OE1-CD-OE2	5.41	135.88	122.90
1	C	52	ALA	CA-C-N	-5.41	113.62	120.60
1	C	52	ALA	C-N-CA	-5.41	113.62	120.60
1	D	551	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	E	211	TYR	N-CA-CB	-5.41	102.69	111.24
1	E	651	HIS	N-CA-C	5.41	117.56	107.99
1	F	509	PHE	CA-C-N	5.41	131.06	122.62
1	F	509	PHE	C-N-CA	5.41	131.06	122.62
1	F	628	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	A	469	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	52	ALA	CA-C-N	-5.41	113.62	120.60
1	B	52	ALA	C-N-CA	-5.41	113.62	120.60
1	B	539	LEU	O-C-N	5.41	130.39	122.39
1	C	370	HIS	O-C-N	5.41	129.64	123.48
1	D	211	TYR	N-CA-CB	-5.41	102.70	111.24
1	D	611	VAL	CA-CB-CG1	5.41	119.59	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	253	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	F	220	PHE	CD1-CE1-CZ	-5.41	110.27	120.00
1	F	279	ASP	CB-CG-OD2	-5.41	105.96	118.40
1	A	220	PHE	CD1-CE1-CZ	-5.41	110.27	120.00
1	A	551	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	B	118	ALA	CA-C-N	-5.41	113.04	120.28
1	B	118	ALA	C-N-CA	-5.41	113.04	120.28
1	B	157	ALA	N-CA-C	-5.41	99.29	110.80
1	B	253	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	B	534	PRO	O-C-N	5.41	129.94	122.64
1	B	576	GLU	OE1-CD-OE2	5.41	135.88	122.90
1	B	611	VAL	CA-CB-CG1	5.41	119.59	110.40
1	C	211	TYR	N-CA-CB	-5.41	102.70	111.24
1	C	414	ASN	CA-C-O	-5.41	114.02	120.56
1	C	469	ASN	CA-CB-CG	-5.41	107.19	112.60
1	C	611	VAL	CA-CB-CG1	5.41	119.59	110.40
1	C	611	VAL	N-CA-CB	-5.41	102.31	111.23
1	E	349	VAL	N-CA-CB	5.41	117.23	110.47
1	F	539	LEU	O-C-N	5.41	130.39	122.39
1	F	551	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	A	576	GLU	OE1-CD-OE2	5.40	135.87	122.90
1	C	533	MET	N-CA-CB	5.40	117.55	109.88
1	D	509	PHE	CA-C-N	5.40	131.05	122.62
1	D	509	PHE	C-N-CA	5.40	131.05	122.62
1	E	38	ASN	CB-CA-C	5.40	118.47	111.01
1	A	211	TYR	N-CA-CB	-5.40	102.70	111.24
1	A	533	MET	N-CA-CB	5.40	117.55	109.88
1	B	141	THR	CA-CB-OG1	5.40	117.70	109.60
1	B	479	ARG	CA-C-N	-5.40	115.65	123.11
1	B	479	ARG	C-N-CA	-5.40	115.65	123.11
1	E	551	HIS	CE1-NE2-CD2	-5.40	103.60	109.00
1	A	450	ALA	N-CA-CB	-5.40	101.43	110.83
1	D	157	ALA	N-CA-C	-5.40	99.30	110.80
1	E	539	LEU	O-C-N	5.40	130.38	122.39
1	F	53	VAL	CA-C-N	-5.40	110.94	120.99
1	F	53	VAL	C-N-CA	-5.40	110.94	120.99
1	F	349	VAL	N-CA-CB	5.40	117.22	110.47
1	F	611	VAL	N-CA-CB	-5.40	102.32	111.23
1	D	611	VAL	N-CA-CB	-5.40	102.32	111.23
1	F	157	ALA	N-CA-C	-5.40	99.30	110.80
1	A	217	GLY	O-C-N	5.40	129.72	122.70
1	A	414	ASN	CA-C-O	-5.40	114.03	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	220	PHE	CD1-CE1-CZ	-5.40	110.28	120.00
1	B	611	VAL	N-CA-CB	-5.40	102.32	111.23
1	C	217	GLY	O-C-N	5.40	129.72	122.70
1	C	256	PHE	CZ-CE2-CD2	-5.40	110.28	120.00
1	D	35	GLU	CB-CG-CD	-5.40	103.42	112.60
1	A	611	VAL	N-CA-CB	-5.40	102.33	111.23
1	B	349	VAL	N-CA-CB	5.40	117.22	110.47
1	C	526	SER	CB-CA-C	-5.40	100.09	109.64
1	D	52	ALA	CA-C-N	-5.40	113.64	120.60
1	D	52	ALA	C-N-CA	-5.40	113.64	120.60
1	D	363	LEU	N-CA-CB	-5.40	103.48	109.74
1	A	157	ALA	N-CA-C	-5.39	99.31	110.80
1	C	563	GLY	O-C-N	5.39	129.71	122.70
1	D	450	ALA	N-CA-CB	-5.39	101.44	110.83
1	F	253	ARG	CD-NE-CZ	-5.39	116.85	124.40
1	F	363	LEU	N-CA-CB	-5.39	103.48	109.74
1	F	576	GLU	OE1-CD-OE2	5.39	135.84	122.90
1	A	651	HIS	N-CA-C	5.39	117.54	107.99
1	B	53	VAL	CA-C-N	-5.39	110.96	120.99
1	B	53	VAL	C-N-CA	-5.39	110.96	120.99
1	C	479	ARG	CA-C-N	-5.39	115.67	123.11
1	C	479	ARG	C-N-CA	-5.39	115.67	123.11
1	E	47	ASN	CA-CB-CG	-5.39	107.21	112.60
1	E	526	SER	CB-CA-C	-5.39	100.10	109.64
1	F	211	TYR	N-CA-CB	-5.39	102.72	111.24
1	C	651	HIS	N-CA-C	5.39	117.53	107.99
1	D	652	HIS	N-CA-C	5.39	117.50	109.25
1	B	190	MET	CA-C-O	-5.39	114.26	120.24
1	B	197	TRP	O-C-N	5.39	128.31	122.11
1	B	211	TYR	N-CA-CB	-5.39	102.72	111.24
1	B	363	LEU	N-CA-CB	-5.39	103.49	109.74
1	B	628	ARG	CD-NE-CZ	-5.39	116.85	124.40
1	C	35	GLU	CB-CG-CD	-5.39	103.44	112.60
1	C	118	ALA	CA-C-N	-5.39	113.06	120.28
1	C	118	ALA	C-N-CA	-5.39	113.06	120.28
1	C	157	ALA	N-CA-C	-5.39	99.32	110.80
1	D	47	ASN	CA-CB-CG	-5.39	107.21	112.60
1	D	89	VAL	N-CA-CB	-5.39	102.34	111.23
1	D	256	PHE	CZ-CE2-CD2	-5.39	110.30	120.00
1	D	318	PRO	CB-CG-CD	-5.39	88.86	106.10
1	E	118	ALA	CA-C-N	-5.39	113.06	120.28
1	E	118	ALA	C-N-CA	-5.39	113.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	256	PHE	CZ-CE2-CD2	-5.39	110.30	120.00
1	E	534	PRO	O-C-N	5.39	129.91	122.64
1	D	118	ALA	CA-C-N	-5.39	113.06	120.28
1	D	118	ALA	C-N-CA	-5.39	113.06	120.28
1	D	370	HIS	O-C-N	5.39	129.62	123.48
1	E	157	ALA	N-CA-C	-5.39	99.32	110.80
1	A	256	PHE	CZ-CE2-CD2	-5.39	110.31	120.00
1	A	370	HIS	O-C-N	5.39	129.62	123.48
1	B	450	ALA	N-CA-CB	-5.39	101.46	110.83
1	C	386	TYR	CA-CB-CG	5.39	123.60	113.90
1	C	450	ALA	N-CA-CB	-5.39	101.46	110.83
1	C	10	LYS	N-CA-C	-5.38	102.48	111.37
1	F	651	HIS	N-CA-C	5.38	117.52	107.99
1	A	526	SER	CB-CA-C	-5.38	100.11	109.64
1	B	414	ASN	CA-C-O	-5.38	114.05	120.56
1	D	190	MET	CA-C-O	-5.38	114.26	120.24
1	E	533	MET	N-CA-CB	5.38	117.52	109.88
1	F	450	ALA	N-CA-CB	-5.38	101.46	110.83
1	A	53	VAL	CA-C-N	-5.38	110.98	120.99
1	A	53	VAL	C-N-CA	-5.38	110.98	120.99
1	A	89	VAL	N-CA-CB	-5.38	102.35	111.23
1	A	118	ALA	CA-C-N	-5.38	113.07	120.28
1	A	118	ALA	C-N-CA	-5.38	113.07	120.28
1	B	217	GLY	O-C-N	5.38	129.70	122.70
1	C	53	VAL	CA-C-N	-5.38	110.98	120.99
1	C	53	VAL	C-N-CA	-5.38	110.98	120.99
1	E	10	LYS	N-CA-C	-5.38	102.49	111.37
1	E	611	VAL	N-CA-CB	-5.38	102.35	111.23
1	F	89	VAL	N-CA-CB	-5.38	102.35	111.23
1	F	526	SER	CB-CA-C	-5.38	100.11	109.64
1	D	53	VAL	CA-C-N	-5.38	110.98	120.99
1	D	53	VAL	C-N-CA	-5.38	110.98	120.99
1	D	479	ARG	CA-C-N	-5.38	115.69	123.11
1	D	479	ARG	C-N-CA	-5.38	115.69	123.11
1	F	414	ASN	CA-C-O	-5.38	114.05	120.56
1	A	318	PRO	CB-CG-CD	-5.38	88.89	106.10
1	A	534	PRO	O-C-N	5.38	129.90	122.64
1	C	197	TRP	O-C-N	5.38	128.30	122.11
1	C	318	PRO	CB-CG-CD	-5.38	88.89	106.10
1	C	551	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
1	D	155	TYR	CB-CA-C	-5.38	100.34	110.67
1	D	319	LYS	CB-CA-C	-5.38	99.25	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	118	ALA	CA-C-N	-5.38	113.07	120.28
1	F	118	ALA	C-N-CA	-5.38	113.07	120.28
1	F	141	THR	CA-CB-CG2	-5.38	101.36	110.50
1	B	89	VAL	N-CA-CB	-5.38	102.36	111.23
1	B	155	TYR	CB-CA-C	-5.38	100.35	110.67
1	B	256	PHE	CZ-CE2-CD2	-5.38	110.32	120.00
1	B	318	PRO	CB-CG-CD	-5.38	88.90	106.10
1	C	363	LEU	N-CA-CB	-5.38	103.50	109.74
1	C	646	VAL	CA-C-O	-5.38	114.71	121.11
1	E	160	THR	CA-CB-CG2	-5.38	101.36	110.50
1	E	563	GLY	O-C-N	5.38	129.69	122.70
1	F	509	PHE	N-CA-C	5.38	117.49	108.73
1	B	509	PHE	N-CA-C	5.38	117.49	108.73
1	B	651	HIS	N-CA-C	5.38	117.50	107.99
1	D	178	GLU	CA-CB-CG	5.38	124.85	114.10
1	D	414	ASN	CA-C-O	-5.38	114.06	120.56
1	D	563	GLY	O-C-N	5.38	129.69	122.70
1	A	479	ARG	CA-C-N	-5.37	115.69	123.11
1	A	479	ARG	C-N-CA	-5.37	115.69	123.11
1	B	319	LYS	CB-CA-C	-5.37	99.26	109.95
1	B	370	HIS	O-C-N	5.37	129.60	123.48
1	B	533	MET	N-CA-CB	5.37	117.51	109.88
1	D	160	THR	CA-CB-CG2	-5.37	101.36	110.50
1	D	386	TYR	CA-CB-CG	5.37	123.57	113.90
1	F	318	PRO	CB-CG-CD	-5.37	88.90	106.10
1	A	10	LYS	N-CA-C	-5.37	102.51	111.37
1	B	178	GLU	CA-CB-CG	5.37	124.84	114.10
1	B	526	SER	CB-CA-C	-5.37	100.13	109.64
1	B	646	VAL	CA-C-O	-5.37	114.72	121.11
1	B	652	HIS	N-CA-C	5.37	117.47	109.25
1	C	652	HIS	N-CA-C	5.37	117.47	109.25
1	D	141	THR	CA-CB-CG2	-5.37	101.37	110.50
1	D	526	SER	CB-CA-C	-5.37	100.13	109.64
1	E	141	THR	CA-CB-CG2	-5.37	101.37	110.50
1	E	190	MET	CA-C-O	-5.37	114.28	120.24
1	E	479	ARG	CA-C-N	-5.37	115.70	123.11
1	E	479	ARG	C-N-CA	-5.37	115.70	123.11
1	D	10	LYS	N-CA-C	-5.37	102.51	111.37
1	E	509	PHE	N-CA-C	5.37	117.48	108.73
1	A	155	TYR	CB-CA-C	-5.37	100.36	110.67
1	B	191	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	563	GLY	O-C-N	5.37	129.68	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	217	GLY	O-C-N	5.37	129.68	122.70
1	D	432	SER	N-CA-CB	-5.37	101.67	110.42
1	E	220	PHE	CD1-CE1-CZ	-5.37	110.34	120.00
1	E	318	PRO	CB-CG-CD	-5.37	88.92	106.10
1	F	190	MET	CA-C-O	-5.37	114.28	120.24
1	F	319	LYS	CB-CA-C	-5.37	99.27	109.95
1	F	534	PRO	O-C-N	5.37	129.89	122.64
1	A	652	HIS	N-CA-C	5.37	117.46	109.25
1	D	28	PRO	N-CD-CG	-5.37	95.15	103.20
1	F	178	GLU	CA-CB-CG	5.37	124.83	114.10
1	A	190	MET	CA-C-O	-5.37	114.28	120.24
1	A	191	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	10	LYS	N-CA-C	-5.37	102.52	111.37
1	C	155	TYR	CB-CA-C	-5.37	100.37	110.67
1	F	479	ARG	CA-C-N	-5.37	115.70	123.11
1	F	479	ARG	C-N-CA	-5.37	115.70	123.11
1	A	141	THR	CA-CB-CG2	-5.36	101.38	110.50
1	A	319	LYS	CB-CA-C	-5.36	99.28	109.95
1	C	89	VAL	N-CA-CB	-5.36	102.38	111.23
1	D	509	PHE	N-CA-C	5.36	117.47	108.73
1	F	155	TYR	CB-CA-C	-5.36	100.37	110.67
1	F	191	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	386	TYR	CA-CB-CG	5.36	123.55	113.90
1	C	28	PRO	N-CD-CG	-5.36	95.16	103.20
1	E	155	TYR	CB-CA-C	-5.36	100.38	110.67
1	E	432	SER	N-CA-CB	-5.36	101.68	110.42
1	A	178	GLU	CA-CB-CG	5.36	124.82	114.10
1	A	509	PHE	N-CA-C	5.36	117.47	108.73
1	E	53	VAL	CA-C-N	-5.36	111.02	120.99
1	E	53	VAL	C-N-CA	-5.36	111.02	120.99
1	E	319	LYS	CB-CA-C	-5.36	99.28	109.95
1	E	370	HIS	O-C-N	5.36	129.59	123.48
1	E	652	HIS	N-CA-C	5.36	117.45	109.25
1	F	24	PRO	CA-C-O	-5.36	110.84	120.60
1	F	432	SER	N-CA-CB	-5.36	101.69	110.42
1	C	534	PRO	O-C-N	5.36	129.87	122.64
1	E	178	GLU	CA-CB-CG	5.36	124.81	114.10
1	E	386	TYR	CA-CB-CG	5.36	123.54	113.90
1	F	256	PHE	CZ-CE2-CD2	-5.36	110.36	120.00
1	A	28	PRO	N-CD-CG	-5.36	95.17	103.20
1	A	563	GLY	O-C-N	5.36	129.66	122.70
1	C	160	THR	CA-CB-CG2	-5.36	101.40	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	370	HIS	CA-C-O	-5.36	114.11	120.43
1	E	362	ASN	CB-CG-OD1	-5.36	110.09	120.80
1	A	160	THR	CA-CB-CG2	-5.35	101.40	110.50
1	E	89	VAL	N-CA-CB	-5.35	102.39	111.23
1	E	646	VAL	CA-C-O	-5.35	114.74	121.11
1	F	90	LEU	O-C-N	-5.35	115.47	122.59
1	F	370	HIS	CA-C-O	-5.35	114.11	120.43
1	F	527	SER	CA-CB-OG	-5.35	100.39	111.10
1	F	644	HIS	CA-C-N	-5.35	115.50	122.94
1	F	644	HIS	C-N-CA	-5.35	115.50	122.94
1	C	644	HIS	CA-C-N	-5.35	115.50	122.94
1	C	644	HIS	C-N-CA	-5.35	115.50	122.94
1	E	213	LEU	CB-CA-C	5.35	118.58	109.53
1	F	10	LYS	N-CA-C	-5.35	102.54	111.37
1	F	160	THR	CA-CB-CG2	-5.35	101.40	110.50
1	C	319	LYS	CB-CA-C	-5.35	99.30	109.95
1	A	386	TYR	CA-CB-CG	5.35	123.53	113.90
1	A	527	SER	CA-CB-OG	-5.35	100.40	111.10
1	E	228	THR	CA-C-O	5.35	126.14	120.10
1	A	646	VAL	CA-C-O	-5.35	114.75	121.11
1	C	141	THR	CA-CB-CG2	-5.35	101.41	110.50
1	C	527	SER	CA-CB-OG	-5.35	100.40	111.10
1	D	527	SER	CA-CB-OG	-5.35	100.41	111.10
1	D	534	PRO	O-C-N	5.35	129.86	122.64
1	F	228	THR	CA-C-O	5.35	126.14	120.10
1	F	652	HIS	N-CA-C	5.35	117.43	109.25
1	A	457	HIS	CB-CA-C	-5.35	98.82	111.65
1	A	432	SER	N-CA-CB	-5.34	101.71	110.42
1	B	141	THR	CA-CB-CG2	-5.34	101.41	110.50
1	C	24	PRO	CA-C-O	-5.34	110.87	120.60
1	C	190	MET	CA-C-O	-5.34	114.31	120.24
1	C	457	HIS	CB-CA-C	-5.34	98.82	111.65
1	C	629	ARG	CD-NE-CZ	-5.34	116.92	124.40
1	D	362	ASN	CB-CG-OD1	-5.34	110.11	120.80
1	D	646	VAL	CA-C-O	-5.34	114.75	121.11
1	E	28	PRO	N-CD-CG	-5.34	95.18	103.20
1	E	78	ARG	CA-CB-CG	-5.34	103.41	114.10
1	E	191	ASN	CA-CB-CG	5.34	117.94	112.60
1	E	629	ARG	CD-NE-CZ	-5.34	116.92	124.40
1	F	28	PRO	N-CD-CG	-5.34	95.18	103.20
1	B	28	PRO	N-CD-CG	-5.34	95.19	103.20
1	B	457	HIS	CB-CA-C	-5.34	98.83	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	509	PHE	N-CA-C	5.34	117.44	108.73
1	E	457	HIS	CB-CA-C	-5.34	98.83	111.65
1	A	370	HIS	CA-C-O	-5.34	114.13	120.43
1	C	178	GLU	CA-CB-CG	5.34	124.78	114.10
1	E	370	HIS	CA-C-O	-5.34	114.13	120.43
1	F	386	TYR	CA-CB-CG	5.34	123.52	113.90
1	A	90	LEU	O-C-N	-5.34	115.49	122.59
1	B	160	THR	CA-CB-CG2	-5.34	101.42	110.50
1	D	78	ARG	CA-CB-CG	-5.34	103.42	114.10
1	F	90	LEU	CB-CA-C	5.34	121.05	110.42
1	F	213	LEU	CB-CA-C	5.34	118.55	109.53
1	F	457	HIS	CB-CA-C	-5.34	98.83	111.65
1	D	213	LEU	CB-CA-C	5.34	118.55	109.53
1	E	344	HIS	O-C-N	-5.34	115.49	122.59
1	B	24	PRO	CA-C-O	-5.34	110.89	120.60
1	B	224	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	B	527	SER	CA-CB-OG	-5.34	100.42	111.10
1	C	117	TYR	CA-CB-CG	5.34	123.51	113.90
1	C	155	TYR	CA-C-N	-5.34	111.45	120.58
1	C	155	TYR	C-N-CA	-5.34	111.45	120.58
1	D	621	PRO	CA-C-O	-5.34	110.89	120.60
1	E	24	PRO	CA-C-O	-5.34	110.89	120.60
1	E	527	SER	CA-CB-OG	-5.34	100.43	111.10
1	A	24	PRO	CA-C-O	-5.33	110.89	120.60
1	B	432	SER	N-CA-CB	-5.33	101.72	110.42
1	F	362	ASN	CB-CG-OD1	-5.33	110.13	120.80
1	A	629	ARG	CD-NE-CZ	-5.33	116.93	124.40
1	B	90	LEU	CB-CA-C	5.33	121.03	110.42
1	B	644	HIS	CA-C-N	-5.33	115.53	122.94
1	B	644	HIS	C-N-CA	-5.33	115.53	122.94
1	C	78	ARG	CA-CB-CG	-5.33	103.43	114.10
1	C	196	THR	CA-CB-OG1	-5.33	101.60	109.60
1	C	432	SER	N-CA-CB	-5.33	101.73	110.42
1	F	78	ARG	CA-CB-CG	-5.33	103.43	114.10
1	F	563	GLY	O-C-N	5.33	129.63	122.70
1	A	362	ASN	CB-CG-OD1	-5.33	110.14	120.80
1	D	90	LEU	O-C-N	-5.33	115.50	122.59
1	D	117	TYR	CA-CB-CG	5.33	123.50	113.90
1	D	370	HIS	CA-C-O	-5.33	114.14	120.43
1	D	457	HIS	CB-CA-C	-5.33	98.86	111.65
1	E	90	LEU	O-C-N	-5.33	115.50	122.59
1	E	196	THR	CA-CB-OG1	-5.33	101.60	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	ARG	CA-CB-CG	-5.33	103.44	114.10
1	A	90	LEU	CB-CA-C	5.33	121.03	110.42
1	A	213	LEU	CB-CA-C	5.33	118.54	109.53
1	E	90	LEU	CB-CA-C	5.33	121.03	110.42
1	E	644	HIS	CA-C-N	-5.33	115.53	122.94
1	E	644	HIS	C-N-CA	-5.33	115.53	122.94
1	F	583	TYR	CA-C-N	-5.33	116.01	123.10
1	F	583	TYR	C-N-CA	-5.33	116.01	123.10
1	A	117	TYR	CA-CB-CG	5.33	123.49	113.90
1	B	155	TYR	CA-C-N	-5.33	111.47	120.58
1	B	155	TYR	C-N-CA	-5.33	111.47	120.58
1	B	362	ASN	CB-CG-OD1	-5.33	110.14	120.80
1	D	191	ASN	CA-CB-CG	5.33	117.93	112.60
1	D	394	HIS	CA-C-O	5.33	126.50	120.00
1	F	144	MET	CA-C-N	-5.33	111.36	121.54
1	F	144	MET	C-N-CA	-5.33	111.36	121.54
1	F	394	HIS	CA-C-O	5.33	126.50	120.00
1	F	646	VAL	CA-C-O	-5.33	114.77	121.11
1	B	213	LEU	CB-CA-C	5.33	118.53	109.53
1	C	90	LEU	O-C-N	-5.33	115.50	122.59
1	C	144	MET	CA-C-N	-5.33	111.37	121.54
1	C	144	MET	C-N-CA	-5.33	111.37	121.54
1	C	213	LEU	CB-CA-C	5.33	118.53	109.53
1	F	196	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	196	THR	CA-CB-OG1	-5.32	101.61	109.60
1	A	644	HIS	CA-C-N	-5.32	115.54	122.94
1	A	644	HIS	C-N-CA	-5.32	115.54	122.94
1	B	117	TYR	CA-CB-CG	5.32	123.48	113.90
1	B	138	TYR	CA-C-N	-5.32	112.56	122.09
1	B	138	TYR	C-N-CA	-5.32	112.56	122.09
1	C	362	ASN	CB-CG-OD1	-5.32	110.15	120.80
1	D	90	LEU	CB-CA-C	5.32	121.02	110.42
1	D	583	TYR	CA-C-N	-5.32	116.02	123.10
1	D	583	TYR	C-N-CA	-5.32	116.02	123.10
1	B	196	THR	CA-CB-OG1	-5.32	101.62	109.60
1	B	370	HIS	CA-C-O	-5.32	114.15	120.43
1	D	196	THR	CA-CB-OG1	-5.32	101.62	109.60
1	E	144	MET	CA-C-N	-5.32	111.38	121.54
1	E	144	MET	C-N-CA	-5.32	111.38	121.54
1	F	138	TYR	CA-C-N	-5.32	112.56	122.09
1	F	138	TYR	C-N-CA	-5.32	112.56	122.09
1	A	621	PRO	CA-C-O	-5.32	110.92	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	78	ARG	CA-CB-CG	-5.32	103.46	114.10
1	B	231	PHE	CE1-CZ-CE2	-5.32	110.42	120.00
1	D	24	PRO	CA-C-O	-5.32	110.92	120.60
1	F	92	GLN	CB-CA-C	5.32	118.53	111.14
1	F	368	MET	CA-C-N	-5.32	114.12	122.95
1	F	368	MET	C-N-CA	-5.32	114.12	122.95
1	F	621	PRO	CA-C-O	-5.32	110.92	120.60
1	F	629	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	A	344	HIS	O-C-N	-5.32	115.52	122.59
1	B	629	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	C	92	GLN	CB-CA-C	5.32	118.53	111.14
1	C	215	ARG	CA-C-N	-5.32	113.15	121.02
1	C	215	ARG	C-N-CA	-5.32	113.15	121.02
1	C	228	THR	CA-C-O	5.32	126.11	120.10
1	E	247	HIS	CG-CD2-NE2	-5.32	101.88	107.20
1	F	117	TYR	CA-CB-CG	5.32	123.47	113.90
1	F	215	ARG	CA-C-N	-5.32	113.15	121.02
1	F	215	ARG	C-N-CA	-5.32	113.15	121.02
1	A	231	PHE	CE1-CZ-CE2	-5.32	110.43	120.00
1	C	344	HIS	O-C-N	-5.32	115.52	122.59
1	E	92	GLN	CB-CA-C	5.32	118.53	111.14
1	E	117	TYR	CA-CB-CG	5.32	123.47	113.90
1	E	368	MET	CA-C-N	-5.32	114.13	122.95
1	E	368	MET	C-N-CA	-5.32	114.13	122.95
1	C	457	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
1	D	215	ARG	CA-C-N	-5.31	113.16	121.02
1	D	215	ARG	C-N-CA	-5.31	113.16	121.02
1	D	344	HIS	O-C-N	-5.31	115.52	122.59
1	D	644	HIS	CA-C-N	-5.31	115.55	122.94
1	D	644	HIS	C-N-CA	-5.31	115.55	122.94
1	A	155	TYR	CA-C-N	-5.31	111.50	120.58
1	A	155	TYR	C-N-CA	-5.31	111.50	120.58
1	A	228	THR	CA-C-O	5.31	126.10	120.10
1	A	539	LEU	N-CA-C	-5.31	106.77	113.20
1	B	621	PRO	CA-C-O	-5.31	110.93	120.60
1	C	231	PHE	CE1-CZ-CE2	-5.31	110.44	120.00
1	D	155	TYR	CA-C-N	-5.31	111.50	120.58
1	D	155	TYR	C-N-CA	-5.31	111.50	120.58
1	E	155	TYR	CA-C-N	-5.31	111.50	120.58
1	E	155	TYR	C-N-CA	-5.31	111.50	120.58
1	B	144	MET	CA-C-N	-5.31	111.40	121.54
1	B	144	MET	C-N-CA	-5.31	111.40	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	144	MET	CA-C-N	-5.31	111.40	121.54
1	D	144	MET	C-N-CA	-5.31	111.40	121.54
1	E	488	ASN	CA-C-N	-5.31	113.40	122.11
1	E	488	ASN	C-N-CA	-5.31	113.40	122.11
1	A	488	ASN	CA-C-N	-5.31	113.40	122.11
1	A	488	ASN	C-N-CA	-5.31	113.40	122.11
1	B	457	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
1	B	539	LEU	N-CA-C	-5.31	106.78	113.20
1	A	394	HIS	CA-C-O	5.31	126.47	120.00
1	C	138	TYR	CA-C-N	-5.31	112.59	122.09
1	C	138	TYR	C-N-CA	-5.31	112.59	122.09
1	D	629	ARG	CD-NE-CZ	-5.31	116.97	124.40
1	E	215	ARG	CA-C-N	-5.31	113.17	121.02
1	E	215	ARG	C-N-CA	-5.31	113.17	121.02
1	A	144	MET	CA-C-N	-5.31	111.41	121.54
1	A	144	MET	C-N-CA	-5.31	111.41	121.54
1	B	215	ARG	CA-C-N	-5.31	113.17	121.02
1	B	215	ARG	C-N-CA	-5.31	113.17	121.02
1	C	90	LEU	CB-CA-C	5.31	120.98	110.42
1	E	193	HIS	CA-C-O	-5.31	114.98	120.92
1	C	539	LEU	N-CA-C	-5.30	106.78	113.20
1	C	621	PRO	CA-C-O	-5.30	110.94	120.60
1	D	488	ASN	CA-C-N	-5.30	113.41	122.11
1	D	488	ASN	C-N-CA	-5.30	113.41	122.11
1	D	539	LEU	N-CA-C	-5.30	106.78	113.20
1	E	138	TYR	CA-C-N	-5.30	112.59	122.09
1	E	138	TYR	C-N-CA	-5.30	112.59	122.09
1	F	231	PHE	CE1-CZ-CE2	-5.30	110.45	120.00
1	F	247	HIS	CG-CD2-NE2	-5.30	101.90	107.20
1	F	344	HIS	O-C-N	-5.30	115.53	122.59
1	A	215	ARG	CA-C-N	-5.30	113.17	121.02
1	A	215	ARG	C-N-CA	-5.30	113.17	121.02
1	B	90	LEU	O-C-N	-5.30	115.54	122.59
1	B	193	HIS	CA-C-O	-5.30	114.98	120.92
1	B	369	GLU	N-CA-CB	5.30	118.64	110.79
1	E	418	ILE	CA-C-O	5.30	126.89	120.74
1	A	138	TYR	CA-C-N	-5.30	112.60	122.09
1	A	138	TYR	C-N-CA	-5.30	112.60	122.09
1	A	583	TYR	CA-C-N	-5.30	116.05	123.10
1	A	583	TYR	C-N-CA	-5.30	116.05	123.10
1	B	488	ASN	CA-C-N	-5.30	113.42	122.11
1	B	488	ASN	C-N-CA	-5.30	113.42	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	507	LYS	O-C-N	5.30	129.83	123.26
1	C	418	ILE	CA-C-O	5.30	126.89	120.74
1	A	92	GLN	CB-CA-C	5.30	118.50	111.14
1	E	199	MET	CG-SD-CE	5.30	112.56	100.90
1	E	539	LEU	N-CA-C	-5.30	106.79	113.20
1	F	488	ASN	CA-C-N	-5.30	113.42	122.11
1	F	488	ASN	C-N-CA	-5.30	113.42	122.11
1	F	539	LEU	N-CA-C	-5.30	106.79	113.20
1	F	640	SER	CA-C-N	-5.30	114.02	122.66
1	F	640	SER	C-N-CA	-5.30	114.02	122.66
1	B	199	MET	CG-SD-CE	5.30	112.56	100.90
1	D	92	GLN	CB-CA-C	5.30	118.50	111.14
1	D	193	HIS	CA-C-O	-5.30	114.99	120.92
1	E	231	PHE	CE1-CZ-CE2	-5.30	110.46	120.00
1	B	344	HIS	O-C-N	-5.30	115.55	122.59
1	B	615	ALA	N-CA-C	5.30	117.85	109.96
1	B	641	ASN	O-C-N	5.30	129.16	122.06
1	C	199	MET	CG-SD-CE	5.30	112.55	100.90
1	D	199	MET	CG-SD-CE	5.30	112.55	100.90
1	D	247	HIS	CG-CD2-NE2	-5.30	101.90	107.20
1	D	369	GLU	N-CA-CB	5.30	118.63	110.79
1	D	457	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
1	F	199	MET	CG-SD-CE	5.30	112.55	100.90
1	A	368	MET	CA-C-N	-5.29	114.16	122.95
1	A	368	MET	C-N-CA	-5.29	114.16	122.95
1	A	640	SER	CA-C-N	-5.29	114.03	122.66
1	A	640	SER	C-N-CA	-5.29	114.03	122.66
1	B	583	TYR	CA-C-N	-5.29	116.06	123.10
1	B	583	TYR	C-N-CA	-5.29	116.06	123.10
1	D	231	PHE	CE1-CZ-CE2	-5.29	110.47	120.00
1	D	469	ASN	CB-CG-ND2	-5.29	108.46	116.40
1	F	457	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
1	A	193	HIS	CA-C-O	-5.29	114.99	120.92
1	A	199	MET	CG-SD-CE	5.29	112.54	100.90
1	B	92	GLN	CB-CA-C	5.29	118.49	111.14
1	D	138	TYR	CA-C-N	-5.29	112.62	122.09
1	D	138	TYR	C-N-CA	-5.29	112.62	122.09
1	E	621	PRO	CA-C-O	-5.29	110.97	120.60
1	F	418	ILE	CA-C-O	5.29	126.88	120.74
1	B	225	HIS	CA-C-N	-5.29	113.25	120.44
1	B	225	HIS	C-N-CA	-5.29	113.25	120.44
1	B	228	THR	CA-C-O	5.29	126.08	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	380	PHE	N-CA-CB	5.29	117.68	110.01
1	C	488	ASN	CA-C-N	-5.29	113.44	122.11
1	C	488	ASN	C-N-CA	-5.29	113.44	122.11
1	E	394	HIS	CA-C-O	5.29	126.45	120.00
1	E	457	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
1	E	615	ALA	N-CA-C	5.29	117.84	109.96
1	F	369	GLU	N-CA-CB	5.29	118.62	110.79
1	F	620	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	C	311	HIS	CA-C-N	-5.29	114.73	122.19
1	C	311	HIS	C-N-CA	-5.29	114.73	122.19
1	F	193	HIS	CA-C-O	-5.29	115.00	120.92
1	B	640	SER	CA-C-N	-5.29	114.05	122.66
1	B	640	SER	C-N-CA	-5.29	114.05	122.66
1	F	237	SER	CA-C-N	-5.29	114.77	122.86
1	F	237	SER	C-N-CA	-5.29	114.77	122.86
1	D	368	MET	CA-C-N	-5.28	114.18	122.95
1	D	368	MET	C-N-CA	-5.28	114.18	122.95
1	D	640	SER	CA-C-N	-5.28	114.05	122.66
1	D	640	SER	C-N-CA	-5.28	114.05	122.66
1	A	9	GLN	CG-CD-NE2	-5.28	108.48	116.40
1	A	225	HIS	CA-C-N	-5.28	113.26	120.44
1	A	225	HIS	C-N-CA	-5.28	113.26	120.44
1	A	247	HIS	CG-CD2-NE2	-5.28	101.92	107.20
1	B	9	GLN	CG-CD-NE2	-5.28	108.48	116.40
1	D	380	PHE	N-CA-CB	5.28	117.67	110.01
1	E	507	LYS	O-C-N	5.28	129.81	123.26
1	B	237	SER	CA-C-N	-5.28	114.78	122.86
1	B	237	SER	C-N-CA	-5.28	114.78	122.86
1	C	641	ASN	O-C-N	5.28	129.14	122.06
1	D	8	ALA	CB-CA-C	5.28	120.93	110.42
1	D	398	PHE	CB-CA-C	5.28	119.01	109.45
1	E	583	TYR	CA-C-N	-5.28	116.08	123.10
1	E	583	TYR	C-N-CA	-5.28	116.08	123.10
1	A	507	LYS	O-C-N	5.28	129.80	123.26
1	B	247	HIS	CG-CD2-NE2	-5.28	101.92	107.20
1	B	368	MET	CA-C-N	-5.28	114.19	122.95
1	B	368	MET	C-N-CA	-5.28	114.19	122.95
1	B	461	THR	CB-CA-C	5.28	120.41	109.38
1	B	501	PHE	CA-CB-CG	5.28	119.08	113.80
1	C	394	HIS	CA-C-O	5.28	126.44	120.00
1	C	438	ASP	CA-CB-CG	-5.28	107.32	112.60
1	D	418	ILE	CA-C-O	5.28	126.86	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	8	ALA	N-CA-CB	-5.28	101.57	110.49
1	A	369	GLU	N-CA-CB	5.28	118.60	110.79
1	B	394	HIS	CA-C-O	5.28	126.44	120.00
1	C	369	GLU	N-CA-CB	5.28	118.60	110.79
1	D	224	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	F	155	TYR	CA-C-N	-5.28	111.56	120.58
1	F	155	TYR	C-N-CA	-5.28	111.56	120.58
1	B	9	GLN	CB-CA-C	-5.27	102.50	111.26
1	C	225	HIS	CA-C-N	-5.27	113.27	120.44
1	C	225	HIS	C-N-CA	-5.27	113.27	120.44
1	C	583	TYR	CA-C-N	-5.27	116.09	123.10
1	C	583	TYR	C-N-CA	-5.27	116.09	123.10
1	D	245	GLU	CB-CG-CD	5.27	121.57	112.60
1	F	9	GLN	CG-CD-NE2	-5.27	108.49	116.40
1	F	51	ALA	N-CA-C	-5.27	105.70	111.82
1	F	308	SER	CA-C-N	-5.27	112.38	121.66
1	F	308	SER	C-N-CA	-5.27	112.38	121.66
1	A	457	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
1	A	615	ALA	N-CA-C	5.27	117.81	109.96
1	B	51	ALA	N-CA-C	-5.27	105.70	111.82
1	C	308	SER	CA-C-N	-5.27	112.38	121.66
1	C	308	SER	C-N-CA	-5.27	112.38	121.66
1	C	368	MET	CA-C-N	-5.27	114.20	122.95
1	C	368	MET	C-N-CA	-5.27	114.20	122.95
1	D	51	ALA	N-CA-C	-5.27	105.70	111.82
1	D	225	HIS	CA-C-N	-5.27	113.27	120.44
1	D	225	HIS	C-N-CA	-5.27	113.27	120.44
1	D	507	LYS	O-C-N	5.27	129.80	123.26
1	E	9	GLN	CG-CD-NE2	-5.27	108.49	116.40
1	B	418	ILE	CA-C-O	5.27	126.86	120.74
1	D	228	THR	CA-C-O	5.27	126.06	120.10
1	F	224	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
1	F	235	ARG	O-C-N	5.27	129.49	122.43
1	A	311	HIS	CA-C-N	-5.27	114.76	122.19
1	A	311	HIS	C-N-CA	-5.27	114.76	122.19
1	C	65	LEU	O-C-N	-5.27	117.16	123.06
1	C	235	ARG	O-C-N	5.27	129.49	122.43
1	C	303	GLY	CA-C-O	-5.27	114.10	119.37
1	C	640	SER	CA-C-N	-5.27	114.07	122.66
1	C	640	SER	C-N-CA	-5.27	114.07	122.66
1	E	303	GLY	CA-C-O	-5.27	114.10	119.37
1	E	380	PHE	N-CA-CB	5.27	117.65	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	640	SER	CA-C-N	-5.27	114.07	122.66
1	E	640	SER	C-N-CA	-5.27	114.07	122.66
1	F	615	ALA	N-CA-C	5.27	117.81	109.96
1	F	641	ASN	O-C-N	5.27	129.12	122.06
1	A	8	ALA	CB-CA-C	5.27	120.90	110.42
1	A	224	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
1	A	235	ARG	O-C-N	5.27	129.49	122.43
1	A	469	ASN	CB-CG-ND2	-5.27	108.50	116.40
1	A	641	ASN	O-C-N	5.27	129.12	122.06
1	B	245	GLU	CB-CG-CD	5.27	121.56	112.60
1	B	542	GLN	CA-CB-CG	-5.27	103.56	114.10
1	C	615	ALA	N-CA-C	5.27	117.81	109.96
1	E	8	ALA	N-CA-CB	-5.27	101.59	110.49
1	E	210	GLY	O-C-N	-5.27	115.85	122.70
1	F	380	PHE	N-CA-CB	5.27	117.65	110.01
1	E	592	ASP	N-CA-C	-5.27	99.58	110.80
1	A	461	THR	CB-CA-C	5.26	120.38	109.38
1	B	123	VAL	CA-CB-CG2	-5.26	101.45	110.40
1	C	461	THR	CB-CA-C	5.26	120.38	109.38
1	D	247	HIS	CB-CA-C	-5.26	99.44	109.66
1	D	592	ASP	N-CA-C	-5.26	99.58	110.80
1	F	8	ALA	CB-CA-C	5.26	120.90	110.42
1	F	469	ASN	CB-CG-ND2	-5.26	108.50	116.40
1	F	507	LYS	O-C-N	5.26	129.79	123.26
1	A	8	ALA	N-CA-CB	-5.26	101.60	110.49
1	A	237	SER	CA-C-N	-5.26	114.81	122.86
1	A	237	SER	C-N-CA	-5.26	114.81	122.86
1	B	235	ARG	N-CA-CB	5.26	119.13	110.39
1	B	420	GLY	CA-C-N	-5.26	114.41	122.62
1	B	420	GLY	C-N-CA	-5.26	114.41	122.62
1	C	592	ASP	N-CA-C	-5.26	99.59	110.80
1	D	65	LEU	O-C-N	-5.26	117.17	123.06
1	D	235	ARG	O-C-N	5.26	129.48	122.43
1	D	641	ASN	O-C-N	5.26	129.11	122.06
1	F	245	GLU	CB-CG-CD	5.26	121.55	112.60
1	A	51	ALA	N-CA-C	-5.26	105.72	111.82
1	B	65	LEU	O-C-N	-5.26	117.17	123.06
1	B	308	SER	CA-C-N	-5.26	112.40	121.66
1	B	308	SER	C-N-CA	-5.26	112.40	121.66
1	B	469	ASN	CB-CG-ND2	-5.26	108.51	116.40
1	C	542	GLN	CA-CB-CG	-5.26	103.58	114.10
1	D	311	HIS	CA-C-N	-5.26	114.77	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	311	HIS	C-N-CA	-5.26	114.77	122.19
1	E	51	ALA	N-CA-C	-5.26	105.72	111.82
1	E	245	GLU	CB-CG-CD	5.26	121.55	112.60
1	F	123	VAL	CA-CB-CG2	-5.26	101.46	110.40
1	F	461	THR	CB-CA-C	5.26	120.38	109.38
1	F	501	PHE	CA-CB-CG	5.26	119.06	113.80
1	C	8	ALA	CB-CA-C	5.26	120.89	110.42
1	C	8	ALA	N-CA-CB	-5.26	101.60	110.49
1	C	501	PHE	CA-CB-CG	5.26	119.06	113.80
1	D	615	ALA	N-CA-C	5.26	117.80	109.96
1	E	272	PRO	O-C-N	5.26	129.29	122.24
1	E	593	THR	O-C-N	5.26	129.58	122.59
1	F	235	ARG	N-CA-CB	5.26	119.12	110.39
1	F	438	ASP	CA-CB-CG	-5.26	107.34	112.60
1	B	8	ALA	CB-CA-C	5.26	120.88	110.42
1	B	592	ASP	N-CA-C	-5.26	99.60	110.80
1	A	123	VAL	CA-CB-CG2	-5.26	101.47	110.40
1	A	620	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	C	243	VAL	CA-C-N	5.26	128.69	120.75
1	C	243	VAL	C-N-CA	5.26	128.69	120.75
1	C	247	HIS	CG-CD2-NE2	-5.26	101.94	107.20
1	C	260	THR	CA-CB-CG2	5.26	119.44	110.50
1	D	308	SER	CA-C-N	-5.26	112.41	121.66
1	D	308	SER	C-N-CA	-5.26	112.41	121.66
1	D	461	THR	CB-CA-C	5.26	120.37	109.38
1	D	482	LEU	O-C-N	5.26	130.98	122.99
1	E	398	PHE	CB-CA-C	5.26	118.96	109.45
1	E	461	THR	CB-CA-C	5.26	120.36	109.38
1	E	641	ASN	O-C-N	5.26	129.10	122.06
1	F	371	PHE	CA-CB-CG	-5.26	108.54	113.80
1	A	380	PHE	N-CA-CB	5.25	117.63	110.01
1	B	247	HIS	CB-CA-C	-5.25	99.47	109.66
1	E	431	TYR	CA-C-O	-5.25	115.48	121.68
1	F	291	ILE	CB-CG1-CD1	-5.25	102.76	113.80
1	A	245	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	418	ILE	CA-C-O	5.25	126.83	120.74
1	A	592	ASP	N-CA-C	-5.25	99.61	110.80
1	B	210	GLY	O-C-N	-5.25	115.87	122.70
1	B	235	ARG	O-C-N	5.25	129.47	122.43
1	B	371	PHE	CA-CB-CG	-5.25	108.55	113.80
1	C	247	HIS	CB-CA-C	-5.25	99.47	109.66
1	C	431	TYR	CA-C-O	-5.25	115.48	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	210	GLY	O-C-N	-5.25	115.87	122.70
1	E	8	ALA	CB-CA-C	5.25	120.88	110.42
1	E	620	ARG	CD-NE-CZ	-5.25	117.04	124.40
1	F	303	GLY	CA-C-O	-5.25	114.12	119.37
1	F	568	MET	CB-CA-C	5.25	119.47	110.01
1	A	9	GLN	CB-CA-C	-5.25	102.54	111.26
1	A	438	ASP	CA-CB-CG	-5.25	107.35	112.60
1	C	123	VAL	CA-CB-CG2	-5.25	101.47	110.40
1	C	224	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	D	9	GLN	CG-CD-NE2	-5.25	108.52	116.40
1	D	46	TYR	CA-C-O	-5.25	114.40	120.49
1	D	438	ASP	CA-CB-CG	-5.25	107.35	112.60
1	E	235	ARG	N-CA-CB	5.25	119.11	110.39
1	E	369	GLU	N-CA-CB	5.25	118.56	110.79
1	F	225	HIS	CA-C-N	-5.25	113.30	120.44
1	F	225	HIS	C-N-CA	-5.25	113.30	120.44
1	F	311	HIS	CA-C-N	-5.25	114.78	122.19
1	F	311	HIS	C-N-CA	-5.25	114.78	122.19
1	F	398	PHE	CB-CA-C	5.25	118.95	109.45
1	F	592	ASP	N-CA-C	-5.25	99.61	110.80
1	A	247	HIS	CB-CA-C	-5.25	99.48	109.66
1	A	308	SER	CA-C-N	-5.25	112.42	121.66
1	A	308	SER	C-N-CA	-5.25	112.42	121.66
1	B	8	ALA	N-CA-CB	-5.25	101.62	110.49
1	B	47	ASN	OD1-CG-ND2	5.25	127.85	122.60
1	B	291	ILE	CB-CG1-CD1	-5.25	102.78	113.80
1	C	9	GLN	CG-CD-NE2	-5.25	108.53	116.40
1	A	501	PHE	CA-CB-CG	5.25	119.05	113.80
1	B	311	HIS	CA-C-N	-5.25	114.79	122.19
1	B	311	HIS	C-N-CA	-5.25	114.79	122.19
1	D	620	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	F	9	GLN	CB-CA-C	-5.25	102.55	111.26
1	F	542	GLN	CA-CB-CG	-5.25	103.60	114.10
1	A	65	LEU	O-C-N	-5.25	117.19	123.06
1	A	210	GLY	O-C-N	-5.25	115.88	122.70
1	A	235	ARG	N-CA-CB	5.25	119.10	110.39
1	C	507	LYS	O-C-N	5.25	129.77	123.26
1	E	43	THR	CA-C-N	-5.25	111.52	121.54
1	E	43	THR	C-N-CA	-5.25	111.52	121.54
1	E	123	VAL	CA-CB-CG2	-5.25	101.48	110.40
1	E	224	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	E	247	HIS	CB-CA-C	-5.25	99.48	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	243	VAL	CA-C-N	5.25	128.67	120.75
1	F	243	VAL	C-N-CA	5.25	128.67	120.75
1	A	398	PHE	CB-CA-C	5.25	118.94	109.45
1	A	431	TYR	CA-C-O	-5.25	115.49	121.68
1	B	260	THR	CA-CB-CG2	5.25	119.42	110.50
1	B	398	PHE	CB-CA-C	5.25	118.94	109.45
1	D	243	VAL	CA-C-N	5.25	128.67	120.75
1	D	243	VAL	C-N-CA	5.25	128.67	120.75
1	E	225	HIS	CA-C-N	-5.25	113.31	120.44
1	E	225	HIS	C-N-CA	-5.25	113.31	120.44
1	A	243	VAL	CA-C-N	5.24	128.67	120.75
1	A	243	VAL	C-N-CA	5.24	128.67	120.75
1	A	542	GLN	CA-CB-CG	-5.24	103.61	114.10
1	D	47	ASN	OD1-CG-ND2	5.24	127.84	122.60
1	D	420	GLY	CA-C-N	-5.24	114.44	122.62
1	D	420	GLY	C-N-CA	-5.24	114.44	122.62
1	D	568	MET	CB-CA-C	5.24	119.45	110.01
1	E	501	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	568	MET	CB-CA-C	5.24	119.45	110.01
1	D	371	PHE	CA-CB-CG	-5.24	108.56	113.80
1	E	311	HIS	CA-C-N	-5.24	114.80	122.19
1	E	311	HIS	C-N-CA	-5.24	114.80	122.19
1	E	420	GLY	CA-C-N	-5.24	114.44	122.62
1	E	420	GLY	C-N-CA	-5.24	114.44	122.62
1	E	542	GLN	CA-CB-CG	-5.24	103.62	114.10
1	C	51	ALA	N-CA-C	-5.24	105.74	111.82
1	C	245	GLU	CB-CG-CD	5.24	121.51	112.60
1	F	482	LEU	O-C-N	5.24	130.96	122.99
1	A	291	ILE	CB-CG1-CD1	-5.24	102.80	113.80
1	B	263	LYS	CA-CB-CG	5.24	124.58	114.10
1	B	431	TYR	CA-C-O	-5.24	115.50	121.68
1	C	235	ARG	N-CA-CB	5.24	119.08	110.39
1	C	327	ILE	CA-C-O	-5.24	115.11	120.71
1	D	250	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	E	291	ILE	CB-CG1-CD1	-5.24	102.80	113.80
1	E	308	SER	CA-C-N	-5.24	112.44	121.66
1	E	308	SER	C-N-CA	-5.24	112.44	121.66
1	E	469	ASN	CB-CG-ND2	-5.24	108.54	116.40
1	A	303	GLY	CA-C-O	-5.24	114.13	119.37
1	E	237	SER	CA-C-N	-5.24	114.85	122.86
1	E	237	SER	C-N-CA	-5.24	114.85	122.86
1	A	260	THR	CA-CB-CG2	5.24	119.40	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	9	GLN	CB-CA-C	-5.24	102.57	111.26
1	C	43	THR	CA-C-N	-5.24	111.54	121.54
1	C	43	THR	C-N-CA	-5.24	111.54	121.54
1	C	193	HIS	CA-C-O	-5.24	115.06	120.92
1	C	250	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	C	291	ILE	CB-CG1-CD1	-5.24	102.81	113.80
1	C	620	ARG	CD-NE-CZ	-5.24	117.07	124.40
1	D	9	GLN	CB-CA-C	-5.24	102.57	111.26
1	D	43	THR	CA-C-N	-5.24	111.54	121.54
1	D	43	THR	C-N-CA	-5.24	111.54	121.54
1	E	9	GLN	CB-CA-C	-5.24	102.57	111.26
1	F	43	THR	CA-C-N	-5.24	111.54	121.54
1	F	43	THR	C-N-CA	-5.24	111.54	121.54
1	F	210	GLY	O-C-N	-5.24	115.89	122.70
1	B	438	ASP	CA-CB-CG	-5.23	107.37	112.60
1	C	237	SER	CA-C-N	-5.23	114.85	122.86
1	C	237	SER	C-N-CA	-5.23	114.85	122.86
1	C	469	ASN	CB-CG-ND2	-5.23	108.55	116.40
1	D	8	ALA	N-CA-CB	-5.23	101.64	110.49
1	D	303	GLY	CA-C-O	-5.23	114.14	119.37
1	D	542	GLN	CA-CB-CG	-5.23	103.63	114.10
1	E	243	VAL	CA-C-N	5.23	128.65	120.75
1	E	243	VAL	C-N-CA	5.23	128.65	120.75
1	A	420	GLY	CA-C-N	-5.23	114.46	122.62
1	A	420	GLY	C-N-CA	-5.23	114.46	122.62
1	B	568	MET	CB-CA-C	5.23	119.43	110.01
1	D	123	VAL	CA-CB-CG2	-5.23	101.50	110.40
1	D	291	ILE	CB-CG1-CD1	-5.23	102.81	113.80
1	E	482	LEU	O-C-N	5.23	130.94	122.99
1	A	43	THR	CA-C-N	-5.23	111.55	121.54
1	A	43	THR	C-N-CA	-5.23	111.55	121.54
1	A	371	PHE	CA-CB-CG	-5.23	108.57	113.80
1	B	93	CYS	CA-CB-SG	-5.23	102.37	114.40
1	B	482	LEU	O-C-N	5.23	130.94	122.99
1	D	471	ASP	CA-C-N	-5.23	111.16	121.41
1	D	471	ASP	C-N-CA	-5.23	111.16	121.41
1	E	260	THR	CA-CB-CG2	5.23	119.39	110.50
1	F	247	HIS	CB-CA-C	-5.23	99.51	109.66
1	B	620	ARG	CD-NE-CZ	-5.23	117.08	124.40
1	E	568	MET	CB-CA-C	5.23	119.42	110.01
1	B	243	VAL	CA-C-N	5.23	128.65	120.75
1	B	243	VAL	C-N-CA	5.23	128.65	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	46	TYR	CA-C-O	-5.23	114.43	120.49
1	F	260	THR	CA-CB-CG2	5.23	119.39	110.50
1	A	353	ARG	NE-CZ-NH2	-5.23	114.50	119.20
1	A	482	LEU	O-C-N	5.23	130.93	122.99
1	B	46	TYR	CA-C-O	-5.23	114.43	120.49
1	F	65	LEU	O-C-N	-5.23	117.21	123.06
1	F	431	TYR	CA-C-O	-5.23	115.51	121.68
1	B	250	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	B	494	THR	N-CA-CB	-5.22	102.60	111.17
1	C	93	CYS	CA-CB-SG	-5.22	102.38	114.40
1	D	93	CYS	CA-CB-SG	-5.22	102.38	114.40
1	D	235	ARG	N-CA-CB	5.22	119.06	110.39
1	E	380	PHE	N-CA-C	-5.22	105.48	111.07
1	E	438	ASP	CA-CB-CG	-5.22	107.38	112.60
1	E	508	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	93	CYS	CA-CB-SG	-5.22	102.39	114.40
1	B	43	THR	CA-C-N	-5.22	111.57	121.54
1	B	43	THR	C-N-CA	-5.22	111.57	121.54
1	B	126	SER	CB-CA-C	-5.22	100.72	109.65
1	C	371	PHE	CA-CB-CG	-5.22	108.58	113.80
1	C	568	MET	CB-CA-C	5.22	119.41	110.01
1	D	237	SER	CA-C-N	-5.22	114.87	122.86
1	D	237	SER	C-N-CA	-5.22	114.87	122.86
1	F	263	LYS	CA-CB-CG	5.22	124.55	114.10
1	A	593	THR	O-C-N	5.22	129.53	122.59
1	C	380	PHE	N-CA-CB	5.22	117.58	110.01
1	D	353	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	E	126	SER	CB-CA-C	-5.22	100.72	109.65
1	E	371	PHE	CA-CB-CG	-5.22	108.58	113.80
1	A	250	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	C	271	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	C	471	ASP	CA-C-N	-5.22	111.18	121.41
1	C	471	ASP	C-N-CA	-5.22	111.18	121.41
1	B	471	ASP	CA-C-N	-5.22	111.18	121.41
1	B	471	ASP	C-N-CA	-5.22	111.18	121.41
1	D	593	THR	O-C-N	5.22	129.53	122.59
1	F	46	TYR	CA-C-O	-5.22	114.44	120.49
1	F	353	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	F	420	GLY	CA-C-N	-5.22	114.48	122.62
1	F	420	GLY	C-N-CA	-5.22	114.48	122.62
1	B	273	ASP	N-CA-CB	-5.22	101.67	110.49
1	C	210	GLY	O-C-N	-5.22	115.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	263	LYS	CA-CB-CG	5.22	124.53	114.10
1	D	343	LEU	CD1-CG-CD2	-5.22	99.33	110.80
1	E	93	CYS	CA-CB-SG	-5.22	102.40	114.40
1	E	384	HIS	N-CA-CB	5.22	118.65	110.46
1	A	126	SER	CB-CA-C	-5.21	100.73	109.65
1	A	263	LYS	CA-CB-CG	5.21	124.53	114.10
1	E	471	ASP	CA-C-N	-5.21	111.19	121.41
1	E	471	ASP	C-N-CA	-5.21	111.19	121.41
1	E	591	LYS	O-C-N	5.21	129.48	122.49
1	F	93	CYS	CA-CB-SG	-5.21	102.41	114.40
1	F	384	HIS	N-CA-CB	5.21	118.64	110.46
1	F	471	ASP	CA-C-N	-5.21	111.19	121.41
1	F	471	ASP	C-N-CA	-5.21	111.19	121.41
1	B	353	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	C	272	PRO	O-C-N	5.21	129.22	122.24
1	C	306	THR	N-CA-CB	-5.21	102.39	110.57
1	C	398	PHE	CB-CA-C	5.21	118.88	109.45
1	D	126	SER	CB-CA-C	-5.21	100.74	109.65
1	E	263	LYS	CA-CB-CG	5.21	124.52	114.10
1	F	126	SER	CB-CA-C	-5.21	100.74	109.65
1	B	2	ALA	CA-C-N	5.21	129.58	122.34
1	B	2	ALA	C-N-CA	5.21	129.58	122.34
1	D	431	TYR	CA-C-O	-5.21	115.53	121.68
1	F	593	THR	O-C-N	5.21	129.52	122.59
1	A	46	TYR	CA-C-O	-5.21	114.45	120.49
1	B	306	THR	N-CA-CB	-5.21	102.39	110.57
1	B	380	PHE	N-CA-C	-5.21	105.50	111.07
1	B	558	TYR	CA-C-N	-5.21	113.35	122.62
1	B	558	TYR	C-N-CA	-5.21	113.35	122.62
1	B	593	THR	O-C-N	5.21	129.52	122.59
1	D	144	MET	CA-CB-CG	5.21	124.52	114.10
1	D	260	THR	CA-CB-CG2	5.21	119.36	110.50
1	D	384	HIS	N-CA-CB	5.21	118.64	110.46
1	D	501	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	47	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	558	TYR	CA-C-N	-5.21	113.35	122.62
1	A	558	TYR	C-N-CA	-5.21	113.35	122.62
1	B	343	LEU	CD1-CG-CD2	-5.21	99.35	110.80
1	E	65	LEU	O-C-N	-5.21	117.23	123.06
1	E	494	THR	N-CA-CB	-5.21	102.63	111.17
1	F	558	TYR	CA-C-N	-5.21	113.35	122.62
1	F	558	TYR	C-N-CA	-5.21	113.35	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	471	ASP	CA-C-N	-5.21	111.21	121.41
1	A	471	ASP	C-N-CA	-5.21	111.21	121.41
1	A	494	THR	N-CA-CB	-5.21	102.63	111.17
1	C	47	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	C	482	LEU	O-C-N	5.21	130.90	122.99
1	A	273	ASP	N-CA-CB	-5.20	101.69	110.49
1	B	303	GLY	CA-C-O	-5.20	114.17	119.37
1	B	384	HIS	N-CA-CB	5.20	118.63	110.46
1	C	263	LYS	CA-CB-CG	5.20	124.51	114.10
1	D	558	TYR	CA-C-N	-5.20	113.36	122.62
1	D	558	TYR	C-N-CA	-5.20	113.36	122.62
1	D	591	LYS	O-C-N	5.20	129.46	122.49
1	E	235	ARG	O-C-N	5.20	129.40	122.43
1	D	273	ASP	N-CA-CB	-5.20	101.70	110.49
1	A	272	PRO	O-C-N	5.20	129.21	122.24
1	C	343	LEU	CD1-CG-CD2	-5.20	99.36	110.80
1	D	327	ILE	CA-C-O	-5.20	115.15	120.71
1	D	494	THR	N-CA-CB	-5.20	102.64	111.17
1	F	144	MET	CA-CB-CG	5.20	124.50	114.10
1	F	494	THR	N-CA-CB	-5.20	102.64	111.17
1	A	343	LEU	CD1-CG-CD2	-5.20	99.36	110.80
1	B	221	PHE	CG-CD2-CE2	5.20	129.54	120.70
1	C	273	ASP	N-CA-CB	-5.20	101.71	110.49
1	C	558	TYR	CA-C-N	-5.20	113.36	122.62
1	C	558	TYR	C-N-CA	-5.20	113.36	122.62
1	D	271	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	C	420	GLY	CA-C-N	-5.20	114.51	122.62
1	C	420	GLY	C-N-CA	-5.20	114.51	122.62
1	E	144	MET	CA-CB-CG	5.20	124.49	114.10
1	F	562	CYS	N-CA-CB	-5.20	102.47	110.16
1	A	306	THR	N-CA-CB	-5.20	102.41	110.57
1	B	271	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	C	353	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	D	272	PRO	O-C-N	5.20	129.20	122.24
1	D	343	LEU	CB-CG-CD1	-5.20	95.12	110.70
1	E	327	ILE	CA-C-O	-5.20	115.15	120.71
1	F	306	THR	N-CA-CB	-5.20	102.41	110.57
1	A	384	HIS	N-CA-CB	5.19	118.61	110.46
1	B	591	LYS	O-C-N	5.19	129.45	122.49
1	D	508	PHE	CA-CB-CG	5.19	118.99	113.80
1	D	562	CYS	N-CA-CB	-5.19	102.47	110.16
1	B	9	GLN	CA-CB-CG	-5.19	103.72	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	272	PRO	O-C-N	5.19	129.20	122.24
1	B	427	ASP	CA-C-N	-5.19	112.81	121.94
1	B	427	ASP	C-N-CA	-5.19	112.81	121.94
1	C	126	SER	CB-CA-C	-5.19	100.77	109.65
1	F	273	ASP	N-CA-CB	-5.19	101.72	110.49
1	F	343	LEU	CB-CG-CD1	-5.19	95.13	110.70
1	A	144	MET	CA-CB-CG	5.19	124.48	114.10
1	E	153	LYS	CA-C-N	-5.19	111.86	120.68
1	E	153	LYS	C-N-CA	-5.19	111.86	120.68
1	A	427	ASP	CA-C-N	-5.19	112.81	121.94
1	A	427	ASP	C-N-CA	-5.19	112.81	121.94
1	B	153	LYS	CA-C-N	-5.19	111.86	120.68
1	B	153	LYS	C-N-CA	-5.19	111.86	120.68
1	C	105	TYR	O-C-N	5.19	127.48	122.09
1	C	427	ASP	CB-CA-C	-5.19	100.10	110.42
1	C	508	PHE	CA-CB-CG	5.19	118.99	113.80
1	E	558	TYR	CA-C-N	-5.19	113.39	122.62
1	E	558	TYR	C-N-CA	-5.19	113.39	122.62
1	F	48	ASP	CB-CG-OD2	-5.19	106.47	118.40
1	A	105	TYR	O-C-N	5.19	127.48	122.09
1	C	343	LEU	CB-CG-CD1	-5.19	95.14	110.70
1	A	153	LYS	CA-C-N	-5.18	111.86	120.68
1	A	153	LYS	C-N-CA	-5.18	111.86	120.68
1	A	327	ILE	CA-C-O	-5.18	115.16	120.71
1	A	343	LEU	CB-CG-CD1	-5.18	95.15	110.70
1	C	153	LYS	CA-C-N	-5.18	111.87	120.68
1	C	153	LYS	C-N-CA	-5.18	111.87	120.68
1	E	343	LEU	CD1-CG-CD2	-5.18	99.39	110.80
1	F	427	ASP	CB-CA-C	-5.18	100.10	110.42
1	A	508	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	343	LEU	CB-CG-CD1	-5.18	95.15	110.70
1	C	9	GLN	CA-CB-CG	-5.18	103.74	114.10
1	D	306	THR	N-CA-CB	-5.18	102.43	110.57
1	E	250	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	F	153	LYS	CA-C-N	-5.18	111.87	120.68
1	F	153	LYS	C-N-CA	-5.18	111.87	120.68
1	F	272	PRO	O-C-N	5.18	129.18	122.24
1	F	343	LEU	CD1-CG-CD2	-5.18	99.40	110.80
1	A	591	LYS	O-C-N	5.18	129.43	122.49
1	B	449	ASN	O-C-N	-5.18	116.42	123.15
1	F	250	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	B	508	PHE	CA-CB-CG	5.18	118.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	611	VAL	CB-CA-C	5.18	119.78	111.29
1	D	48	ASP	CB-CG-OD2	-5.18	106.48	118.40
1	E	48	ASP	CB-CG-OD2	-5.18	106.49	118.40
1	E	306	THR	N-CA-CB	-5.18	102.44	110.57
1	F	105	TYR	O-C-N	5.18	127.48	122.09
1	D	105	TYR	O-C-N	5.18	127.47	122.09
1	D	427	ASP	CA-C-N	-5.18	112.83	121.94
1	D	427	ASP	C-N-CA	-5.18	112.83	121.94
1	A	48	ASP	CB-CG-OD2	-5.18	106.49	118.40
1	A	562	CYS	N-CA-CB	-5.18	102.50	110.16
1	B	144	MET	CA-CB-CG	5.18	124.45	114.10
1	D	521	ARG	CD-NE-CZ	-5.18	117.15	124.40
1	E	273	ASP	N-CA-CB	-5.18	101.74	110.49
1	E	343	LEU	CB-CG-CD1	-5.18	95.17	110.70
1	F	427	ASP	CA-C-N	-5.18	112.83	121.94
1	F	427	ASP	C-N-CA	-5.18	112.83	121.94
1	A	9	GLN	CA-CB-CG	-5.17	103.75	114.10
1	A	271	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	C	596	HIS	CA-CB-CG	-5.17	108.62	113.80
1	D	2	ALA	CA-C-N	5.17	129.53	122.34
1	D	2	ALA	C-N-CA	5.17	129.53	122.34
1	E	253	ARG	CB-CA-C	5.17	118.93	110.96
1	E	427	ASP	CA-C-N	-5.17	112.83	121.94
1	E	427	ASP	C-N-CA	-5.17	112.83	121.94
1	F	187	ASP	CA-C-O	5.17	126.96	121.16
1	F	508	PHE	CA-CB-CG	5.17	118.97	113.80
1	C	2	ALA	CA-C-N	5.17	129.53	122.34
1	C	2	ALA	C-N-CA	5.17	129.53	122.34
1	C	221	PHE	CG-CD2-CE2	5.17	129.49	120.70
1	E	180	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	E	353	ARG	NE-CZ-NH2	-5.17	114.54	119.20
1	A	221	PHE	CG-CD2-CE2	5.17	129.49	120.70
1	B	596	HIS	CA-CB-CG	-5.17	108.63	113.80
1	C	494	THR	N-CA-CB	-5.17	102.69	111.17
1	D	453	HIS	N-CA-C	5.17	117.04	108.20
1	F	271	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	F	272	PRO	N-CA-C	5.17	120.56	113.84
1	A	2	ALA	CA-C-N	5.17	129.53	122.34
1	A	2	ALA	C-N-CA	5.17	129.53	122.34
1	B	562	CYS	N-CA-CB	-5.17	102.51	110.16
1	C	427	ASP	CA-C-N	-5.17	112.84	121.94
1	C	427	ASP	C-N-CA	-5.17	112.84	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	221	PHE	CG-CD2-CE2	5.17	129.49	120.70
1	D	611	VAL	CB-CA-C	5.17	119.77	111.29
1	E	453	HIS	N-CA-C	5.17	117.04	108.20
1	F	9	GLN	CA-CB-CG	-5.17	103.76	114.10
1	A	427	ASP	CB-CA-C	-5.17	100.14	110.42
1	C	48	ASP	CB-CG-OD2	-5.17	106.51	118.40
1	C	144	MET	CA-CB-CG	5.17	124.44	114.10
1	C	449	ASN	O-C-N	-5.17	116.43	123.15
1	C	562	CYS	N-CA-CB	-5.17	102.51	110.16
1	C	611	VAL	CB-CA-C	5.17	119.77	111.29
1	D	427	ASP	CB-CA-C	-5.17	100.13	110.42
1	E	9	GLN	CA-CB-CG	-5.17	103.76	114.10
1	F	453	HIS	N-CA-C	5.17	117.04	108.20
1	C	593	THR	O-C-N	5.17	129.46	122.59
1	E	272	PRO	N-CA-C	5.17	120.56	113.84
1	F	178	GLU	N-CA-C	-5.17	99.80	110.80
1	F	380	PHE	N-CA-C	-5.17	105.54	111.07
1	F	449	ASN	O-C-N	-5.17	116.43	123.15
1	B	322	GLU	OE1-CD-OE2	-5.17	110.50	122.90
1	D	152	ASP	CA-C-O	-5.17	114.03	119.97
1	D	178	GLU	N-CA-C	-5.17	99.80	110.80
1	A	453	HIS	N-CA-C	5.16	117.03	108.20
1	B	180	ARG	CA-C-N	-5.16	112.68	121.97
1	B	180	ARG	C-N-CA	-5.16	112.68	121.97
1	B	272	PRO	N-CA-C	5.16	120.55	113.84
1	B	521	ARG	CD-NE-CZ	-5.16	117.17	124.40
1	C	46	TYR	CA-C-O	-5.16	114.50	120.49
1	D	9	GLN	CA-CB-CG	-5.16	103.77	114.10
1	D	449	ASN	O-C-N	-5.16	116.44	123.15
1	F	591	LYS	O-C-N	5.16	129.41	122.49
1	A	380	PHE	N-CA-C	-5.16	105.55	111.07
1	B	152	ASP	CA-C-O	-5.16	114.03	119.97
1	C	591	LYS	O-C-N	5.16	129.41	122.49
1	E	221	PHE	CG-CD2-CE2	5.16	129.48	120.70
1	B	327	ILE	CA-C-O	-5.16	115.19	120.71
1	B	427	ASP	CB-CA-C	-5.16	100.15	110.42
1	C	152	ASP	CA-C-O	-5.16	114.04	119.97
1	C	384	HIS	N-CA-CB	5.16	118.56	110.46
1	F	9	GLN	N-CA-C	-5.16	105.20	112.12
1	F	221	PHE	CG-CD2-CE2	5.16	129.47	120.70
1	A	178	GLU	N-CA-C	-5.16	99.81	110.80
1	B	16	HIS	CA-C-N	5.16	127.15	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	16	HIS	C-N-CA	5.16	127.15	120.44
1	D	153	LYS	CA-C-N	-5.16	111.91	120.68
1	D	153	LYS	C-N-CA	-5.16	111.91	120.68
1	E	47	ASN	OD1-CG-ND2	5.16	127.76	122.60
1	E	427	ASP	CB-CA-C	-5.16	100.15	110.42
1	E	562	CYS	N-CA-CB	-5.16	102.53	110.16
1	B	539	LEU	CB-CG-CD2	-5.16	95.23	110.70
1	A	354	GLN	CG-CD-NE2	5.16	124.13	116.40
1	A	596	HIS	CA-CB-CG	-5.16	108.64	113.80
1	B	48	ASP	CB-CG-OD2	-5.16	106.54	118.40
1	B	177	ARG	CG-CD-NE	-5.16	100.66	112.00
1	D	354	GLN	CG-CD-NE2	5.16	124.13	116.40
1	E	9	GLN	N-CA-C	-5.16	105.21	112.12
1	F	2	ALA	CA-C-N	5.16	129.51	122.34
1	F	2	ALA	C-N-CA	5.16	129.51	122.34
1	F	596	HIS	CA-CB-CG	-5.16	108.64	113.80
1	C	453	HIS	N-CA-C	5.15	117.01	108.20
1	D	272	PRO	N-CA-C	5.15	120.54	113.84
1	D	370	HIS	ND1-CE1-NE2	5.15	113.55	108.40
1	D	380	PHE	N-CA-C	-5.15	105.56	111.07
1	E	271	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	F	16	HIS	CA-C-N	5.15	127.14	120.44
1	F	16	HIS	C-N-CA	5.15	127.14	120.44
1	F	152	ASP	CA-C-O	-5.15	114.04	119.97
1	F	177	ARG	CG-CD-NE	-5.15	100.66	112.00
1	A	449	ASN	O-C-N	-5.15	116.45	123.15
1	A	611	VAL	CB-CA-C	5.15	119.74	111.29
1	B	180	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	B	187	ASP	CA-C-O	5.15	126.93	121.16
1	B	216	LYS	CA-C-O	-5.15	114.78	120.70
1	B	634	ARG	CB-CA-C	5.15	120.67	110.42
1	D	66	LEU	CA-C-O	-5.15	116.09	121.55
1	A	258	PRO	CA-C-N	-5.15	114.57	122.61
1	A	258	PRO	C-N-CA	-5.15	114.57	122.61
1	C	16	HIS	CA-C-N	5.15	127.14	120.44
1	C	16	HIS	C-N-CA	5.15	127.14	120.44
1	C	178	GLU	N-CA-C	-5.15	99.83	110.80
1	D	634	ARG	CB-CA-C	5.15	120.67	110.42
1	E	216	LYS	CA-C-O	-5.15	114.78	120.70
1	E	596	HIS	CA-CB-CG	-5.15	108.65	113.80
1	F	611	VAL	CB-CA-C	5.15	119.73	111.29
1	B	105	TYR	O-C-N	5.15	127.44	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	29	ASP	CA-C-O	5.15	126.23	120.82
1	D	539	LEU	CB-CG-CD2	-5.15	95.25	110.70
1	E	16	HIS	CA-C-N	5.15	127.13	120.44
1	E	16	HIS	C-N-CA	5.15	127.13	120.44
1	F	354	GLN	CG-CD-NE2	5.15	124.12	116.40
1	A	187	ASP	CA-C-O	5.15	126.93	121.16
1	A	253	ARG	CB-CA-C	5.15	118.89	110.96
1	A	272	PRO	N-CA-C	5.15	120.53	113.84
1	B	178	GLU	N-CA-C	-5.15	99.83	110.80
1	C	9	GLN	N-CA-C	-5.15	105.22	112.12
1	C	180	ARG	CA-C-N	-5.15	112.70	121.97
1	C	180	ARG	C-N-CA	-5.15	112.70	121.97
1	C	546	ALA	CA-C-N	-5.15	113.00	121.34
1	C	546	ALA	C-N-CA	-5.15	113.00	121.34
1	C	634	ARG	CB-CA-C	5.15	120.66	110.42
1	D	253	ARG	CB-CA-C	5.15	118.89	110.96
1	D	258	PRO	CA-C-N	-5.15	114.58	122.61
1	D	258	PRO	C-N-CA	-5.15	114.58	122.61
1	E	634	ARG	CB-CA-C	5.15	120.66	110.42
1	F	180	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	F	182	ALA	N-CA-C	5.15	116.89	111.28
1	F	327	ILE	CA-C-O	-5.15	115.20	120.71
1	A	539	LEU	CB-CG-CD2	-5.15	95.26	110.70
1	E	76	ASN	CB-CA-C	-5.15	102.85	110.67
1	E	539	LEU	CB-CG-CD2	-5.15	95.26	110.70
1	A	16	HIS	CA-C-N	5.14	127.13	120.44
1	A	16	HIS	C-N-CA	5.14	127.13	120.44
1	B	76	ASN	CB-CA-C	-5.14	102.85	110.67
1	C	177	ARG	CG-CD-NE	-5.14	100.68	112.00
1	C	322	GLU	OE1-CD-OE2	-5.14	110.55	122.90
1	D	100	ARG	CB-CG-CD	5.14	123.13	111.30
1	D	182	ALA	N-CA-C	5.14	116.89	111.28
1	F	47	ASN	OD1-CG-ND2	5.14	127.75	122.60
1	A	177	ARG	CG-CD-NE	-5.14	100.69	112.00
1	B	253	ARG	CB-CA-C	5.14	118.88	110.96
1	B	453	HIS	N-CA-C	5.14	116.99	108.20
1	C	354	GLN	CG-CD-NE2	5.14	124.11	116.40
1	D	152	ASP	OD1-CG-OD2	-5.14	110.56	122.90
1	D	322	GLU	OE1-CD-OE2	-5.14	110.56	122.90
1	F	253	ARG	CB-CA-C	5.14	118.88	110.96
1	F	521	ARG	CD-NE-CZ	-5.14	117.20	124.40
1	B	66	LEU	CA-C-O	-5.14	116.10	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	254	GLU	CG-CD-OE2	5.14	130.22	118.40
1	E	2	ALA	CA-C-N	5.14	129.49	122.34
1	E	2	ALA	C-N-CA	5.14	129.49	122.34
1	E	66	LEU	CA-C-O	-5.14	116.10	121.55
1	F	225	HIS	CA-C-O	5.14	125.88	119.97
1	F	322	GLU	OE1-CD-OE2	-5.14	110.56	122.90
1	A	634	ARG	CB-CA-C	5.14	120.65	110.42
1	B	546	ALA	CA-C-N	-5.14	113.01	121.34
1	B	546	ALA	C-N-CA	-5.14	113.01	121.34
1	C	182	ALA	N-CA-C	5.14	116.88	111.28
1	C	304	TYR	N-CA-CB	-5.14	102.61	111.55
1	E	177	ARG	CG-CD-NE	-5.14	100.69	112.00
1	E	180	ARG	CA-C-N	-5.14	112.72	121.97
1	E	180	ARG	C-N-CA	-5.14	112.72	121.97
1	E	182	ALA	N-CA-C	5.14	116.88	111.28
1	F	180	ARG	CA-C-N	-5.14	112.72	121.97
1	F	180	ARG	C-N-CA	-5.14	112.72	121.97
1	F	254	GLU	CG-CD-OE2	5.14	130.22	118.40
1	F	301	ASP	CA-C-O	-5.14	114.06	119.97
1	F	634	ARG	CB-CA-C	5.14	120.65	110.42
1	A	322	GLU	OE1-CD-OE2	-5.14	110.57	122.90
1	D	16	HIS	CA-C-N	5.14	127.12	120.44
1	D	16	HIS	C-N-CA	5.14	127.12	120.44
1	D	526	SER	CA-C-O	-5.14	115.89	121.44
1	E	152	ASP	OD1-CG-OD2	-5.14	110.57	122.90
1	E	178	GLU	N-CA-C	-5.14	99.86	110.80
1	E	526	SER	CA-C-O	-5.14	115.89	121.44
1	A	370	HIS	ND1-CE1-NE2	5.14	113.54	108.40
1	B	354	GLN	CG-CD-NE2	5.14	124.11	116.40
1	C	29	ASP	CA-C-O	5.14	126.21	120.82
1	C	152	ASP	OD1-CG-OD2	-5.14	110.57	122.90
1	C	539	LEU	CB-CG-CD2	-5.14	95.29	110.70
1	E	322	GLU	OE1-CD-OE2	-5.14	110.57	122.90
1	F	66	LEU	CA-C-O	-5.14	116.11	121.55
1	F	258	PRO	CA-C-N	-5.14	114.60	122.61
1	F	258	PRO	C-N-CA	-5.14	114.60	122.61
1	A	9	GLN	N-CA-C	-5.13	105.24	112.12
1	A	152	ASP	CA-C-O	-5.13	114.06	119.97
1	D	76	ASN	CB-CA-C	-5.13	102.86	110.67
1	E	29	ASP	CA-C-O	5.13	126.21	120.82
1	E	105	TYR	O-C-N	5.13	127.43	122.09
1	E	373	THR	O-C-N	-5.13	116.49	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	611	VAL	CB-CA-C	5.13	119.71	111.29
1	F	508	PHE	CA-C-O	-5.13	115.24	120.99
1	F	539	LEU	CB-CG-CD2	-5.13	95.29	110.70
1	A	521	ARG	CD-NE-CZ	-5.13	117.21	124.40
1	D	177	ARG	CG-CD-NE	-5.13	100.71	112.00
1	F	50	GLY	O-C-N	5.13	126.67	122.51
1	F	526	SER	CA-C-O	-5.13	115.90	121.44
1	A	76	ASN	CB-CA-C	-5.13	102.87	110.67
1	A	152	ASP	OD1-CG-OD2	-5.13	110.59	122.90
1	B	152	ASP	OD1-CG-OD2	-5.13	110.59	122.90
1	C	76	ASN	CB-CA-C	-5.13	102.87	110.67
1	C	272	PRO	N-CA-C	5.13	120.51	113.84
1	C	308	SER	CB-CA-C	-5.13	101.14	110.63
1	F	100	ARG	CB-CG-CD	5.13	123.10	111.30
1	F	370	HIS	ND1-CE1-NE2	5.13	113.53	108.40
1	B	182	ALA	N-CA-C	5.13	116.87	111.28
1	C	301	ASP	CA-C-O	-5.13	114.07	119.97
1	C	380	PHE	N-CA-C	-5.13	105.58	111.07
1	A	100	ARG	CB-CG-CD	5.13	123.10	111.30
1	A	180	ARG	CA-C-N	-5.13	112.74	121.97
1	A	180	ARG	C-N-CA	-5.13	112.74	121.97
1	A	182	ALA	N-CA-C	5.13	116.87	111.28
1	B	100	ARG	CB-CG-CD	5.13	123.10	111.30
1	B	308	SER	CB-CA-C	-5.13	101.14	110.63
1	B	481	PHE	N-CA-C	5.13	118.47	110.32
1	D	546	ALA	CA-C-N	-5.13	113.03	121.34
1	D	546	ALA	C-N-CA	-5.13	113.03	121.34
1	E	225	HIS	CA-C-O	5.13	125.87	119.97
1	E	546	ALA	CA-C-N	-5.13	113.03	121.34
1	E	546	ALA	C-N-CA	-5.13	113.03	121.34
1	F	76	ASN	CB-CA-C	-5.13	102.88	110.67
1	F	373	THR	O-C-N	-5.13	116.50	122.09
1	F	628	ARG	NH1-CZ-NH2	5.13	125.97	119.30
1	A	29	ASP	CA-C-O	5.13	126.20	120.82
1	B	258	PRO	CA-C-N	-5.13	114.61	122.61
1	B	258	PRO	C-N-CA	-5.13	114.61	122.61
1	C	253	ARG	CB-CA-C	5.13	118.86	110.96
1	C	258	PRO	CA-C-N	-5.13	114.61	122.61
1	C	258	PRO	C-N-CA	-5.13	114.61	122.61
1	D	267	GLU	CG-CD-OE2	5.13	130.19	118.40
1	E	100	ARG	CB-CG-CD	5.13	123.09	111.30
1	E	258	PRO	CA-C-N	-5.12	114.61	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	258	PRO	C-N-CA	-5.12	114.61	122.61
1	F	29	ASP	CA-C-O	5.12	126.20	120.82
1	A	180	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	B	9	GLN	N-CA-C	-5.12	105.26	112.12
1	B	370	HIS	ND1-CE1-NE2	5.12	113.52	108.40
1	B	628	ARG	N-CA-C	5.12	117.94	109.85
1	C	187	ASP	CA-C-O	5.12	126.90	121.16
1	C	373	THR	O-C-N	-5.12	116.51	122.09
1	D	301	ASP	CA-C-O	-5.12	114.08	119.97
1	D	628	ARG	N-CA-C	5.12	117.94	109.85
1	E	152	ASP	CA-C-O	-5.12	114.08	119.97
1	F	308	SER	CB-CA-C	-5.12	101.15	110.63
1	A	50	GLY	O-C-N	5.12	126.66	122.51
1	C	254	GLU	CG-CD-OE2	5.12	130.18	118.40
1	D	295	ARG	N-CA-C	-5.12	105.70	111.28
1	D	308	SER	CB-CA-C	-5.12	101.16	110.63
1	E	267	GLU	CG-CD-OE2	5.12	130.18	118.40
1	E	521	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	F	152	ASP	OD1-CG-OD2	-5.12	110.61	122.90
1	A	304	TYR	N-CA-CB	-5.12	102.64	111.55
1	B	29	ASP	CA-C-O	5.12	126.20	120.82
1	B	622	LEU	O-C-N	-5.12	117.25	123.29
1	C	216	LYS	CA-C-O	-5.12	114.81	120.70
1	D	9	GLN	N-CA-C	-5.12	105.26	112.12
1	F	385	LYS	CB-CG-CD	-5.12	99.52	111.30
1	A	546	ALA	CA-C-N	-5.12	113.05	121.34
1	A	546	ALA	C-N-CA	-5.12	113.05	121.34
1	D	187	ASP	CA-C-O	5.12	126.89	121.16
1	E	187	ASP	CA-C-O	5.12	126.89	121.16
1	F	538	SER	CA-C-O	-5.12	113.19	120.51
1	A	254	GLU	CG-CD-OE2	5.12	130.17	118.40
1	A	308	SER	CB-CA-C	-5.12	101.16	110.63
1	A	385	LYS	CB-CG-CD	-5.12	99.53	111.30
1	A	526	SER	CA-C-O	-5.12	115.91	121.44
1	C	100	ARG	CB-CG-CD	5.12	123.07	111.30
1	E	370	HIS	ND1-CE1-NE2	5.12	113.52	108.40
1	B	538	SER	CA-C-O	-5.12	113.19	120.51
1	C	63	HIS	CA-C-O	5.12	127.83	120.51
1	F	628	ARG	N-CA-C	5.12	117.93	109.85
1	A	216	LYS	CA-C-O	-5.11	114.82	120.70
1	B	254	GLU	CG-CD-OE2	5.11	130.16	118.40
1	B	526	SER	CA-C-O	-5.11	115.92	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	50	GLY	O-C-N	5.11	126.65	122.51
1	D	304	TYR	N-CA-CB	-5.11	102.65	111.55
1	D	385	LYS	CB-CG-CD	-5.11	99.54	111.30
1	D	596	HIS	CA-CB-CG	-5.11	108.69	113.80
1	F	546	ALA	CA-C-N	-5.11	113.06	121.34
1	F	546	ALA	C-N-CA	-5.11	113.06	121.34
1	A	301	ASP	CA-C-O	-5.11	114.09	119.97
1	C	370	HIS	ND1-CE1-NE2	5.11	113.51	108.40
1	F	216	LYS	CA-C-O	-5.11	114.82	120.70
1	A	66	LEU	CA-C-O	-5.11	116.13	121.55
1	C	267	GLU	CG-CD-OE2	5.11	130.15	118.40
1	C	521	ARG	CD-NE-CZ	-5.11	117.24	124.40
1	D	50	GLY	O-C-N	5.11	126.65	122.51
1	D	481	PHE	N-CA-C	5.11	118.45	110.32
1	E	301	ASP	CA-C-O	-5.11	114.09	119.97
1	E	354	GLN	CG-CD-NE2	5.11	124.06	116.40
1	E	385	LYS	CB-CG-CD	-5.11	99.55	111.30
1	E	449	ASN	O-C-N	-5.11	116.51	123.15
1	A	63	HIS	CA-C-O	5.11	127.82	120.51
1	B	350	MET	CB-CG-SD	-5.11	97.37	112.70
1	D	216	LYS	CA-C-O	-5.11	114.83	120.70
1	A	508	PHE	CA-C-O	-5.11	115.27	120.99
1	B	295	ARG	N-CA-C	-5.11	105.71	111.28
1	C	385	LYS	CB-CG-CD	-5.11	99.55	111.30
1	E	308	SER	CB-CA-C	-5.11	101.18	110.63
1	F	304	TYR	N-CA-CB	-5.11	102.66	111.55
1	A	225	HIS	CA-C-O	5.11	125.84	119.97
1	C	481	PHE	N-CA-C	5.11	118.44	110.32
1	C	628	ARG	NH1-CZ-NH2	5.11	125.94	119.30
1	F	615	ALA	N-CA-CB	-5.11	101.44	109.51
1	A	523	SER	CB-CA-C	-5.10	100.26	110.42
1	E	254	GLU	CG-CD-OE2	5.10	130.14	118.40
1	E	628	ARG	N-CA-C	5.10	117.91	109.85
1	A	267	GLU	CG-CD-OE2	5.10	130.13	118.40
1	A	373	THR	O-C-N	-5.10	116.53	122.09
1	B	385	LYS	CB-CG-CD	-5.10	99.57	111.30
1	B	523	SER	CB-CA-C	-5.10	100.27	110.42
1	C	66	LEU	CA-C-O	-5.10	116.14	121.55
1	C	267	GLU	CG-CD-OE1	-5.10	106.66	118.40
1	C	523	SER	CB-CA-C	-5.10	100.27	110.42
1	D	180	ARG	CA-C-N	-5.10	112.78	121.97
1	D	180	ARG	C-N-CA	-5.10	112.78	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	523	SER	CB-CA-C	-5.10	100.26	110.42
1	E	350	MET	CB-CG-SD	-5.10	97.39	112.70
1	F	235	ARG	CB-CG-CD	-5.10	99.56	111.30
1	F	267	GLU	CG-CD-OE2	5.10	130.14	118.40
1	F	496	ASP	CB-CA-C	5.10	120.58	110.42
1	A	481	PHE	N-CA-C	5.10	118.43	110.32
1	A	628	ARG	N-CA-C	5.10	117.91	109.85
1	B	304	TYR	N-CA-CB	-5.10	102.67	111.55
1	B	373	THR	O-C-N	-5.10	116.53	122.09
1	C	526	SER	CA-C-O	-5.10	115.93	121.44
1	D	267	GLU	CG-CD-OE1	-5.10	106.67	118.40
1	B	225	HIS	CA-C-O	5.10	125.83	119.97
1	E	295	ARG	N-CA-C	-5.10	105.72	111.28
1	E	304	TYR	N-CA-CB	-5.10	102.68	111.55
1	E	622	LEU	O-C-N	-5.10	117.27	123.29
1	D	628	ARG	NH1-CZ-NH2	5.10	125.93	119.30
1	E	267	GLU	CG-CD-OE1	-5.10	106.67	118.40
1	E	523	SER	CB-CA-C	-5.10	100.28	110.42
1	B	267	GLU	CG-CD-OE2	5.10	130.12	118.40
1	C	235	ARG	CB-CG-CD	-5.10	99.58	111.30
1	D	350	MET	CB-CG-SD	-5.10	97.41	112.70
1	F	523	SER	CB-CA-C	-5.10	100.28	110.42
1	A	295	ARG	N-CA-C	-5.09	105.73	111.28
1	A	350	MET	CB-CG-SD	-5.09	97.41	112.70
1	C	615	ALA	N-CA-CB	-5.09	101.46	109.51
1	C	622	LEU	O-C-N	-5.09	117.28	123.29
1	D	235	ARG	CB-CG-CD	-5.09	99.58	111.30
1	E	481	PHE	N-CA-C	5.09	118.42	110.32
1	E	628	ARG	NH1-CZ-NH2	5.09	125.92	119.30
1	F	312	THR	N-CA-C	-5.09	101.00	109.46
1	B	496	ASP	CB-CA-C	5.09	120.56	110.42
1	B	628	ARG	NH1-CZ-NH2	5.09	125.92	119.30
1	C	350	MET	CB-CG-SD	-5.09	97.42	112.70
1	D	63	HIS	CA-C-O	5.09	127.79	120.51
1	A	267	GLU	CG-CD-OE1	-5.09	106.69	118.40
1	D	224	HIS	CA-CB-CG	5.09	118.89	113.80
1	F	295	ARG	N-CA-C	-5.09	105.73	111.28
1	A	235	ARG	CB-CG-CD	-5.09	99.59	111.30
1	A	538	SER	CA-C-O	-5.09	113.23	120.51
1	B	63	HIS	CA-C-O	5.09	127.79	120.51
1	E	235	ARG	CB-CG-CD	-5.09	99.59	111.30
1	F	367	VAL	CA-CB-CG1	5.09	119.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	481	PHE	N-CA-C	5.09	118.41	110.32
1	A	628	ARG	NH1-CZ-NH2	5.09	125.91	119.30
1	D	538	SER	CA-C-O	-5.09	113.23	120.51
1	E	50	GLY	O-C-N	5.09	126.63	122.51
1	E	508	PHE	CA-C-O	-5.09	115.29	120.99
1	E	538	SER	CA-C-O	-5.09	113.23	120.51
1	F	350	MET	CB-CG-SD	-5.09	97.44	112.70
1	A	496	ASP	CB-CA-C	5.09	120.54	110.42
1	B	50	GLY	O-C-N	5.09	126.63	122.51
1	B	267	GLU	CG-CD-OE1	-5.09	106.70	118.40
1	C	180	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	E	367	VAL	CA-CB-CG1	5.09	119.05	110.40
1	F	63	HIS	CA-C-O	5.09	127.78	120.51
1	F	215	ARG	NH1-CZ-NH2	5.09	125.91	119.30
1	B	534	PRO	CA-C-O	-5.08	111.35	120.60
1	C	508	PHE	CA-C-O	-5.08	115.30	120.99
1	D	357	PRO	O-C-N	5.08	129.50	122.64
1	A	215	ARG	NH1-CZ-NH2	5.08	125.91	119.30
1	C	200	ASP	OD1-CG-OD2	-5.08	110.70	122.90
1	C	225	HIS	CA-C-O	5.08	125.82	119.97
1	E	534	PRO	CA-C-O	-5.08	111.35	120.60
1	C	295	ARG	N-CA-C	-5.08	105.74	111.28
1	C	496	ASP	CB-CA-C	5.08	120.53	110.42
1	D	496	ASP	CB-CA-C	5.08	120.53	110.42
1	D	508	PHE	CA-C-O	-5.08	115.30	120.99
1	B	215	ARG	NH1-CZ-NH2	5.08	125.90	119.30
1	B	528	VAL	CA-CB-CG1	-5.08	101.77	110.40
1	B	615	ALA	N-CA-CB	-5.08	101.49	109.51
1	C	224	HIS	CA-CB-CG	5.08	118.88	113.80
1	E	63	HIS	CA-C-O	5.08	127.77	120.51
1	A	615	ALA	N-CA-CB	-5.08	101.49	109.51
1	C	357	PRO	O-C-N	5.08	129.49	122.64
1	A	367	VAL	CA-CB-CG1	5.08	119.03	110.40
1	B	235	ARG	CB-CG-CD	-5.08	99.63	111.30
1	B	306	THR	CB-CA-C	5.08	118.50	109.72
1	C	312	THR	N-CA-C	-5.08	101.03	109.46
1	C	367	VAL	CA-CB-CG1	5.08	119.03	110.40
1	C	628	ARG	N-CA-C	5.08	117.87	109.85
1	D	180	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	D	534	PRO	CA-C-O	-5.08	111.36	120.60
1	E	215	ARG	NH1-CZ-NH2	5.08	125.90	119.30
1	B	367	VAL	CA-CB-CG1	5.07	119.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	482	LEU	N-CA-C	-5.07	97.10	107.70
1	D	367	VAL	CA-CB-CG1	5.07	119.02	110.40
1	D	373	THR	O-C-N	-5.07	116.56	122.09
1	E	496	ASP	CB-CA-C	5.07	120.52	110.42
1	F	12	GLN	CA-CB-CG	5.07	124.25	114.10
1	A	312	THR	N-CA-C	-5.07	101.04	109.46
1	A	534	PRO	CA-C-O	-5.07	111.37	120.60
1	E	615	ALA	N-CA-CB	-5.07	101.50	109.51
1	F	146	THR	O-C-N	5.07	128.74	123.06
1	A	622	LEU	O-C-N	-5.07	117.31	123.29
1	C	306	THR	CB-CA-C	5.07	118.49	109.72
1	E	200	ASP	OD1-CG-OD2	-5.07	110.73	122.90
1	F	267	GLU	CG-CD-OE1	-5.07	106.74	118.40
1	A	357	PRO	O-C-N	5.07	129.48	122.64
1	D	225	HIS	CA-C-O	5.07	125.80	119.97
1	D	312	THR	N-CA-C	-5.07	101.05	109.46
1	D	200	ASP	OD1-CG-OD2	-5.07	110.74	122.90
1	D	615	ALA	N-CA-CB	-5.07	101.50	109.51
1	F	29	ASP	N-CA-C	-5.07	105.65	111.07
1	A	200	ASP	OD1-CG-OD2	-5.07	110.74	122.90
1	B	29	ASP	N-CA-C	-5.07	105.65	111.07
1	B	508	PHE	CA-C-O	-5.07	115.32	120.99
1	A	224	HIS	CA-CB-CG	5.06	118.86	113.80
1	F	357	PRO	O-C-N	5.06	129.48	122.64
1	C	353	ARG	N-CA-C	-5.06	106.95	113.02
1	D	42	ASP	CA-C-O	5.06	127.75	120.51
1	E	12	GLN	CA-CB-CG	5.06	124.22	114.10
1	E	306	THR	CB-CA-C	5.06	118.48	109.72
1	E	650	VAL	CG1-CB-CG2	5.06	121.94	110.80
1	A	528	VAL	CA-CB-CG1	-5.06	101.80	110.40
1	B	200	ASP	OD1-CG-OD2	-5.06	110.75	122.90
1	C	528	VAL	CA-CB-CG1	-5.06	101.80	110.40
1	A	12	GLN	CA-CB-CG	5.06	124.22	114.10
1	A	482	LEU	N-CA-C	-5.06	97.13	107.70
1	B	357	PRO	O-C-N	5.06	129.47	122.64
1	C	538	SER	CA-C-O	-5.06	113.27	120.51
1	D	622	LEU	O-C-N	-5.06	117.32	123.29
1	E	29	ASP	N-CA-C	-5.06	105.66	111.07
1	F	353	ARG	N-CA-C	-5.06	106.95	113.02
1	A	306	THR	CB-CA-C	5.06	118.47	109.72
1	A	29	ASP	N-CA-C	-5.06	105.66	111.07
1	B	301	ASP	CA-C-O	-5.06	114.16	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	482	LEU	N-CA-C	-5.06	97.13	107.70
1	E	312	THR	N-CA-C	-5.06	101.07	109.46
1	C	478	PHE	N-CA-CB	5.05	117.57	110.24
1	E	14	ILE	CB-CA-C	5.05	118.13	111.81
1	E	42	ASP	CA-C-O	5.05	127.74	120.51
1	E	224	HIS	CA-CB-CG	5.05	118.85	113.80
1	F	14	ILE	CB-CA-C	5.05	118.13	111.81
1	F	200	ASP	OD1-CG-OD2	-5.05	110.77	122.90
1	F	534	PRO	CA-C-O	-5.05	111.40	120.60
1	B	312	THR	N-CA-C	-5.05	101.07	109.46
1	D	541	GLU	CB-CG-CD	5.05	121.19	112.60
1	C	12	GLN	CA-CB-CG	5.05	124.20	114.10
1	C	333	TYR	CB-CG-CD1	5.05	128.38	120.80
1	D	29	ASP	N-CA-C	-5.05	105.66	111.07
1	D	482	LEU	N-CA-C	-5.05	97.14	107.70
1	F	541	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	14	ILE	CB-CA-C	5.05	118.12	111.81
1	A	353	ARG	N-CA-C	-5.05	106.96	113.02
1	C	534	PRO	CA-C-O	-5.05	111.41	120.60
1	D	528	VAL	CA-CB-CG1	-5.05	101.82	110.40
1	F	528	VAL	CA-CB-CG1	-5.05	101.82	110.40
1	B	650	VAL	CG1-CB-CG2	5.05	121.91	110.80
1	E	528	VAL	CA-CB-CG1	-5.05	101.82	110.40
1	A	333	TYR	CB-CG-CD1	5.05	128.37	120.80
1	B	12	GLN	CA-CB-CG	5.05	124.19	114.10
1	C	127	LYS	N-CA-CB	-5.05	102.42	109.94
1	D	478	PHE	N-CA-CB	5.05	117.56	110.24
1	E	333	TYR	CB-CG-CD1	5.05	128.37	120.80
1	F	482	LEU	N-CA-C	-5.05	97.15	107.70
1	A	650	VAL	CG1-CB-CG2	5.04	121.90	110.80
1	F	224	HIS	CA-CB-CG	5.04	118.84	113.80
1	F	289	LEU	CB-CA-C	5.04	120.46	111.03
1	A	42	ASP	CA-C-O	5.04	127.72	120.51
1	C	650	VAL	CG1-CB-CG2	5.04	121.89	110.80
1	D	12	GLN	CA-CB-CG	5.04	124.19	114.10
1	D	215	ARG	NH1-CZ-NH2	5.04	125.86	119.30
1	C	42	ASP	CA-C-O	5.04	127.72	120.51
1	D	14	ILE	CB-CA-C	5.04	118.11	111.81
1	D	424	THR	CA-CB-CG2	-5.04	101.93	110.50
1	E	357	PRO	O-C-N	5.04	129.45	122.64
1	B	353	ARG	N-CA-C	-5.04	106.97	113.02
1	E	482	LEU	N-CA-C	-5.04	97.17	107.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	LYS	N-CA-CB	-5.04	102.43	109.94
1	B	541	GLU	CB-CG-CD	5.04	121.17	112.60
1	D	127	LYS	N-CA-CB	-5.04	102.43	109.94
1	D	306	THR	CB-CA-C	5.04	118.44	109.72
1	D	333	TYR	CB-CG-CD1	5.04	128.36	120.80
1	D	463	LYS	CA-CB-CG	-5.04	104.02	114.10
1	D	650	VAL	CG1-CB-CG2	5.04	121.88	110.80
1	F	306	THR	CB-CA-C	5.04	118.44	109.72
1	F	424	THR	CA-CB-CG2	-5.04	101.93	110.50
1	F	622	LEU	O-C-N	-5.04	117.34	123.29
1	F	650	VAL	CG1-CB-CG2	5.04	121.88	110.80
1	A	289	LEU	CB-CA-C	5.04	120.45	111.03
1	B	463	LYS	CB-CG-CD	5.04	122.88	111.30
1	F	42	ASP	CA-C-O	5.04	127.71	120.51
1	E	245	GLU	OE1-CD-OE2	-5.04	110.81	122.90
1	E	289	LEU	CB-CA-C	5.04	120.44	111.03
1	F	333	TYR	CB-CG-CD1	5.04	128.35	120.80
1	B	245	GLU	OE1-CD-OE2	-5.03	110.82	122.90
1	C	215	ARG	NH1-CZ-NH2	5.03	125.84	119.30
1	D	245	GLU	OE1-CD-OE2	-5.03	110.82	122.90
1	D	397	SER	CA-CB-OG	-5.03	101.03	111.10
1	F	463	LYS	CB-CG-CD	5.03	122.88	111.30
1	A	397	SER	CA-CB-OG	-5.03	101.04	111.10
1	D	289	LEU	CB-CA-C	5.03	120.44	111.03
1	F	397	SER	CA-CB-OG	-5.03	101.04	111.10
1	B	14	ILE	CB-CA-C	5.03	118.10	111.81
1	C	397	SER	CA-CB-OG	-5.03	101.04	111.10
1	F	245	GLU	OE1-CD-OE2	-5.03	110.83	122.90
1	F	287	HIS	CA-C-O	5.03	125.57	119.38
1	B	42	ASP	CA-C-O	5.03	127.70	120.51
1	B	478	PHE	N-CA-CB	5.03	117.53	110.24
1	E	127	LYS	N-CA-CB	-5.03	102.45	109.94
1	A	245	GLU	OE1-CD-OE2	-5.03	110.83	122.90
1	B	333	TYR	CB-CG-CD1	5.03	128.34	120.80
1	C	245	GLU	OE1-CD-OE2	-5.03	110.83	122.90
1	E	463	LYS	CB-CG-CD	5.03	122.86	111.30
1	B	397	SER	CA-CB-OG	-5.03	101.05	111.10
1	C	463	LYS	CA-CB-CG	-5.03	104.05	114.10
1	A	541	GLU	CB-CG-CD	5.02	121.14	112.60
1	E	541	GLU	CB-CG-CD	5.02	121.14	112.60
1	C	29	ASP	N-CA-C	-5.02	105.70	111.07
1	C	289	LEU	CB-CA-C	5.02	120.42	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	541	GLU	CB-CG-CD	5.02	121.14	112.60
1	D	304	TYR	N-CA-C	5.02	117.30	109.52
1	E	397	SER	CA-CB-OG	-5.02	101.06	111.10
1	E	424	THR	CA-CB-CG2	-5.02	101.96	110.50
1	F	127	LYS	N-CA-CB	-5.02	102.45	109.94
1	B	127	LYS	N-CA-CB	-5.02	102.46	109.94
1	A	463	LYS	CA-CB-CG	-5.02	104.06	114.10
1	B	289	LEU	CB-CA-C	5.02	120.42	111.03
1	E	463	LYS	CA-CB-CG	-5.02	104.06	114.10
1	A	304	TYR	N-CA-C	5.02	117.30	109.52
1	A	424	THR	CA-CB-CG2	-5.02	101.97	110.50
1	A	478	PHE	N-CA-CB	5.02	117.52	110.24
1	B	424	THR	CA-CB-CG2	-5.02	101.97	110.50
1	B	463	LYS	CA-CB-CG	-5.02	104.06	114.10
1	C	14	ILE	CB-CA-C	5.02	118.08	111.81
1	C	424	THR	CA-CB-CG2	-5.02	101.97	110.50
1	D	132	ILE	CB-CA-C	-5.02	104.36	111.28
1	D	353	ARG	N-CA-C	-5.02	107.00	113.02
1	E	353	ARG	N-CA-C	-5.02	107.00	113.02
1	B	224	HIS	CA-CB-CG	5.02	118.82	113.80
1	A	463	LYS	CB-CG-CD	5.01	122.83	111.30
1	B	287	HIS	CA-C-O	5.01	125.55	119.38
1	F	495	LEU	CD1-CG-CD2	-5.01	99.77	110.80
1	C	390	ILE	CA-CB-CG1	5.01	118.92	110.40
1	B	304	TYR	N-CA-C	5.01	117.29	109.52
1	D	287	HIS	CA-C-O	5.01	125.54	119.38
1	F	390	ILE	CA-C-N	-5.01	113.62	120.44
1	F	390	ILE	C-N-CA	-5.01	113.62	120.44
1	F	390	ILE	CA-CB-CG1	5.01	118.92	110.40
1	F	463	LYS	CA-CB-CG	-5.01	104.08	114.10
1	F	478	PHE	N-CA-CB	5.01	117.50	110.24
1	C	390	ILE	CA-C-N	-5.01	113.63	120.44
1	C	390	ILE	C-N-CA	-5.01	113.63	120.44
1	F	304	TYR	N-CA-C	5.01	117.28	109.52
1	E	391	PHE	CA-C-O	-5.01	115.54	120.70
1	A	390	ILE	CA-C-N	-5.01	113.63	120.44
1	A	390	ILE	C-N-CA	-5.01	113.63	120.44
1	A	495	LEU	CD1-CG-CD2	-5.01	99.79	110.80
1	B	391	PHE	CA-C-O	-5.01	115.54	120.70
1	D	391	PHE	CA-C-O	-5.01	115.54	120.70
1	E	37	PHE	O-C-N	5.01	128.77	122.86
1	E	495	LEU	CD1-CG-CD2	-5.01	99.78	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	HIS	CA-C-O	5.00	125.54	119.38
1	C	495	LEU	CD1-CG-CD2	-5.00	99.79	110.80
1	A	390	ILE	CA-CB-CG1	5.00	118.91	110.40
1	D	390	ILE	CA-C-N	-5.00	113.64	120.44
1	D	390	ILE	C-N-CA	-5.00	113.64	120.44
1	A	476	ALA	CA-C-N	-5.00	115.77	122.42
1	A	476	ALA	C-N-CA	-5.00	115.77	122.42
1	B	495	LEU	CD1-CG-CD2	-5.00	99.80	110.80

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	A	177	ARG	Sidechain
1	A	215	ARG	Sidechain
1	A	454	ARG	Sidechain
1	A	499	ARG	Sidechain
1	A	620	ARG	Sidechain
1	A	628	ARG	Sidechain
1	B	100	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	215	ARG	Sidechain
1	B	454	ARG	Sidechain
1	B	499	ARG	Sidechain
1	B	620	ARG	Sidechain
1	B	628	ARG	Sidechain
1	C	100	ARG	Sidechain
1	C	177	ARG	Sidechain
1	C	215	ARG	Sidechain
1	C	454	ARG	Sidechain
1	C	499	ARG	Sidechain
1	C	620	ARG	Sidechain
1	C	628	ARG	Sidechain
1	D	100	ARG	Sidechain
1	D	177	ARG	Sidechain
1	D	215	ARG	Sidechain
1	D	454	ARG	Sidechain
1	D	499	ARG	Sidechain
1	D	620	ARG	Sidechain
1	D	628	ARG	Sidechain
1	E	100	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	177	ARG	Sidechain
1	E	215	ARG	Sidechain
1	E	454	ARG	Sidechain
1	E	499	ARG	Sidechain
1	E	620	ARG	Sidechain
1	E	628	ARG	Sidechain
1	F	100	ARG	Sidechain
1	F	177	ARG	Sidechain
1	F	215	ARG	Sidechain
1	F	454	ARG	Sidechain
1	F	499	ARG	Sidechain
1	F	620	ARG	Sidechain
1	F	628	ARG	Sidechain

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	5239	0	4950	600	1
1	B	5239	0	4950	587	0
1	C	5239	0	4950	591	0
1	D	5239	0	4950	610	0
1	E	5239	0	4950	589	1
1	F	5239	0	4950	572	0
2	G	28	0	25	6	0
2	H	28	0	25	6	0
2	I	28	0	25	6	0
2	J	28	0	25	6	0
2	K	28	0	25	6	0
2	L	28	0	25	6	0
3	A	2	0	0	0	0
4	A	176	0	0	32	0
4	B	4	0	0	1	0
4	C	2	0	0	0	0
4	E	3	0	0	1	0
4	F	1	0	0	0	0
All	All	31790	0	29850	3505	1

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 57.

All (3505) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:HG22	1:B:141:THR:HG23	1.20	1.18
1:A:140:ILE:HG22	1:A:141:THR:HG23	1.20	1.17
1:F:140:ILE:HG22	1:F:141:THR:HG23	1.20	1.17
1:E:140:ILE:HG22	1:E:141:THR:HG23	1.20	1.15
1:D:140:ILE:HG22	1:D:141:THR:HG23	1.20	1.15
1:C:140:ILE:HG22	1:C:141:THR:HG23	1.20	1.12
1:E:59:GLU:OE1	1:E:64:ARG:HD3	1.54	1.08
1:D:59:GLU:OE1	1:D:64:ARG:HD3	1.54	1.07
1:F:414:ASN:HD22	1:F:466:MET:HA	1.20	1.07
1:B:59:GLU:OE1	1:B:64:ARG:HD3	1.54	1.06
1:A:59:GLU:OE1	1:A:64:ARG:HD3	1.54	1.05
1:F:59:GLU:OE1	1:F:64:ARG:HD3	1.54	1.05
1:C:59:GLU:OE1	1:C:64:ARG:HD3	1.54	1.05
1:D:634:ARG:HH21	1:F:64:ARG:HD2	1.22	1.05
1:E:513:PRO:HG3	1:E:517:GLU:HB2	1.39	1.05
1:E:414:ASN:HD22	1:E:466:MET:HA	1.20	1.04
1:A:411:MET:HG2	4:A:834:HOH:O	1.57	1.04
1:D:414:ASN:HD22	1:D:466:MET:HA	1.20	1.04
1:F:513:PRO:HG3	1:F:517:GLU:HB2	1.40	1.04
1:D:513:PRO:HG3	1:D:517:GLU:HB2	1.39	1.03
2:G:2:NAG:C8	2:G:2:NAG:HN2	1.72	1.03
2:K:2:NAG:C8	2:K:2:NAG:HN2	1.72	1.03
1:C:414:ASN:HD22	1:C:466:MET:HA	1.20	1.03
1:C:513:PRO:HG3	1:C:517:GLU:HB2	1.40	1.03
2:H:2:NAG:C8	2:H:2:NAG:HN2	1.72	1.03
2:J:2:NAG:C8	2:J:2:NAG:HN2	1.72	1.03
1:A:414:ASN:HD22	1:A:466:MET:HA	1.20	1.03
1:C:487:ASP:HB3	1:C:489:ASN:H	1.22	1.03
1:B:513:PRO:HG3	1:B:517:GLU:HB2	1.39	1.02
1:C:175:LYS:O	1:D:491:ILE:HD11	1.57	1.02
1:F:487:ASP:HB3	1:F:489:ASN:H	1.22	1.02
2:L:2:NAG:HN2	2:L:2:NAG:C8	1.72	1.02
2:I:2:NAG:HN2	2:I:2:NAG:C8	1.72	1.01
1:A:487:ASP:HB3	1:A:489:ASN:H	1.22	1.01
1:A:513:PRO:HG3	1:A:517:GLU:HB2	1.39	1.00
1:B:414:ASN:HD22	1:B:466:MET:HA	1.20	1.00
1:A:273:ASP:OD2	1:B:360:LYS:HE3	1.61	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:ASP:HB3	1:E:489:ASN:H	1.22	1.00
1:C:491:ILE:CD1	1:D:175:LYS:HB2	1.93	0.99
1:D:487:ASP:HB3	1:D:489:ASN:H	1.22	0.99
1:B:487:ASP:HB3	1:B:489:ASN:H	1.22	0.98
1:C:252:ILE:HG13	1:C:275:ILE:HG22	1.47	0.97
1:F:252:ILE:HG13	1:F:275:ILE:HG22	1.47	0.96
1:A:360:LYS:HE3	1:B:273:ASP:OD2	1.65	0.96
1:D:252:ILE:HG13	1:D:275:ILE:HG22	1.47	0.96
1:C:175:LYS:HB2	1:D:491:ILE:CD1	1.96	0.96
1:E:585:ALA:HB1	1:E:642:ILE:HG12	1.49	0.95
1:E:252:ILE:HG13	1:E:275:ILE:HG22	1.47	0.94
1:B:585:ALA:HB1	1:B:642:ILE:HG12	1.49	0.94
1:C:585:ALA:HB1	1:C:642:ILE:HG12	1.49	0.94
1:F:585:ALA:HB1	1:F:642:ILE:HG12	1.49	0.93
1:B:252:ILE:HG13	1:B:275:ILE:HG22	1.47	0.93
1:F:634:ARG:HG2	1:F:634:ARG:HH11	1.35	0.92
1:A:585:ALA:HB1	1:A:642:ILE:HG12	1.49	0.92
1:E:634:ARG:HG2	1:E:634:ARG:HH11	1.35	0.92
1:D:585:ALA:HB1	1:D:642:ILE:HG12	1.49	0.92
1:A:252:ILE:HG13	1:A:275:ILE:HG22	1.47	0.92
1:F:165:THR:HG22	1:F:449:ASN:HB2	1.52	0.92
1:E:165:THR:HG22	1:E:449:ASN:HB2	1.52	0.91
1:C:491:ILE:HD11	1:D:175:LYS:HB2	1.53	0.91
1:A:634:ARG:HG2	1:A:634:ARG:HH11	1.35	0.91
1:C:634:ARG:HH11	1:C:634:ARG:HG2	1.34	0.91
1:B:165:THR:HG22	1:B:449:ASN:HB2	1.52	0.91
1:D:634:ARG:HG2	1:D:634:ARG:HH11	1.35	0.91
1:B:634:ARG:HG2	1:B:634:ARG:HH11	1.35	0.91
2:J:1:NAG:C8	2:J:1:NAG:HN2	1.84	0.91
1:A:165:THR:HG22	1:A:449:ASN:HB2	1.52	0.90
2:L:1:NAG:C8	2:L:1:NAG:HN2	1.84	0.90
1:C:165:THR:HG22	1:C:449:ASN:HB2	1.52	0.90
2:G:1:NAG:C8	2:G:1:NAG:HN2	1.84	0.90
2:K:1:NAG:HN2	2:K:1:NAG:C8	1.84	0.90
1:E:272:PRO:O	1:E:273:ASP:HB3	1.71	0.90
1:E:533:MET:H	1:E:533:MET:HE3	1.37	0.90
2:H:1:NAG:C8	2:H:1:NAG:HN2	1.84	0.90
1:D:165:THR:HG22	1:D:449:ASN:HB2	1.52	0.90
1:D:533:MET:HE3	1:D:533:MET:H	1.37	0.90
2:I:1:NAG:HN2	2:I:1:NAG:C8	1.84	0.89
1:D:313:ILE:HD11	1:D:323:LEU:HD13	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:LYS:HG2	1:E:96:TRP:CE2	2.08	0.89
1:B:313:ILE:HD11	1:B:323:LEU:HD13	1.55	0.89
1:C:10:LYS:HG2	1:C:96:TRP:CE2	2.08	0.89
1:A:138:TYR:CE2	1:A:188:ILE:HD12	2.08	0.89
1:A:313:ILE:HD11	1:A:323:LEU:HD13	1.55	0.89
1:B:272:PRO:O	1:B:273:ASP:HB3	1.71	0.88
1:E:138:TYR:CE2	1:E:188:ILE:HD12	2.08	0.88
1:F:313:ILE:HD11	1:F:323:LEU:HD13	1.55	0.88
1:B:138:TYR:CE2	1:B:188:ILE:HD12	2.08	0.88
1:D:606:HIS:HD2	1:D:608:GLN:HG2	1.39	0.88
1:E:313:ILE:HD11	1:E:323:LEU:HD13	1.55	0.88
1:A:10:LYS:HG2	1:A:96:TRP:CE2	2.08	0.88
1:A:533:MET:HE3	1:A:533:MET:H	1.37	0.88
1:C:313:ILE:HD11	1:C:323:LEU:HD13	1.55	0.88
1:D:272:PRO:O	1:D:273:ASP:HB3	1.71	0.88
1:F:533:MET:HE3	1:F:533:MET:H	1.37	0.88
1:F:138:TYR:CE2	1:F:188:ILE:HD12	2.08	0.88
1:C:138:TYR:CE2	1:C:188:ILE:HD12	2.08	0.88
1:C:606:HIS:HD2	1:C:608:GLN:HG2	1.39	0.88
1:D:138:TYR:CE2	1:D:188:ILE:HD12	2.08	0.88
1:A:272:PRO:O	1:A:273:ASP:HB3	1.71	0.88
1:B:10:LYS:HG2	1:B:96:TRP:CE2	2.08	0.88
1:C:493:LEU:HD13	1:C:498:ALA:HB2	1.56	0.88
1:D:493:LEU:HD13	1:D:498:ALA:HB2	1.56	0.88
1:E:606:HIS:HD2	1:E:608:GLN:HG2	1.39	0.88
1:B:533:MET:HE3	1:B:533:MET:H	1.37	0.87
1:F:272:PRO:O	1:F:273:ASP:HB3	1.71	0.87
1:F:493:LEU:HD13	1:F:498:ALA:HB2	1.56	0.87
1:A:493:LEU:HD13	1:A:498:ALA:HB2	1.56	0.87
1:C:272:PRO:O	1:C:273:ASP:HB3	1.71	0.87
1:D:10:LYS:HG2	1:D:96:TRP:CE2	2.08	0.87
1:C:533:MET:HE3	1:C:533:MET:H	1.37	0.87
1:F:10:LYS:HG2	1:F:96:TRP:CE2	2.08	0.87
1:E:493:LEU:HD13	1:E:498:ALA:HB2	1.56	0.87
1:B:493:LEU:HD13	1:B:498:ALA:HB2	1.56	0.86
1:B:606:HIS:HD2	1:B:608:GLN:HG2	1.39	0.86
1:A:140:ILE:HG22	1:A:141:THR:CG2	2.04	0.86
1:D:272:PRO:HG2	1:E:272:PRO:HG2	1.55	0.86
1:F:606:HIS:HD2	1:F:608:GLN:HG2	1.39	0.86
1:F:76:ASN:HB3	1:F:79:GLN:HB2	1.57	0.86
1:F:239:TRP:CZ2	1:F:574:LYS:HG2	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:ILE:HG22	1:E:141:THR:CG2	2.04	0.86
1:B:76:ASN:HB3	1:B:79:GLN:HB2	1.58	0.85
1:A:456:ASN:HD22	1:A:457:HIS:H	1.24	0.85
1:C:239:TRP:CZ2	1:C:574:LYS:HG2	2.10	0.85
1:D:239:TRP:CZ2	1:D:574:LYS:HG2	2.10	0.85
1:B:239:TRP:CZ2	1:B:574:LYS:HG2	2.10	0.85
1:B:456:ASN:HD22	1:B:457:HIS:H	1.24	0.85
1:A:239:TRP:CZ2	1:A:574:LYS:HG2	2.10	0.85
1:A:606:HIS:HD2	1:A:608:GLN:HG2	1.39	0.85
1:C:175:LYS:O	1:D:491:ILE:CD1	2.25	0.85
1:C:175:LYS:C	1:D:491:ILE:HD11	2.02	0.85
1:C:76:ASN:HB3	1:C:79:GLN:HB2	1.58	0.85
1:C:140:ILE:HG22	1:C:141:THR:CG2	2.04	0.85
1:B:140:ILE:HG22	1:B:141:THR:CG2	2.04	0.85
1:E:239:TRP:CZ2	1:E:574:LYS:HG2	2.10	0.85
1:E:76:ASN:HB3	1:E:79:GLN:HB2	1.58	0.84
1:A:76:ASN:HB3	1:A:79:GLN:HB2	1.57	0.84
1:D:140:ILE:HG22	1:D:141:THR:CG2	2.04	0.84
1:C:456:ASN:HD22	1:C:457:HIS:H	1.24	0.83
1:E:120:TYR:CD2	1:E:134:LEU:HD13	2.13	0.83
1:B:366:GLY:H	1:B:369:GLU:HG3	1.43	0.83
1:D:120:TYR:CD2	1:D:134:LEU:HD13	2.13	0.83
1:F:456:ASN:HD22	1:F:457:HIS:H	1.24	0.83
1:A:120:TYR:CD2	1:A:134:LEU:HD13	2.13	0.83
1:A:366:GLY:H	1:A:369:GLU:HG3	1.44	0.83
1:D:456:ASN:HD22	1:D:457:HIS:H	1.24	0.83
1:E:414:ASN:ND2	1:E:466:MET:HA	1.94	0.83
1:F:366:GLY:H	1:F:369:GLU:HG3	1.43	0.83
1:F:140:ILE:HG22	1:F:141:THR:CG2	2.04	0.83
1:B:414:ASN:ND2	1:B:466:MET:HA	1.94	0.83
1:D:414:ASN:ND2	1:D:466:MET:HA	1.94	0.83
1:C:414:ASN:ND2	1:C:466:MET:HA	1.94	0.82
1:F:414:ASN:ND2	1:F:466:MET:HA	1.94	0.82
1:F:120:TYR:CD2	1:F:134:LEU:HD13	2.13	0.82
1:B:120:TYR:CD2	1:B:134:LEU:HD13	2.13	0.82
1:C:120:TYR:CD2	1:C:134:LEU:HD13	2.14	0.82
1:C:462:TYR:O	1:C:520:GLU:HA	1.80	0.82
1:D:366:GLY:H	1:D:369:GLU:HG3	1.43	0.82
1:F:462:TYR:O	1:F:520:GLU:HA	1.80	0.82
1:D:76:ASN:HB3	1:D:79:GLN:HB2	1.58	0.82
1:D:462:TYR:O	1:D:520:GLU:HA	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLN:HG3	1:C:15:ASN:HD21	1.45	0.82
1:E:11:GLN:HG3	1:E:15:ASN:HD21	1.45	0.82
1:E:283:VAL:O	1:E:284:ALA:HB2	1.80	0.81
1:A:462:TYR:O	1:A:520:GLU:HA	1.80	0.81
1:A:283:VAL:O	1:A:284:ALA:HB2	1.80	0.81
1:B:462:TYR:O	1:B:520:GLU:HA	1.80	0.81
1:E:366:GLY:H	1:E:369:GLU:HG3	1.43	0.81
1:E:462:TYR:O	1:E:520:GLU:HA	1.80	0.81
1:F:11:GLN:HG3	1:F:15:ASN:HD21	1.45	0.81
1:E:456:ASN:HD22	1:E:457:HIS:H	1.24	0.81
1:C:366:GLY:H	1:C:369:GLU:HG3	1.44	0.81
1:F:606:HIS:HB3	1:F:608:GLN:H	1.46	0.81
1:C:576:GLU:OE1	1:D:576:GLU:OE1	1.98	0.81
1:A:414:ASN:ND2	1:A:466:MET:HA	1.94	0.81
1:D:559:GLU:O	1:D:560:ARG:HG3	1.81	0.81
1:E:606:HIS:HB3	1:E:608:GLN:H	1.46	0.80
1:C:283:VAL:O	1:C:284:ALA:HB2	1.80	0.80
1:B:559:GLU:O	1:B:560:ARG:HG3	1.81	0.80
1:B:606:HIS:HB3	1:B:608:GLN:H	1.46	0.80
1:C:559:GLU:O	1:C:560:ARG:HG3	1.81	0.80
1:F:283:VAL:O	1:F:284:ALA:HB2	1.80	0.80
1:B:11:GLN:HG3	1:B:15:ASN:HD21	1.45	0.80
1:D:11:GLN:HG3	1:D:15:ASN:HD21	1.45	0.80
1:A:639:VAL:HG23	1:A:641:ASN:ND2	1.98	0.79
1:E:559:GLU:O	1:E:560:ARG:HG3	1.81	0.79
1:A:559:GLU:O	1:A:560:ARG:HG3	1.81	0.79
1:F:639:VAL:HG23	1:F:641:ASN:ND2	1.98	0.79
1:F:559:GLU:O	1:F:560:ARG:HG3	1.81	0.79
1:C:272:PRO:HG2	1:F:272:PRO:HG2	1.64	0.79
1:C:606:HIS:HB3	1:C:608:GLN:H	1.46	0.79
1:D:283:VAL:O	1:D:284:ALA:HB2	1.80	0.79
1:F:295:ARG:HG2	1:F:339:TYR:CZ	2.18	0.79
1:D:606:HIS:HB3	1:D:608:GLN:H	1.46	0.79
1:E:639:VAL:HG23	1:E:641:ASN:ND2	1.98	0.79
1:B:295:ARG:HG2	1:B:339:TYR:CZ	2.18	0.79
1:A:295:ARG:HG2	1:A:339:TYR:CZ	2.18	0.79
1:C:187:ASP:OD1	1:C:189:GLY:N	2.16	0.79
1:E:187:ASP:OD1	1:E:189:GLY:N	2.16	0.79
1:A:316:ARG:HD3	4:A:829:HOH:O	1.81	0.78
1:A:408:PHE:N	1:A:641:ASN:OD1	2.16	0.78
1:D:295:ARG:HG2	1:D:339:TYR:CZ	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASP:OD1	1:B:189:GLY:N	2.16	0.78
1:B:639:VAL:HG23	1:B:641:ASN:ND2	1.98	0.78
1:D:639:VAL:HG23	1:D:641:ASN:ND2	1.98	0.78
1:E:239:TRP:CH2	1:E:574:LYS:HG2	2.19	0.78
1:D:239:TRP:CH2	1:D:574:LYS:HG2	2.19	0.78
1:E:8:ALA:HA	1:E:553:LEU:HD12	1.66	0.78
1:E:295:ARG:HG2	1:E:339:TYR:CZ	2.18	0.78
1:E:408:PHE:N	1:E:641:ASN:OD1	2.16	0.78
1:E:298:GLU:OE2	4:E:792:HOH:O	2.02	0.78
1:A:11:GLN:HG3	1:A:15:ASN:HD21	1.45	0.78
1:A:606:HIS:HB3	1:A:608:GLN:H	1.46	0.78
1:B:283:VAL:O	1:B:284:ALA:HB2	1.80	0.78
1:F:239:TRP:CH2	1:F:574:LYS:HG2	2.19	0.78
1:C:295:ARG:HG2	1:C:339:TYR:CZ	2.18	0.78
1:A:237:SER:HB3	1:A:573:SER:HA	1.67	0.78
1:A:551:HIS:CD2	1:A:552:ASP:N	2.52	0.78
1:B:408:PHE:N	1:B:641:ASN:OD1	2.16	0.78
1:B:551:HIS:CD2	1:B:552:ASP:N	2.52	0.78
1:C:239:TRP:CH2	1:C:574:LYS:HG2	2.19	0.78
1:C:606:HIS:CD2	1:C:608:GLN:HG2	2.19	0.78
1:C:639:VAL:HG23	1:C:641:ASN:ND2	1.98	0.78
1:D:606:HIS:CD2	1:D:608:GLN:HG2	2.19	0.78
1:D:7:ASN:C	1:D:9:GLN:H	1.92	0.77
1:D:473:GLU:HA	1:D:512:VAL:O	1.84	0.77
1:F:408:PHE:N	1:F:641:ASN:OD1	2.17	0.77
1:F:473:GLU:HA	1:F:512:VAL:O	1.84	0.77
1:A:557:ALA:HB3	1:A:558:TYR:CD1	2.20	0.77
1:B:237:SER:HB3	1:B:573:SER:HA	1.66	0.77
1:B:606:HIS:CD2	1:B:608:GLN:HG2	2.19	0.77
1:C:7:ASN:C	1:C:9:GLN:H	1.92	0.77
1:C:8:ALA:HA	1:C:553:LEU:HD12	1.66	0.77
1:E:7:ASN:C	1:E:9:GLN:H	1.92	0.77
1:F:7:ASN:C	1:F:9:GLN:H	1.93	0.77
1:A:239:TRP:CH2	1:A:574:LYS:HG2	2.19	0.77
1:B:150:VAL:HG21	1:B:168:VAL:HG12	1.67	0.77
1:E:317:GLN:HB2	1:E:318:PRO:HD2	1.66	0.77
1:A:7:ASN:C	1:A:9:GLN:H	1.92	0.77
1:B:239:TRP:CH2	1:B:574:LYS:HG2	2.19	0.77
1:C:557:ALA:HB3	1:C:558:TYR:CD1	2.20	0.77
1:D:150:VAL:HG21	1:D:168:VAL:HG12	1.67	0.77
1:A:174:LYS:O	1:A:175:LYS:HG2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:HIS:CD2	1:A:608:GLN:HG2	2.19	0.77
1:C:174:LYS:O	1:C:175:LYS:HG2	1.85	0.77
1:C:175:LYS:HB2	1:D:491:ILE:HG12	1.66	0.77
1:D:317:GLN:HB2	1:D:318:PRO:HD2	1.66	0.77
1:D:551:HIS:CD2	1:D:552:ASP:N	2.52	0.77
1:D:557:ALA:HB3	1:D:558:TYR:CD1	2.20	0.77
1:E:150:VAL:HG21	1:E:168:VAL:HG12	1.67	0.77
1:E:551:HIS:CD2	1:E:552:ASP:N	2.52	0.77
1:F:174:LYS:O	1:F:175:LYS:HG2	1.85	0.77
1:A:187:ASP:OD1	1:A:189:GLY:N	2.16	0.77
1:B:557:ALA:HB3	1:B:558:TYR:CD1	2.20	0.77
1:F:150:VAL:HG21	1:F:168:VAL:HG12	1.67	0.77
1:A:150:VAL:HG21	1:A:168:VAL:HG12	1.67	0.77
1:A:473:GLU:HA	1:A:512:VAL:O	1.84	0.77
1:D:174:LYS:O	1:D:175:LYS:HG2	1.85	0.77
1:D:408:PHE:N	1:D:641:ASN:OD1	2.16	0.77
1:F:237:SER:HB3	1:F:573:SER:HA	1.66	0.77
1:F:551:HIS:CD2	1:F:552:ASP:N	2.52	0.77
1:B:317:GLN:HB2	1:B:318:PRO:HD2	1.66	0.76
1:C:237:SER:HB3	1:C:573:SER:HA	1.66	0.76
1:C:585:ALA:CB	1:C:642:ILE:HG12	2.15	0.76
1:D:8:ALA:HA	1:D:553:LEU:HD12	1.66	0.76
1:C:408:PHE:N	1:C:641:ASN:OD1	2.17	0.76
1:E:473:GLU:HA	1:E:512:VAL:O	1.84	0.76
1:A:317:GLN:HB2	1:A:318:PRO:HD2	1.66	0.76
1:D:585:ALA:CB	1:D:642:ILE:HG12	2.15	0.76
1:E:174:LYS:O	1:E:175:LYS:HG2	1.85	0.76
1:E:606:HIS:CD2	1:E:608:GLN:HG2	2.19	0.76
1:F:8:ALA:HA	1:F:553:LEU:HD12	1.66	0.76
1:F:187:ASP:OD1	1:F:189:GLY:N	2.16	0.76
1:F:317:GLN:HB2	1:F:318:PRO:HD2	1.66	0.76
1:A:521:ARG:HD3	4:A:864:HOH:O	1.86	0.76
1:B:201:PHE:HB3	1:B:216:LYS:CD	2.16	0.76
1:C:551:HIS:CD2	1:C:552:ASP:N	2.52	0.76
1:E:557:ALA:HB3	1:E:558:TYR:CD1	2.20	0.76
1:A:8:ALA:HA	1:A:553:LEU:HD12	1.66	0.76
1:B:7:ASN:C	1:B:9:GLN:H	1.92	0.76
1:B:174:LYS:O	1:B:175:LYS:HG2	1.85	0.76
1:B:473:GLU:HA	1:B:512:VAL:O	1.84	0.76
1:B:585:ALA:CB	1:B:642:ILE:HG12	2.15	0.76
1:C:150:VAL:HG21	1:C:168:VAL:HG12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:GLU:HA	1:C:512:VAL:O	1.84	0.76
1:F:86:LEU:O	1:F:86:LEU:HD23	1.86	0.76
1:C:86:LEU:O	1:C:86:LEU:HD23	1.86	0.76
1:D:201:PHE:HB3	1:D:216:LYS:CD	2.16	0.76
1:F:606:HIS:CD2	1:F:608:GLN:HG2	2.19	0.76
1:A:201:PHE:HB3	1:A:216:LYS:CD	2.16	0.76
1:D:272:PRO:HG2	1:E:272:PRO:CG	2.16	0.76
1:F:557:ALA:HB3	1:F:558:TYR:CD1	2.20	0.76
1:B:37:PHE:CE2	1:B:101:SER:HB3	2.21	0.76
1:C:317:GLN:HB2	1:C:318:PRO:HD2	1.66	0.76
1:F:201:PHE:HB3	1:F:216:LYS:CD	2.16	0.76
1:B:174:LYS:C	1:B:175:LYS:HG2	2.11	0.76
1:C:37:PHE:CE2	1:C:101:SER:HB3	2.21	0.76
1:C:201:PHE:HB3	1:C:216:LYS:CD	2.16	0.76
1:D:174:LYS:C	1:D:175:LYS:HG2	2.11	0.76
1:E:37:PHE:CE2	1:E:101:SER:HB3	2.21	0.76
1:E:585:ALA:CB	1:E:642:ILE:HG12	2.15	0.76
1:A:37:PHE:CE2	1:A:101:SER:HB3	2.21	0.76
1:B:413:VAL:CG2	1:B:466:MET:HE3	2.16	0.76
1:D:237:SER:HB3	1:D:573:SER:HA	1.66	0.76
1:E:201:PHE:HB3	1:E:216:LYS:CD	2.16	0.76
1:A:585:ALA:CB	1:A:642:ILE:HG12	2.15	0.75
1:D:533:MET:HB3	1:D:534:PRO:HD2	1.68	0.75
1:F:585:ALA:CB	1:F:642:ILE:HG12	2.15	0.75
1:A:84:LEU:HD11	1:A:204:TRP:CE2	2.21	0.75
1:C:413:VAL:CG2	1:C:466:MET:HE3	2.16	0.75
1:D:84:LEU:HD11	1:D:204:TRP:CE2	2.21	0.75
1:E:65:LEU:HD21	1:E:110:MET:HE2	1.69	0.75
1:F:533:MET:HB3	1:F:534:PRO:HD2	1.68	0.75
1:A:379:SER:HB3	4:A:719:HOH:O	1.85	0.75
1:B:533:MET:HB3	1:B:534:PRO:HD2	1.68	0.75
1:D:413:VAL:CG2	1:D:466:MET:HE3	2.16	0.75
1:D:634:ARG:HE	1:F:64:ARG:NE	1.84	0.75
1:E:237:SER:HB3	1:E:573:SER:HA	1.67	0.75
1:E:533:MET:HB3	1:E:534:PRO:HD2	1.68	0.75
1:A:533:MET:HB3	1:A:534:PRO:HD2	1.68	0.75
1:C:65:LEU:HD21	1:C:110:MET:HE2	1.69	0.75
1:C:175:LYS:HB2	1:D:491:ILE:CG1	2.16	0.75
1:C:220:PHE:CE2	1:C:329:GLU:HB2	2.22	0.75
1:D:65:LEU:HD21	1:D:110:MET:HE2	1.69	0.75
1:E:174:LYS:C	1:E:175:LYS:HG2	2.11	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:VAL:CG2	1:E:466:MET:HE3	2.17	0.75
1:C:174:LYS:C	1:C:175:LYS:HG2	2.11	0.75
1:D:408:PHE:HB3	1:D:641:ASN:OD1	1.87	0.75
1:D:495:LEU:HD23	1:D:630:ILE:HG21	1.68	0.75
1:A:392:LYS:O	1:A:396:ASP:HB2	1.87	0.75
1:B:220:PHE:CE2	1:B:329:GLU:HB2	2.22	0.75
1:E:84:LEU:HD11	1:E:204:TRP:CE2	2.21	0.75
1:E:408:PHE:HB3	1:E:641:ASN:OD1	1.87	0.75
1:D:634:ARG:HH21	1:F:64:ARG:CD	1.98	0.75
1:F:408:PHE:HB3	1:F:641:ASN:OD1	1.87	0.75
1:F:413:VAL:CG2	1:F:466:MET:HE3	2.17	0.75
1:B:8:ALA:HA	1:B:553:LEU:HD12	1.66	0.75
1:D:86:LEU:HD23	1:D:86:LEU:O	1.86	0.75
1:A:174:LYS:C	1:A:175:LYS:HG2	2.11	0.74
1:B:86:LEU:HD23	1:B:86:LEU:O	1.86	0.74
1:B:185:GLY:O	1:B:375:THR:HG22	1.87	0.74
1:C:408:PHE:HB3	1:C:641:ASN:OD1	1.87	0.74
1:D:392:LYS:O	1:D:396:ASP:HB2	1.87	0.74
1:E:86:LEU:HD23	1:E:86:LEU:O	1.86	0.74
1:F:65:LEU:HD21	1:F:110:MET:HE2	1.69	0.74
1:F:392:LYS:O	1:F:396:ASP:HB2	1.87	0.74
1:A:413:VAL:CG2	1:A:466:MET:HE3	2.17	0.74
1:C:533:MET:HB3	1:C:534:PRO:HD2	1.68	0.74
1:D:185:GLY:O	1:D:375:THR:HG22	1.87	0.74
1:F:174:LYS:C	1:F:175:LYS:HG2	2.11	0.74
1:A:86:LEU:O	1:A:86:LEU:HD23	1.86	0.74
1:A:220:PHE:CE2	1:A:329:GLU:HB2	2.22	0.74
1:B:392:LYS:O	1:B:396:ASP:HB2	1.87	0.74
1:A:235:ARG:NH2	4:A:705:HOH:O	1.98	0.74
1:C:495:LEU:HD23	1:C:630:ILE:HG21	1.68	0.74
1:F:37:PHE:CE2	1:F:101:SER:HB3	2.21	0.74
1:C:84:LEU:HD11	1:C:204:TRP:CE2	2.21	0.74
1:D:283:VAL:HG11	1:D:349:VAL:HB	1.70	0.74
1:E:185:GLY:O	1:E:375:THR:HG22	1.87	0.74
1:F:220:PHE:CE2	1:F:329:GLU:HB2	2.22	0.74
1:A:408:PHE:HB3	1:A:641:ASN:OD1	1.87	0.74
1:E:220:PHE:CE2	1:E:329:GLU:HB2	2.22	0.74
1:B:408:PHE:HB3	1:B:641:ASN:OD1	1.87	0.74
1:C:261:SER:OG	1:C:267:GLU:HG2	1.88	0.74
1:C:392:LYS:O	1:C:396:ASP:HB2	1.87	0.74
1:D:37:PHE:CE2	1:D:101:SER:HB3	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ARG:HD2	1:E:360:LYS:HB3	1.68	0.74
1:F:84:LEU:HD11	1:F:204:TRP:CE2	2.21	0.74
1:A:261:SER:OG	1:A:267:GLU:HG2	1.88	0.74
1:A:495:LEU:HD23	1:A:630:ILE:HG21	1.68	0.74
1:B:84:LEU:HD11	1:B:204:TRP:CE2	2.21	0.74
1:B:495:LEU:HD23	1:B:630:ILE:HG21	1.68	0.74
1:E:261:SER:OG	1:E:267:GLU:HG2	1.88	0.74
1:E:392:LYS:O	1:E:396:ASP:HB2	1.87	0.74
1:D:220:PHE:CE2	1:D:329:GLU:HB2	2.22	0.73
1:E:413:VAL:HG22	1:E:466:MET:HE3	1.70	0.73
1:E:495:LEU:HD23	1:E:630:ILE:HG21	1.68	0.73
1:F:185:GLY:O	1:F:375:THR:HG22	1.87	0.73
1:A:413:VAL:HG22	1:A:466:MET:HE3	1.70	0.73
1:B:283:VAL:HG11	1:B:349:VAL:HB	1.70	0.73
1:C:185:GLY:O	1:C:375:THR:HG22	1.87	0.73
1:B:207:ASP:OD2	1:B:212:HIS:HB2	1.89	0.73
1:D:272:PRO:CG	1:E:272:PRO:HG2	2.18	0.73
1:E:207:ASP:OD2	1:E:212:HIS:HB2	1.89	0.73
1:E:412:VAL:HG22	1:E:412:VAL:O	1.89	0.73
1:B:413:VAL:HG22	1:B:466:MET:HE3	1.70	0.73
1:D:187:ASP:OD1	1:D:189:GLY:N	2.16	0.73
1:D:522:SER:O	1:D:523:SER:C	2.32	0.73
1:D:634:ARG:HE	1:F:64:ARG:CZ	2.01	0.73
1:F:495:LEU:HD23	1:F:630:ILE:HG21	1.68	0.73
1:A:185:GLY:O	1:A:375:THR:HG22	1.87	0.73
1:A:412:VAL:O	1:A:412:VAL:HG22	1.89	0.73
1:C:86:LEU:CD2	1:C:90:LEU:HD22	2.19	0.73
1:C:175:LYS:HB2	1:D:491:ILE:HD11	1.71	0.73
1:F:522:SER:O	1:F:523:SER:C	2.32	0.73
1:A:86:LEU:CD2	1:A:90:LEU:HD22	2.19	0.73
1:C:465:THR:HG23	1:C:518:THR:OG1	1.89	0.73
1:D:413:VAL:HG22	1:D:466:MET:HE3	1.70	0.73
1:A:207:ASP:OD2	1:A:212:HIS:HB2	1.89	0.73
1:A:522:SER:O	1:A:523:SER:C	2.32	0.73
1:B:65:LEU:HD21	1:B:110:MET:HE2	1.69	0.73
1:C:413:VAL:HG22	1:C:466:MET:HE3	1.70	0.73
1:A:465:THR:HG23	1:A:518:THR:OG1	1.89	0.73
1:E:86:LEU:CD2	1:E:90:LEU:HD22	2.19	0.73
1:F:413:VAL:HG22	1:F:466:MET:HE3	1.70	0.73
1:B:412:VAL:HG22	1:B:412:VAL:O	1.89	0.73
1:D:307:ASP:HA	1:D:336:ASN:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:SER:OG	1:F:267:GLU:HG2	1.88	0.72
1:F:307:ASP:HA	1:F:336:ASN:HB2	1.71	0.72
1:A:307:ASP:HA	1:A:336:ASN:HB2	1.71	0.72
1:B:261:SER:OG	1:B:267:GLU:HG2	1.88	0.72
1:D:207:ASP:OD2	1:D:212:HIS:HB2	1.89	0.72
1:D:261:SER:OG	1:D:267:GLU:HG2	1.88	0.72
1:D:10:LYS:HG2	1:D:96:TRP:CD2	2.25	0.72
1:F:465:THR:HG23	1:F:518:THR:OG1	1.89	0.72
1:A:65:LEU:HD21	1:A:110:MET:HE2	1.69	0.72
1:C:207:ASP:OD2	1:C:212:HIS:HB2	1.89	0.72
1:D:465:THR:HG23	1:D:518:THR:OG1	1.89	0.72
1:F:207:ASP:OD2	1:F:212:HIS:HB2	1.89	0.72
1:B:86:LEU:CD2	1:B:90:LEU:HD22	2.19	0.72
1:A:10:LYS:HG2	1:A:96:TRP:CD2	2.25	0.72
1:A:283:VAL:HG11	1:A:349:VAL:HB	1.70	0.72
1:B:465:THR:HG23	1:B:518:THR:OG1	1.89	0.72
1:D:86:LEU:CD2	1:D:90:LEU:HD22	2.19	0.72
1:F:86:LEU:CD2	1:F:90:LEU:HD22	2.19	0.72
1:B:10:LYS:HG2	1:B:96:TRP:CD2	2.25	0.72
1:C:307:ASP:HA	1:C:336:ASN:HB2	1.71	0.72
1:F:10:LYS:HG2	1:F:96:TRP:CD2	2.25	0.72
2:J:2:NAG:C8	2:J:2:NAG:N2	2.52	0.72
1:D:412:VAL:O	1:D:412:VAL:HG22	1.89	0.72
1:E:10:LYS:HG2	1:E:96:TRP:CD2	2.25	0.72
1:E:353:ARG:C	1:E:355:GLY:H	1.97	0.72
1:F:283:VAL:HG11	1:F:349:VAL:HB	1.70	0.72
1:C:283:VAL:HG11	1:C:349:VAL:HB	1.70	0.71
1:B:307:ASP:HA	1:B:336:ASN:HB2	1.71	0.71
1:B:353:ARG:C	1:B:355:GLY:H	1.97	0.71
1:E:307:ASP:HA	1:E:336:ASN:HB2	1.71	0.71
1:E:465:THR:HG23	1:E:518:THR:OG1	1.89	0.71
1:C:10:LYS:HG2	1:C:96:TRP:CD2	2.25	0.71
1:C:412:VAL:O	1:C:412:VAL:HG22	1.89	0.71
1:D:537:GLN:O	1:D:540:LYS:N	2.23	0.71
1:B:565:PRO:HB2	1:B:568:MET:CG	2.21	0.71
1:C:353:ARG:C	1:C:355:GLY:H	1.97	0.71
1:F:565:PRO:HB2	1:F:568:MET:CG	2.21	0.71
1:D:477:THR:HB	1:D:479:ARG:NH1	2.06	0.71
1:D:569:LEU:HD23	1:D:570:LEU:HD13	1.73	0.71
1:E:253:ARG:NH1	1:E:274:ASN:OD1	2.24	0.71
1:A:477:THR:HB	1:A:479:ARG:NH1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:THR:HB	1:E:479:ARG:NH1	2.06	0.71
1:B:167:ASN:OD1	1:B:451:ARG:NE	2.24	0.71
1:C:487:ASP:HB3	1:C:490:GLY:H	1.56	0.71
2:I:2:NAG:C8	2:I:2:NAG:N2	2.52	0.71
1:B:123:VAL:HG11	1:B:134:LEU:HD21	1.73	0.71
1:C:477:THR:HB	1:C:479:ARG:NH1	2.06	0.71
1:E:283:VAL:HG11	1:E:349:VAL:HB	1.70	0.71
1:E:522:SER:O	1:E:523:SER:C	2.32	0.71
1:A:177:ARG:NH1	1:A:179:GLN:HG3	2.06	0.71
1:C:569:LEU:HD23	1:C:570:LEU:HD13	1.73	0.71
1:D:353:ARG:C	1:D:355:GLY:H	1.97	0.71
1:A:123:VAL:HG11	1:A:134:LEU:HD21	1.72	0.70
1:C:177:ARG:NH1	1:C:179:GLN:HG3	2.06	0.70
1:C:253:ARG:NH1	1:C:274:ASN:OD1	2.24	0.70
1:E:167:ASN:OD1	1:E:451:ARG:NE	2.24	0.70
1:E:565:PRO:HB2	1:E:568:MET:HG2	1.74	0.70
1:B:253:ARG:NH1	1:B:274:ASN:OD1	2.24	0.70
1:B:537:GLN:O	1:B:540:LYS:N	2.23	0.70
1:D:167:ASN:OD1	1:D:451:ARG:NE	2.24	0.70
1:E:177:ARG:NH1	1:E:179:GLN:HG3	2.06	0.70
1:E:487:ASP:HB3	1:E:490:GLY:H	1.56	0.70
1:C:522:SER:O	1:C:523:SER:C	2.32	0.70
1:F:177:ARG:NH1	1:F:179:GLN:HG3	2.06	0.70
1:F:253:ARG:NH1	1:F:274:ASN:OD1	2.24	0.70
1:F:463:LYS:HG2	1:F:520:GLU:HB2	1.73	0.70
1:F:537:GLN:O	1:F:540:LYS:N	2.23	0.70
1:A:76:ASN:O	1:A:77:THR:C	2.32	0.70
1:A:253:ARG:NH1	1:A:274:ASN:OD1	2.24	0.70
1:A:353:ARG:C	1:A:355:GLY:H	1.97	0.70
1:D:253:ARG:NH1	1:D:274:ASN:OD1	2.24	0.70
1:D:565:PRO:HB2	1:D:568:MET:HG2	1.74	0.70
1:F:295:ARG:HG2	1:F:339:TYR:CE1	2.27	0.70
1:B:177:ARG:NH1	1:B:179:GLN:HG3	2.06	0.70
1:C:56:LEU:HD21	1:C:110:MET:HE3	1.74	0.70
1:D:565:PRO:HB2	1:D:568:MET:CG	2.21	0.70
1:E:353:ARG:C	1:E:355:GLY:N	2.49	0.70
1:E:463:LYS:HG2	1:E:520:GLU:HB2	1.73	0.70
1:E:569:LEU:HD23	1:E:570:LEU:HD13	1.73	0.70
1:F:353:ARG:C	1:F:355:GLY:H	1.97	0.70
1:A:81:LYS:HD2	4:A:793:HOH:O	1.90	0.70
1:A:487:ASP:HB3	1:A:490:GLY:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:PRO:HB2	1:A:568:MET:CG	2.21	0.70
1:B:152:ASP:OD1	4:B:679:HOH:O	2.10	0.70
1:B:487:ASP:HB3	1:B:490:GLY:H	1.56	0.70
1:E:123:VAL:HG11	1:E:134:LEU:HD21	1.72	0.70
1:E:565:PRO:HB2	1:E:568:MET:CG	2.21	0.70
1:D:123:VAL:HG11	1:D:134:LEU:HD21	1.73	0.70
1:D:295:ARG:HG2	1:D:339:TYR:CE1	2.26	0.70
1:F:56:LEU:HD21	1:F:110:MET:HE3	1.74	0.70
1:A:167:ASN:OD1	1:A:451:ARG:NE	2.24	0.70
1:A:411:MET:CG	4:A:834:HOH:O	2.22	0.70
1:B:56:LEU:HD21	1:B:110:MET:HE3	1.74	0.70
1:F:477:THR:HB	1:F:479:ARG:NH1	2.06	0.70
1:B:569:LEU:HD23	1:B:570:LEU:HD13	1.73	0.70
1:C:295:ARG:HG2	1:C:339:TYR:CE1	2.27	0.70
1:D:177:ARG:NH1	1:D:179:GLN:HG3	2.06	0.70
1:D:424:THR:O	1:D:651:HIS:ND1	2.23	0.70
1:F:412:VAL:O	1:F:412:VAL:HG22	1.89	0.70
1:A:56:LEU:HD21	1:A:110:MET:HE3	1.74	0.70
1:A:569:LEU:HD23	1:A:570:LEU:HD13	1.73	0.70
1:B:295:ARG:HG2	1:B:339:TYR:CE1	2.27	0.70
1:B:477:THR:HB	1:B:479:ARG:NH1	2.06	0.70
1:C:565:PRO:HB2	1:C:568:MET:CG	2.21	0.70
2:H:1:NAG:C8	2:H:1:NAG:N2	2.55	0.70
2:L:1:NAG:C8	2:L:1:NAG:N2	2.55	0.70
1:C:123:VAL:HG11	1:C:134:LEU:HD21	1.73	0.69
1:D:121:VAL:HG23	1:D:199:MET:HG2	1.74	0.69
1:F:487:ASP:HB3	1:F:490:GLY:H	1.56	0.69
1:F:569:LEU:HD23	1:F:570:LEU:HD13	1.73	0.69
1:A:382:ARG:HD2	4:A:712:HOH:O	1.91	0.69
1:A:463:LYS:HG2	1:A:520:GLU:HB2	1.73	0.69
1:C:167:ASN:OD1	1:C:451:ARG:NE	2.24	0.69
1:D:76:ASN:O	1:D:77:THR:C	2.32	0.69
1:A:59:GLU:OE1	1:A:64:ARG:CD	2.38	0.69
1:A:295:ARG:HG2	1:A:339:TYR:CE1	2.27	0.69
1:B:76:ASN:O	1:B:77:THR:C	2.32	0.69
1:B:487:ASP:HB3	1:B:489:ASN:N	2.04	0.69
1:C:353:ARG:C	1:C:355:GLY:N	2.49	0.69
1:E:8:ALA:CA	1:E:553:LEU:HD12	2.23	0.69
1:E:473:GLU:C	1:E:474:ARG:HG2	2.17	0.69
2:H:2:NAG:C8	2:H:2:NAG:N2	2.52	0.69
1:C:76:ASN:O	1:C:77:THR:C	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:THR:O	1:B:651:HIS:ND1	2.23	0.69
1:C:463:LYS:HG2	1:C:520:GLU:HB2	1.73	0.69
1:D:89:VAL:O	1:D:91:ASN:N	2.26	0.69
1:D:353:ARG:C	1:D:355:GLY:N	2.49	0.69
1:E:537:GLN:O	1:E:540:LYS:N	2.23	0.69
1:B:59:GLU:OE1	1:B:64:ARG:CD	2.38	0.69
1:B:463:LYS:HG2	1:B:520:GLU:HB2	1.73	0.69
1:B:473:GLU:C	1:B:474:ARG:HG2	2.18	0.69
1:B:565:PRO:HB2	1:B:568:MET:HG2	1.74	0.69
1:E:121:VAL:HG23	1:E:199:MET:HG2	1.74	0.69
1:E:295:ARG:HG2	1:E:339:TYR:CE1	2.27	0.69
2:K:1:NAG:C8	2:K:1:NAG:N2	2.55	0.69
1:A:8:ALA:CA	1:A:553:LEU:HD12	2.23	0.69
1:B:89:VAL:O	1:B:91:ASN:N	2.26	0.69
1:B:522:SER:O	1:B:523:SER:C	2.32	0.69
1:C:89:VAL:O	1:C:91:ASN:N	2.26	0.69
1:C:368:MET:HE1	1:C:380:PHE:HA	1.75	0.69
1:C:565:PRO:HB2	1:C:568:MET:HG2	1.74	0.69
1:E:69:ARG:N	1:E:112:GLU:OE2	2.25	0.69
1:F:565:PRO:HB2	1:F:568:MET:HG2	1.74	0.69
2:G:1:NAG:C8	2:G:1:NAG:N2	2.55	0.69
2:J:1:NAG:C8	2:J:1:NAG:N2	2.55	0.69
1:A:473:GLU:C	1:A:474:ARG:HG2	2.17	0.69
1:D:463:LYS:HG2	1:D:520:GLU:HB2	1.73	0.69
1:D:487:ASP:HB3	1:D:490:GLY:H	1.56	0.69
1:E:368:MET:HE1	1:E:380:PHE:HA	1.75	0.69
1:B:8:ALA:CA	1:B:553:LEU:HD12	2.23	0.69
1:B:69:ARG:N	1:B:112:GLU:OE2	2.25	0.69
1:B:121:VAL:HG23	1:B:199:MET:HG2	1.74	0.69
1:F:59:GLU:OE1	1:F:64:ARG:CD	2.38	0.69
1:F:368:MET:HE1	1:F:380:PHE:HA	1.75	0.69
1:B:307:ASP:OD2	1:B:311:HIS:HB2	1.93	0.68
1:C:535:SER:HB3	1:C:538:SER:HB3	1.76	0.68
1:E:56:LEU:HD21	1:E:110:MET:HE3	1.74	0.68
1:F:121:VAL:HG23	1:F:199:MET:HG2	1.74	0.68
1:A:89:VAL:O	1:A:91:ASN:N	2.26	0.68
1:A:565:PRO:HB2	1:A:568:MET:HG2	1.74	0.68
1:C:537:GLN:O	1:C:540:LYS:N	2.24	0.68
1:F:89:VAL:O	1:F:91:ASN:N	2.26	0.68
1:F:123:VAL:HG11	1:F:134:LEU:HD21	1.73	0.68
1:A:69:ARG:N	1:A:112:GLU:OE2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ALA:CA	1:C:553:LEU:HD12	2.23	0.68
1:C:473:GLU:C	1:C:474:ARG:HG2	2.17	0.68
1:E:535:SER:HB3	1:E:538:SER:HB3	1.76	0.68
1:F:76:ASN:O	1:F:77:THR:C	2.32	0.68
1:C:121:VAL:HG23	1:C:199:MET:HG2	1.74	0.68
1:D:59:GLU:OE1	1:D:64:ARG:CD	2.38	0.68
1:D:61:ASN:C	1:D:63:HIS:H	2.02	0.68
1:F:353:ARG:C	1:F:355:GLY:N	2.49	0.68
1:A:368:MET:HE1	1:A:380:PHE:HA	1.75	0.68
1:D:535:SER:HB3	1:D:538:SER:HB3	1.76	0.68
1:F:8:ALA:CA	1:F:553:LEU:HD12	2.23	0.68
1:F:167:ASN:OD1	1:F:451:ARG:NE	2.24	0.68
1:F:307:ASP:OD2	1:F:311:HIS:HB2	1.93	0.68
1:F:473:GLU:C	1:F:474:ARG:HG2	2.17	0.68
1:A:353:ARG:C	1:A:355:GLY:N	2.49	0.68
1:C:59:GLU:OE1	1:C:64:ARG:CD	2.38	0.68
1:C:84:LEU:HD11	1:C:204:TRP:CZ2	2.29	0.68
1:D:8:ALA:CA	1:D:553:LEU:HD12	2.23	0.68
1:D:56:LEU:HD21	1:D:110:MET:HE3	1.74	0.68
1:D:84:LEU:HD11	1:D:204:TRP:CZ2	2.29	0.68
1:D:368:MET:HE1	1:D:380:PHE:HA	1.75	0.68
1:B:353:ARG:C	1:B:355:GLY:N	2.49	0.68
1:E:89:VAL:O	1:E:91:ASN:N	2.26	0.68
1:E:84:LEU:HD11	1:E:204:TRP:CZ2	2.29	0.68
1:F:69:ARG:N	1:F:112:GLU:OE2	2.26	0.68
1:A:84:LEU:HD11	1:A:204:TRP:CZ2	2.29	0.68
1:A:573:SER:N	4:A:857:HOH:O	2.27	0.68
1:E:487:ASP:HB3	1:E:489:ASN:N	2.04	0.68
1:A:360:LYS:CE	1:B:273:ASP:OD2	2.41	0.68
1:D:159:MET:HE1	1:E:155:TYR:CD1	2.28	0.68
1:D:473:GLU:C	1:D:474:ARG:HG2	2.17	0.68
1:B:414:ASN:ND2	1:B:467:SER:H	1.93	0.67
1:C:7:ASN:O	1:C:9:GLN:N	2.27	0.67
1:C:61:ASN:C	1:C:63:HIS:H	2.02	0.67
1:C:278:GLU:H	1:C:354:GLN:HE22	1.42	0.67
1:C:307:ASP:OD2	1:C:311:HIS:HB2	1.93	0.67
1:F:7:ASN:O	1:F:9:GLN:N	2.28	0.67
1:A:7:ASN:O	1:A:9:GLN:N	2.27	0.67
1:E:7:ASN:O	1:E:9:GLN:N	2.27	0.67
1:F:84:LEU:HD11	1:F:204:TRP:CZ2	2.29	0.67
2:I:1:NAG:C8	2:I:1:NAG:N2	2.55	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:NAG:C8	2:K:2:NAG:N2	2.52	0.67
1:A:121:VAL:HG23	1:A:199:MET:HG2	1.74	0.67
1:D:278:GLU:H	1:D:354:GLN:HE22	1.42	0.67
1:A:537:GLN:O	1:A:540:LYS:N	2.23	0.67
1:D:307:ASP:OD2	1:D:311:HIS:HB2	1.93	0.67
1:D:639:VAL:HG23	1:D:641:ASN:HD22	1.60	0.67
1:E:307:ASP:OD2	1:E:311:HIS:HB2	1.93	0.67
1:A:182:ALA:O	1:A:186:GLU:HB2	1.95	0.67
1:A:424:THR:O	1:A:651:HIS:ND1	2.23	0.67
1:B:368:MET:HE1	1:B:380:PHE:HA	1.75	0.67
1:D:7:ASN:O	1:D:9:GLN:N	2.28	0.67
1:E:182:ALA:O	1:E:186:GLU:HB2	1.95	0.67
1:F:535:SER:HB3	1:F:538:SER:HB3	1.76	0.67
2:G:2:NAG:C8	2:G:2:NAG:N2	2.52	0.67
2:L:2:NAG:C8	2:L:2:NAG:N2	2.52	0.67
1:A:572:LYS:N	4:A:857:HOH:O	2.28	0.67
1:B:278:GLU:H	1:B:354:GLN:HE22	1.42	0.67
1:B:182:ALA:O	1:B:186:GLU:HB2	1.95	0.67
1:B:535:SER:HB3	1:B:538:SER:HB3	1.76	0.67
1:C:424:THR:O	1:C:651:HIS:ND1	2.23	0.67
1:E:414:ASN:ND2	1:E:467:SER:H	1.93	0.67
1:E:639:VAL:HG23	1:E:641:ASN:HD22	1.60	0.67
1:A:535:SER:HB3	1:A:538:SER:HB3	1.76	0.67
1:C:634:ARG:HH21	1:E:64:ARG:HD2	1.59	0.67
1:F:278:GLU:H	1:F:354:GLN:HE22	1.42	0.67
1:A:61:ASN:C	1:A:63:HIS:H	2.02	0.67
1:A:307:ASP:OD2	1:A:311:HIS:HB2	1.93	0.67
1:C:639:VAL:HG23	1:C:641:ASN:HD22	1.60	0.67
1:D:414:ASN:ND2	1:D:467:SER:H	1.93	0.67
1:E:61:ASN:C	1:E:63:HIS:H	2.02	0.66
1:B:84:LEU:HD11	1:B:204:TRP:CZ2	2.29	0.66
1:C:414:ASN:ND2	1:C:467:SER:H	1.93	0.66
1:D:182:ALA:O	1:D:186:GLU:HB2	1.95	0.66
1:F:414:ASN:ND2	1:F:467:SER:H	1.93	0.66
1:B:551:HIS:O	1:B:552:ASP:HB3	1.96	0.66
1:C:551:HIS:O	1:C:552:ASP:HB3	1.96	0.66
1:D:183:TYR:OH	1:D:234:GLU:OE1	2.11	0.66
1:C:182:ALA:O	1:C:186:GLU:HB2	1.95	0.66
1:E:424:THR:O	1:E:651:HIS:ND1	2.23	0.66
1:F:424:THR:O	1:F:651:HIS:ND1	2.23	0.66
1:A:48:ASP:CB	1:A:92:GLN:HE21	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:OD2	1:B:360:LYS:CE	2.41	0.66
1:A:475:LEU:HB2	1:A:590:ASP:OD1	1.96	0.66
1:B:7:ASN:O	1:B:9:GLN:N	2.28	0.66
1:D:177:ARG:CD	1:E:360:LYS:HB3	2.25	0.66
1:D:551:HIS:O	1:D:552:ASP:HB3	1.96	0.66
1:F:182:ALA:O	1:F:186:GLU:HB2	1.95	0.66
1:B:61:ASN:C	1:B:63:HIS:H	2.02	0.66
1:D:48:ASP:CB	1:D:92:GLN:HE21	2.09	0.66
1:F:1:ASP:HB2	1:F:4:GLY:H	1.61	0.66
1:A:639:VAL:HG23	1:A:641:ASN:HD22	1.60	0.66
1:C:491:ILE:HD11	1:D:175:LYS:O	1.96	0.66
1:D:475:LEU:HB2	1:D:590:ASP:OD1	1.96	0.66
1:D:487:ASP:HB3	1:D:489:ASN:N	2.04	0.66
1:F:183:TYR:OH	1:F:234:GLU:OE1	2.11	0.66
1:A:414:ASN:ND2	1:A:467:SER:H	1.93	0.66
1:C:1:ASP:HB2	1:C:4:GLY:H	1.61	0.66
1:B:48:ASP:CB	1:B:92:GLN:HE21	2.09	0.66
1:E:76:ASN:O	1:E:77:THR:C	2.32	0.66
1:F:61:ASN:C	1:F:63:HIS:H	2.02	0.66
1:C:634:ARG:HH11	1:C:634:ARG:CG	2.09	0.65
1:E:183:TYR:OH	1:E:234:GLU:OE1	2.11	0.65
1:F:48:ASP:CB	1:F:92:GLN:HE21	2.09	0.65
1:F:475:LEU:HB2	1:F:590:ASP:OD1	1.96	0.65
1:A:1:ASP:HB2	1:A:4:GLY:H	1.61	0.65
1:C:475:LEU:HB2	1:C:590:ASP:OD1	1.96	0.65
1:D:1:ASP:HB2	1:D:4:GLY:H	1.61	0.65
1:F:639:VAL:HG23	1:F:641:ASN:HD22	1.60	0.65
1:B:165:THR:CG2	1:B:449:ASN:HB2	2.27	0.65
1:D:19:ASP:O	1:D:20:LYS:C	2.40	0.65
1:E:59:GLU:OE1	1:E:64:ARG:CD	2.38	0.65
1:A:571:PRO:C	4:A:857:HOH:O	2.39	0.65
1:C:529:THR:O	1:C:530:VAL:HG23	1.97	0.65
1:D:69:ARG:N	1:D:112:GLU:OE2	2.25	0.65
1:F:512:VAL:CG1	1:F:513:PRO:HD2	2.27	0.65
1:A:353:ARG:O	1:A:355:GLY:N	2.30	0.65
1:B:414:ASN:HD21	1:B:467:SER:H	1.45	0.65
1:C:48:ASP:CB	1:C:92:GLN:HE21	2.09	0.65
1:C:69:ARG:N	1:C:112:GLU:OE2	2.25	0.65
1:C:414:ASN:HD21	1:C:467:SER:H	1.45	0.65
1:E:414:ASN:HD21	1:E:467:SER:H	1.45	0.65
1:E:512:VAL:CG1	1:E:513:PRO:HD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:446:VAL:HG13	1:F:446:VAL:O	1.97	0.65
1:A:278:GLU:H	1:A:354:GLN:HE22	1.42	0.65
1:A:414:ASN:HD21	1:A:467:SER:H	1.45	0.65
1:B:40:LEU:HD11	1:B:54:GLU:HG3	1.79	0.65
1:B:475:LEU:HB2	1:B:590:ASP:OD1	1.96	0.65
1:B:512:VAL:CG1	1:B:513:PRO:HD2	2.27	0.65
1:D:512:VAL:CG1	1:D:513:PRO:HD2	2.27	0.65
1:F:414:ASN:HD21	1:F:467:SER:H	1.45	0.65
1:A:19:ASP:O	1:A:20:LYS:C	2.40	0.65
1:A:551:HIS:O	1:A:552:ASP:HB3	1.96	0.65
1:B:19:ASP:O	1:B:20:LYS:C	2.40	0.65
1:B:353:ARG:O	1:B:355:GLY:N	2.30	0.65
1:C:40:LEU:HD11	1:C:54:GLU:HG3	1.79	0.65
1:E:39:PRO:HB3	1:E:102:ASN:HD21	1.62	0.65
1:E:475:LEU:HB2	1:E:590:ASP:OD1	1.96	0.65
1:F:353:ARG:O	1:F:355:GLY:N	2.30	0.65
1:A:529:THR:O	1:A:530:VAL:HG23	1.97	0.65
1:C:487:ASP:HB3	1:C:489:ASN:N	2.04	0.65
1:C:551:HIS:HD2	1:C:552:ASP:HA	1.62	0.65
1:E:278:GLU:H	1:E:354:GLN:HE22	1.42	0.65
1:B:46:TYR:CE2	1:B:53:VAL:HG21	2.32	0.65
1:D:39:PRO:HB3	1:D:102:ASN:HD21	1.62	0.65
1:F:19:ASP:O	1:F:20:LYS:C	2.40	0.65
1:F:529:THR:O	1:F:530:VAL:HG23	1.97	0.65
1:B:455:LEU:HG	1:B:456:ASN:N	2.13	0.64
1:B:529:THR:O	1:B:530:VAL:HG23	1.97	0.64
1:D:40:LEU:HD11	1:D:54:GLU:HG3	1.79	0.64
1:E:48:ASP:CB	1:E:92:GLN:HE21	2.09	0.64
1:E:446:VAL:O	1:E:446:VAL:HG13	1.97	0.64
1:E:466:MET:HG3	1:E:466:MET:O	1.97	0.64
1:F:148:SER:HB2	1:F:259:LEU:O	1.97	0.64
1:B:148:SER:HB2	1:B:259:LEU:O	1.97	0.64
1:C:353:ARG:O	1:C:355:GLY:N	2.30	0.64
1:D:529:THR:O	1:D:530:VAL:HG23	1.97	0.64
1:D:551:HIS:HD2	1:D:552:ASP:HA	1.62	0.64
1:E:1:ASP:HB2	1:E:4:GLY:H	1.61	0.64
1:B:446:VAL:O	1:B:446:VAL:HG13	1.97	0.64
1:B:551:HIS:HD2	1:B:552:ASP:HA	1.62	0.64
1:C:19:ASP:O	1:C:20:LYS:C	2.40	0.64
1:C:39:PRO:HB3	1:C:102:ASN:HD21	1.62	0.64
1:D:353:ARG:O	1:D:355:GLY:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:ARG:O	1:E:355:GLY:N	2.30	0.64
1:E:551:HIS:O	1:E:552:ASP:HB3	1.96	0.64
1:A:39:PRO:HB3	1:A:102:ASN:HD21	1.62	0.64
1:A:446:VAL:HG13	1:A:446:VAL:O	1.97	0.64
1:D:455:LEU:HG	1:D:456:ASN:N	2.13	0.64
1:A:40:LEU:HD11	1:A:54:GLU:HG3	1.79	0.64
1:A:512:VAL:CG1	1:A:513:PRO:HD2	2.27	0.64
1:A:551:HIS:HD2	1:A:552:ASP:HA	1.62	0.64
1:B:1:ASP:HB2	1:B:4:GLY:H	1.61	0.64
1:C:148:SER:HB2	1:C:259:LEU:O	1.97	0.64
1:D:414:ASN:HD21	1:D:467:SER:H	1.45	0.64
1:D:466:MET:HG3	1:D:466:MET:O	1.97	0.64
1:E:165:THR:CG2	1:E:449:ASN:HB2	2.27	0.64
1:F:551:HIS:O	1:F:552:ASP:HB3	1.96	0.64
1:C:512:VAL:CG1	1:C:513:PRO:HD2	2.27	0.64
1:F:40:LEU:HD11	1:F:54:GLU:HG3	1.79	0.64
1:F:46:TYR:CE2	1:F:53:VAL:HG21	2.32	0.64
1:F:165:THR:CG2	1:F:449:ASN:HB2	2.27	0.64
1:B:466:MET:HG3	1:B:466:MET:O	1.97	0.64
1:B:639:VAL:HG23	1:B:641:ASN:HD22	1.60	0.64
1:D:46:TYR:CE2	1:D:53:VAL:HG21	2.32	0.64
1:F:487:ASP:HB3	1:F:489:ASN:N	2.04	0.64
1:A:148:SER:HB2	1:A:259:LEU:O	1.97	0.64
1:B:39:PRO:HB3	1:B:102:ASN:HD21	1.62	0.64
1:E:46:TYR:CE2	1:E:53:VAL:HG21	2.32	0.64
1:A:26:LYS:NZ	4:A:732:HOH:O	2.28	0.64
1:B:89:VAL:O	1:B:90:LEU:C	2.41	0.64
1:E:40:LEU:HD11	1:E:54:GLU:HG3	1.79	0.64
1:E:148:SER:HB2	1:E:259:LEU:O	1.97	0.64
1:F:593:THR:C	1:F:595:GLY:H	2.06	0.64
1:A:46:TYR:CE2	1:A:53:VAL:HG21	2.32	0.64
1:A:255:GLY:HA2	1:A:271:ARG:NH1	2.13	0.64
1:A:487:ASP:HB3	1:A:489:ASN:N	2.04	0.64
1:C:46:TYR:CE2	1:C:53:VAL:HG21	2.32	0.64
1:C:89:VAL:O	1:C:90:LEU:C	2.41	0.64
1:C:593:THR:C	1:C:595:GLY:H	2.06	0.64
1:E:89:VAL:O	1:E:90:LEU:C	2.41	0.64
1:A:466:MET:HG3	1:A:466:MET:O	1.97	0.63
1:B:593:THR:C	1:B:595:GLY:H	2.06	0.63
1:F:255:GLY:HA2	1:F:271:ARG:NH1	2.14	0.63
1:F:551:HIS:HD2	1:F:552:ASP:HA	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:VAL:O	1:D:446:VAL:HG13	1.97	0.63
1:E:168:VAL:CG2	1:E:452:VAL:HG12	2.29	0.63
1:E:300:ILE:HG12	1:E:324:LEU:HD11	1.81	0.63
1:B:29:ASP:OD1	1:B:29:ASP:N	2.31	0.63
1:B:168:VAL:CG2	1:B:452:VAL:HG12	2.29	0.63
1:B:255:GLY:HA2	1:B:271:ARG:NH1	2.13	0.63
1:C:446:VAL:HG13	1:C:446:VAL:O	1.97	0.63
1:D:593:THR:C	1:D:595:GLY:H	2.06	0.63
1:F:300:ILE:HG12	1:F:324:LEU:HD11	1.81	0.63
1:B:300:ILE:HG12	1:B:324:LEU:HD11	1.81	0.63
1:E:19:ASP:O	1:E:20:LYS:C	2.40	0.63
1:E:593:THR:C	1:E:595:GLY:H	2.06	0.63
1:F:466:MET:HG3	1:F:466:MET:O	1.97	0.63
1:E:533:MET:CB	1:E:534:PRO:HD2	2.28	0.63
1:E:551:HIS:HD2	1:E:552:ASP:HA	1.62	0.63
1:F:455:LEU:HG	1:F:456:ASN:N	2.13	0.63
1:A:183:TYR:OH	1:A:234:GLU:OE1	2.11	0.63
1:B:5:THR:HG23	1:B:10:LYS:HE3	1.81	0.63
1:C:300:ILE:HG12	1:C:324:LEU:HD11	1.81	0.63
1:D:148:SER:HB2	1:D:259:LEU:O	1.97	0.63
1:E:255:GLY:HA2	1:E:271:ARG:NH1	2.14	0.63
1:E:529:THR:O	1:E:530:VAL:HG23	1.97	0.63
1:A:5:THR:HG23	1:A:10:LYS:HE3	1.81	0.63
1:A:455:LEU:HG	1:A:456:ASN:N	2.13	0.63
1:A:593:THR:C	1:A:595:GLY:H	2.06	0.63
1:D:300:ILE:HG12	1:D:324:LEU:HD11	1.81	0.63
1:D:380:PHE:CE2	1:D:384:HIS:CE1	2.87	0.63
1:F:150:VAL:HG12	1:F:433:LEU:HD11	1.81	0.63
1:A:239:TRP:CH2	1:A:574:LYS:HE3	2.34	0.63
1:C:255:GLY:HA2	1:C:271:ARG:NH1	2.14	0.63
1:D:486:GLU:HA	1:D:492:THR:HA	1.81	0.63
1:E:634:ARG:HH11	1:E:634:ARG:CG	2.09	0.63
1:F:5:THR:HG23	1:F:10:LYS:HE3	1.81	0.63
1:F:39:PRO:HB3	1:F:102:ASN:HD21	1.62	0.63
1:F:402:THR:HG23	1:F:405:ASN:OD1	1.99	0.63
1:A:89:VAL:O	1:A:90:LEU:C	2.41	0.63
1:B:380:PHE:CE2	1:B:384:HIS:CE1	2.87	0.63
1:C:239:TRP:CH2	1:C:574:LYS:HE3	2.34	0.62
1:D:89:VAL:O	1:D:90:LEU:C	2.41	0.62
1:D:168:VAL:CG2	1:D:452:VAL:HG12	2.28	0.62
1:D:254:GLU:OE2	1:E:360:LYS:NZ	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:486:GLU:HA	1:E:492:THR:HA	1.81	0.62
1:E:512:VAL:HG13	1:E:513:PRO:HD2	1.81	0.62
1:F:89:VAL:O	1:F:90:LEU:C	2.41	0.62
1:C:262:TYR:CE1	1:C:268:PHE:CE1	2.88	0.62
1:C:455:LEU:HG	1:C:456:ASN:N	2.13	0.62
1:C:466:MET:HG3	1:C:466:MET:O	1.97	0.62
1:D:239:TRP:CH2	1:D:574:LYS:HE3	2.34	0.62
1:E:150:VAL:HG12	1:E:433:LEU:HD11	1.81	0.62
1:F:168:VAL:CG2	1:F:452:VAL:HG12	2.29	0.62
1:B:402:THR:HG23	1:B:405:ASN:OD1	1.99	0.62
1:C:168:VAL:CG2	1:C:452:VAL:HG12	2.28	0.62
1:C:183:TYR:OH	1:C:234:GLU:OE1	2.11	0.62
1:C:486:GLU:HA	1:C:492:THR:HA	1.81	0.62
1:E:380:PHE:CE2	1:E:384:HIS:CE1	2.87	0.62
1:E:455:LEU:HG	1:E:456:ASN:N	2.13	0.62
1:A:168:VAL:CG2	1:A:452:VAL:HG12	2.29	0.62
1:A:300:ILE:HG12	1:A:324:LEU:HD11	1.81	0.62
1:D:512:VAL:HG13	1:D:513:PRO:HD2	1.81	0.62
1:E:262:TYR:CE1	1:E:268:PHE:CE1	2.88	0.62
1:E:239:TRP:CH2	1:E:574:LYS:HE3	2.34	0.62
1:A:301:ASP:OD2	1:A:393:LYS:NZ	2.33	0.62
1:A:402:THR:HG23	1:A:405:ASN:OD1	1.99	0.62
1:B:486:GLU:HA	1:B:492:THR:HA	1.81	0.62
1:B:512:VAL:HG13	1:B:513:PRO:HD2	1.81	0.62
1:C:380:PHE:CE2	1:C:384:HIS:CE1	2.87	0.62
1:D:62:ASP:O	1:D:63:HIS:HD2	1.83	0.62
1:D:402:THR:HG23	1:D:405:ASN:OD1	1.99	0.62
1:F:512:VAL:HG13	1:F:513:PRO:HD2	1.81	0.62
1:A:29:ASP:OD1	1:A:29:ASP:N	2.31	0.62
1:E:127:LYS:NZ	1:E:211:TYR:HE2	1.98	0.62
1:A:150:VAL:HG12	1:A:433:LEU:HD11	1.81	0.62
1:A:165:THR:CG2	1:A:449:ASN:HB2	2.27	0.62
1:A:380:PHE:CE2	1:A:384:HIS:CE1	2.87	0.62
1:A:486:GLU:HA	1:A:492:THR:HA	1.81	0.62
1:B:239:TRP:CH2	1:B:574:LYS:HE3	2.34	0.62
1:C:62:ASP:O	1:C:63:HIS:HD2	1.83	0.62
1:E:62:ASP:O	1:E:63:HIS:HD2	1.83	0.62
1:A:5:THR:HG22	1:A:6:GLY:H	1.65	0.62
1:A:7:ASN:C	1:A:9:GLN:N	2.55	0.62
1:A:256:PHE:CD2	1:A:378:PRO:HD3	2.35	0.62
1:C:5:THR:HG22	1:C:6:GLY:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:THR:HG23	1:E:10:LYS:HE3	1.81	0.62
1:F:239:TRP:CH2	1:F:574:LYS:HE3	2.34	0.62
1:B:256:PHE:CD2	1:B:378:PRO:HD3	2.35	0.62
1:D:127:LYS:NZ	1:D:211:TYR:HE2	1.98	0.62
1:D:262:TYR:CE1	1:D:268:PHE:CE1	2.88	0.62
1:D:316:ARG:HH21	1:F:338:GLN:NE2	1.98	0.62
1:E:5:THR:HG22	1:E:6:GLY:H	1.65	0.62
1:F:62:ASP:O	1:F:63:HIS:HD2	1.83	0.62
1:F:380:PHE:CE2	1:F:384:HIS:CE1	2.87	0.62
1:E:256:PHE:CD2	1:E:378:PRO:HD3	2.35	0.61
1:E:402:THR:HG23	1:E:405:ASN:OD1	1.99	0.61
1:F:262:TYR:CE1	1:F:268:PHE:CE1	2.88	0.61
1:F:486:GLU:HA	1:F:492:THR:HA	1.81	0.61
1:F:487:ASP:HB3	1:F:490:GLY:N	2.15	0.61
1:A:485:ILE:HD12	1:A:579:GLU:O	2.01	0.61
1:A:512:VAL:HG13	1:A:513:PRO:HD2	1.81	0.61
1:B:127:LYS:NZ	1:B:211:TYR:HE2	1.98	0.61
1:C:150:VAL:HG12	1:C:433:LEU:HD11	1.81	0.61
1:D:5:THR:HG23	1:D:10:LYS:HE3	1.81	0.61
1:D:120:TYR:O	1:D:124:ILE:HG13	2.00	0.61
1:D:485:ILE:HD12	1:D:579:GLU:O	2.01	0.61
1:F:256:PHE:CD2	1:F:378:PRO:HD3	2.35	0.61
1:C:32:ASP:HB2	1:C:36:ASN:HD22	1.65	0.61
1:C:127:LYS:NZ	1:C:211:TYR:HE2	1.98	0.61
1:C:256:PHE:CD2	1:C:378:PRO:HD3	2.35	0.61
1:C:272:PRO:HG2	1:F:272:PRO:CG	2.30	0.61
1:D:32:ASP:HB2	1:D:36:ASN:HD22	1.65	0.61
1:F:120:TYR:O	1:F:124:ILE:HG13	2.00	0.61
1:A:262:TYR:CE1	1:A:268:PHE:CE1	2.88	0.61
1:B:150:VAL:HG12	1:B:433:LEU:HD11	1.81	0.61
1:B:485:ILE:HD12	1:B:579:GLU:O	2.01	0.61
1:C:5:THR:HG23	1:C:10:LYS:HE3	1.81	0.61
1:C:165:THR:CG2	1:C:449:ASN:HB2	2.27	0.61
1:C:533:MET:CB	1:C:534:PRO:HD2	2.28	0.61
1:D:150:VAL:HG12	1:D:433:LEU:HD11	1.81	0.61
1:D:255:GLY:HA2	1:D:271:ARG:NH1	2.13	0.61
1:D:256:PHE:CD2	1:D:378:PRO:HD3	2.35	0.61
1:D:301:ASP:OD2	1:D:393:LYS:NZ	2.33	0.61
1:F:485:ILE:HD12	1:F:579:GLU:O	2.01	0.61
1:F:533:MET:CB	1:F:534:PRO:HD2	2.28	0.61
1:A:256:PHE:CE2	1:A:377:ASP:HA	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:HD2	1:F:360:LYS:HB3	1.82	0.61
1:C:301:ASP:OD2	1:C:393:LYS:NZ	2.33	0.61
1:C:512:VAL:HG13	1:C:513:PRO:HD2	1.81	0.61
1:E:485:ILE:HD12	1:E:579:GLU:O	2.01	0.61
1:B:487:ASP:HB3	1:B:490:GLY:N	2.15	0.61
1:D:634:ARG:NH2	1:F:64:ARG:HD2	2.06	0.61
1:F:5:THR:HG22	1:F:6:GLY:H	1.65	0.61
1:B:32:ASP:HB2	1:B:36:ASN:HD22	1.65	0.61
1:B:301:ASP:OD2	1:B:393:LYS:NZ	2.33	0.61
1:C:402:THR:HG23	1:C:405:ASN:OD1	1.99	0.61
1:F:86:LEU:HD22	1:F:90:LEU:HD22	1.83	0.61
1:A:120:TYR:O	1:A:124:ILE:HG13	2.00	0.61
1:B:62:ASP:O	1:B:63:HIS:HD2	1.83	0.61
1:B:262:TYR:CE1	1:B:268:PHE:CE1	2.88	0.61
1:C:256:PHE:CE2	1:C:377:ASP:HA	2.36	0.61
1:D:5:THR:HG22	1:D:6:GLY:H	1.65	0.61
1:F:634:ARG:HH11	1:F:634:ARG:CG	2.09	0.61
1:D:256:PHE:CE2	1:D:377:ASP:HA	2.36	0.61
1:D:634:ARG:HH11	1:D:634:ARG:CG	2.09	0.61
1:E:86:LEU:HD22	1:E:90:LEU:CD2	2.31	0.61
1:F:256:PHE:CE2	1:F:377:ASP:HA	2.36	0.61
1:A:62:ASP:O	1:A:63:HIS:HD2	1.83	0.60
1:A:127:LYS:NZ	1:A:211:TYR:HE2	1.98	0.60
1:B:634:ARG:HH11	1:B:634:ARG:CG	2.09	0.60
1:C:485:ILE:HD12	1:C:579:GLU:O	2.01	0.60
1:C:487:ASP:HB3	1:C:490:GLY:N	2.15	0.60
1:E:487:ASP:HB3	1:E:490:GLY:N	2.15	0.60
1:F:32:ASP:HB2	1:F:36:ASN:HD22	1.65	0.60
1:A:32:ASP:HB2	1:A:36:ASN:HD22	1.65	0.60
1:A:86:LEU:HD22	1:A:90:LEU:CD2	2.31	0.60
1:B:300:ILE:CD1	1:B:390:ILE:HG22	2.31	0.60
1:C:86:LEU:HD22	1:C:90:LEU:CD2	2.31	0.60
1:C:120:TYR:O	1:C:124:ILE:HG13	2.00	0.60
1:C:535:SER:OG	1:C:536:PHE:N	2.34	0.60
1:D:86:LEU:HD22	1:D:90:LEU:CD2	2.31	0.60
1:D:487:ASP:HB3	1:D:490:GLY:N	2.15	0.60
1:E:120:TYR:O	1:E:124:ILE:HG13	2.00	0.60
1:A:487:ASP:HB3	1:A:490:GLY:N	2.15	0.60
1:B:121:VAL:CG2	1:B:199:MET:HG2	2.32	0.60
1:C:576:GLU:CD	1:D:576:GLU:OE1	2.44	0.60
1:E:121:VAL:CG2	1:E:199:MET:HG2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ILE:HG22	1:E:133:VAL:N	2.16	0.60
1:E:256:PHE:CE2	1:E:377:ASP:HA	2.36	0.60
1:B:86:LEU:HD22	1:B:90:LEU:CD2	2.31	0.60
1:C:300:ILE:CD1	1:C:390:ILE:HG22	2.31	0.60
1:D:165:THR:CG2	1:D:449:ASN:HB2	2.27	0.60
1:D:300:ILE:CD1	1:D:390:ILE:HG22	2.31	0.60
1:E:7:ASN:C	1:E:9:GLN:N	2.55	0.60
1:F:127:LYS:NZ	1:F:211:TYR:HE2	1.98	0.60
1:A:283:VAL:O	1:A:284:ALA:CB	2.49	0.60
1:A:479:ARG:NH2	1:A:618:ASP:OD2	2.35	0.60
1:B:132:ILE:HG22	1:B:133:VAL:N	2.16	0.60
1:C:86:LEU:HD22	1:C:90:LEU:HD22	1.83	0.60
1:C:272:PRO:CG	1:F:272:PRO:HG2	2.31	0.60
1:D:479:ARG:NH2	1:D:618:ASP:OD2	2.35	0.60
1:E:403:HIS:C	1:E:405:ASN:N	2.59	0.60
1:E:479:ARG:NH2	1:E:618:ASP:OD2	2.35	0.60
1:F:300:ILE:CD1	1:F:390:ILE:HG22	2.31	0.60
1:A:367:VAL:O	1:A:373:THR:HG22	2.02	0.60
1:B:183:TYR:OH	1:B:234:GLU:HB3	2.02	0.60
1:D:591:LYS:HA	1:D:594:GLU:HB2	1.84	0.60
1:B:535:SER:OG	1:B:536:PHE:N	2.34	0.60
1:B:591:LYS:HA	1:B:594:GLU:HB2	1.84	0.60
1:C:132:ILE:HG22	1:C:133:VAL:N	2.16	0.60
1:C:429:PHE:HB3	1:C:452:VAL:HG23	1.84	0.60
1:C:529:THR:C	1:C:530:VAL:HG23	2.27	0.60
1:F:121:VAL:CG2	1:F:199:MET:HG2	2.32	0.60
1:A:300:ILE:CD1	1:A:390:ILE:HG22	2.31	0.60
1:D:7:ASN:C	1:D:9:GLN:N	2.55	0.60
1:E:429:PHE:HB3	1:E:452:VAL:HG23	1.84	0.60
1:E:529:THR:C	1:E:530:VAL:HG23	2.27	0.60
1:F:86:LEU:HD22	1:F:90:LEU:CD2	2.31	0.60
1:F:529:THR:C	1:F:530:VAL:HG23	2.27	0.60
1:B:479:ARG:NH2	1:B:618:ASP:OD2	2.35	0.60
1:B:624:TYR:CE1	1:B:625:PRO:HB3	2.37	0.60
1:C:367:VAL:O	1:C:373:THR:HG22	2.02	0.60
1:C:479:ARG:NH2	1:C:618:ASP:OD2	2.34	0.60
1:D:183:TYR:OH	1:D:234:GLU:HB3	2.02	0.60
1:D:367:VAL:O	1:D:373:THR:HG22	2.02	0.60
1:E:32:ASP:HB2	1:E:36:ASN:HD22	1.65	0.60
1:E:301:ASP:OD2	1:E:393:LYS:NZ	2.33	0.60
1:F:301:ASP:OD2	1:F:393:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:VAL:CG2	1:A:199:MET:HG2	2.32	0.60
1:A:591:LYS:HB2	1:A:591:LYS:NZ	2.17	0.60
1:B:120:TYR:O	1:B:124:ILE:HG13	2.00	0.60
1:B:256:PHE:CE2	1:B:377:ASP:HA	2.36	0.60
1:B:429:PHE:HB3	1:B:452:VAL:HG23	1.84	0.60
1:B:529:THR:C	1:B:530:VAL:HG23	2.27	0.60
1:C:260:THR:HG22	1:C:268:PHE:CE2	2.37	0.60
1:D:529:THR:C	1:D:530:VAL:HG23	2.27	0.60
1:D:535:SER:OG	1:D:536:PHE:N	2.34	0.60
1:D:606:HIS:HD2	1:D:608:GLN:CG	2.14	0.60
1:E:160:THR:O	1:E:161:GLN:HB2	2.02	0.60
1:E:183:TYR:OH	1:E:234:GLU:HB3	2.02	0.60
1:E:300:ILE:CD1	1:E:390:ILE:HG22	2.31	0.60
1:F:183:TYR:OH	1:F:234:GLU:HB3	2.02	0.60
1:A:160:THR:O	1:A:161:GLN:HB2	2.02	0.59
1:A:575:PRO:HD2	1:A:576:GLU:HG3	1.84	0.59
1:C:591:LYS:HA	1:C:594:GLU:HB2	1.84	0.59
1:D:86:LEU:HD22	1:D:90:LEU:HD22	1.83	0.59
1:D:624:TYR:CE1	1:D:625:PRO:HB3	2.37	0.59
1:E:535:SER:OG	1:E:536:PHE:N	2.34	0.59
1:F:479:ARG:NH2	1:F:618:ASP:OD2	2.35	0.59
1:A:86:LEU:HD22	1:A:90:LEU:HD22	1.83	0.59
1:B:86:LEU:HD22	1:B:90:LEU:HD22	1.83	0.59
1:C:575:PRO:HD2	1:C:576:GLU:HG3	1.84	0.59
1:D:38:ASN:C	1:D:40:LEU:H	2.10	0.59
1:D:496:ASP:OD1	1:D:499:ARG:HD3	2.03	0.59
1:F:591:LYS:NZ	1:F:591:LYS:HB2	2.17	0.59
1:B:5:THR:HG22	1:B:6:GLY:H	1.65	0.59
1:D:76:ASN:HD22	1:D:79:GLN:H	1.51	0.59
1:D:121:VAL:CG2	1:D:199:MET:HG2	2.32	0.59
1:D:132:ILE:HG22	1:D:133:VAL:N	2.16	0.59
1:D:168:VAL:HG21	1:D:452:VAL:HG12	1.84	0.59
1:F:535:SER:OG	1:F:536:PHE:N	2.34	0.59
1:B:575:PRO:HD2	1:B:576:GLU:HG3	1.84	0.59
1:C:624:TYR:CE1	1:C:625:PRO:HB3	2.37	0.59
1:E:86:LEU:HD22	1:E:90:LEU:HD22	1.83	0.59
1:E:367:VAL:O	1:E:373:THR:HG22	2.02	0.59
1:E:491:ILE:HG22	1:E:491:ILE:O	2.03	0.59
1:F:367:VAL:O	1:F:373:THR:HG22	2.02	0.59
1:F:591:LYS:HA	1:F:594:GLU:HB2	1.84	0.59
1:A:132:ILE:HG22	1:A:133:VAL:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:OD1	1:A:309:ASP:N	2.34	0.59
1:A:491:ILE:O	1:A:491:ILE:HG22	2.03	0.59
1:B:168:VAL:HG21	1:B:452:VAL:HG12	1.84	0.59
1:B:468:ASN:HD22	1:B:514:SER:HA	1.67	0.59
1:C:121:VAL:CG2	1:C:199:MET:HG2	2.32	0.59
1:C:591:LYS:HB2	1:C:591:LYS:NZ	2.17	0.59
1:F:429:PHE:HB3	1:F:452:VAL:HG23	1.84	0.59
1:A:529:THR:C	1:A:530:VAL:HG23	2.27	0.59
1:B:403:HIS:C	1:B:405:ASN:N	2.59	0.59
1:C:496:ASP:OD1	1:C:499:ARG:HD3	2.03	0.59
1:F:76:ASN:HD22	1:F:79:GLN:H	1.51	0.59
1:A:168:VAL:HG21	1:A:452:VAL:HG12	1.84	0.59
1:A:496:ASP:OD1	1:A:499:ARG:HD3	2.03	0.59
1:A:591:LYS:HA	1:A:594:GLU:HB2	1.84	0.59
1:B:269:PRO:HB3	1:B:363:LEU:HD23	1.85	0.59
1:B:574:LYS:HD3	1:B:578:MET:SD	2.43	0.59
1:C:76:ASN:HD22	1:C:79:GLN:H	1.51	0.59
1:C:160:THR:O	1:C:161:GLN:HB2	2.02	0.59
1:C:168:VAL:HG21	1:C:452:VAL:HG12	1.84	0.59
1:D:429:PHE:HB3	1:D:452:VAL:HG23	1.84	0.59
1:E:168:VAL:HG21	1:E:452:VAL:HG12	1.84	0.59
1:E:591:LYS:HB2	1:E:591:LYS:NZ	2.17	0.59
1:A:183:TYR:OH	1:A:234:GLU:HB3	2.02	0.59
1:A:535:SER:OG	1:A:536:PHE:N	2.34	0.59
1:C:183:TYR:OH	1:C:234:GLU:HB3	2.02	0.59
1:C:470:ASN:CB	1:C:474:ARG:HD3	2.33	0.59
1:C:491:ILE:O	1:C:491:ILE:HG22	2.03	0.59
1:D:48:ASP:HB3	1:D:92:GLN:NE2	2.18	0.59
1:D:403:HIS:C	1:D:405:ASN:N	2.59	0.59
1:D:574:LYS:HD3	1:D:578:MET:SD	2.43	0.59
1:F:78:ARG:O	1:F:79:GLN:C	2.45	0.59
1:F:260:THR:HG22	1:F:268:PHE:CE2	2.37	0.59
1:C:403:HIS:C	1:C:405:ASN:N	2.59	0.59
1:D:56:LEU:HD11	1:D:110:MET:CE	2.33	0.59
1:E:207:ASP:OD2	1:E:212:HIS:CB	2.51	0.59
1:E:575:PRO:HD2	1:E:576:GLU:HG3	1.84	0.59
1:F:132:ILE:HG22	1:F:133:VAL:N	2.16	0.59
1:A:574:LYS:HD3	1:A:578:MET:SD	2.43	0.59
1:B:160:THR:O	1:B:161:GLN:HB2	2.02	0.59
1:D:260:THR:HG22	1:D:268:PHE:CE2	2.37	0.59
1:E:48:ASP:HB3	1:E:92:GLN:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:LEU:HD11	1:E:110:MET:CE	2.33	0.59
1:A:38:ASN:C	1:A:40:LEU:H	2.10	0.58
1:A:76:ASN:HD22	1:A:79:GLN:H	1.51	0.58
1:A:260:THR:HG22	1:A:268:PHE:CE2	2.37	0.58
1:A:533:MET:HG2	4:A:781:HOH:O	2.02	0.58
1:A:624:TYR:CE1	1:A:625:PRO:HB3	2.37	0.58
1:B:260:THR:HG22	1:B:268:PHE:CE2	2.37	0.58
1:C:38:ASN:C	1:C:40:LEU:H	2.10	0.58
1:E:634:ARG:HG2	1:E:634:ARG:NH1	2.14	0.58
1:F:269:PRO:HB3	1:F:363:LEU:HD23	1.85	0.58
1:F:468:ASN:HD22	1:F:514:SER:HA	1.67	0.58
1:F:574:LYS:HD3	1:F:578:MET:SD	2.43	0.58
1:A:269:PRO:HB3	1:A:363:LEU:HD23	1.85	0.58
1:C:468:ASN:HD22	1:C:514:SER:HA	1.67	0.58
1:D:283:VAL:O	1:D:284:ALA:CB	2.49	0.58
1:D:470:ASN:CB	1:D:474:ARG:HD3	2.33	0.58
1:D:491:ILE:O	1:D:491:ILE:HG22	2.03	0.58
1:E:574:LYS:HD3	1:E:578:MET:SD	2.43	0.58
1:F:48:ASP:HB3	1:F:92:GLN:NE2	2.18	0.58
1:F:624:TYR:CE1	1:F:625:PRO:HB3	2.37	0.58
1:C:48:ASP:HB3	1:C:92:GLN:NE2	2.18	0.58
1:C:78:ARG:O	1:C:79:GLN:C	2.45	0.58
1:D:272:PRO:HG2	1:E:272:PRO:CD	2.33	0.58
1:D:634:ARG:HG2	1:D:634:ARG:NH1	2.14	0.58
1:E:470:ASN:CB	1:E:474:ARG:HD3	2.33	0.58
1:E:551:HIS:HD2	1:E:552:ASP:CA	2.16	0.58
1:A:48:ASP:HB3	1:A:92:GLN:NE2	2.18	0.58
1:A:429:PHE:HB3	1:A:452:VAL:HG23	1.84	0.58
1:B:496:ASP:OD1	1:B:499:ARG:HD3	2.03	0.58
1:C:207:ASP:OD2	1:C:212:HIS:CB	2.51	0.58
1:E:591:LYS:HA	1:E:594:GLU:HB2	1.84	0.58
1:F:160:THR:O	1:F:161:GLN:HB2	2.02	0.58
1:A:634:ARG:HH11	1:A:634:ARG:CG	2.09	0.58
1:B:491:ILE:HG22	1:B:491:ILE:O	2.03	0.58
1:C:56:LEU:HD11	1:C:110:MET:CE	2.33	0.58
1:C:360:LYS:HE3	1:F:273:ASP:OD2	2.03	0.58
1:D:160:THR:O	1:D:161:GLN:HB2	2.02	0.58
1:D:269:PRO:HB3	1:D:363:LEU:HD23	1.85	0.58
1:E:38:ASN:C	1:E:40:LEU:H	2.10	0.58
1:E:624:TYR:CE1	1:E:625:PRO:HB3	2.37	0.58
1:F:38:ASN:C	1:F:40:LEU:H	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:PHE:CD1	1:B:256:PHE:C	2.82	0.58
1:C:269:PRO:HB3	1:C:363:LEU:HD23	1.85	0.58
1:C:573:SER:HB2	1:C:578:MET:HG3	1.86	0.58
1:C:574:LYS:HD3	1:C:578:MET:SD	2.43	0.58
1:C:629:ARG:HH11	1:C:629:ARG:HG3	1.69	0.58
1:D:468:ASN:HD22	1:D:514:SER:HA	1.67	0.58
1:D:591:LYS:HB2	1:D:591:LYS:NZ	2.17	0.58
1:E:606:HIS:HD2	1:E:608:GLN:CG	2.14	0.58
1:A:470:ASN:CB	1:A:474:ARG:HD3	2.33	0.58
1:B:367:VAL:O	1:B:373:THR:HG22	2.02	0.58
1:D:207:ASP:OD2	1:D:212:HIS:CB	2.51	0.58
1:E:256:PHE:CD1	1:E:256:PHE:C	2.82	0.58
1:E:260:THR:HG22	1:E:268:PHE:CE2	2.37	0.58
1:B:11:GLN:O	1:B:15:ASN:ND2	2.37	0.58
1:B:38:ASN:C	1:B:40:LEU:H	2.10	0.58
1:B:78:ARG:O	1:B:79:GLN:C	2.45	0.58
1:D:46:TYR:CD2	1:D:53:VAL:HG21	2.39	0.58
1:E:496:ASP:OD1	1:E:499:ARG:HD3	2.03	0.58
1:F:56:LEU:HD11	1:F:110:MET:CE	2.33	0.58
1:F:403:HIS:C	1:F:405:ASN:N	2.59	0.58
1:F:496:ASP:OD1	1:F:499:ARG:HD3	2.03	0.58
1:B:43:THR:HG23	1:B:49:HIS:C	2.29	0.58
1:B:48:ASP:HB3	1:B:92:GLN:NE2	2.18	0.58
1:B:207:ASP:OD2	1:B:212:HIS:CB	2.51	0.58
1:B:591:LYS:HB2	1:B:591:LYS:NZ	2.17	0.58
1:E:235:ARG:O	1:E:240:LEU:HB2	2.04	0.58
1:F:168:VAL:HG21	1:F:452:VAL:HG12	1.84	0.58
1:F:175:LYS:O	1:F:176:ASN:HB2	2.04	0.58
1:F:256:PHE:CD1	1:F:256:PHE:C	2.82	0.58
1:F:551:HIS:HD2	1:F:552:ASP:CA	2.16	0.58
1:A:403:HIS:C	1:A:405:ASN:N	2.59	0.58
1:B:56:LEU:HD11	1:B:110:MET:CE	2.33	0.58
1:B:551:HIS:HD2	1:B:552:ASP:CA	2.16	0.58
1:B:573:SER:HB2	1:B:578:MET:HG3	1.86	0.58
1:C:175:LYS:O	1:C:176:ASN:HB2	2.04	0.58
1:D:575:PRO:HD2	1:D:576:GLU:HG3	1.84	0.58
1:F:491:ILE:O	1:F:491:ILE:HG22	2.03	0.58
1:F:575:PRO:HD2	1:F:576:GLU:HG3	1.84	0.58
1:A:11:GLN:O	1:A:15:ASN:ND2	2.37	0.57
1:A:56:LEU:HD11	1:A:110:MET:CE	2.33	0.57
1:B:183:TYR:OH	1:B:234:GLU:OE1	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ARG:O	1:D:240:LEU:HB2	2.04	0.57
1:D:551:HIS:HD2	1:D:552:ASP:CA	2.16	0.57
1:F:207:ASP:OD2	1:F:212:HIS:CB	2.51	0.57
1:A:468:ASN:HD22	1:A:514:SER:HA	1.67	0.57
1:B:76:ASN:HD22	1:B:79:GLN:H	1.51	0.57
1:D:256:PHE:C	1:D:256:PHE:CD1	2.82	0.57
1:D:522:SER:O	1:D:524:LYS:N	2.38	0.57
1:F:470:ASN:CB	1:F:474:ARG:HD3	2.33	0.57
1:A:95:GLU:HA	1:A:128:LEU:HD21	1.86	0.57
1:A:470:ASN:ND2	1:A:474:ARG:HD3	2.20	0.57
1:A:629:ARG:HH11	1:A:629:ARG:HG3	1.69	0.57
1:D:48:ASP:HB3	1:D:92:GLN:HE21	1.69	0.57
1:E:175:LYS:O	1:E:176:ASN:HB2	2.04	0.57
1:E:468:ASN:HD22	1:E:514:SER:HA	1.67	0.57
1:E:629:ARG:HG3	1:E:629:ARG:HH11	1.69	0.57
1:A:46:TYR:CD2	1:A:53:VAL:HG21	2.39	0.57
1:B:470:ASN:CB	1:B:474:ARG:HD3	2.33	0.57
1:D:573:SER:HB2	1:D:578:MET:HG3	1.86	0.57
1:E:78:ARG:O	1:E:79:GLN:C	2.45	0.57
1:E:573:SER:HB2	1:E:578:MET:HG3	1.86	0.57
1:F:470:ASN:ND2	1:F:474:ARG:HD3	2.20	0.57
1:A:551:HIS:HD2	1:A:552:ASP:CA	2.16	0.57
1:B:46:TYR:CD2	1:B:53:VAL:HG21	2.39	0.57
1:C:551:HIS:HD2	1:C:552:ASP:CA	2.16	0.57
1:F:11:GLN:O	1:F:15:ASN:ND2	2.37	0.57
1:F:46:TYR:CD2	1:F:53:VAL:HG21	2.39	0.57
1:F:522:SER:O	1:F:524:LYS:N	2.38	0.57
1:F:573:SER:HB2	1:F:578:MET:HG3	1.86	0.57
1:E:11:GLN:O	1:E:15:ASN:ND2	2.37	0.57
1:E:43:THR:HG23	1:E:49:HIS:C	2.29	0.57
1:E:76:ASN:HD22	1:E:79:GLN:H	1.51	0.57
1:E:269:PRO:HB3	1:E:363:LEU:HD23	1.85	0.57
1:F:235:ARG:O	1:F:240:LEU:HB2	2.04	0.57
1:F:606:HIS:HD2	1:F:608:GLN:CG	2.14	0.57
1:F:629:ARG:HH11	1:F:629:ARG:HG3	1.69	0.57
1:A:256:PHE:C	1:A:256:PHE:CD1	2.82	0.57
1:A:522:SER:O	1:A:524:LYS:N	2.38	0.57
1:B:425:PHE:CE1	1:B:456:ASN:HB3	2.40	0.57
1:C:7:ASN:C	1:C:9:GLN:N	2.55	0.57
1:C:283:VAL:O	1:C:284:ALA:CB	2.49	0.57
1:C:43:THR:HG23	1:C:49:HIS:C	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:TYR:CD2	1:C:53:VAL:HG21	2.39	0.57
1:C:175:LYS:CB	1:D:491:ILE:HG12	2.34	0.57
1:C:256:PHE:CD1	1:C:256:PHE:C	2.82	0.57
1:D:11:GLN:O	1:D:15:ASN:ND2	2.37	0.57
1:F:43:THR:HG23	1:F:49:HIS:C	2.29	0.57
1:A:235:ARG:O	1:A:240:LEU:HB2	2.04	0.57
1:E:46:TYR:CD2	1:E:53:VAL:HG21	2.39	0.57
1:E:522:SER:O	1:E:524:LYS:N	2.38	0.57
1:F:74:LEU:HG	1:F:74:LEU:O	2.05	0.57
1:A:61:ASN:C	1:A:63:HIS:N	2.62	0.57
1:C:173:THR:HG22	1:C:174:LYS:O	2.05	0.57
1:C:235:ARG:O	1:C:240:LEU:HB2	2.04	0.57
1:C:470:ASN:ND2	1:C:474:ARG:HD3	2.20	0.57
1:C:522:SER:O	1:C:524:LYS:N	2.38	0.57
1:D:156:SER:OG	1:E:438:ASP:OD1	2.23	0.57
1:D:307:ASP:OD1	1:D:309:ASP:N	2.34	0.57
1:D:425:PHE:CE1	1:D:456:ASN:HB3	2.40	0.57
1:F:477:THR:HB	1:F:479:ARG:HH12	1.70	0.57
1:A:173:THR:HG22	1:A:174:LYS:O	2.05	0.56
1:A:175:LYS:O	1:A:176:ASN:HB2	2.04	0.56
1:A:207:ASP:OD2	1:A:212:HIS:CB	2.51	0.56
1:A:354:GLN:HA	1:A:354:GLN:NE2	2.20	0.56
1:B:59:GLU:HG3	1:B:85:MET:HE1	1.87	0.56
1:B:89:VAL:O	1:B:92:GLN:N	2.38	0.56
1:B:629:ARG:HG3	1:B:629:ARG:HH11	1.69	0.56
1:C:11:GLN:O	1:C:15:ASN:ND2	2.37	0.56
1:C:425:PHE:CE1	1:C:456:ASN:HB3	2.40	0.56
1:D:74:LEU:O	1:D:74:LEU:HG	2.05	0.56
1:D:173:THR:HG22	1:D:174:LYS:O	2.05	0.56
1:D:533:MET:CB	1:D:534:PRO:HD2	2.28	0.56
1:E:48:ASP:HB3	1:E:92:GLN:HE21	1.69	0.56
1:E:173:THR:HG22	1:E:174:LYS:O	2.05	0.56
1:F:48:ASP:HB3	1:F:92:GLN:HE21	1.69	0.56
1:F:59:GLU:HG3	1:F:85:MET:HE1	1.87	0.56
1:A:48:ASP:HB3	1:A:92:GLN:HE21	1.69	0.56
1:B:74:LEU:HG	1:B:74:LEU:O	2.05	0.56
1:E:61:ASN:C	1:E:63:HIS:N	2.62	0.56
1:A:59:GLU:HG3	1:A:85:MET:HE1	1.87	0.56
1:A:101:SER:O	1:A:104:ALA:HB3	2.06	0.56
1:A:271:ARG:NH2	1:A:377:ASP:OD1	2.39	0.56
1:A:425:PHE:CE1	1:A:456:ASN:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:THR:HB	1:A:479:ARG:HH12	1.70	0.56
1:B:235:ARG:O	1:B:240:LEU:HB2	2.04	0.56
1:C:95:GLU:HA	1:C:128:LEU:HD21	1.86	0.56
1:C:271:ARG:NH2	1:C:377:ASP:OD1	2.39	0.56
1:D:89:VAL:O	1:D:92:GLN:N	2.38	0.56
1:D:89:VAL:C	1:D:91:ASN:N	2.63	0.56
1:D:95:GLU:HA	1:D:128:LEU:HD21	1.87	0.56
1:D:101:SER:O	1:D:104:ALA:HB3	2.06	0.56
1:D:175:LYS:O	1:D:176:ASN:HB2	2.04	0.56
1:D:629:ARG:HH11	1:D:629:ARG:HG3	1.69	0.56
1:F:101:SER:O	1:F:104:ALA:HB3	2.05	0.56
1:F:173:THR:HG22	1:F:174:LYS:O	2.05	0.56
1:F:354:GLN:HA	1:F:354:GLN:NE2	2.20	0.56
1:B:101:SER:O	1:B:104:ALA:HB3	2.05	0.56
1:C:487:ASP:O	1:C:488:ASN:HB3	2.06	0.56
1:E:470:ASN:ND2	1:E:474:ARG:HD3	2.20	0.56
1:A:78:ARG:O	1:A:79:GLN:C	2.45	0.56
1:A:89:VAL:O	1:A:92:GLN:N	2.38	0.56
1:B:95:GLU:HA	1:B:128:LEU:HD21	1.87	0.56
1:C:61:ASN:C	1:C:63:HIS:N	2.62	0.56
1:C:74:LEU:HG	1:C:74:LEU:O	2.05	0.56
1:D:470:ASN:ND2	1:D:474:ARG:HD3	2.20	0.56
1:E:59:GLU:HG3	1:E:85:MET:HE1	1.87	0.56
1:E:307:ASP:OD1	1:E:309:ASP:N	2.34	0.56
1:B:173:THR:HG22	1:B:174:LYS:O	2.05	0.56
1:B:482:LEU:HB2	1:B:505:LEU:HD22	1.87	0.56
1:B:522:SER:O	1:B:524:LYS:N	2.38	0.56
1:C:89:VAL:O	1:C:92:GLN:N	2.38	0.56
1:C:354:GLN:HA	1:C:354:GLN:NE2	2.20	0.56
1:D:43:THR:HG23	1:D:49:HIS:C	2.29	0.56
1:D:477:THR:HB	1:D:479:ARG:HH12	1.70	0.56
1:F:237:SER:HB3	1:F:573:SER:CA	2.36	0.56
1:B:61:ASN:C	1:B:63:HIS:N	2.62	0.56
1:B:271:ARG:NH2	1:B:377:ASP:OD1	2.39	0.56
1:C:477:THR:HB	1:C:479:ARG:HH12	1.70	0.56
1:D:29:ASP:OD1	1:D:29:ASP:N	2.31	0.56
1:F:237:SER:HA	1:F:574:LYS:HD2	1.88	0.56
1:A:174:LYS:O	1:A:175:LYS:CG	2.54	0.56
1:B:470:ASN:ND2	1:B:474:ARG:HD3	2.20	0.56
1:C:634:ARG:HG2	1:C:634:ARG:NH1	2.14	0.56
1:D:237:SER:HA	1:D:574:LYS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:GLU:O	1:D:323:LEU:C	2.49	0.56
1:E:89:VAL:O	1:E:92:GLN:N	2.38	0.56
1:E:271:ARG:NH2	1:E:377:ASP:OD1	2.39	0.56
1:E:412:VAL:HB	1:E:640:SER:HB2	1.88	0.56
1:F:412:VAL:HB	1:F:640:SER:HB2	1.88	0.56
1:A:43:THR:HG23	1:A:49:HIS:C	2.29	0.56
1:B:89:VAL:C	1:B:91:ASN:N	2.63	0.56
1:B:106:PHE:O	1:B:107:ARG:C	2.49	0.56
1:B:237:SER:HA	1:B:574:LYS:HD2	1.88	0.56
1:C:89:VAL:C	1:C:91:ASN:N	2.63	0.56
1:D:59:GLU:HG3	1:D:85:MET:HE1	1.87	0.56
1:E:29:ASP:O	1:E:33:ILE:HG13	2.06	0.56
1:E:89:VAL:C	1:E:91:ASN:N	2.63	0.56
1:E:477:THR:HB	1:E:479:ARG:HH12	1.70	0.56
1:F:283:VAL:O	1:F:284:ALA:CB	2.49	0.56
1:A:74:LEU:O	1:A:74:LEU:HG	2.05	0.56
1:A:533:MET:H	1:A:533:MET:CE	2.16	0.56
1:B:29:ASP:O	1:B:33:ILE:HG13	2.06	0.56
1:B:322:GLU:O	1:B:323:LEU:C	2.49	0.56
1:D:13:ASP:CG	1:D:100:ARG:HD2	2.31	0.56
1:E:13:ASP:CG	1:E:100:ARG:HD2	2.31	0.56
1:E:74:LEU:HG	1:E:74:LEU:O	2.05	0.56
1:F:29:ASP:O	1:F:33:ILE:HG13	2.06	0.56
1:F:76:ASN:CB	1:F:79:GLN:HB2	2.34	0.56
1:F:95:GLU:HA	1:F:128:LEU:HD21	1.86	0.56
1:F:482:LEU:HB2	1:F:505:LEU:HD22	1.87	0.56
1:D:413:VAL:HG23	1:D:466:MET:HE3	1.88	0.55
1:A:237:SER:HA	1:A:574:LYS:HD2	1.88	0.55
1:A:482:LEU:HB2	1:A:505:LEU:HD22	1.87	0.55
1:A:573:SER:HB2	1:A:578:MET:HG3	1.86	0.55
1:B:13:ASP:CG	1:B:100:ARG:HD2	2.31	0.55
1:C:414:ASN:ND2	1:C:467:SER:N	2.54	0.55
1:C:634:ARG:HE	1:E:64:ARG:NE	2.04	0.55
1:E:95:GLU:HA	1:E:128:LEU:HD21	1.86	0.55
1:E:101:SER:O	1:E:104:ALA:HB3	2.06	0.55
1:E:354:GLN:NE2	1:E:354:GLN:HA	2.20	0.55
1:F:13:ASP:CG	1:F:100:ARG:HD2	2.31	0.55
1:F:89:VAL:O	1:F:92:GLN:N	2.38	0.55
1:F:437:VAL:HG23	1:F:437:VAL:O	2.07	0.55
1:A:230:ARG:NE	4:A:751:HOH:O	2.19	0.55
1:C:101:SER:O	1:C:104:ALA:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LYS:O	1:C:175:LYS:CG	2.54	0.55
1:C:526:SER:OG	1:C:527:SER:N	2.40	0.55
1:E:463:LYS:HG2	1:E:520:GLU:CB	2.36	0.55
1:F:321:ILE:O	1:F:321:ILE:HG12	2.07	0.55
1:F:463:LYS:HG2	1:F:520:GLU:CB	2.36	0.55
1:A:551:HIS:O	1:A:552:ASP:CB	2.55	0.55
1:C:321:ILE:O	1:C:321:ILE:HG12	2.07	0.55
1:D:414:ASN:ND2	1:D:467:SER:N	2.54	0.55
1:E:86:LEU:HD23	1:E:86:LEU:C	2.30	0.55
1:E:237:SER:HB3	1:E:573:SER:CA	2.36	0.55
1:E:425:PHE:CE1	1:E:456:ASN:HB3	2.40	0.55
1:E:624:TYR:CD1	1:E:625:PRO:HB3	2.42	0.55
1:B:412:VAL:HB	1:B:640:SER:HB2	1.88	0.55
1:C:482:LEU:HB2	1:C:505:LEU:HD22	1.87	0.55
1:D:68:GLN:HB3	1:D:69:ARG:NH1	2.22	0.55
1:D:271:ARG:NH2	1:D:377:ASP:OD1	2.39	0.55
1:E:487:ASP:O	1:E:488:ASN:HB3	2.06	0.55
1:F:425:PHE:CE1	1:F:456:ASN:HB3	2.40	0.55
1:A:66:LEU:HD13	1:A:111:ASN:ND2	2.22	0.55
1:A:606:HIS:HD2	1:A:608:GLN:CG	2.14	0.55
1:A:634:ARG:HG2	1:A:634:ARG:NH1	2.14	0.55
1:B:48:ASP:HB3	1:B:92:GLN:HE21	1.69	0.55
1:B:175:LYS:O	1:B:176:ASN:HB2	2.04	0.55
1:B:354:GLN:NE2	1:B:354:GLN:HA	2.20	0.55
1:C:491:ILE:HD11	1:D:175:LYS:C	2.32	0.55
1:D:61:ASN:C	1:D:63:HIS:N	2.62	0.55
1:D:78:ARG:O	1:D:79:GLN:C	2.45	0.55
1:D:437:VAL:HG23	1:D:437:VAL:O	2.07	0.55
1:E:237:SER:HA	1:E:574:LYS:HD2	1.88	0.55
1:E:321:ILE:O	1:E:321:ILE:HG12	2.07	0.55
1:F:66:LEU:HD13	1:F:111:ASN:ND2	2.22	0.55
1:A:29:ASP:O	1:A:33:ILE:HG13	2.06	0.55
1:A:86:LEU:HD23	1:A:86:LEU:C	2.30	0.55
1:A:127:LYS:NZ	1:A:211:TYR:CE2	2.75	0.55
1:B:237:SER:CB	1:B:573:SER:HA	2.37	0.55
1:D:29:ASP:O	1:D:33:ILE:HG13	2.06	0.55
1:D:66:LEU:HD13	1:D:111:ASN:ND2	2.22	0.55
1:D:237:SER:HB3	1:D:573:SER:CA	2.36	0.55
1:D:487:ASP:O	1:D:488:ASN:HB3	2.06	0.55
1:D:551:HIS:O	1:D:552:ASP:CB	2.55	0.55
1:A:403:HIS:C	1:A:405:ASN:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:VAL:HG23	1:A:437:VAL:O	2.07	0.55
1:D:321:ILE:O	1:D:321:ILE:HG12	2.07	0.55
1:D:482:LEU:HB2	1:D:505:LEU:HD22	1.87	0.55
1:E:482:LEU:HB2	1:E:505:LEU:HD22	1.87	0.55
1:F:307:ASP:OD1	1:F:309:ASP:N	2.34	0.55
1:F:353:ARG:O	1:F:354:GLN:C	2.49	0.55
1:A:321:ILE:O	1:A:321:ILE:HG12	2.07	0.55
1:A:412:VAL:HB	1:A:640:SER:HB2	1.88	0.55
1:A:624:TYR:CD1	1:A:625:PRO:HB3	2.42	0.55
1:B:48:ASP:CA	1:B:92:GLN:HE21	2.20	0.55
1:C:76:ASN:CB	1:C:79:GLN:HB2	2.34	0.55
1:E:413:VAL:HG23	1:E:466:MET:HE3	1.88	0.55
1:F:127:LYS:NZ	1:F:211:TYR:CE2	2.75	0.55
1:F:414:ASN:ND2	1:F:467:SER:N	2.54	0.55
1:F:484:PRO:HD2	1:F:498:ALA:HB1	1.89	0.55
1:F:487:ASP:O	1:F:488:ASN:HB3	2.06	0.55
1:A:13:ASP:CG	1:A:100:ARG:HD2	2.31	0.55
1:A:68:GLN:HB3	1:A:69:ARG:NH1	2.22	0.55
1:A:76:ASN:CB	1:A:79:GLN:HB2	2.34	0.55
1:A:106:PHE:O	1:A:107:ARG:C	2.49	0.55
1:A:237:SER:HB3	1:A:573:SER:CA	2.36	0.55
1:A:487:ASP:O	1:A:488:ASN:HB3	2.06	0.55
1:B:484:PRO:HD2	1:B:498:ALA:HB1	1.89	0.55
1:C:13:ASP:CG	1:C:100:ARG:HD2	2.31	0.55
1:C:59:GLU:HG3	1:C:85:MET:HE1	1.87	0.55
1:C:237:SER:HB3	1:C:573:SER:CA	2.36	0.55
1:C:606:HIS:HD2	1:C:608:GLN:CG	2.14	0.55
1:D:412:VAL:HB	1:D:640:SER:HB2	1.88	0.55
1:D:463:LYS:HG2	1:D:520:GLU:CB	2.36	0.55
1:D:484:PRO:HD2	1:D:498:ALA:HB1	1.89	0.55
1:D:526:SER:OG	1:D:527:SER:N	2.40	0.55
1:E:66:LEU:HD13	1:E:111:ASN:ND2	2.22	0.55
1:E:484:PRO:HD2	1:E:498:ALA:HB1	1.89	0.55
1:E:522:SER:C	1:E:524:LYS:N	2.63	0.55
1:F:533:MET:H	1:F:533:MET:CE	2.16	0.55
1:B:66:LEU:HD13	1:B:111:ASN:ND2	2.22	0.54
1:B:437:VAL:HG23	1:B:437:VAL:O	2.07	0.54
1:C:48:ASP:HB3	1:C:92:GLN:HE21	1.69	0.54
1:C:307:ASP:OD1	1:C:309:ASP:N	2.34	0.54
1:C:353:ARG:O	1:C:354:GLN:C	2.49	0.54
1:C:463:LYS:HG2	1:C:520:GLU:CB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:ILE:HD11	1:E:462:TYR:CE1	2.43	0.54
1:E:437:VAL:HG23	1:E:437:VAL:O	2.07	0.54
1:F:271:ARG:NH2	1:F:377:ASP:OD1	2.39	0.54
1:A:158:LYS:O	1:A:159:MET:C	2.49	0.54
1:A:413:VAL:HG23	1:A:466:MET:HE3	1.88	0.54
1:A:414:ASN:ND2	1:A:467:SER:N	2.54	0.54
1:A:463:LYS:HG2	1:A:520:GLU:CB	2.36	0.54
1:B:283:VAL:O	1:B:284:ALA:CB	2.49	0.54
1:B:624:TYR:CD1	1:B:625:PRO:HB3	2.42	0.54
1:C:237:SER:HA	1:C:574:LYS:HD2	1.88	0.54
1:C:412:VAL:HB	1:C:640:SER:HB2	1.88	0.54
1:C:533:MET:H	1:C:533:MET:CE	2.16	0.54
1:E:96:TRP:O	1:E:97:TYR:C	2.51	0.54
1:E:106:PHE:O	1:E:107:ARG:C	2.49	0.54
1:E:414:ASN:ND2	1:E:467:SER:N	2.54	0.54
1:F:48:ASP:CA	1:F:92:GLN:HE21	2.20	0.54
2:H:1:NAG:H3	2:H:1:NAG:O7	2.07	0.54
2:J:1:NAG:O7	2:J:1:NAG:H3	2.08	0.54
1:A:89:VAL:C	1:A:91:ASN:N	2.63	0.54
1:B:86:LEU:HD23	1:B:86:LEU:C	2.30	0.54
1:B:237:SER:HB3	1:B:573:SER:CA	2.36	0.54
1:B:313:ILE:O	1:B:313:ILE:HG13	2.07	0.54
1:B:414:ASN:ND2	1:B:467:SER:N	2.54	0.54
1:C:418:ILE:HD11	1:C:462:TYR:CE1	2.43	0.54
1:C:425:PHE:N	1:C:456:ASN:O	2.39	0.54
1:C:484:PRO:HD2	1:C:498:ALA:HB1	1.89	0.54
1:E:68:GLN:HB3	1:E:69:ARG:NH1	2.22	0.54
1:E:574:LYS:HE2	1:E:578:MET:HG2	1.90	0.54
1:F:106:PHE:O	1:F:107:ARG:C	2.49	0.54
1:A:235:ARG:CZ	4:A:705:HOH:O	2.48	0.54
1:B:418:ILE:HD11	1:B:462:TYR:CE1	2.43	0.54
1:B:487:ASP:O	1:B:488:ASN:HB3	2.06	0.54
1:B:526:SER:OG	1:B:527:SER:N	2.40	0.54
1:C:624:TYR:CD1	1:C:625:PRO:HB3	2.42	0.54
1:D:158:LYS:O	1:D:159:MET:C	2.49	0.54
1:D:477:THR:HG23	1:D:509:PHE:CD1	2.43	0.54
1:D:624:TYR:CD1	1:D:625:PRO:HB3	2.42	0.54
1:E:29:ASP:OD1	1:E:29:ASP:N	2.31	0.54
1:A:161:GLN:HG3	1:B:443:ILE:HD13	1.90	0.54
1:A:473:GLU:HG3	1:A:473:GLU:O	2.08	0.54
1:B:174:LYS:O	1:B:175:LYS:CG	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLN:HB3	1:C:69:ARG:NH1	2.22	0.54
1:C:437:VAL:HG23	1:C:437:VAL:O	2.07	0.54
1:C:477:THR:HG23	1:C:509:PHE:CD1	2.43	0.54
1:D:127:LYS:NZ	1:D:211:TYR:CE2	2.75	0.54
1:F:68:GLN:HB3	1:F:69:ARG:NH1	2.22	0.54
1:F:403:HIS:C	1:F:405:ASN:H	2.15	0.54
1:A:353:ARG:O	1:A:354:GLN:C	2.49	0.54
1:A:574:LYS:HE2	1:A:578:MET:HG2	1.90	0.54
1:B:463:LYS:HG2	1:B:520:GLU:CB	2.36	0.54
1:D:12:GLN:OE1	1:D:547:VAL:HG21	2.08	0.54
1:D:354:GLN:HA	1:D:354:GLN:NE2	2.20	0.54
1:D:403:HIS:C	1:D:405:ASN:H	2.15	0.54
1:E:158:LYS:O	1:E:159:MET:C	2.49	0.54
1:E:477:THR:HG23	1:E:509:PHE:CD1	2.43	0.54
1:E:526:SER:OG	1:E:527:SER:N	2.40	0.54
1:F:89:VAL:C	1:F:91:ASN:N	2.63	0.54
1:F:418:ILE:HD11	1:F:462:TYR:CE1	2.43	0.54
1:A:551:HIS:HD2	1:A:552:ASP:N	2.05	0.54
1:B:96:TRP:O	1:B:97:TYR:C	2.50	0.54
1:C:48:ASP:CA	1:C:92:GLN:HE21	2.20	0.54
1:C:473:GLU:HG3	1:C:473:GLU:O	2.08	0.54
1:C:611:VAL:HG12	1:C:612:HIS:HD2	1.73	0.54
1:D:126:SER:OG	1:D:127:LYS:N	2.41	0.54
1:D:220:PHE:CZ	1:D:329:GLU:HB2	2.43	0.54
1:E:127:LYS:NZ	1:E:211:TYR:CE2	2.75	0.54
1:E:174:LYS:O	1:E:175:LYS:CG	2.54	0.54
1:E:521:ARG:HG2	1:E:522:SER:N	2.23	0.54
1:A:48:ASP:CA	1:A:92:GLN:HE21	2.20	0.54
1:A:138:TYR:CD2	1:A:188:ILE:HD12	2.43	0.54
1:A:570:LEU:N	4:A:858:HOH:O	2.40	0.54
1:A:592:ASP:C	1:A:594:GLU:H	2.16	0.54
1:A:628:ARG:O	1:A:629:ARG:C	2.50	0.54
1:B:12:GLN:OE1	1:B:547:VAL:HG21	2.08	0.54
1:B:127:LYS:NZ	1:B:211:TYR:CE2	2.75	0.54
1:B:413:VAL:HG23	1:B:466:MET:HE3	1.88	0.54
1:B:477:THR:HG23	1:B:509:PHE:CD1	2.43	0.54
1:C:12:GLN:OE1	1:C:547:VAL:HG21	2.08	0.54
1:C:66:LEU:HD13	1:C:111:ASN:ND2	2.22	0.54
1:C:367:VAL:HG23	1:C:373:THR:O	2.08	0.54
1:C:620:ARG:HG3	1:C:624:TYR:CD2	2.43	0.54
1:D:37:PHE:CZ	1:D:101:SER:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ILE:O	1:D:313:ILE:HG13	2.07	0.54
1:D:620:ARG:HG3	1:D:624:TYR:CD2	2.43	0.54
1:F:624:TYR:CD1	1:F:625:PRO:HB3	2.42	0.54
1:A:307:ASP:C	1:A:336:ASN:HD22	2.16	0.54
1:A:418:ILE:HD11	1:A:462:TYR:CE1	2.43	0.54
1:A:521:ARG:HB3	4:A:864:HOH:O	2.07	0.54
1:B:7:ASN:C	1:B:9:GLN:N	2.55	0.54
1:B:68:GLN:HB3	1:B:69:ARG:NH1	2.22	0.54
1:B:158:LYS:O	1:B:159:MET:C	2.49	0.54
1:B:574:LYS:HE2	1:B:578:MET:HG2	1.90	0.54
1:C:220:PHE:CZ	1:C:329:GLU:HB2	2.43	0.54
1:D:106:PHE:O	1:D:107:ARG:C	2.49	0.54
1:E:283:VAL:O	1:E:284:ALA:CB	2.49	0.54
1:E:324:LEU:O	1:E:328:ILE:HG13	2.08	0.54
1:E:533:MET:H	1:E:533:MET:CE	2.16	0.54
1:E:611:VAL:HG12	1:E:612:HIS:HD2	1.73	0.54
1:F:37:PHE:CZ	1:F:101:SER:HB3	2.43	0.54
1:F:526:SER:OG	1:F:527:SER:N	2.40	0.54
1:A:322:GLU:O	1:A:323:LEU:C	2.49	0.54
1:A:425:PHE:N	1:A:456:ASN:O	2.39	0.54
1:A:526:SER:OG	1:A:527:SER:N	2.40	0.54
1:B:321:ILE:HG12	1:B:321:ILE:O	2.07	0.54
1:B:434:ILE:C	1:B:436:ALA:H	2.16	0.54
1:B:620:ARG:HG3	1:B:624:TYR:CD2	2.43	0.54
1:C:127:LYS:NZ	1:C:211:TYR:CE2	2.75	0.54
1:D:592:ASP:C	1:D:594:GLU:H	2.16	0.54
1:F:367:VAL:HG23	1:F:373:THR:O	2.08	0.54
1:F:592:ASP:C	1:F:594:GLU:H	2.16	0.54
1:F:611:VAL:HG12	1:F:612:HIS:HD2	1.73	0.54
2:G:1:NAG:O7	2:G:1:NAG:H3	2.08	0.54
1:A:324:LEU:O	1:A:328:ILE:HG13	2.08	0.53
1:A:477:THR:HG23	1:A:509:PHE:CD1	2.43	0.53
1:C:37:PHE:CE2	1:C:101:SER:CB	2.92	0.53
1:C:86:LEU:HD23	1:C:86:LEU:C	2.30	0.53
1:D:324:LEU:O	1:D:328:ILE:HG13	2.08	0.53
1:D:521:ARG:HG2	1:D:522:SER:N	2.23	0.53
1:D:611:VAL:HG12	1:D:612:HIS:HD2	1.73	0.53
1:E:126:SER:OG	1:E:127:LYS:N	2.41	0.53
1:E:313:ILE:O	1:E:313:ILE:HG13	2.07	0.53
1:E:322:GLU:O	1:E:323:LEU:C	2.49	0.53
1:F:220:PHE:CZ	1:F:329:GLU:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324:LEU:O	1:F:328:ILE:HG13	2.08	0.53
1:A:256:PHE:CZ	1:A:258:PRO:HB3	2.44	0.53
1:A:484:PRO:HD2	1:A:498:ALA:HB1	1.89	0.53
1:B:76:ASN:CB	1:B:79:GLN:HB2	2.34	0.53
1:B:126:SER:OG	1:B:127:LYS:N	2.41	0.53
1:C:37:PHE:CZ	1:C:101:SER:HB3	2.43	0.53
1:C:403:HIS:C	1:C:405:ASN:H	2.15	0.53
1:C:434:ILE:C	1:C:436:ALA:H	2.16	0.53
1:C:551:HIS:O	1:C:552:ASP:CB	2.55	0.53
1:D:48:ASP:CA	1:D:92:GLN:HE21	2.20	0.53
1:D:367:VAL:HG23	1:D:373:THR:O	2.08	0.53
1:E:12:GLN:OE1	1:E:547:VAL:HG21	2.08	0.53
1:E:278:GLU:H	1:E:354:GLN:NE2	2.06	0.53
1:E:551:HIS:O	1:E:552:ASP:CB	2.55	0.53
1:F:174:LYS:O	1:F:175:LYS:CG	2.54	0.53
1:F:322:GLU:O	1:F:323:LEU:C	2.49	0.53
1:A:12:GLN:OE1	1:A:547:VAL:HG21	2.08	0.53
1:B:278:GLU:H	1:B:354:GLN:NE2	2.06	0.53
1:C:29:ASP:O	1:C:33:ILE:HG13	2.06	0.53
1:D:187:ASP:OD1	1:D:187:ASP:C	2.52	0.53
1:D:522:SER:C	1:D:524:LYS:N	2.63	0.53
1:E:48:ASP:CA	1:E:92:GLN:HE21	2.20	0.53
1:E:256:PHE:CZ	1:E:258:PRO:HB3	2.44	0.53
1:F:158:LYS:O	1:F:159:MET:C	2.49	0.53
1:F:237:SER:CB	1:F:573:SER:HA	2.37	0.53
1:F:434:ILE:C	1:F:436:ALA:N	2.66	0.53
1:F:522:SER:C	1:F:524:LYS:N	2.63	0.53
2:L:1:NAG:O7	2:L:1:NAG:H3	2.08	0.53
1:A:201:PHE:HB3	1:A:216:LYS:HD3	1.90	0.53
1:A:278:GLU:H	1:A:354:GLN:NE2	2.06	0.53
1:A:367:VAL:HG23	1:A:373:THR:O	2.08	0.53
1:B:353:ARG:O	1:B:354:GLN:C	2.49	0.53
1:B:367:VAL:HG23	1:B:373:THR:O	2.08	0.53
1:B:411:MET:C	1:B:412:VAL:HG12	2.34	0.53
1:C:138:TYR:CD2	1:C:188:ILE:HD12	2.43	0.53
1:C:201:PHE:HB3	1:C:216:LYS:HD3	1.90	0.53
1:C:324:LEU:O	1:C:328:ILE:HG13	2.08	0.53
1:C:574:LYS:HE2	1:C:578:MET:HG2	1.90	0.53
1:D:237:SER:CB	1:D:573:SER:HA	2.37	0.53
1:D:628:ARG:O	1:D:629:ARG:C	2.50	0.53
1:F:609:CYS:C	1:F:611:VAL:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:620:ARG:HG3	1:F:624:TYR:CD2	2.43	0.53
1:B:256:PHE:CZ	1:B:258:PRO:HB3	2.44	0.53
1:C:106:PHE:O	1:C:107:ARG:C	2.49	0.53
1:C:256:PHE:CZ	1:C:258:PRO:HB3	2.44	0.53
1:D:21:ILE:HG13	1:D:21:ILE:O	2.08	0.53
1:D:411:MET:C	1:D:412:VAL:HG12	2.34	0.53
1:D:418:ILE:HD11	1:D:462:TYR:CE1	2.43	0.53
1:D:434:ILE:C	1:D:436:ALA:N	2.66	0.53
1:E:201:PHE:HB3	1:E:216:LYS:HD3	1.90	0.53
1:E:220:PHE:CZ	1:E:329:GLU:HB2	2.43	0.53
1:E:313:ILE:C	1:E:313:ILE:HD12	2.34	0.53
1:E:403:HIS:C	1:E:405:ASN:H	2.15	0.53
1:F:21:ILE:O	1:F:21:ILE:HG13	2.09	0.53
1:F:313:ILE:HG13	1:F:313:ILE:O	2.07	0.53
1:F:403:HIS:O	1:F:405:ASN:N	2.42	0.53
1:F:424:THR:HA	1:F:456:ASN:O	2.09	0.53
2:K:1:NAG:H3	2:K:1:NAG:O7	2.08	0.53
1:A:21:ILE:HG13	1:A:21:ILE:O	2.09	0.53
1:A:313:ILE:HG13	1:A:313:ILE:O	2.07	0.53
1:B:307:ASP:OD1	1:B:309:ASP:N	2.34	0.53
1:B:477:THR:HB	1:B:479:ARG:HH12	1.70	0.53
1:B:521:ARG:HG2	1:B:522:SER:N	2.23	0.53
1:C:413:VAL:HG23	1:C:466:MET:HE3	1.88	0.53
1:C:592:ASP:C	1:C:594:GLU:H	2.16	0.53
1:D:551:HIS:HD2	1:D:552:ASP:N	2.05	0.53
1:E:197:TRP:NE1	1:E:223:VAL:HG21	2.24	0.53
1:F:7:ASN:C	1:F:9:GLN:N	2.55	0.53
1:F:256:PHE:CZ	1:F:258:PRO:HB3	2.44	0.53
1:F:425:PHE:N	1:F:456:ASN:O	2.39	0.53
1:A:338:GLN:NE2	1:E:316:ARG:HH21	2.07	0.53
1:B:7:ASN:O	1:B:8:ALA:C	2.51	0.53
1:B:197:TRP:NE1	1:B:223:VAL:HG21	2.24	0.53
1:B:220:PHE:CZ	1:B:329:GLU:HB2	2.43	0.53
1:B:307:ASP:C	1:B:336:ASN:HD22	2.16	0.53
1:B:611:VAL:HG12	1:B:612:HIS:HD2	1.73	0.53
1:C:424:THR:HA	1:C:456:ASN:O	2.09	0.53
1:C:521:ARG:HG2	1:C:522:SER:N	2.23	0.53
1:C:609:CYS:C	1:C:611:VAL:H	2.17	0.53
1:D:76:ASN:CB	1:D:79:GLN:HB2	2.34	0.53
1:E:307:ASP:C	1:E:336:ASN:HD22	2.16	0.53
1:E:434:ILE:C	1:E:436:ALA:N	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:620:ARG:HG3	1:E:624:TYR:CD2	2.43	0.53
1:F:45:ILE:O	1:F:94:LYS:HD3	2.09	0.53
1:F:313:ILE:C	1:F:313:ILE:HD12	2.34	0.53
1:F:521:ARG:HG2	1:F:522:SER:N	2.23	0.53
1:A:248:TRP:CH2	1:A:289:LEU:HD13	2.44	0.53
1:A:303:GLY:O	1:A:315:ILE:HG12	2.09	0.53
1:A:313:ILE:HD12	1:A:313:ILE:C	2.34	0.53
1:B:37:PHE:CZ	1:B:101:SER:HB3	2.43	0.53
1:B:45:ILE:O	1:B:94:LYS:HD3	2.09	0.53
1:B:248:TRP:CH2	1:B:289:LEU:HD13	2.44	0.53
1:C:31:LYS:O	1:C:34:ALA:HB3	2.09	0.53
1:C:307:ASP:C	1:C:336:ASN:HD22	2.16	0.53
1:C:403:HIS:O	1:C:405:ASN:N	2.42	0.53
1:C:633:GLU:C	1:C:635:VAL:N	2.66	0.53
1:D:45:ILE:O	1:D:94:LYS:HD3	2.09	0.53
1:D:174:LYS:O	1:D:175:LYS:CG	2.54	0.53
1:E:37:PHE:CZ	1:E:101:SER:HB3	2.43	0.53
1:F:12:GLN:OE1	1:F:547:VAL:HG21	2.08	0.53
1:F:307:ASP:C	1:F:336:ASN:HD22	2.16	0.53
1:F:477:THR:HG23	1:F:509:PHE:CD1	2.43	0.53
1:F:574:LYS:HE2	1:F:578:MET:HG2	1.89	0.53
2:I:1:NAG:H3	2:I:1:NAG:O7	2.07	0.53
1:A:17:LEU:HD21	1:A:103:ALA:O	2.09	0.53
1:A:37:PHE:CZ	1:A:101:SER:HB3	2.43	0.53
1:A:620:ARG:HG3	1:A:624:TYR:CD2	2.43	0.53
1:B:403:HIS:C	1:B:405:ASN:H	2.15	0.53
1:B:592:ASP:C	1:B:594:GLU:H	2.16	0.53
1:C:248:TRP:CH2	1:C:289:LEU:HD13	2.44	0.53
1:C:278:GLU:H	1:C:354:GLN:NE2	2.06	0.53
1:D:31:LYS:O	1:D:34:ALA:HB3	2.09	0.53
1:D:197:TRP:NE1	1:D:223:VAL:HG21	2.24	0.53
1:D:307:ASP:C	1:D:336:ASN:HD22	2.16	0.53
1:D:313:ILE:C	1:D:313:ILE:HD12	2.34	0.53
1:D:574:LYS:HE2	1:D:578:MET:HG2	1.90	0.53
1:E:17:LEU:HD21	1:E:103:ALA:O	2.09	0.53
1:E:31:LYS:O	1:E:34:ALA:HB3	2.09	0.53
1:E:353:ARG:O	1:E:354:GLN:C	2.49	0.53
1:E:411:MET:C	1:E:412:VAL:HG12	2.34	0.53
1:E:473:GLU:HG3	1:E:473:GLU:O	2.08	0.53
1:E:592:ASP:C	1:E:594:GLU:H	2.16	0.53
1:F:7:ASN:O	1:F:8:ALA:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:LEU:HD21	1:F:103:ALA:O	2.09	0.53
1:F:126:SER:OG	1:F:127:LYS:N	2.41	0.53
1:A:31:LYS:O	1:A:34:ALA:HB3	2.09	0.53
1:A:45:ILE:O	1:A:94:LYS:HD3	2.09	0.53
1:A:126:SER:OG	1:A:127:LYS:N	2.41	0.53
1:A:317:GLN:CB	1:A:318:PRO:HD2	2.36	0.53
1:A:403:HIS:O	1:A:405:ASN:N	2.42	0.53
1:A:434:ILE:C	1:A:436:ALA:H	2.16	0.53
1:B:138:TYR:CD2	1:B:188:ILE:HD12	2.43	0.53
1:B:424:THR:HA	1:B:456:ASN:O	2.09	0.53
1:B:425:PHE:N	1:B:456:ASN:O	2.39	0.53
1:C:38:ASN:C	1:C:40:LEU:N	2.67	0.53
1:C:45:ILE:O	1:C:94:LYS:HD3	2.09	0.53
1:C:78:ARG:HD3	1:C:82:GLU:OE2	2.10	0.53
1:C:303:GLY:O	1:C:315:ILE:HG12	2.09	0.53
1:C:313:ILE:C	1:C:313:ILE:HD12	2.34	0.53
1:C:313:ILE:HG13	1:C:313:ILE:O	2.07	0.53
1:D:86:LEU:HD23	1:D:86:LEU:C	2.30	0.53
1:D:201:PHE:HB3	1:D:216:LYS:HD3	1.90	0.53
1:D:256:PHE:CZ	1:D:258:PRO:HB3	2.44	0.53
1:E:21:ILE:O	1:E:21:ILE:HG13	2.09	0.53
1:E:38:ASN:C	1:E:40:LEU:N	2.67	0.53
1:E:303:GLY:O	1:E:315:ILE:HG12	2.09	0.53
1:E:479:ARG:HD2	1:E:587:THR:CG2	2.39	0.53
1:F:197:TRP:NE1	1:F:223:VAL:HG21	2.24	0.53
1:A:197:TRP:NE1	1:A:223:VAL:HG21	2.24	0.52
1:B:473:GLU:O	1:B:473:GLU:HG3	2.08	0.52
1:B:633:GLU:C	1:B:635:VAL:N	2.66	0.52
1:C:4:GLY:HA2	1:C:95:GLU:OE1	2.09	0.52
1:C:187:ASP:OD1	1:C:187:ASP:C	2.52	0.52
1:C:479:ARG:HD2	1:C:587:THR:CG2	2.39	0.52
1:C:487:ASP:CB	1:C:489:ASN:H	2.10	0.52
1:C:591:LYS:HB2	1:C:591:LYS:HZ2	1.74	0.52
1:D:473:GLU:O	1:D:473:GLU:HG3	2.08	0.52
1:D:557:ALA:HB3	1:D:558:TYR:CE1	2.44	0.52
1:E:37:PHE:CE2	1:E:101:SER:CB	2.92	0.52
1:E:78:ARG:HD3	1:E:82:GLU:OE2	2.09	0.52
1:E:398:PHE:HB3	1:E:399:PRO:HD2	1.92	0.52
1:F:278:GLU:H	1:F:354:GLN:NE2	2.06	0.52
1:F:303:GLY:O	1:F:315:ILE:HG12	2.09	0.52
1:A:187:ASP:OD1	1:A:187:ASP:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ILE:C	1:A:436:ALA:N	2.66	0.52
1:A:557:ALA:HB3	1:A:558:TYR:CE1	2.44	0.52
1:A:609:CYS:C	1:A:611:VAL:H	2.17	0.52
1:B:4:GLY:HA2	1:B:95:GLU:OE1	2.09	0.52
1:B:78:ARG:HD3	1:B:82:GLU:OE2	2.09	0.52
1:B:307:ASP:OD1	1:B:307:ASP:C	2.53	0.52
1:B:324:LEU:O	1:B:328:ILE:HG13	2.08	0.52
1:B:628:ARG:O	1:B:629:ARG:C	2.50	0.52
1:E:138:TYR:CD2	1:E:188:ILE:HD12	2.43	0.52
1:E:367:VAL:HG23	1:E:373:THR:O	2.08	0.52
1:E:425:PHE:N	1:E:456:ASN:O	2.39	0.52
1:E:633:GLU:C	1:E:635:VAL:N	2.66	0.52
1:F:187:ASP:OD1	1:F:187:ASP:C	2.52	0.52
1:F:248:TRP:CH2	1:F:289:LEU:HD13	2.44	0.52
1:F:473:GLU:HG3	1:F:473:GLU:O	2.08	0.52
1:F:557:ALA:HB3	1:F:558:TYR:CE1	2.44	0.52
1:F:628:ARG:O	1:F:629:ARG:C	2.50	0.52
1:A:78:ARG:HD3	1:A:82:GLU:OE2	2.09	0.52
1:B:17:LEU:HD21	1:B:103:ALA:O	2.09	0.52
1:B:187:ASP:OD1	1:B:187:ASP:C	2.52	0.52
1:C:551:HIS:HD2	1:C:552:ASP:N	2.05	0.52
1:D:96:TRP:O	1:D:97:TYR:C	2.51	0.52
1:D:303:GLY:O	1:D:315:ILE:HG12	2.09	0.52
1:E:403:HIS:O	1:E:405:ASN:N	2.42	0.52
1:F:78:ARG:HD3	1:F:82:GLU:OE2	2.09	0.52
1:A:96:TRP:O	1:A:97:TYR:C	2.51	0.52
1:B:403:HIS:O	1:B:405:ASN:N	2.42	0.52
1:B:533:MET:H	1:B:533:MET:CE	2.16	0.52
1:F:52:ALA:HB1	1:F:89:VAL:HG23	1.91	0.52
1:F:551:HIS:O	1:F:552:ASP:CB	2.55	0.52
1:A:220:PHE:CZ	1:A:329:GLU:HB2	2.43	0.52
1:B:479:ARG:HD2	1:B:587:THR:HG21	1.92	0.52
1:B:609:CYS:C	1:B:611:VAL:H	2.17	0.52
1:C:138:TYR:CZ	1:C:188:ILE:HD12	2.45	0.52
1:C:479:ARG:HD2	1:C:587:THR:HG21	1.92	0.52
1:D:248:TRP:CH2	1:D:289:LEU:HD13	2.44	0.52
1:E:4:GLY:HA2	1:E:95:GLU:OE1	2.09	0.52
1:E:7:ASN:O	1:E:8:ALA:C	2.51	0.52
1:E:248:TRP:CH2	1:E:289:LEU:HD13	2.44	0.52
1:F:413:VAL:HG23	1:F:466:MET:HE3	1.89	0.52
1:A:52:ALA:HB1	1:A:89:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:CD	4:A:829:HOH:O	2.48	0.52
1:A:479:ARG:HD2	1:A:587:THR:HG21	1.92	0.52
1:A:521:ARG:HG2	1:A:522:SER:N	2.23	0.52
1:A:522:SER:C	1:A:524:LYS:N	2.63	0.52
1:A:533:MET:CB	1:A:534:PRO:HD2	2.28	0.52
1:B:201:PHE:HB3	1:B:216:LYS:HD3	1.90	0.52
1:C:317:GLN:CB	1:C:318:PRO:HD2	2.36	0.52
1:C:322:GLU:O	1:C:323:LEU:C	2.49	0.52
1:C:522:SER:C	1:C:524:LYS:N	2.63	0.52
1:D:609:CYS:C	1:D:611:VAL:H	2.17	0.52
1:E:45:ILE:O	1:E:94:LYS:HD3	2.09	0.52
1:B:31:LYS:O	1:B:34:ALA:HB3	2.09	0.52
1:B:593:THR:C	1:B:595:GLY:N	2.68	0.52
1:C:17:LEU:HD21	1:C:103:ALA:O	2.09	0.52
1:C:158:LYS:O	1:C:159:MET:C	2.49	0.52
1:D:4:GLY:HA2	1:D:95:GLU:OE1	2.09	0.52
1:D:78:ARG:HD3	1:D:82:GLU:OE2	2.09	0.52
1:E:307:ASP:OD1	1:E:307:ASP:C	2.53	0.52
1:F:138:TYR:CD2	1:F:188:ILE:HD12	2.43	0.52
1:F:434:ILE:C	1:F:436:ALA:H	2.16	0.52
1:A:343:LEU:HD11	4:A:861:HOH:O	2.09	0.52
1:A:479:ARG:HD2	1:A:587:THR:CG2	2.39	0.52
1:B:434:ILE:C	1:B:436:ALA:N	2.66	0.52
1:B:557:ALA:HB3	1:B:558:TYR:CE1	2.44	0.52
1:D:37:PHE:CE2	1:D:101:SER:CB	2.91	0.52
1:E:187:ASP:OD1	1:E:187:ASP:C	2.52	0.52
1:E:609:CYS:C	1:E:611:VAL:H	2.17	0.52
1:F:4:GLY:HA2	1:F:95:GLU:OE1	2.09	0.52
1:A:398:PHE:HB3	1:A:399:PRO:HD2	1.91	0.52
1:A:424:THR:HA	1:A:456:ASN:O	2.09	0.52
1:B:21:ILE:HG13	1:B:21:ILE:O	2.09	0.52
1:C:197:TRP:NE1	1:C:223:VAL:HG21	2.24	0.52
1:C:593:THR:C	1:C:595:GLY:N	2.68	0.52
1:D:353:ARG:O	1:D:354:GLN:C	2.49	0.52
1:D:403:HIS:O	1:D:405:ASN:N	2.42	0.52
1:D:551:HIS:CD2	1:D:551:HIS:C	2.88	0.52
1:E:319:LYS:O	1:E:320:GLY:C	2.53	0.52
1:F:201:PHE:HB3	1:F:216:LYS:HD3	1.90	0.52
1:F:417:ALA:O	1:F:463:LYS:N	2.37	0.52
1:F:479:ARG:HD2	1:F:587:THR:CG2	2.39	0.52
1:A:138:TYR:CZ	1:A:188:ILE:HD12	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:HIS:CD2	1:A:551:HIS:C	2.88	0.52
1:A:633:GLU:C	1:A:635:VAL:N	2.66	0.52
1:B:479:ARG:HD2	1:B:587:THR:CG2	2.39	0.52
1:C:21:ILE:O	1:C:21:ILE:HG13	2.09	0.52
1:C:398:PHE:HB3	1:C:399:PRO:HD2	1.91	0.52
1:D:455:LEU:HG	1:D:456:ASN:H	1.75	0.52
2:G:1:NAG:C8	2:G:1:NAG:C7	2.88	0.52
1:A:307:ASP:OD1	1:A:307:ASP:C	2.53	0.51
1:B:303:GLY:O	1:B:315:ILE:HG12	2.09	0.51
1:C:557:ALA:HB3	1:C:558:TYR:CE1	2.44	0.51
1:D:307:ASP:OD1	1:D:307:ASP:C	2.53	0.51
1:D:424:THR:HA	1:D:456:ASN:O	2.09	0.51
1:E:52:ALA:HB1	1:E:89:VAL:HG23	1.91	0.51
1:E:430:GLN:HA	1:E:450:ALA:O	2.10	0.51
1:F:96:TRP:O	1:F:97:TYR:C	2.51	0.51
1:F:398:PHE:HB3	1:F:399:PRO:HD2	1.91	0.51
2:L:1:NAG:C8	2:L:1:NAG:C7	2.88	0.51
1:A:280:VAL:HA	1:A:357:PRO:HB3	1.93	0.51
1:A:430:GLN:HA	1:A:450:ALA:O	2.10	0.51
1:A:571:PRO:HB2	4:A:857:HOH:O	2.09	0.51
1:B:269:PRO:HB3	1:B:363:LEU:CD2	2.41	0.51
1:B:280:VAL:HA	1:B:357:PRO:HB3	1.93	0.51
1:B:313:ILE:C	1:B:313:ILE:HD12	2.34	0.51
1:C:441:GLU:C	1:C:443:ILE:H	2.18	0.51
1:D:17:LEU:HD21	1:D:103:ALA:O	2.09	0.51
1:D:593:THR:C	1:D:595:GLY:N	2.68	0.51
1:E:237:SER:CB	1:E:573:SER:HA	2.37	0.51
1:E:424:THR:HA	1:E:456:ASN:O	2.09	0.51
1:F:31:LYS:O	1:F:34:ALA:HB3	2.09	0.51
1:F:551:HIS:HD2	1:F:552:ASP:N	2.05	0.51
2:J:1:NAG:C8	2:J:1:NAG:C7	2.88	0.51
1:A:625:PRO:C	1:A:626:LEU:HD23	2.36	0.51
1:B:513:PRO:CG	1:B:517:GLU:HB2	2.27	0.51
1:B:625:PRO:C	1:B:626:LEU:HD23	2.36	0.51
1:C:337:VAL:HG13	1:C:338:GLN:N	2.25	0.51
1:C:411:MET:C	1:C:412:VAL:HG12	2.34	0.51
1:C:576:GLU:OE1	1:D:576:GLU:CD	2.53	0.51
1:D:52:ALA:HB1	1:D:89:VAL:HG23	1.91	0.51
1:D:425:PHE:N	1:D:456:ASN:O	2.39	0.51
1:F:29:ASP:OD1	1:F:29:ASP:N	2.31	0.51
2:H:1:NAG:C8	2:H:1:NAG:C7	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1:NAG:C8	2:K:1:NAG:C7	2.88	0.51
1:A:4:GLY:HA2	1:A:95:GLU:OE1	2.09	0.51
1:A:156:SER:OG	1:B:438:ASP:OD1	2.27	0.51
1:D:38:ASN:C	1:D:40:LEU:N	2.67	0.51
1:D:262:TYR:OH	1:D:370:HIS:NE2	2.32	0.51
1:D:272:PRO:CD	1:E:272:PRO:HG2	2.41	0.51
1:D:353:ARG:NE	1:D:369:GLU:OE2	2.43	0.51
1:D:366:GLY:N	1:D:369:GLU:HG3	2.21	0.51
1:E:434:ILE:C	1:E:436:ALA:H	2.16	0.51
1:E:487:ASP:CB	1:E:489:ASN:H	2.09	0.51
1:E:551:HIS:CD2	1:E:551:HIS:C	2.88	0.51
1:A:269:PRO:HB3	1:A:363:LEU:CD2	2.41	0.51
1:A:593:THR:C	1:A:595:GLY:N	2.68	0.51
1:B:411:MET:SD	1:B:411:MET:N	2.83	0.51
1:B:430:GLN:HA	1:B:450:ALA:O	2.10	0.51
1:B:533:MET:CB	1:B:534:PRO:HD2	2.28	0.51
1:C:96:TRP:O	1:C:97:TYR:C	2.50	0.51
1:C:307:ASP:OD1	1:C:307:ASP:C	2.53	0.51
1:C:628:ARG:O	1:C:629:ARG:C	2.50	0.51
1:D:8:ALA:HA	1:D:553:LEU:CD1	2.40	0.51
1:D:48:ASP:OD2	1:D:51:ALA:HB3	2.11	0.51
1:D:430:GLN:HA	1:D:450:ALA:O	2.10	0.51
1:E:625:PRO:C	1:E:626:LEU:HD23	2.36	0.51
1:F:138:TYR:CZ	1:F:188:ILE:HD12	2.45	0.51
1:F:300:ILE:CD1	1:F:390:ILE:CG2	2.89	0.51
1:A:285:HIS:HB2	1:A:288:ASP:CG	2.36	0.51
1:B:52:ALA:HB1	1:B:89:VAL:HG23	1.91	0.51
1:B:201:PHE:HB3	1:B:216:LYS:HD2	1.92	0.51
1:B:366:GLY:N	1:B:369:GLU:HG3	2.21	0.51
1:C:126:SER:OG	1:C:127:LYS:N	2.41	0.51
1:D:280:VAL:HA	1:D:357:PRO:HB3	1.93	0.51
1:D:434:ILE:C	1:D:436:ALA:H	2.16	0.51
1:D:479:ARG:HD2	1:D:587:THR:CG2	2.39	0.51
1:E:48:ASP:OD2	1:E:51:ALA:HB3	2.11	0.51
1:E:269:PRO:HB3	1:E:363:LEU:CD2	2.41	0.51
1:F:285:HIS:HB2	1:F:288:ASP:CG	2.36	0.51
2:I:1:NAG:C8	2:I:1:NAG:C7	2.88	0.51
1:A:300:ILE:CD1	1:A:390:ILE:CG2	2.89	0.51
1:C:269:PRO:HB3	1:C:363:LEU:CD2	2.41	0.51
1:C:280:VAL:HA	1:C:357:PRO:HB3	1.93	0.51
1:C:300:ILE:CD1	1:C:390:ILE:CG2	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:TYR:CD2	1:D:188:ILE:HD12	2.43	0.51
1:D:269:PRO:HB3	1:D:363:LEU:CD2	2.41	0.51
1:D:337:VAL:HG13	1:D:338:GLN:N	2.25	0.51
1:D:418:ILE:HD11	1:D:462:TYR:HE1	1.76	0.51
1:D:591:LYS:HB2	1:D:591:LYS:HZ2	1.74	0.51
1:E:76:ASN:HD22	1:E:79:GLN:HG3	1.76	0.51
1:E:557:ALA:HB3	1:E:558:TYR:CE1	2.44	0.51
1:F:280:VAL:HA	1:F:357:PRO:HB3	1.93	0.51
1:F:430:GLN:HA	1:F:450:ALA:O	2.10	0.51
1:F:625:PRO:C	1:F:626:LEU:HD23	2.36	0.51
1:F:634:ARG:HG2	1:F:634:ARG:NH1	2.14	0.51
1:A:102:ASN:O	1:A:104:ALA:N	2.44	0.51
1:A:611:VAL:HG12	1:A:612:HIS:HD2	1.73	0.51
1:B:37:PHE:CE2	1:B:101:SER:CB	2.92	0.51
1:B:337:VAL:HG13	1:B:338:GLN:N	2.25	0.51
1:B:487:ASP:CB	1:B:489:ASN:H	2.09	0.51
1:B:606:HIS:HD2	1:B:608:GLN:CG	2.14	0.51
1:C:417:ALA:O	1:C:463:LYS:N	2.37	0.51
1:C:430:GLN:HA	1:C:450:ALA:O	2.10	0.51
1:C:625:PRO:C	1:C:626:LEU:HD23	2.36	0.51
1:D:278:GLU:H	1:D:354:GLN:NE2	2.06	0.51
1:E:138:TYR:CZ	1:E:188:ILE:HD12	2.45	0.51
1:E:280:VAL:HA	1:E:357:PRO:HB3	1.93	0.51
1:F:307:ASP:OD1	1:F:307:ASP:C	2.53	0.51
1:F:366:GLY:N	1:F:369:GLU:HG3	2.22	0.51
1:A:37:PHE:CE2	1:A:101:SER:CB	2.91	0.51
1:A:48:ASP:OD2	1:A:51:ALA:HB3	2.11	0.51
1:B:71:TRP:CZ3	1:B:365:PRO:HG2	2.46	0.51
1:B:454:ARG:CZ	1:B:567:ARG:HD2	2.41	0.51
1:C:52:ALA:HB1	1:C:89:VAL:HG23	1.92	0.51
1:C:285:HIS:HB2	1:C:288:ASP:CG	2.36	0.51
1:C:546:ALA:HB1	1:C:552:ASP:OD1	2.11	0.51
1:D:7:ASN:O	1:D:8:ALA:C	2.51	0.51
1:D:177:ARG:HD2	1:E:360:LYS:O	2.11	0.51
1:D:300:ILE:CD1	1:D:390:ILE:CG2	2.89	0.51
1:F:580:PHE:CD2	1:F:649:ILE:HG13	2.46	0.51
1:A:418:ILE:HD11	1:A:462:TYR:HE1	1.76	0.51
1:A:138:TYR:O	1:A:142:PRO:HG3	2.11	0.50
1:A:454:ARG:CZ	1:A:567:ARG:HD2	2.41	0.50
1:B:138:TYR:O	1:B:142:PRO:HG3	2.11	0.50
1:B:398:PHE:HB3	1:B:399:PRO:HD2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:TRP:CZ3	1:C:365:PRO:HG2	2.46	0.50
1:D:102:ASN:O	1:D:104:ALA:N	2.44	0.50
1:D:285:HIS:HB2	1:D:288:ASP:CG	2.36	0.50
1:D:398:PHE:HB3	1:D:399:PRO:HD2	1.92	0.50
1:D:479:ARG:HD2	1:D:587:THR:HG21	1.92	0.50
1:D:625:PRO:C	1:D:626:LEU:HD23	2.36	0.50
1:E:454:ARG:CZ	1:E:567:ARG:HD2	2.41	0.50
1:E:580:PHE:CD2	1:E:649:ILE:HG13	2.46	0.50
1:E:593:THR:C	1:E:595:GLY:N	2.68	0.50
1:E:628:ARG:O	1:E:629:ARG:C	2.50	0.50
1:F:71:TRP:CZ3	1:F:365:PRO:HG2	2.46	0.50
1:F:479:ARG:HD2	1:F:587:THR:HG21	1.92	0.50
1:F:593:THR:C	1:F:595:GLY:N	2.68	0.50
1:B:300:ILE:CD1	1:B:390:ILE:CG2	2.89	0.50
1:B:319:LYS:O	1:B:320:GLY:C	2.53	0.50
1:B:402:THR:N	1:B:405:ASN:HB2	2.27	0.50
1:B:417:ALA:O	1:B:463:LYS:N	2.37	0.50
1:B:564:ILE:HB	1:B:565:PRO:CD	2.42	0.50
1:C:454:ARG:CZ	1:C:567:ARG:HD2	2.41	0.50
1:D:279:ASP:OD1	1:D:286:VAL:N	2.42	0.50
1:E:546:ALA:HB1	1:E:552:ASP:OD1	2.11	0.50
1:F:48:ASP:OD2	1:F:51:ALA:HB3	2.11	0.50
1:F:86:LEU:HD23	1:F:86:LEU:C	2.30	0.50
1:F:455:LEU:HG	1:F:456:ASN:H	1.75	0.50
1:F:551:HIS:CD2	1:F:551:HIS:C	2.88	0.50
1:A:13:ASP:OD1	1:A:100:ARG:NE	2.43	0.50
1:A:580:PHE:CD2	1:A:649:ILE:HG13	2.46	0.50
1:B:262:TYR:OH	1:B:370:HIS:NE2	2.32	0.50
1:B:479:ARG:HH11	1:B:587:THR:CG2	2.24	0.50
1:B:551:HIS:CD2	1:B:551:HIS:C	2.88	0.50
1:C:138:TYR:O	1:C:142:PRO:HG3	2.12	0.50
1:C:506:ASP:OD1	1:C:507:LYS:N	2.44	0.50
1:C:580:PHE:CD2	1:C:649:ILE:HG13	2.46	0.50
1:D:71:TRP:CZ3	1:D:365:PRO:HG2	2.47	0.50
1:E:317:GLN:CB	1:E:318:PRO:HD2	2.36	0.50
1:E:455:LEU:HG	1:E:456:ASN:H	1.75	0.50
1:A:402:THR:N	1:A:405:ASN:HB2	2.27	0.50
1:B:580:PHE:CD2	1:B:649:ILE:HG13	2.46	0.50
1:C:48:ASP:OD2	1:C:51:ALA:HB3	2.11	0.50
1:D:138:TYR:O	1:D:142:PRO:HG3	2.11	0.50
1:D:564:ILE:HB	1:D:565:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:632:ASP:O	1:D:635:VAL:HG23	2.12	0.50
1:E:285:HIS:HB2	1:E:288:ASP:CG	2.36	0.50
1:F:61:ASN:C	1:F:63:HIS:N	2.62	0.50
1:F:411:MET:C	1:F:412:VAL:HG12	2.34	0.50
1:A:7:ASN:O	1:A:8:ALA:C	2.51	0.50
1:A:506:ASP:OD1	1:A:507:LYS:N	2.44	0.50
1:B:455:LEU:HG	1:B:456:ASN:H	1.75	0.50
1:C:402:THR:N	1:C:405:ASN:HB2	2.27	0.50
1:D:316:ARG:HH21	1:F:338:GLN:HE22	1.58	0.50
1:D:454:ARG:CZ	1:D:567:ARG:HD2	2.41	0.50
1:E:71:TRP:CZ3	1:E:365:PRO:HG2	2.47	0.50
1:E:479:ARG:HD2	1:E:587:THR:HG21	1.92	0.50
1:E:479:ARG:HH11	1:E:587:THR:CG2	2.25	0.50
1:F:479:ARG:HH11	1:F:587:THR:CG2	2.24	0.50
1:A:173:THR:HG22	1:A:176:ASN:HB2	1.94	0.50
1:A:479:ARG:HH11	1:A:587:THR:CG2	2.25	0.50
1:B:38:ASN:C	1:B:40:LEU:N	2.67	0.50
1:B:285:HIS:HB2	1:B:288:ASP:CG	2.36	0.50
1:B:592:ASP:C	1:B:594:GLU:N	2.70	0.50
1:C:8:ALA:CB	1:C:553:LEU:HD12	2.42	0.50
1:C:29:ASP:OD1	1:C:29:ASP:N	2.31	0.50
1:C:434:ILE:C	1:C:436:ALA:N	2.66	0.50
1:C:455:LEU:HG	1:C:456:ASN:H	1.75	0.50
1:D:8:ALA:CB	1:D:553:LEU:HD12	2.42	0.50
1:D:13:ASP:OD1	1:D:100:ARG:NE	2.43	0.50
1:E:402:THR:N	1:E:405:ASN:HB2	2.27	0.50
1:E:418:ILE:HD11	1:E:462:TYR:HE1	1.76	0.50
1:E:564:ILE:HB	1:E:565:PRO:CD	2.42	0.50
1:F:8:ALA:CB	1:F:553:LEU:HD12	2.42	0.50
1:C:237:SER:CB	1:C:573:SER:HA	2.37	0.50
1:C:418:ILE:HD11	1:C:462:TYR:HE1	1.76	0.50
1:D:72:TYR:HA	1:D:79:GLN:OE1	2.12	0.50
1:D:319:LYS:O	1:D:320:GLY:C	2.53	0.50
1:D:402:THR:N	1:D:405:ASN:HB2	2.27	0.50
1:F:76:ASN:HD22	1:F:79:GLN:HG3	1.76	0.50
1:F:222:TRP:CH2	1:F:226:GLN:NE2	2.80	0.50
1:F:543:ALA:HA	1:F:553:LEU:HD11	1.94	0.50
1:A:11:GLN:HG3	1:A:15:ASN:ND2	2.22	0.50
1:A:411:MET:C	1:A:412:VAL:HG12	2.34	0.50
1:A:455:LEU:HG	1:A:456:ASN:H	1.75	0.50
1:B:76:ASN:HD22	1:B:79:GLN:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:HIS:O	1:B:552:ASP:CB	2.55	0.50
1:C:319:LYS:O	1:C:320:GLY:C	2.53	0.50
1:D:222:TRP:CZ2	1:D:226:GLN:NE2	2.80	0.50
1:D:546:ALA:HB1	1:D:552:ASP:OD1	2.11	0.50
1:D:555:LEU:H	1:D:555:LEU:HD12	1.77	0.50
1:E:97:TYR:O	1:E:101:SER:HB2	2.12	0.50
1:E:300:ILE:CD1	1:E:390:ILE:CG2	2.89	0.50
1:E:555:LEU:O	1:E:557:ALA:N	2.45	0.50
1:F:173:THR:HG22	1:F:176:ASN:HB2	1.94	0.50
1:F:269:PRO:HB3	1:F:363:LEU:CD2	2.40	0.50
1:F:454:ARG:CZ	1:F:567:ARG:HD2	2.41	0.50
1:F:555:LEU:H	1:F:555:LEU:HD12	1.77	0.50
1:B:8:ALA:CB	1:B:553:LEU:HD12	2.42	0.50
1:B:138:TYR:CZ	1:B:188:ILE:HD12	2.45	0.50
1:B:479:ARG:NH1	1:B:587:THR:OG1	2.45	0.50
1:C:97:TYR:O	1:C:101:SER:HB2	2.12	0.50
1:E:8:ALA:HA	1:E:553:LEU:CD1	2.40	0.50
1:E:138:TYR:O	1:E:142:PRO:HG3	2.11	0.50
1:E:533:MET:CB	1:E:534:PRO:CD	2.90	0.50
1:F:72:TYR:HA	1:F:79:GLN:OE1	2.12	0.50
1:F:83:ALA:HB2	1:F:114:GLU:HA	1.94	0.50
1:F:374:ALA:C	1:F:376:ARG:N	2.70	0.50
1:F:428:GLU:HG3	1:F:453:HIS:CD2	2.47	0.50
1:F:555:LEU:O	1:F:557:ALA:N	2.45	0.50
1:F:632:ASP:O	1:F:635:VAL:HG23	2.12	0.50
1:A:38:ASN:C	1:A:40:LEU:N	2.67	0.49
1:A:72:TYR:HA	1:A:79:GLN:OE1	2.12	0.49
1:A:173:THR:CG2	1:A:176:ASN:HB2	2.42	0.49
1:A:237:SER:CB	1:A:573:SER:HA	2.37	0.49
1:B:83:ALA:HB2	1:B:114:GLU:HA	1.94	0.49
1:B:227:LEU:N	1:B:227:LEU:CD1	2.75	0.49
1:C:76:ASN:HD22	1:C:79:GLN:HG3	1.76	0.49
1:C:83:ALA:HB2	1:C:114:GLU:HA	1.94	0.49
1:C:102:ASN:O	1:C:104:ALA:N	2.44	0.49
1:C:222:TRP:CZ2	1:C:226:GLN:NE2	2.80	0.49
1:C:551:HIS:CD2	1:C:551:HIS:C	2.88	0.49
1:D:201:PHE:HB3	1:D:216:LYS:HD2	1.92	0.49
1:D:374:ALA:C	1:D:376:ARG:N	2.70	0.49
1:D:428:GLU:HG3	1:D:453:HIS:CD2	2.47	0.49
1:D:506:ASP:OD1	1:D:507:LYS:N	2.44	0.49
1:D:533:MET:CB	1:D:534:PRO:CD	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:HIS:O	1:E:288:ASP:HB2	2.12	0.49
1:E:543:ALA:HA	1:E:553:LEU:HD11	1.94	0.49
1:E:592:ASP:C	1:E:594:GLU:N	2.70	0.49
1:E:632:ASP:O	1:E:635:VAL:HG23	2.12	0.49
1:F:13:ASP:OD1	1:F:100:ARG:NE	2.43	0.49
1:F:424:THR:HA	1:F:457:HIS:HA	1.94	0.49
1:A:71:TRP:CZ3	1:A:365:PRO:HG2	2.46	0.49
1:B:48:ASP:OD2	1:B:51:ALA:HB3	2.11	0.49
1:B:70:HIS:ND1	1:B:71:TRP:N	2.60	0.49
1:B:222:TRP:CH2	1:B:226:GLN:NE2	2.80	0.49
1:B:533:MET:CB	1:B:534:PRO:CD	2.90	0.49
1:B:632:ASP:O	1:B:635:VAL:HG23	2.12	0.49
1:C:8:ALA:HA	1:C:553:LEU:CD1	2.40	0.49
1:C:72:TYR:HA	1:C:79:GLN:OE1	2.12	0.49
1:C:173:THR:HG22	1:C:176:ASN:HB2	1.94	0.49
1:C:424:THR:HA	1:C:457:HIS:HA	1.94	0.49
1:D:11:GLN:HG3	1:D:15:ASN:ND2	2.22	0.49
1:E:72:TYR:HA	1:E:79:GLN:OE1	2.12	0.49
1:E:506:ASP:OD1	1:E:507:LYS:N	2.44	0.49
1:E:555:LEU:H	1:E:555:LEU:HD12	1.77	0.49
1:F:138:TYR:O	1:F:142:PRO:HG3	2.12	0.49
1:F:546:ALA:HB1	1:F:552:ASP:OD1	2.11	0.49
1:F:560:ARG:NH1	1:F:606:HIS:N	2.60	0.49
1:A:222:TRP:CH2	1:A:226:GLN:NE2	2.80	0.49
1:A:316:ARG:HH21	1:C:338:GLN:NE2	2.11	0.49
1:A:374:ALA:C	1:A:376:ARG:N	2.70	0.49
1:A:428:GLU:HG3	1:A:453:HIS:CD2	2.47	0.49
1:A:533:MET:CB	1:A:534:PRO:CD	2.90	0.49
1:B:222:TRP:CZ2	1:B:226:GLN:NE2	2.80	0.49
1:B:551:HIS:HD2	1:B:552:ASP:N	2.05	0.49
1:C:70:HIS:ND1	1:C:71:TRP:N	2.60	0.49
1:C:533:MET:CB	1:C:534:PRO:CD	2.90	0.49
1:C:560:ARG:NH1	1:C:606:HIS:N	2.60	0.49
1:D:173:THR:CG2	1:D:176:ASN:HB2	2.42	0.49
1:D:222:TRP:CH2	1:D:226:GLN:NE2	2.80	0.49
1:D:285:HIS:O	1:D:288:ASP:HB2	2.12	0.49
1:D:479:ARG:HH11	1:D:587:THR:CG2	2.25	0.49
1:D:580:PHE:CD2	1:D:649:ILE:HG13	2.46	0.49
1:E:8:ALA:CB	1:E:553:LEU:HD12	2.42	0.49
1:F:506:ASP:OD1	1:F:507:LYS:N	2.44	0.49
1:F:533:MET:CB	1:F:534:PRO:CD	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:CB	1:A:553:LEU:HD12	2.42	0.49
1:A:479:ARG:NH1	1:A:587:THR:OG1	2.45	0.49
1:A:589:GLY:O	1:A:593:THR:OG1	2.30	0.49
1:B:72:TYR:HA	1:B:79:GLN:OE1	2.12	0.49
1:B:175:LYS:O	1:B:176:ASN:CB	2.60	0.49
1:B:555:LEU:H	1:B:555:LEU:HD12	1.77	0.49
1:C:201:PHE:HB3	1:C:216:LYS:HD2	1.92	0.49
1:C:222:TRP:CH2	1:C:226:GLN:NE2	2.80	0.49
1:C:428:GLU:HG3	1:C:453:HIS:CD2	2.47	0.49
1:C:564:ILE:HB	1:C:565:PRO:CD	2.42	0.49
1:C:592:ASP:C	1:C:594:GLU:N	2.70	0.49
1:D:76:ASN:HD22	1:D:79:GLN:HG3	1.76	0.49
1:D:83:ALA:HB2	1:D:114:GLU:HA	1.94	0.49
1:D:402:THR:O	1:D:405:ASN:HB2	2.13	0.49
1:D:633:GLU:C	1:D:635:VAL:N	2.66	0.49
1:F:37:PHE:CE2	1:F:101:SER:CB	2.91	0.49
1:F:279:ASP:OD1	1:F:286:VAL:N	2.42	0.49
1:F:353:ARG:NE	1:F:369:GLU:OE2	2.43	0.49
1:F:633:GLU:C	1:F:635:VAL:N	2.66	0.49
1:A:319:LYS:O	1:A:320:GLY:C	2.53	0.49
1:A:424:THR:HA	1:A:457:HIS:HA	1.94	0.49
1:A:546:ALA:HB1	1:A:552:ASP:OD1	2.11	0.49
1:A:564:ILE:HB	1:A:565:PRO:CD	2.42	0.49
1:B:97:TYR:O	1:B:101:SER:HB2	2.12	0.49
1:B:102:ASN:O	1:B:104:ALA:N	2.44	0.49
1:B:173:THR:HG22	1:B:176:ASN:HB2	1.94	0.49
1:B:227:LEU:N	1:B:227:LEU:HD12	2.27	0.49
1:B:285:HIS:O	1:B:288:ASP:HB2	2.12	0.49
1:B:428:GLU:HG3	1:B:453:HIS:CD2	2.47	0.49
1:B:546:ALA:HB1	1:B:552:ASP:OD1	2.11	0.49
1:C:173:THR:CG2	1:C:176:ASN:HB2	2.42	0.49
1:C:227:LEU:N	1:C:227:LEU:CD1	2.75	0.49
1:C:479:ARG:HH11	1:C:587:THR:CG2	2.25	0.49
1:D:543:ALA:HA	1:D:553:LEU:HD11	1.94	0.49
1:E:16:HIS:CD2	1:E:27:TYR:CE2	3.01	0.49
1:E:424:THR:HA	1:E:457:HIS:HA	1.94	0.49
1:F:69:ARG:HA	1:F:264:TYR:CD2	2.48	0.49
1:F:285:HIS:O	1:F:288:ASP:HB2	2.12	0.49
1:F:402:THR:N	1:F:405:ASN:HB2	2.27	0.49
1:F:564:ILE:HB	1:F:565:PRO:CD	2.42	0.49
1:A:555:LEU:H	1:A:555:LEU:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:HIS:CD2	1:B:27:TYR:CE2	3.01	0.49
1:B:217:GLY:H	1:B:220:PHE:H	1.61	0.49
1:C:285:HIS:O	1:C:288:ASP:HB2	2.12	0.49
1:C:589:GLY:O	1:C:593:THR:OG1	2.30	0.49
1:D:195:VAL:HG22	1:D:196:THR:N	2.28	0.49
1:D:227:LEU:CD1	1:D:227:LEU:N	2.75	0.49
1:D:560:ARG:NH1	1:D:606:HIS:N	2.60	0.49
1:E:83:ALA:HB2	1:E:114:GLU:HA	1.94	0.49
1:E:173:THR:HG22	1:E:176:ASN:HB2	1.94	0.49
1:E:402:THR:O	1:E:405:ASN:HB2	2.13	0.49
1:E:594:GLU:HG2	1:E:594:GLU:O	2.13	0.49
1:F:70:HIS:ND1	1:F:71:TRP:N	2.60	0.49
1:A:543:ALA:HA	1:A:553:LEU:HD11	1.94	0.49
1:B:48:ASP:C	1:B:50:GLY:N	2.69	0.49
1:B:506:ASP:OD1	1:B:507:LYS:N	2.44	0.49
1:B:522:SER:C	1:B:524:LYS:N	2.63	0.49
1:B:538:SER:O	1:B:542:GLN:HG3	2.13	0.49
1:C:11:GLN:HG3	1:C:15:ASN:ND2	2.22	0.49
1:C:13:ASP:OD1	1:C:100:ARG:NE	2.43	0.49
1:C:69:ARG:HA	1:C:264:TYR:CD2	2.48	0.49
1:C:463:LYS:CG	1:C:520:GLU:HG3	2.43	0.49
1:C:632:ASP:O	1:C:635:VAL:HG23	2.12	0.49
1:D:16:HIS:CD2	1:D:27:TYR:CE2	3.01	0.49
1:D:138:TYR:CZ	1:D:188:ILE:HD12	2.45	0.49
1:D:443:ILE:HD13	1:E:161:GLN:HG3	1.95	0.49
1:D:463:LYS:CG	1:D:520:GLU:HG3	2.43	0.49
1:D:479:ARG:NH1	1:D:587:THR:OG1	2.45	0.49
1:E:222:TRP:CZ2	1:E:226:GLN:NE2	2.80	0.49
1:E:227:LEU:N	1:E:227:LEU:CD1	2.75	0.49
1:E:538:SER:O	1:E:542:GLN:HG3	2.13	0.49
1:F:173:THR:CG2	1:F:176:ASN:HB2	2.42	0.49
1:F:357:PRO:HB2	1:F:358:HIS:CE1	2.48	0.49
1:F:479:ARG:NH1	1:F:587:THR:OG1	2.45	0.49
1:A:16:HIS:CD2	1:A:27:TYR:CE2	3.01	0.49
1:A:188:ILE:HG23	4:A:720:HOH:O	2.12	0.49
1:A:222:TRP:CZ2	1:A:226:GLN:NE2	2.80	0.49
1:A:313:ILE:HD12	1:A:314:ASP:O	2.13	0.49
1:A:357:PRO:HB2	1:A:358:HIS:CE1	2.48	0.49
1:A:402:THR:O	1:A:405:ASN:HB2	2.13	0.49
1:A:487:ASP:CB	1:A:489:ASN:H	2.09	0.49
1:A:555:LEU:O	1:A:557:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ARG:NH1	1:A:606:HIS:N	2.60	0.49
1:A:585:ALA:HA	1:A:642:ILE:HA	1.95	0.49
1:A:632:ASP:O	1:A:635:VAL:HG23	2.12	0.49
1:B:173:THR:CG2	1:B:176:ASN:HB2	2.42	0.49
1:B:313:ILE:HD12	1:B:314:ASP:O	2.13	0.49
1:B:555:LEU:O	1:B:557:ALA:N	2.45	0.49
1:C:479:ARG:NH1	1:C:587:THR:OG1	2.45	0.49
1:E:76:ASN:ND2	1:E:79:GLN:HG3	2.28	0.49
1:E:357:PRO:HB2	1:E:358:HIS:CE1	2.48	0.49
1:F:402:THR:O	1:F:405:ASN:HB2	2.13	0.49
1:F:418:ILE:HD11	1:F:462:TYR:HE1	1.76	0.49
1:A:70:HIS:ND1	1:A:71:TRP:N	2.60	0.49
1:A:76:ASN:HD22	1:A:79:GLN:HG3	1.76	0.49
1:B:8:ALA:HA	1:B:553:LEU:CD1	2.40	0.49
1:B:353:ARG:NE	1:B:369:GLU:OE2	2.43	0.49
1:B:374:ALA:C	1:B:376:ARG:N	2.69	0.49
1:C:313:ILE:HD12	1:C:314:ASP:O	2.13	0.49
1:C:543:ALA:HA	1:C:553:LEU:HD11	1.94	0.49
1:D:270:VAL:HG13	1:E:270:VAL:HG13	1.94	0.49
1:D:424:THR:HA	1:D:457:HIS:HA	1.94	0.49
1:D:589:GLY:O	1:D:593:THR:OG1	2.30	0.49
1:D:594:GLU:O	1:D:594:GLU:HG2	2.13	0.49
1:E:217:GLY:H	1:E:220:PHE:H	1.61	0.49
1:E:222:TRP:CH2	1:E:226:GLN:NE2	2.80	0.49
1:E:428:GLU:HG3	1:E:453:HIS:CD2	2.47	0.49
1:F:16:HIS:CD2	1:F:27:TYR:CE2	3.01	0.49
1:F:222:TRP:CZ2	1:F:226:GLN:NE2	2.80	0.49
1:F:227:LEU:N	1:F:227:LEU:CD1	2.75	0.49
1:F:592:ASP:C	1:F:594:GLU:N	2.70	0.49
1:A:76:ASN:ND2	1:A:79:GLN:HG3	2.28	0.49
1:A:178:GLU:OE1	4:A:705:HOH:O	2.19	0.49
1:A:465:THR:O	1:A:466:MET:HB3	2.12	0.49
1:B:357:PRO:HB2	1:B:358:HIS:CE1	2.48	0.49
1:B:418:ILE:HD11	1:B:462:TYR:HE1	1.76	0.49
1:B:594:GLU:HG2	1:B:594:GLU:O	2.13	0.49
1:C:374:ALA:C	1:C:376:ARG:N	2.69	0.49
1:C:555:LEU:O	1:C:557:ALA:N	2.45	0.49
1:C:555:LEU:HD12	1:C:555:LEU:H	1.77	0.49
1:D:313:ILE:HD12	1:D:314:ASP:O	2.13	0.49
1:E:70:HIS:ND1	1:E:71:TRP:N	2.60	0.49
1:E:102:ASN:O	1:E:104:ALA:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:ARG:NH1	1:E:587:THR:OG1	2.45	0.49
1:E:642:ILE:HG21	1:E:642:ILE:HD13	1.63	0.49
1:F:76:ASN:O	1:F:78:ARG:N	2.46	0.49
1:F:102:ASN:O	1:F:104:ALA:N	2.44	0.49
1:F:319:LYS:O	1:F:320:GLY:C	2.53	0.49
1:A:108:GLU:OE1	1:A:108:GLU:HA	2.13	0.48
1:A:285:HIS:O	1:A:288:ASP:HB2	2.12	0.48
1:B:69:ARG:HA	1:B:264:TYR:CD2	2.48	0.48
1:C:414:ASN:HD21	1:C:467:SER:N	2.10	0.48
1:C:491:ILE:CG1	1:D:175:LYS:HB2	2.42	0.48
1:D:173:THR:HG22	1:D:176:ASN:HB2	1.94	0.48
1:D:538:SER:O	1:D:542:GLN:HG3	2.13	0.48
1:E:313:ILE:HD12	1:E:314:ASP:O	2.13	0.48
1:A:57:MET:O	1:A:61:ASN:HB2	2.13	0.48
1:A:69:ARG:HA	1:A:264:TYR:CD2	2.48	0.48
1:A:76:ASN:O	1:A:78:ARG:N	2.46	0.48
1:A:83:ALA:HB2	1:A:114:GLU:HA	1.94	0.48
1:A:227:LEU:N	1:A:227:LEU:CD1	2.75	0.48
1:A:538:SER:O	1:A:542:GLN:HG3	2.13	0.48
1:B:195:VAL:HG22	1:B:196:THR:N	2.28	0.48
1:B:560:ARG:NH1	1:B:606:HIS:N	2.60	0.48
1:C:353:ARG:NE	1:C:369:GLU:OE2	2.43	0.48
1:D:70:HIS:ND1	1:D:71:TRP:N	2.61	0.48
1:E:76:ASN:CB	1:E:79:GLN:HB2	2.34	0.48
1:E:173:THR:CG2	1:E:176:ASN:HB2	2.42	0.48
1:E:227:LEU:N	1:E:227:LEU:HD12	2.27	0.48
1:E:262:TYR:OH	1:E:370:HIS:NE2	2.32	0.48
1:F:201:PHE:HB3	1:F:216:LYS:HD2	1.92	0.48
1:F:217:GLY:H	1:F:220:PHE:H	1.61	0.48
1:F:594:GLU:O	1:F:594:GLU:HG2	2.13	0.48
1:A:551:HIS:C	1:A:552:ASP:OD1	2.57	0.48
1:C:76:ASN:O	1:C:78:ARG:N	2.46	0.48
1:C:357:PRO:HB2	1:C:358:HIS:CE1	2.48	0.48
1:C:555:LEU:O	1:C:556:SER:C	2.54	0.48
1:D:300:ILE:HD11	1:D:390:ILE:HG22	1.95	0.48
1:D:374:ALA:C	1:D:376:ARG:H	2.22	0.48
1:D:551:HIS:C	1:D:552:ASP:OD1	2.57	0.48
1:E:374:ALA:C	1:E:376:ARG:H	2.22	0.48
1:F:38:ASN:C	1:F:40:LEU:N	2.67	0.48
1:F:76:ASN:ND2	1:F:79:GLN:HG3	2.28	0.48
1:F:97:TYR:O	1:F:101:SER:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:LEU:N	1:F:227:LEU:HD12	2.27	0.48
1:F:544:ASP:O	1:F:547:VAL:HG23	2.14	0.48
1:A:300:ILE:HD11	1:A:390:ILE:HG22	1.95	0.48
1:B:57:MET:O	1:B:61:ASN:HB2	2.13	0.48
1:B:296:ILE:HG23	1:B:296:ILE:HD12	1.42	0.48
1:C:16:HIS:CD2	1:C:27:TYR:CE2	3.01	0.48
1:C:217:GLY:H	1:C:220:PHE:H	1.61	0.48
1:C:443:ILE:HD13	1:F:161:GLN:HG3	1.95	0.48
1:D:57:MET:O	1:D:61:ASN:HB2	2.13	0.48
1:D:175:LYS:O	1:D:176:ASN:CB	2.60	0.48
1:D:555:LEU:O	1:D:557:ALA:N	2.45	0.48
1:E:69:ARG:HA	1:E:264:TYR:CD2	2.48	0.48
1:E:195:VAL:HG22	1:E:196:THR:N	2.28	0.48
1:B:108:GLU:OE1	1:B:108:GLU:HA	2.13	0.48
1:B:402:THR:O	1:B:405:ASN:HB2	2.13	0.48
1:B:493:LEU:HA	1:B:497:GLU:OE1	2.14	0.48
1:B:543:ALA:HA	1:B:553:LEU:HD11	1.94	0.48
1:B:585:ALA:HA	1:B:642:ILE:HA	1.95	0.48
1:C:493:LEU:HA	1:C:497:GLU:OE1	2.14	0.48
1:D:97:TYR:O	1:D:101:SER:HB2	2.12	0.48
1:D:513:PRO:CG	1:D:517:GLU:HB2	2.27	0.48
1:E:57:MET:O	1:E:61:ASN:HB2	2.13	0.48
1:E:374:ALA:C	1:E:376:ARG:N	2.69	0.48
1:E:493:LEU:HA	1:E:497:GLU:OE1	2.14	0.48
1:E:560:ARG:NH1	1:E:606:HIS:N	2.60	0.48
1:F:313:ILE:HD12	1:F:314:ASP:O	2.13	0.48
1:F:463:LYS:CG	1:F:520:GLU:HG3	2.43	0.48
1:A:97:TYR:O	1:A:101:SER:HB2	2.12	0.48
1:A:227:LEU:N	1:A:227:LEU:HD12	2.27	0.48
1:A:374:ALA:C	1:A:376:ARG:H	2.22	0.48
1:A:487:ASP:O	1:A:488:ASN:CB	2.62	0.48
1:B:165:THR:HA	1:B:449:ASN:O	2.14	0.48
1:B:403:HIS:O	1:B:404:ASP:C	2.57	0.48
1:B:487:ASP:O	1:B:488:ASN:CB	2.62	0.48
1:C:57:MET:O	1:C:61:ASN:HB2	2.13	0.48
1:C:175:LYS:O	1:C:176:ASN:CB	2.60	0.48
1:C:225:HIS:HD2	1:C:388:ASP:OD2	1.97	0.48
1:C:402:THR:O	1:C:405:ASN:HB2	2.13	0.48
1:C:433:LEU:HD23	1:C:433:LEU:HA	1.56	0.48
1:D:69:ARG:HA	1:D:264:TYR:CD2	2.48	0.48
1:D:487:ASP:O	1:D:488:ASN:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:MET:H	1:D:533:MET:CE	2.16	0.48
1:D:564:ILE:HB	1:D:565:PRO:HD2	1.96	0.48
1:E:175:LYS:O	1:E:176:ASN:CB	2.60	0.48
1:F:57:MET:O	1:F:61:ASN:HB2	2.13	0.48
1:A:493:LEU:HA	1:A:497:GLU:OE1	2.14	0.48
1:A:544:ASP:O	1:A:547:VAL:HG23	2.14	0.48
1:B:56:LEU:HD21	1:B:110:MET:CE	2.44	0.48
1:B:76:ASN:O	1:B:78:ARG:N	2.46	0.48
1:B:463:LYS:CG	1:B:520:GLU:HG3	2.43	0.48
1:C:108:GLU:OE1	1:C:108:GLU:HA	2.13	0.48
1:C:487:ASP:O	1:C:488:ASN:CB	2.62	0.48
1:D:76:ASN:O	1:D:78:ARG:N	2.46	0.48
1:D:123:VAL:CG1	1:D:134:LEU:HD21	2.43	0.48
1:D:227:LEU:N	1:D:227:LEU:HD12	2.28	0.48
1:D:585:ALA:HA	1:D:642:ILE:HA	1.95	0.48
1:E:225:HIS:HD2	1:E:388:ASP:OD2	1.97	0.48
1:E:279:ASP:OD1	1:E:286:VAL:N	2.42	0.48
1:E:441:GLU:C	1:E:443:ILE:H	2.18	0.48
1:E:551:HIS:C	1:E:552:ASP:OD1	2.57	0.48
1:F:493:LEU:HA	1:F:497:GLU:OE1	2.14	0.48
1:F:585:ALA:HA	1:F:642:ILE:HA	1.95	0.48
1:A:487:ASP:OD2	1:A:489:ASN:HB2	2.14	0.48
1:B:190:MET:HG3	1:B:568:MET:HE2	1.96	0.48
1:B:296:ILE:HA	1:B:296:ILE:HD13	1.38	0.48
1:B:424:THR:HA	1:B:457:HIS:HA	1.94	0.48
1:C:195:VAL:HG22	1:C:196:THR:N	2.28	0.48
1:C:594:GLU:O	1:C:594:GLU:HG2	2.13	0.48
1:D:5:THR:HG22	1:D:6:GLY:O	2.14	0.48
1:D:108:GLU:OE1	1:D:108:GLU:HA	2.13	0.48
1:D:165:THR:HA	1:D:449:ASN:O	2.14	0.48
1:D:357:PRO:HB2	1:D:358:HIS:CE1	2.48	0.48
1:D:508:PHE:CE2	1:D:521:ARG:CD	2.97	0.48
1:E:201:PHE:HB3	1:E:216:LYS:HD2	1.92	0.48
1:E:491:ILE:O	1:E:492:THR:CG2	2.62	0.48
1:E:508:PHE:CE2	1:E:521:ARG:CD	2.97	0.48
1:E:564:ILE:HB	1:E:565:PRO:HD2	1.96	0.48
1:E:585:ALA:HA	1:E:642:ILE:HA	1.95	0.48
1:E:589:GLY:O	1:E:593:THR:OG1	2.30	0.48
1:F:441:GLU:C	1:F:443:ILE:H	2.18	0.48
1:F:465:THR:O	1:F:466:MET:HB3	2.12	0.48
1:A:224:HIS:O	1:A:228:THR:OG1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:GLN:NE2	4:A:820:HOH:O	2.31	0.48
1:B:5:THR:HG22	1:B:6:GLY:O	2.14	0.48
1:B:300:ILE:HD11	1:B:390:ILE:HG22	1.95	0.48
1:C:458:ASN:O	1:C:459:GLU:C	2.56	0.48
1:C:487:ASP:OD2	1:C:489:ASN:HB2	2.14	0.48
1:C:491:ILE:O	1:C:492:THR:CG2	2.62	0.48
1:C:544:ASP:O	1:C:547:VAL:HG23	2.14	0.48
1:C:564:ILE:HB	1:C:565:PRO:HD2	1.96	0.48
1:C:585:ALA:HA	1:C:642:ILE:HA	1.95	0.48
1:D:41:GLY:O	1:D:42:ASP:HB2	2.13	0.48
1:D:76:ASN:ND2	1:D:79:GLN:HG3	2.28	0.48
1:D:478:PHE:CZ	1:D:519:ILE:HD12	2.49	0.48
1:D:487:ASP:CB	1:D:489:ASN:H	2.09	0.48
1:E:337:VAL:HG13	1:E:338:GLN:N	2.25	0.48
1:F:165:THR:HA	1:F:449:ASN:O	2.14	0.48
1:F:195:VAL:HG22	1:F:196:THR:N	2.28	0.48
1:A:337:VAL:HG13	1:A:338:GLN:N	2.25	0.48
1:A:441:GLU:C	1:A:443:ILE:H	2.18	0.48
1:A:594:GLU:O	1:A:594:GLU:HG2	2.13	0.48
1:B:589:GLY:O	1:B:593:THR:OG1	2.30	0.48
1:B:591:LYS:HB2	1:B:591:LYS:HZ3	1.77	0.48
1:C:76:ASN:ND2	1:C:79:GLN:HG3	2.28	0.48
1:C:374:ALA:C	1:C:376:ARG:H	2.22	0.48
1:C:411:MET:N	1:C:411:MET:SD	2.83	0.48
1:D:190:MET:HG3	1:D:568:MET:HE2	1.96	0.48
1:D:592:ASP:C	1:D:594:GLU:N	2.70	0.48
1:E:392:LYS:HA	1:E:395:THR:HB	1.96	0.48
1:E:434:ILE:HD11	1:E:447:GLU:HA	1.96	0.48
1:E:578:MET:SD	1:E:580:PHE:CZ	3.07	0.48
1:F:300:ILE:HD11	1:F:390:ILE:HG22	1.95	0.48
1:A:217:GLY:H	1:A:220:PHE:H	1.61	0.47
1:B:41:GLY:O	1:B:42:ASP:HB2	2.13	0.47
1:B:508:PHE:CE2	1:B:521:ARG:CD	2.97	0.47
1:B:551:HIS:C	1:B:552:ASP:OD1	2.57	0.47
1:B:578:MET:SD	1:B:580:PHE:CZ	3.07	0.47
1:C:239:TRP:CZ3	1:C:574:LYS:NZ	2.79	0.47
1:C:538:SER:O	1:C:542:GLN:HG3	2.13	0.47
1:C:551:HIS:C	1:C:552:ASP:OD1	2.57	0.47
1:D:150:VAL:CG2	1:D:168:VAL:HG12	2.42	0.47
1:D:177:ARG:NH1	1:E:361:PHE:HE1	2.12	0.47
1:D:217:GLY:H	1:D:220:PHE:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:ASP:O	1:D:547:VAL:HG23	2.14	0.47
1:E:513:PRO:CG	1:E:517:GLU:HB2	2.27	0.47
1:F:392:LYS:HA	1:F:395:THR:HB	1.96	0.47
1:F:551:HIS:C	1:F:552:ASP:OD1	2.57	0.47
1:F:555:LEU:O	1:F:556:SER:C	2.54	0.47
1:F:589:GLY:O	1:F:593:THR:OG1	2.30	0.47
1:A:366:GLY:N	1:A:369:GLU:HG3	2.22	0.47
1:A:463:LYS:CG	1:A:520:GLU:HG3	2.43	0.47
1:C:56:LEU:HD21	1:C:110:MET:CE	2.44	0.47
1:C:392:LYS:HA	1:C:395:THR:HB	1.96	0.47
1:C:513:PRO:CG	1:C:517:GLU:HB2	2.27	0.47
1:D:40:LEU:HA	1:D:40:LEU:HD12	1.52	0.47
1:D:392:LYS:HA	1:D:395:THR:HB	1.96	0.47
1:D:491:ILE:O	1:D:492:THR:CG2	2.62	0.47
1:E:76:ASN:O	1:E:78:ARG:N	2.46	0.47
1:E:165:THR:HA	1:E:449:ASN:O	2.14	0.47
1:E:296:ILE:HG23	1:E:296:ILE:HD12	1.42	0.47
1:E:544:ASP:O	1:E:547:VAL:HG23	2.14	0.47
1:F:317:GLN:CB	1:F:318:PRO:HD2	2.36	0.47
1:F:434:ILE:HD11	1:F:447:GLU:HA	1.96	0.47
1:F:458:ASN:O	1:F:459:GLU:C	2.56	0.47
1:A:175:LYS:O	1:A:176:ASN:CB	2.60	0.47
1:A:458:ASN:O	1:A:459:GLU:C	2.56	0.47
1:B:279:ASP:OD1	1:B:286:VAL:N	2.42	0.47
1:B:366:GLY:O	1:B:367:VAL:C	2.57	0.47
1:B:419:ASP:HB2	1:B:463:LYS:HZ2	1.79	0.47
1:C:165:THR:HA	1:C:449:ASN:O	2.14	0.47
1:C:403:HIS:O	1:C:404:ASP:C	2.57	0.47
1:D:403:HIS:O	1:D:404:ASP:C	2.57	0.47
1:D:487:ASP:OD2	1:D:489:ASN:HB2	2.14	0.47
1:E:30:LEU:HD23	1:E:30:LEU:HA	1.55	0.47
1:E:41:GLY:O	1:E:42:ASP:HB2	2.13	0.47
1:E:463:LYS:CG	1:E:520:GLU:HG3	2.43	0.47
1:F:62:ASP:O	1:F:63:HIS:C	2.57	0.47
1:F:451:ARG:HH11	1:F:451:ARG:HD3	1.47	0.47
1:F:491:ILE:O	1:F:492:THR:CG2	2.62	0.47
1:F:538:SER:O	1:F:542:GLN:HG3	2.13	0.47
1:A:195:VAL:HG22	1:A:196:THR:N	2.28	0.47
1:A:225:HIS:HD2	1:A:388:ASP:OD2	1.97	0.47
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.54	0.47
1:A:434:ILE:HD11	1:A:447:GLU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:LEU:HA	1:A:553:LEU:HD23	1.55	0.47
1:B:434:ILE:HD11	1:B:447:GLU:HA	1.96	0.47
1:B:564:ILE:HB	1:B:565:PRO:HD2	1.96	0.47
1:D:225:HIS:HD2	1:D:388:ASP:OD2	1.97	0.47
1:D:315:ILE:HG13	1:D:315:ILE:O	2.15	0.47
1:D:493:LEU:HA	1:D:497:GLU:OE1	2.14	0.47
1:D:578:MET:SD	1:D:580:PHE:CZ	3.07	0.47
1:E:40:LEU:HA	1:E:40:LEU:HD12	1.52	0.47
1:E:403:HIS:O	1:E:404:ASP:C	2.57	0.47
1:F:315:ILE:HG13	1:F:315:ILE:O	2.15	0.47
1:F:508:PHE:CE2	1:F:521:ARG:CD	2.97	0.47
1:A:5:THR:HG22	1:A:6:GLY:O	2.14	0.47
1:A:165:THR:HA	1:A:449:ASN:O	2.14	0.47
1:A:290:GLU:HG2	4:A:749:HOH:O	2.14	0.47
1:A:465:THR:HG23	1:A:518:THR:HG1	1.78	0.47
1:B:11:GLN:HG3	1:B:15:ASN:ND2	2.21	0.47
1:B:13:ASP:OD1	1:B:100:ARG:NE	2.43	0.47
1:B:441:GLU:C	1:B:443:ILE:H	2.18	0.47
1:C:62:ASP:HB2	1:C:64:ARG:HG2	1.97	0.47
1:C:227:LEU:N	1:C:227:LEU:HD12	2.27	0.47
1:C:578:MET:SD	1:C:580:PHE:CZ	3.07	0.47
1:D:56:LEU:HD21	1:D:110:MET:CE	2.44	0.47
1:D:555:LEU:O	1:D:556:SER:C	2.54	0.47
1:E:5:THR:HG22	1:E:6:GLY:O	2.14	0.47
1:E:11:GLN:HG3	1:E:15:ASN:ND2	2.22	0.47
1:E:405:ASN:HD22	1:E:405:ASN:HA	1.45	0.47
1:E:417:ALA:O	1:E:463:LYS:N	2.37	0.47
1:F:11:GLN:HG3	1:F:15:ASN:ND2	2.22	0.47
1:F:41:GLY:O	1:F:42:ASP:HB2	2.13	0.47
1:F:411:MET:SD	1:F:411:MET:N	2.83	0.47
1:B:225:HIS:HD2	1:B:388:ASP:OD2	1.97	0.47
1:B:458:ASN:O	1:B:459:GLU:C	2.56	0.47
1:B:478:PHE:CZ	1:B:519:ILE:HD12	2.49	0.47
1:B:533:MET:HB3	1:B:534:PRO:CD	2.43	0.47
1:C:434:ILE:HD11	1:C:447:GLU:HA	1.96	0.47
1:C:478:PHE:CZ	1:C:519:ILE:HD12	2.49	0.47
1:C:508:PHE:CE2	1:C:521:ARG:CD	2.97	0.47
1:C:586:VAL:O	1:C:641:ASN:HB2	2.15	0.47
1:D:316:ARG:HE	1:F:338:GLN:HE22	1.63	0.47
1:E:106:PHE:O	1:E:109:ARG:N	2.43	0.47
1:F:108:GLU:OE1	1:F:108:GLU:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:478:PHE:CZ	1:F:519:ILE:HD12	2.49	0.47
1:F:553:LEU:HA	1:F:553:LEU:HD23	1.55	0.47
1:F:578:MET:SD	1:F:580:PHE:CZ	3.07	0.47
1:A:45:ILE:C	1:A:94:LYS:HD3	2.40	0.47
1:A:62:ASP:HB2	1:A:64:ARG:HG2	1.97	0.47
1:A:78:ARG:HD3	1:A:78:ARG:HH11	1.31	0.47
1:A:154:ALA:O	1:A:157:ALA:HB3	2.15	0.47
1:A:190:MET:HG3	1:A:568:MET:HE2	1.96	0.47
1:A:201:PHE:HB3	1:A:216:LYS:HD2	1.92	0.47
1:A:273:ASP:CG	1:B:360:LYS:HE3	2.39	0.47
1:A:366:GLY:O	1:A:367:VAL:C	2.57	0.47
1:A:491:ILE:O	1:A:492:THR:CG2	2.62	0.47
1:A:508:PHE:CE2	1:A:521:ARG:CD	2.97	0.47
1:A:586:VAL:O	1:A:641:ASN:HB2	2.15	0.47
1:A:592:ASP:C	1:A:594:GLU:N	2.70	0.47
1:B:45:ILE:C	1:B:94:LYS:HD3	2.40	0.47
1:B:76:ASN:ND2	1:B:79:GLN:HG3	2.28	0.47
1:B:239:TRP:CZ3	1:B:574:LYS:NZ	2.79	0.47
1:B:487:ASP:OD2	1:B:489:ASN:HB2	2.14	0.47
1:C:5:THR:HG22	1:C:6:GLY:O	2.14	0.47
1:C:190:MET:HG3	1:C:568:MET:HE2	1.96	0.47
1:C:451:ARG:HH11	1:C:451:ARG:HD3	1.47	0.47
1:C:592:ASP:O	1:C:594:GLU:N	2.45	0.47
1:C:653:LEU:HA	1:C:653:LEU:HD12	1.47	0.47
1:D:62:ASP:HB2	1:D:64:ARG:HG2	1.97	0.47
1:D:106:PHE:O	1:D:109:ARG:N	2.43	0.47
1:D:414:ASN:HD21	1:D:467:SER:N	2.10	0.47
1:D:533:MET:HB3	1:D:534:PRO:CD	2.43	0.47
1:D:653:LEU:HD12	1:D:653:LEU:HA	1.47	0.47
1:E:62:ASP:HB2	1:E:64:ARG:HG2	1.97	0.47
1:E:115:PHE:O	1:E:116:VAL:C	2.57	0.47
1:E:154:ALA:HB1	1:E:448:ILE:HG21	1.97	0.47
1:E:366:GLY:O	1:E:367:VAL:C	2.57	0.47
1:E:540:LYS:O	1:E:541:GLU:C	2.58	0.47
1:E:586:VAL:O	1:E:641:ASN:HB2	2.15	0.47
1:F:45:ILE:C	1:F:94:LYS:HD3	2.40	0.47
1:F:190:MET:HG3	1:F:568:MET:HE2	1.96	0.47
1:F:225:HIS:HD2	1:F:388:ASP:OD2	1.97	0.47
1:F:296:ILE:HA	1:F:296:ILE:HD13	1.38	0.47
1:F:374:ALA:C	1:F:376:ARG:H	2.22	0.47
1:F:540:LYS:O	1:F:541:GLU:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:632:ASP:C	1:F:634:ARG:N	2.73	0.47
1:A:222:TRP:CD1	1:A:622:LEU:HD23	2.50	0.47
1:B:115:PHE:O	1:B:116:VAL:C	2.57	0.47
1:B:491:ILE:O	1:B:492:THR:CG2	2.62	0.47
1:B:620:ARG:HG3	1:B:624:TYR:CG	2.50	0.47
1:C:45:ILE:C	1:C:94:LYS:HD3	2.40	0.47
1:C:540:LYS:O	1:C:541:GLU:C	2.58	0.47
1:E:222:TRP:CD1	1:E:622:LEU:HD23	2.50	0.47
1:E:315:ILE:O	1:E:315:ILE:HG13	2.15	0.47
1:E:458:ASN:O	1:E:459:GLU:C	2.56	0.47
1:F:197:TRP:CD1	1:F:223:VAL:HG21	2.50	0.47
1:F:414:ASN:HD21	1:F:467:SER:N	2.10	0.47
1:F:586:VAL:O	1:F:641:ASN:HB2	2.15	0.47
1:A:41:GLY:O	1:A:42:ASP:HB2	2.13	0.47
1:A:392:LYS:HA	1:A:395:THR:HB	1.96	0.47
1:A:540:LYS:O	1:A:541:GLU:C	2.58	0.47
1:B:197:TRP:CD1	1:B:223:VAL:HG21	2.50	0.47
1:B:540:LYS:O	1:B:541:GLU:C	2.58	0.47
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.55	0.47
1:C:41:GLY:O	1:C:42:ASP:HB2	2.13	0.47
1:C:62:ASP:O	1:C:63:HIS:C	2.57	0.47
1:D:62:ASP:O	1:D:63:HIS:C	2.57	0.47
1:D:154:ALA:O	1:D:157:ALA:HB3	2.15	0.47
1:D:434:ILE:HD11	1:D:447:GLU:HA	1.96	0.47
1:E:465:THR:O	1:E:466:MET:HB3	2.12	0.47
1:E:478:PHE:CZ	1:E:519:ILE:HD12	2.49	0.47
1:F:56:LEU:HD21	1:F:110:MET:CE	2.44	0.47
1:F:487:ASP:OD2	1:F:489:ASN:HB2	2.14	0.47
1:F:620:ARG:HG3	1:F:624:TYR:CG	2.50	0.47
1:A:8:ALA:HA	1:A:553:LEU:CD1	2.40	0.47
1:A:353:ARG:NE	1:A:369:GLU:OE2	2.43	0.47
1:A:478:PHE:CZ	1:A:519:ILE:HD12	2.49	0.47
1:A:578:MET:SD	1:A:580:PHE:CZ	3.07	0.47
1:B:222:TRP:CD1	1:B:622:LEU:HD23	2.50	0.47
1:C:7:ASN:O	1:C:8:ALA:C	2.51	0.47
1:C:154:ALA:O	1:C:157:ALA:HB3	2.15	0.47
1:C:156:SER:O	1:C:157:ALA:C	2.58	0.47
1:C:262:TYR:OH	1:C:370:HIS:NE2	2.32	0.47
1:D:170:PHE:HD1	1:D:170:PHE:HA	1.53	0.47
1:D:623:GLY:O	1:D:626:LEU:N	2.39	0.47
1:E:45:ILE:C	1:E:94:LYS:HD3	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:LEU:HA	1:E:65:LEU:HD12	1.72	0.47
1:E:108:GLU:HA	1:E:108:GLU:OE1	2.13	0.47
1:E:150:VAL:CG2	1:E:168:VAL:HG12	2.42	0.47
1:E:300:ILE:HD11	1:E:390:ILE:HG22	1.95	0.47
1:E:620:ARG:HG3	1:E:624:TYR:CG	2.50	0.47
1:F:5:THR:HG22	1:F:6:GLY:O	2.14	0.47
1:F:8:ALA:HA	1:F:553:LEU:CD1	2.40	0.47
1:F:123:VAL:CG1	1:F:134:LEU:HD21	2.43	0.47
1:A:403:HIS:O	1:A:404:ASP:C	2.57	0.46
1:A:564:ILE:HB	1:A:565:PRO:HD2	1.96	0.46
1:B:123:VAL:CG1	1:B:134:LEU:HD21	2.43	0.46
1:B:154:ALA:HB1	1:B:448:ILE:HG21	1.97	0.46
1:C:222:TRP:CD1	1:C:622:LEU:CD2	2.98	0.46
1:C:366:GLY:O	1:C:367:VAL:C	2.57	0.46
1:C:399:PRO:HA	1:C:400:PRO:HD3	1.59	0.46
1:D:620:ARG:HG3	1:D:624:TYR:CG	2.50	0.46
1:E:86:LEU:HD21	1:E:90:LEU:HD22	1.97	0.46
1:E:555:LEU:O	1:E:556:SER:C	2.54	0.46
1:E:623:GLY:O	1:E:626:LEU:N	2.39	0.46
1:F:222:TRP:CD1	1:F:622:LEU:CD2	2.98	0.46
1:F:337:VAL:HG13	1:F:338:GLN:N	2.25	0.46
1:F:564:ILE:HB	1:F:565:PRO:HD2	1.96	0.46
1:F:614:GLU:H	1:F:614:GLU:HG3	1.15	0.46
1:A:295:ARG:HH11	1:A:295:ARG:HD2	1.31	0.46
1:A:555:LEU:O	1:A:556:SER:C	2.54	0.46
1:B:42:ASP:O	1:B:45:ILE:HG12	2.16	0.46
1:B:170:PHE:HD1	1:B:170:PHE:HA	1.53	0.46
1:B:317:GLN:CB	1:B:318:PRO:HD2	2.36	0.46
1:B:374:ALA:C	1:B:376:ARG:H	2.21	0.46
1:B:392:LYS:HA	1:B:395:THR:HB	1.96	0.46
1:B:586:VAL:O	1:B:641:ASN:HB2	2.15	0.46
1:C:40:LEU:HD12	1:C:40:LEU:HA	1.52	0.46
1:E:190:MET:HG3	1:E:568:MET:HE2	1.96	0.46
1:E:222:TRP:CD1	1:E:622:LEU:CD2	2.98	0.46
1:F:222:TRP:CD1	1:F:622:LEU:HD23	2.50	0.46
1:A:279:ASP:OD1	1:A:286:VAL:N	2.42	0.46
1:B:544:ASP:O	1:B:547:VAL:HG23	2.14	0.46
1:C:222:TRP:CD1	1:C:622:LEU:HD23	2.50	0.46
1:C:300:ILE:HD11	1:C:390:ILE:HG22	1.95	0.46
1:D:465:THR:O	1:D:466:MET:HB3	2.12	0.46
1:E:42:ASP:O	1:E:45:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:THR:HG22	1:E:268:PHE:CD2	2.51	0.46
1:E:353:ARG:NE	1:E:369:GLU:OE2	2.43	0.46
1:E:487:ASP:OD2	1:E:489:ASN:HB2	2.14	0.46
1:F:537:GLN:O	1:F:538:SER:C	2.59	0.46
1:A:62:ASP:O	1:A:63:HIS:C	2.57	0.46
1:B:156:SER:O	1:B:157:ALA:C	2.58	0.46
1:B:260:THR:HG22	1:B:268:PHE:CD2	2.51	0.46
1:C:42:ASP:O	1:C:45:ILE:HG12	2.16	0.46
1:C:80:ARG:HH11	1:C:80:ARG:HD2	1.24	0.46
1:C:405:ASN:HD22	1:C:405:ASN:HA	1.45	0.46
1:D:642:ILE:HD13	1:D:642:ILE:HG21	1.63	0.46
1:E:16:HIS:HB3	1:E:30:LEU:CD1	2.46	0.46
1:E:48:ASP:C	1:E:50:GLY:N	2.69	0.46
1:E:487:ASP:O	1:E:488:ASN:CB	2.62	0.46
1:F:30:LEU:HA	1:F:30:LEU:HD23	1.55	0.46
1:F:642:ILE:HG21	1:F:642:ILE:HD13	1.63	0.46
1:A:150:VAL:CG2	1:A:168:VAL:HG12	2.42	0.46
1:A:262:TYR:OH	1:A:370:HIS:NE2	2.32	0.46
1:A:315:ILE:HG13	1:A:315:ILE:O	2.15	0.46
1:A:414:ASN:HD21	1:A:467:SER:N	2.10	0.46
1:B:16:HIS:HB3	1:B:30:LEU:CD1	2.46	0.46
1:B:62:ASP:HB2	1:B:64:ARG:HG2	1.97	0.46
1:C:197:TRP:CD1	1:C:223:VAL:HG21	2.50	0.46
1:D:45:ILE:C	1:D:94:LYS:HD3	2.40	0.46
1:D:222:TRP:CD1	1:D:622:LEU:CD2	2.98	0.46
1:D:441:GLU:C	1:D:443:ILE:H	2.18	0.46
1:D:540:LYS:O	1:D:541:GLU:C	2.58	0.46
1:F:62:ASP:HB2	1:F:64:ARG:HG2	1.97	0.46
1:F:154:ALA:HB1	1:F:448:ILE:HG21	1.97	0.46
1:F:175:LYS:O	1:F:176:ASN:CB	2.60	0.46
1:A:86:LEU:HD21	1:A:90:LEU:HD22	1.98	0.46
1:A:470:ASN:CG	1:A:474:ARG:HD3	2.41	0.46
1:D:48:ASP:C	1:D:50:GLY:N	2.70	0.46
1:D:127:LYS:HZ1	1:D:211:TYR:HE2	1.63	0.46
1:D:586:VAL:O	1:D:641:ASN:HB2	2.15	0.46
1:E:62:ASP:O	1:E:63:HIS:C	2.57	0.46
1:E:156:SER:O	1:E:157:ALA:C	2.58	0.46
1:E:470:ASN:CG	1:E:474:ARG:HD3	2.41	0.46
1:F:260:THR:HG22	1:F:268:PHE:CD2	2.51	0.46
1:A:417:ALA:O	1:A:463:LYS:N	2.37	0.46
1:A:591:LYS:HB2	1:A:591:LYS:HZ2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ASN:ND2	1:A:641:ASN:H	2.14	0.46
1:B:20:LYS:HZ1	1:B:20:LYS:HG3	1.73	0.46
1:B:62:ASP:O	1:B:63:HIS:C	2.57	0.46
1:C:9:GLN:O	1:C:10:LYS:C	2.58	0.46
1:D:12:GLN:HA	1:D:15:ASN:HD22	1.81	0.46
1:D:16:HIS:HB3	1:D:30:LEU:CD1	2.46	0.46
1:D:197:TRP:CD1	1:D:223:VAL:HG21	2.50	0.46
1:D:222:TRP:CD1	1:D:622:LEU:HD23	2.50	0.46
1:D:458:ASN:O	1:D:459:GLU:C	2.56	0.46
1:E:451:ARG:HH11	1:E:451:ARG:HD3	1.47	0.46
1:F:42:ASP:O	1:F:45:ILE:HG12	2.16	0.46
1:A:16:HIS:HB3	1:A:30:LEU:CD1	2.46	0.46
1:A:42:ASP:O	1:A:45:ILE:HG12	2.16	0.46
1:A:260:THR:HG22	1:A:268:PHE:CD2	2.51	0.46
1:A:620:ARG:HG3	1:A:624:TYR:CG	2.50	0.46
1:B:469:ASN:HD22	1:B:469:ASN:HA	1.40	0.46
1:C:315:ILE:O	1:C:315:ILE:HG13	2.15	0.46
1:C:470:ASN:CG	1:C:474:ARG:HD3	2.41	0.46
1:C:512:VAL:HA	1:C:513:PRO:HD2	1.59	0.46
1:D:42:ASP:O	1:D:45:ILE:HG12	2.16	0.46
1:D:271:ARG:HA	1:D:272:PRO:HD3	1.69	0.46
1:F:366:GLY:O	1:F:367:VAL:C	2.57	0.46
1:A:9:GLN:O	1:A:10:LYS:C	2.58	0.46
1:A:156:SER:O	1:A:157:ALA:C	2.58	0.46
1:A:159:MET:HE1	1:B:155:TYR:CD1	2.51	0.46
1:A:197:TRP:CD1	1:A:223:VAL:HG21	2.50	0.46
1:A:419:ASP:HB2	1:A:463:LYS:HZ2	1.81	0.46
1:B:154:ALA:O	1:B:157:ALA:HB3	2.15	0.46
1:B:408:PHE:CD1	1:B:588:ASP:HB2	2.51	0.46
1:B:433:LEU:HD23	1:B:433:LEU:HA	1.56	0.46
1:B:470:ASN:CG	1:B:474:ARG:HD3	2.41	0.46
1:C:12:GLN:HA	1:C:15:ASN:HD22	1.81	0.46
1:C:16:HIS:HB3	1:C:30:LEU:CD1	2.46	0.46
1:C:275:ILE:HG21	1:C:275:ILE:HD13	1.54	0.46
1:C:408:PHE:CD1	1:C:588:ASP:HB2	2.51	0.46
1:D:260:THR:HG22	1:D:268:PHE:CD2	2.51	0.46
1:E:13:ASP:OD1	1:E:100:ARG:NE	2.43	0.46
1:E:99:PHE:O	1:E:100:ARG:C	2.59	0.46
1:E:154:ALA:O	1:E:157:ALA:HB3	2.15	0.46
1:E:239:TRP:HH2	1:E:574:LYS:HE3	1.81	0.46
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ALA:HB1	1:A:448:ILE:HG21	1.97	0.46
1:A:222:TRP:CD1	1:A:622:LEU:CD2	2.98	0.46
1:A:592:ASP:O	1:A:594:GLU:N	2.45	0.46
1:B:29:ASP:O	1:B:30:LEU:C	2.59	0.46
1:B:86:LEU:HD21	1:B:90:LEU:HD22	1.97	0.46
1:B:127:LYS:HZ1	1:B:211:TYR:HE2	1.64	0.46
1:B:251:ILE:H	1:B:251:ILE:HG12	1.45	0.46
1:B:315:ILE:O	1:B:315:ILE:HG13	2.15	0.46
1:C:465:THR:O	1:C:466:MET:HB3	2.12	0.46
1:C:620:ARG:HG3	1:C:624:TYR:CG	2.50	0.46
1:D:99:PHE:O	1:D:100:ARG:C	2.59	0.46
1:D:154:ALA:HB1	1:D:448:ILE:HG21	1.97	0.46
1:D:222:TRP:O	1:D:223:VAL:C	2.59	0.46
1:D:275:ILE:HG21	1:D:275:ILE:HD13	1.54	0.46
1:D:451:ARG:HH11	1:D:451:ARG:HD3	1.47	0.46
1:E:9:GLN:O	1:E:10:LYS:C	2.58	0.46
1:E:197:TRP:CD1	1:E:223:VAL:HG21	2.50	0.46
1:E:219:LEU:HD12	1:E:219:LEU:HA	1.81	0.46
1:F:16:HIS:HB3	1:F:30:LEU:CD1	2.46	0.46
1:A:199:MET:HE3	4:A:774:HOH:O	2.16	0.45
1:B:140:ILE:C	1:B:141:THR:HG23	2.42	0.45
1:B:222:TRP:O	1:B:223:VAL:C	2.59	0.45
1:C:154:ALA:HB1	1:C:448:ILE:HG21	1.97	0.45
1:C:239:TRP:HH2	1:C:574:LYS:HE3	1.81	0.45
1:D:417:ALA:O	1:D:463:LYS:N	2.37	0.45
1:D:470:ASN:CG	1:D:474:ARG:HD3	2.41	0.45
1:E:32:ASP:O	1:E:36:ASN:HB2	2.16	0.45
1:E:238:ASN:C	1:E:240:LEU:N	2.73	0.45
1:F:12:GLN:HA	1:F:15:ASN:HD22	1.81	0.45
1:F:403:HIS:O	1:F:404:ASP:C	2.57	0.45
1:F:528:VAL:H	1:F:528:VAL:HG13	1.51	0.45
1:F:543:ALA:O	1:F:547:VAL:HG22	2.16	0.45
1:A:192:ILE:HA	1:A:192:ILE:HD13	1.48	0.45
1:A:408:PHE:CD1	1:A:588:ASP:HB2	2.51	0.45
1:A:543:ALA:O	1:A:547:VAL:HG22	2.16	0.45
1:B:32:ASP:O	1:B:36:ASN:HB2	2.16	0.45
1:B:577:GLY:CA	1:B:650:VAL:HG13	2.47	0.45
1:C:48:ASP:C	1:C:50:GLY:N	2.69	0.45
1:C:233:PHE:O	1:C:234:GLU:C	2.59	0.45
1:C:279:ASP:OD1	1:C:286:VAL:N	2.42	0.45
1:C:366:GLY:N	1:C:369:GLU:HG3	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:ARG:HH11	1:D:567:ARG:HD3	1.42	0.45
1:D:577:GLY:CA	1:D:650:VAL:HG13	2.47	0.45
1:D:641:ASN:ND2	1:D:641:ASN:H	2.14	0.45
1:E:12:GLN:HA	1:E:15:ASN:HD22	1.81	0.45
1:E:29:ASP:O	1:E:30:LEU:C	2.59	0.45
1:E:275:ILE:HG21	1:E:275:ILE:HD13	1.54	0.45
1:E:414:ASN:HD21	1:E:467:SER:N	2.10	0.45
1:A:68:GLN:HB3	1:A:69:ARG:HH11	1.82	0.45
1:A:99:PHE:O	1:A:100:ARG:C	2.59	0.45
1:A:577:GLY:CA	1:A:650:VAL:HG13	2.47	0.45
1:B:80:ARG:HH11	1:B:80:ARG:HD2	1.24	0.45
1:B:222:TRP:CD1	1:B:622:LEU:CD2	2.98	0.45
1:C:105:TYR:O	1:C:109:ARG:NE	2.46	0.45
1:C:224:HIS:O	1:C:228:THR:OG1	2.30	0.45
1:D:86:LEU:HD21	1:D:90:LEU:HD22	1.98	0.45
1:F:127:LYS:H	1:F:127:LYS:HG2	0.97	0.45
1:F:154:ALA:O	1:F:157:ALA:HB3	2.15	0.45
1:F:224:HIS:O	1:F:228:THR:OG1	2.30	0.45
1:F:238:ASN:C	1:F:240:LEU:N	2.73	0.45
1:F:470:ASN:CG	1:F:474:ARG:HD3	2.41	0.45
1:A:32:ASP:O	1:A:36:ASN:HB2	2.16	0.45
1:A:238:ASN:C	1:A:240:LEU:N	2.73	0.45
1:A:251:ILE:H	1:A:251:ILE:HG12	1.45	0.45
1:A:272:PRO:HG2	1:B:272:PRO:HG2	1.99	0.45
1:A:423:ILE:HG23	1:A:458:ASN:CG	2.41	0.45
1:B:30:LEU:HD23	1:B:30:LEU:HA	1.55	0.45
1:D:32:ASP:O	1:D:36:ASN:HB2	2.16	0.45
1:D:68:GLN:HB3	1:D:69:ARG:HH11	1.81	0.45
1:D:543:ALA:O	1:D:547:VAL:HG22	2.16	0.45
1:E:127:LYS:HZ1	1:E:211:TYR:HE2	1.63	0.45
1:E:132:ILE:H	1:E:132:ILE:HG13	1.46	0.45
1:E:408:PHE:CD1	1:E:588:ASP:HB2	2.51	0.45
1:F:239:TRP:CZ3	1:F:574:LYS:NZ	2.79	0.45
1:F:577:GLY:CA	1:F:650:VAL:HG13	2.47	0.45
1:A:411:MET:SD	1:A:411:MET:N	2.83	0.45
1:A:537:GLN:O	1:A:538:SER:C	2.59	0.45
1:A:567:ARG:HH11	1:A:567:ARG:HD3	1.42	0.45
1:B:27:TYR:HA	1:B:28:PRO:HD2	1.60	0.45
1:C:32:ASP:HB2	1:C:36:ASN:ND2	2.32	0.45
1:C:106:PHE:O	1:C:108:GLU:N	2.50	0.45
1:C:140:ILE:C	1:C:141:THR:HG23	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:ARG:HA	1:C:272:PRO:HD3	1.69	0.45
1:D:360:LYS:HE3	1:E:273:ASP:OD2	2.16	0.45
1:D:411:MET:N	1:D:411:MET:SD	2.83	0.45
1:D:537:GLN:O	1:D:538:SER:C	2.59	0.45
1:E:78:ARG:HD3	1:E:78:ARG:HH11	1.31	0.45
1:A:12:GLN:HA	1:A:15:ASN:HD22	1.81	0.45
1:A:127:LYS:HZ1	1:A:211:TYR:HE2	1.63	0.45
1:D:39:PRO:HB2	1:D:53:VAL:CG1	2.47	0.45
1:D:106:PHE:O	1:D:108:GLU:N	2.50	0.45
1:D:159:MET:HE1	1:E:155:TYR:CE1	2.52	0.45
1:D:437:VAL:H	1:D:437:VAL:HG22	1.44	0.45
1:E:423:ILE:HG23	1:E:458:ASN:CG	2.41	0.45
1:E:543:ALA:O	1:E:547:VAL:HG22	2.16	0.45
1:F:40:LEU:HD12	1:F:40:LEU:HA	1.52	0.45
1:F:275:ILE:HD13	1:F:275:ILE:HG21	1.54	0.45
1:B:12:GLN:HA	1:B:15:ASN:HD22	1.81	0.45
1:B:478:PHE:CZ	1:B:519:ILE:CD1	3.00	0.45
1:B:495:LEU:HD13	1:B:583:TYR:OH	2.17	0.45
1:C:260:THR:HG22	1:C:268:PHE:CD2	2.51	0.45
1:C:533:MET:HB3	1:C:534:PRO:CD	2.43	0.45
1:D:580:PHE:HD2	1:D:649:ILE:HG13	1.82	0.45
1:E:105:TYR:O	1:E:109:ARG:NE	2.46	0.45
1:F:32:ASP:HB2	1:F:36:ASN:ND2	2.32	0.45
1:F:192:ILE:HD12	1:F:192:ILE:HG23	1.72	0.45
1:A:311:HIS:HD2	1:A:311:HIS:HA	1.65	0.45
1:A:533:MET:HB3	1:A:534:PRO:CD	2.43	0.45
1:B:543:ALA:O	1:B:547:VAL:HG22	2.16	0.45
1:B:641:ASN:ND2	1:B:641:ASN:H	2.14	0.45
1:C:177:ARG:HE	1:C:177:ARG:HB3	1.41	0.45
1:C:423:ILE:HG23	1:C:458:ASN:CG	2.41	0.45
1:D:478:PHE:CZ	1:D:519:ILE:CD1	3.00	0.45
1:E:127:LYS:H	1:E:127:LYS:HG2	0.97	0.45
1:E:512:VAL:HA	1:E:513:PRO:HD2	1.59	0.45
1:F:86:LEU:HD21	1:F:90:LEU:HD22	1.98	0.45
1:F:106:PHE:O	1:F:108:GLU:N	2.50	0.45
1:F:156:SER:O	1:F:157:ALA:C	2.58	0.45
1:A:39:PRO:HB2	1:A:53:VAL:CG1	2.47	0.45
1:A:111:ASN:C	1:A:111:ASN:OD1	2.59	0.45
1:C:32:ASP:O	1:C:36:ASN:HB2	2.16	0.45
1:C:68:GLN:HB3	1:C:69:ARG:HH11	1.81	0.45
1:C:238:ASN:C	1:C:240:LEU:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ILE:CD1	1:D:175:LYS:O	2.63	0.45
1:C:576:GLU:HG3	1:C:576:GLU:H	1.20	0.45
1:C:577:GLY:CA	1:C:650:VAL:HG13	2.47	0.45
1:D:238:ASN:C	1:D:240:LEU:N	2.73	0.45
1:D:239:TRP:CZ3	1:D:574:LYS:NZ	2.79	0.45
1:D:632:ASP:C	1:D:634:ARG:N	2.73	0.45
1:E:106:PHE:O	1:E:108:GLU:N	2.50	0.45
1:E:224:HIS:O	1:E:228:THR:OG1	2.30	0.45
1:E:537:GLN:O	1:E:538:SER:C	2.59	0.45
1:E:567:ARG:HH11	1:E:567:ARG:HD3	1.42	0.45
1:F:32:ASP:O	1:F:36:ASN:HB2	2.16	0.45
1:F:78:ARG:HD3	1:F:78:ARG:HH11	1.31	0.45
1:F:405:ASN:HD22	1:F:405:ASN:HA	1.45	0.45
1:F:408:PHE:CD1	1:F:588:ASP:HB2	2.51	0.45
1:F:487:ASP:O	1:F:488:ASN:CB	2.62	0.45
1:A:301:ASP:CB	1:C:295:ARG:NH2	2.80	0.45
1:B:316:ARG:HH21	1:D:338:GLN:NE2	2.15	0.45
1:B:576:GLU:HG3	1:B:576:GLU:H	1.20	0.45
1:C:39:PRO:HB2	1:C:53:VAL:CG1	2.47	0.45
1:C:192:ILE:HD13	1:C:192:ILE:HA	1.48	0.45
1:D:139:GLN:OE1	1:D:536:PHE:N	2.40	0.45
1:E:10:LYS:HA	1:E:96:TRP:CE2	2.52	0.45
1:F:111:ASN:C	1:F:111:ASN:OD1	2.59	0.45
1:F:533:MET:HB3	1:F:534:PRO:CD	2.43	0.45
1:A:139:GLN:OE1	1:A:536:PHE:N	2.40	0.44
1:A:192:ILE:HG23	1:A:192:ILE:HD12	1.72	0.44
1:B:105:TYR:O	1:B:109:ARG:NE	2.46	0.44
1:B:414:ASN:HD21	1:B:467:SER:N	2.10	0.44
1:B:555:LEU:O	1:B:556:SER:C	2.54	0.44
1:B:630:ILE:HG21	1:B:630:ILE:HD13	1.71	0.44
1:C:111:ASN:C	1:C:111:ASN:OD1	2.60	0.44
1:C:115:PHE:O	1:C:116:VAL:C	2.57	0.44
1:C:123:VAL:CG1	1:C:134:LEU:HD21	2.43	0.44
1:E:39:PRO:HB2	1:E:53:VAL:CG1	2.47	0.44
1:E:222:TRP:O	1:E:223:VAL:C	2.59	0.44
1:E:469:ASN:HD22	1:E:469:ASN:HA	1.40	0.44
1:E:580:PHE:HD2	1:E:649:ILE:HG13	1.82	0.44
1:A:56:LEU:HD21	1:A:110:MET:CE	2.44	0.44
1:A:106:PHE:O	1:A:108:GLU:N	2.50	0.44
1:A:296:ILE:HA	1:A:296:ILE:HD13	1.38	0.44
1:B:39:PRO:HB2	1:B:53:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:PRO:HA	1:B:400:PRO:HD3	1.59	0.44
1:B:423:ILE:HG23	1:B:458:ASN:CG	2.41	0.44
1:B:537:GLN:O	1:B:538:SER:C	2.59	0.44
1:C:27:TYR:HA	1:C:28:PRO:HD2	1.60	0.44
1:C:580:PHE:HD2	1:C:649:ILE:HG13	1.82	0.44
1:C:592:ASP:O	1:C:619:ASN:ND2	2.40	0.44
1:D:50:GLY:C	1:D:53:VAL:HG23	2.43	0.44
1:D:156:SER:O	1:D:157:ALA:C	2.58	0.44
1:D:295:ARG:HH11	1:D:295:ARG:HD2	1.31	0.44
1:E:123:VAL:CG1	1:E:134:LEU:HD21	2.43	0.44
1:E:239:TRP:CZ3	1:E:574:LYS:NZ	2.79	0.44
1:F:150:VAL:CG2	1:F:168:VAL:HG12	2.42	0.44
1:F:641:ASN:ND2	1:F:641:ASN:H	2.14	0.44
1:A:40:LEU:HA	1:A:40:LEU:HD12	1.52	0.44
1:A:338:GLN:HE22	1:E:316:ARG:HE	1.65	0.44
1:A:447:GLU:HG3	4:A:726:HOH:O	2.16	0.44
1:A:653:LEU:HD12	1:A:653:LEU:HA	1.47	0.44
1:B:291:ILE:HD12	1:B:291:ILE:HG21	1.77	0.44
1:D:27:TYR:HA	1:D:28:PRO:HD2	1.60	0.44
1:D:495:LEU:HD13	1:D:583:TYR:OH	2.17	0.44
1:E:11:GLN:HE21	1:E:11:GLN:HB2	1.21	0.44
1:E:239:TRP:CH2	1:E:574:LYS:CE	3.01	0.44
1:E:577:GLY:CA	1:E:650:VAL:HG13	2.47	0.44
1:F:9:GLN:O	1:F:10:LYS:C	2.58	0.44
1:F:423:ILE:HG23	1:F:458:ASN:CG	2.41	0.44
1:B:139:GLN:OE1	1:B:536:PHE:N	2.40	0.44
1:B:150:VAL:CG2	1:B:168:VAL:HG12	2.42	0.44
1:C:543:ALA:O	1:C:547:VAL:HG22	2.16	0.44
1:E:592:ASP:O	1:E:619:ASN:ND2	2.41	0.44
1:A:10:LYS:HA	1:A:96:TRP:CE2	2.52	0.44
1:A:50:GLY:C	1:A:53:VAL:HG23	2.43	0.44
1:B:68:GLN:HB3	1:B:69:ARG:HH11	1.81	0.44
1:B:106:PHE:O	1:B:108:GLU:N	2.50	0.44
1:B:307:ASP:CG	1:B:311:HIS:HB2	2.43	0.44
1:B:624:TYR:HA	1:B:625:PRO:HA	1.77	0.44
1:B:642:ILE:HG21	1:B:642:ILE:HD13	1.63	0.44
1:C:491:ILE:HD13	1:D:175:LYS:HB2	1.92	0.44
1:D:78:ARG:HD3	1:D:78:ARG:HH11	1.31	0.44
1:D:111:ASN:OD1	1:D:111:ASN:C	2.59	0.44
1:D:318:PRO:C	1:D:320:GLY:H	2.23	0.44
1:D:408:PHE:CD1	1:D:588:ASP:HB2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:ILE:HG23	1:D:458:ASN:CG	2.41	0.44
1:E:139:GLN:OE1	1:E:536:PHE:N	2.40	0.44
1:E:478:PHE:CZ	1:E:519:ILE:CD1	3.00	0.44
1:E:614:GLU:H	1:E:614:GLU:HG3	1.15	0.44
1:F:39:PRO:HB2	1:F:53:VAL:CG1	2.47	0.44
1:F:386:TYR:O	1:F:387:MET:C	2.61	0.44
1:A:43:THR:O	1:A:44:SER:CB	2.63	0.44
1:A:48:ASP:C	1:A:50:GLY:N	2.69	0.44
1:A:155:TYR:CD1	1:B:159:MET:HE1	2.52	0.44
1:A:173:THR:O	1:A:176:ASN:HB2	2.18	0.44
1:A:399:PRO:HA	1:A:400:PRO:HD3	1.59	0.44
1:B:465:THR:O	1:B:466:MET:HB3	2.12	0.44
1:D:553:LEU:HA	1:D:553:LEU:HD23	1.55	0.44
1:E:173:THR:O	1:E:176:ASN:HB2	2.18	0.44
1:F:10:LYS:HA	1:F:96:TRP:CE2	2.53	0.44
1:F:29:ASP:O	1:F:30:LEU:C	2.59	0.44
1:F:68:GLN:HB3	1:F:69:ARG:HH11	1.82	0.44
1:F:580:PHE:HD2	1:F:649:ILE:HG13	1.82	0.44
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.55	0.44
1:A:115:PHE:O	1:A:116:VAL:C	2.57	0.44
1:A:478:PHE:CZ	1:A:519:ILE:CD1	3.00	0.44
1:B:111:ASN:OD1	1:B:111:ASN:C	2.59	0.44
1:B:238:ASN:C	1:B:240:LEU:N	2.73	0.44
1:B:634:ARG:HG2	1:B:634:ARG:NH1	2.14	0.44
1:C:10:LYS:HA	1:C:96:TRP:CE2	2.52	0.44
1:C:50:GLY:C	1:C:53:VAL:HG23	2.43	0.44
1:C:99:PHE:O	1:C:100:ARG:C	2.59	0.44
1:C:173:THR:O	1:C:176:ASN:HB2	2.18	0.44
1:C:222:TRP:O	1:C:223:VAL:C	2.59	0.44
1:C:495:LEU:HD13	1:C:583:TYR:OH	2.17	0.44
1:D:10:LYS:HA	1:D:96:TRP:CE2	2.53	0.44
1:D:178:GLU:O	1:D:178:GLU:HG3	2.18	0.44
1:E:56:LEU:HD21	1:E:110:MET:CE	2.44	0.44
1:E:68:GLN:HB3	1:E:69:ARG:HH11	1.82	0.44
1:E:295:ARG:NE	1:E:339:TYR:CE1	2.86	0.44
1:E:632:ASP:C	1:E:634:ARG:N	2.73	0.44
1:F:495:LEU:HD13	1:F:583:TYR:OH	2.17	0.44
1:A:239:TRP:CH2	1:A:574:LYS:CE	3.01	0.44
1:A:513:PRO:CG	1:A:517:GLU:HB2	2.27	0.44
1:B:50:GLY:C	1:B:53:VAL:HG23	2.43	0.44
1:B:405:ASN:HD22	1:B:405:ASN:HA	1.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:GLN:O	1:D:10:LYS:C	2.58	0.44
1:D:127:LYS:H	1:D:127:LYS:HG2	0.97	0.44
1:D:256:PHE:HA	1:E:361:PHE:CE1	2.52	0.44
1:E:111:ASN:C	1:E:111:ASN:OD1	2.60	0.44
1:E:275:ILE:HG23	1:E:276:HIS:N	2.33	0.44
1:E:411:MET:SD	1:E:411:MET:N	2.83	0.44
1:E:433:LEU:HD23	1:E:433:LEU:HA	1.55	0.44
1:E:487:ASP:C	1:E:489:ASN:H	2.26	0.44
1:F:115:PHE:O	1:F:116:VAL:C	2.57	0.44
1:F:178:GLU:O	1:F:178:GLU:HG3	2.18	0.44
1:F:222:TRP:O	1:F:223:VAL:C	2.59	0.44
1:F:239:TRP:CH2	1:F:574:LYS:CE	3.00	0.44
1:F:478:PHE:CZ	1:F:519:ILE:CD1	3.00	0.44
1:F:513:PRO:CG	1:F:517:GLU:HB2	2.27	0.44
1:A:32:ASP:HB2	1:A:36:ASN:ND2	2.32	0.44
1:A:487:ASP:C	1:A:489:ASN:H	2.26	0.44
1:B:239:TRP:CH2	1:B:574:LYS:CE	3.01	0.44
1:B:318:PRO:C	1:B:320:GLY:N	2.74	0.44
1:B:624:TYR:CD1	1:B:624:TYR:C	2.96	0.44
1:C:275:ILE:HG23	1:C:276:HIS:N	2.33	0.44
1:C:478:PHE:CZ	1:C:519:ILE:CD1	3.00	0.44
1:D:177:ARG:CG	1:E:360:LYS:HB3	2.48	0.44
1:D:296:ILE:HD12	1:D:296:ILE:HG23	1.42	0.44
1:A:483:CYS:HB3	4:A:763:HOH:O	2.18	0.43
1:A:495:LEU:HD13	1:A:583:TYR:OH	2.17	0.43
1:B:99:PHE:O	1:B:100:ARG:C	2.59	0.43
1:B:178:GLU:HG3	1:B:178:GLU:O	2.18	0.43
1:C:48:ASP:OD1	1:C:92:GLN:HG3	2.18	0.43
1:C:295:ARG:NE	1:C:339:TYR:CE1	2.86	0.43
1:C:300:ILE:H	1:C:300:ILE:HG13	1.60	0.43
1:C:641:ASN:ND2	1:C:641:ASN:H	2.14	0.43
1:D:494:THR:O	1:D:495:LEU:C	2.61	0.43
1:E:495:LEU:HD13	1:E:583:TYR:OH	2.17	0.43
1:E:624:TYR:HA	1:E:625:PRO:HA	1.77	0.43
1:F:239:TRP:HZ3	1:F:574:LYS:HZ2	1.59	0.43
1:F:295:ARG:NE	1:F:339:TYR:CE1	2.86	0.43
1:F:345:ASN:O	1:F:346:THR:C	2.60	0.43
1:F:494:THR:O	1:F:495:LEU:C	2.61	0.43
1:A:211:TYR:CE1	1:A:612:HIS:HA	2.53	0.43
1:A:318:PRO:C	1:A:320:GLY:N	2.73	0.43
1:B:10:LYS:HA	1:B:96:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASP:HB2	1:B:36:ASN:ND2	2.32	0.43
1:B:40:LEU:HA	1:B:40:LEU:HD12	1.52	0.43
1:B:386:TYR:O	1:B:387:MET:C	2.61	0.43
1:B:425:PHE:C	1:B:425:PHE:CD1	2.96	0.43
1:C:78:ARG:HD3	1:C:78:ARG:HH11	1.32	0.43
1:C:215:ARG:NE	1:C:218:GLU:OE2	2.45	0.43
1:C:307:ASP:CG	1:C:311:HIS:HB2	2.43	0.43
1:C:386:TYR:O	1:C:387:MET:C	2.61	0.43
1:C:425:PHE:CD1	1:C:425:PHE:C	2.97	0.43
1:C:624:TYR:CD1	1:C:624:TYR:C	2.96	0.43
1:D:48:ASP:OD1	1:D:92:GLN:HG3	2.18	0.43
1:F:48:ASP:OD1	1:F:92:GLN:HG3	2.18	0.43
1:A:105:TYR:O	1:A:109:ARG:NE	2.46	0.43
1:A:136:PRO:O	1:A:137:LEU:C	2.61	0.43
1:B:65:LEU:HD12	1:B:82:GLU:HG2	2.00	0.43
1:D:84:LEU:HD11	1:D:204:TRP:CD2	2.54	0.43
1:D:295:ARG:NE	1:D:339:TYR:CE1	2.86	0.43
1:D:307:ASP:CG	1:D:311:HIS:HB2	2.43	0.43
1:E:32:ASP:HB2	1:E:36:ASN:ND2	2.32	0.43
1:E:48:ASP:OD1	1:E:92:GLN:HG3	2.18	0.43
1:E:65:LEU:HD12	1:E:82:GLU:HG2	2.00	0.43
1:E:211:TYR:CE1	1:E:612:HIS:HA	2.53	0.43
1:E:271:ARG:HA	1:E:272:PRO:HD3	1.69	0.43
1:E:624:TYR:CD1	1:E:624:TYR:C	2.96	0.43
1:E:641:ASN:ND2	1:E:641:ASN:H	2.14	0.43
1:F:50:GLY:C	1:F:53:VAL:HG23	2.43	0.43
1:F:624:TYR:CD1	1:F:624:TYR:C	2.96	0.43
1:A:300:ILE:HG12	1:A:324:LEU:CD1	2.48	0.43
1:B:132:ILE:H	1:B:132:ILE:HG13	1.46	0.43
1:C:66:LEU:HD21	1:C:70:HIS:ND1	2.34	0.43
1:C:312:THR:O	1:C:312:THR:OG1	2.33	0.43
1:C:494:THR:O	1:C:495:LEU:C	2.61	0.43
1:D:239:TRP:CH2	1:D:574:LYS:CE	3.01	0.43
1:E:50:GLY:C	1:E:53:VAL:HG23	2.43	0.43
1:F:551:HIS:CD2	1:F:552:ASP:CA	2.99	0.43
1:F:591:LYS:HB2	1:F:591:LYS:HZ3	1.83	0.43
1:A:106:PHE:O	1:A:109:ARG:N	2.43	0.43
1:A:275:ILE:HG23	1:A:276:HIS:N	2.33	0.43
1:A:386:TYR:CE1	4:A:861:HOH:O	2.72	0.43
1:A:469:ASN:HD22	1:A:469:ASN:HA	1.40	0.43
1:A:576:GLU:HG3	1:A:576:GLU:H	1.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:PHE:HD2	1:A:649:ILE:HG13	1.82	0.43
1:A:642:ILE:HG21	1:A:642:ILE:HD13	1.63	0.43
1:C:239:TRP:CH2	1:C:574:LYS:CE	3.01	0.43
1:D:624:TYR:CD1	1:D:624:TYR:C	2.96	0.43
1:E:56:LEU:O	1:E:57:MET:C	2.62	0.43
1:E:494:THR:O	1:E:495:LEU:C	2.61	0.43
1:A:29:ASP:O	1:A:30:LEU:C	2.59	0.43
1:A:632:ASP:C	1:A:634:ARG:N	2.73	0.43
1:B:84:LEU:HD11	1:B:204:TRP:CD2	2.54	0.43
1:B:127:LYS:H	1:B:127:LYS:HG2	0.97	0.43
1:B:224:HIS:O	1:B:228:THR:OG1	2.30	0.43
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.82	0.43
1:C:553:LEU:HD23	1:C:553:LEU:HA	1.55	0.43
1:C:614:GLU:H	1:C:614:GLU:HG3	1.15	0.43
1:D:233:PHE:O	1:D:234:GLU:C	2.59	0.43
1:D:386:TYR:O	1:D:387:MET:C	2.61	0.43
1:E:486:GLU:HA	1:E:492:THR:H	1.84	0.43
1:F:271:ARG:NH2	1:F:377:ASP:OD2	2.52	0.43
1:A:295:ARG:NE	1:A:339:TYR:CE1	2.86	0.43
1:A:296:ILE:HG23	1:A:296:ILE:HD12	1.42	0.43
1:A:300:ILE:H	1:A:300:ILE:HG13	1.60	0.43
1:A:307:ASP:CG	1:A:311:HIS:HB2	2.43	0.43
1:A:624:TYR:CD1	1:A:624:TYR:C	2.96	0.43
1:B:494:THR:O	1:B:495:LEU:C	2.61	0.43
1:C:367:VAL:HA	1:C:373:THR:CG2	2.49	0.43
1:D:32:ASP:HB2	1:D:36:ASN:ND2	2.32	0.43
1:D:78:ARG:NH1	1:D:82:GLU:OE2	2.52	0.43
1:D:366:GLY:O	1:D:367:VAL:C	2.57	0.43
1:E:345:ASN:O	1:E:346:THR:C	2.60	0.43
1:E:399:PRO:HA	1:E:400:PRO:HD3	1.59	0.43
1:E:533:MET:HB3	1:E:534:PRO:CD	2.43	0.43
1:A:48:ASP:OD1	1:A:92:GLN:HG3	2.18	0.43
1:A:178:GLU:HG3	1:A:178:GLU:O	2.18	0.43
1:A:650:VAL:HG12	1:A:651:HIS:H	1.84	0.43
1:B:158:LYS:HD3	1:B:158:LYS:HA	1.72	0.43
1:B:173:THR:O	1:B:176:ASN:HB2	2.18	0.43
1:B:192:ILE:HA	1:B:192:ILE:HD13	1.48	0.43
1:D:86:LEU:CD2	1:D:86:LEU:C	2.92	0.43
1:D:136:PRO:O	1:D:137:LEU:C	2.61	0.43
1:D:190:MET:HG3	1:D:568:MET:CE	2.49	0.43
1:D:486:GLU:HA	1:D:492:THR:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:HIS:HD2	1:E:311:HIS:HA	1.65	0.43
1:F:65:LEU:HD12	1:F:82:GLU:HG2	2.00	0.43
1:F:239:TRP:HH2	1:F:574:LYS:HE3	1.81	0.43
1:F:469:ASN:HD22	1:F:469:ASN:HA	1.40	0.43
1:A:66:LEU:HD21	1:A:70:HIS:ND1	2.34	0.43
1:A:233:PHE:O	1:A:234:GLU:C	2.59	0.43
1:B:56:LEU:O	1:B:57:MET:C	2.62	0.43
1:B:275:ILE:HG23	1:B:276:HIS:N	2.33	0.43
1:B:295:ARG:NE	1:B:339:TYR:CE1	2.86	0.43
1:C:211:TYR:CE1	1:C:612:HIS:HA	2.53	0.43
1:C:345:ASN:O	1:C:346:THR:C	2.60	0.43
1:C:380:PHE:CD1	1:C:380:PHE:C	2.97	0.43
1:D:115:PHE:O	1:D:116:VAL:C	2.57	0.43
1:D:192:ILE:HG23	1:D:192:ILE:HD12	1.72	0.43
1:D:300:ILE:HG12	1:D:324:LEU:CD1	2.48	0.43
1:D:630:ILE:HG21	1:D:630:ILE:HD13	1.71	0.43
1:E:178:GLU:O	1:E:178:GLU:HG3	2.18	0.43
1:E:233:PHE:O	1:E:234:GLU:C	2.59	0.43
1:E:380:PHE:CD1	1:E:380:PHE:C	2.97	0.43
1:F:275:ILE:HG23	1:F:276:HIS:N	2.33	0.43
1:A:56:LEU:O	1:A:57:MET:C	2.62	0.43
1:A:65:LEU:HD12	1:A:82:GLU:HG2	2.00	0.43
1:A:405:ASN:HD22	1:A:405:ASN:HA	1.45	0.43
1:B:136:PRO:O	1:B:137:LEU:C	2.61	0.43
1:B:236:LEU:HA	1:B:236:LEU:HD12	1.83	0.43
1:B:300:ILE:H	1:B:300:ILE:HG13	1.60	0.43
1:C:65:LEU:HD12	1:C:65:LEU:HA	1.71	0.43
1:C:630:ILE:HG21	1:C:630:ILE:HD13	1.71	0.43
1:D:173:THR:O	1:D:176:ASN:HB2	2.18	0.43
1:E:136:PRO:O	1:E:137:LEU:C	2.61	0.43
1:E:307:ASP:CG	1:E:311:HIS:HB2	2.43	0.43
1:F:66:LEU:HD21	1:F:70:HIS:ND1	2.34	0.43
1:F:190:MET:HG3	1:F:568:MET:CE	2.49	0.43
1:F:291:ILE:HD12	1:F:291:ILE:HG21	1.77	0.43
1:F:307:ASP:CG	1:F:311:HIS:HB2	2.43	0.43
1:F:367:VAL:HA	1:F:373:THR:CG2	2.49	0.43
1:F:419:ASP:HB2	1:F:463:LYS:HZ2	1.84	0.43
1:A:86:LEU:CD2	1:A:86:LEU:C	2.92	0.42
1:A:123:VAL:CG1	1:A:134:LEU:HD21	2.43	0.42
1:A:367:VAL:HA	1:A:373:THR:CG2	2.49	0.42
1:A:390:ILE:HD11	4:A:861:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ILE:HD13	1:B:161:GLN:HG3	2.00	0.42
1:B:86:LEU:CD2	1:B:86:LEU:C	2.92	0.42
1:B:211:TYR:CE1	1:B:612:HIS:HA	2.53	0.42
1:B:380:PHE:CD1	1:B:380:PHE:C	2.97	0.42
1:B:650:VAL:HG12	1:B:651:HIS:H	1.84	0.42
1:C:136:PRO:O	1:C:137:LEU:C	2.61	0.42
1:C:150:VAL:CG2	1:C:168:VAL:HG12	2.41	0.42
1:C:537:GLN:O	1:C:538:SER:C	2.59	0.42
1:C:632:ASP:C	1:C:634:ARG:N	2.73	0.42
1:D:80:ARG:HH11	1:D:80:ARG:HD2	1.24	0.42
1:D:211:TYR:CE1	1:D:612:HIS:HA	2.53	0.42
1:D:215:ARG:NE	1:D:218:GLU:OE2	2.44	0.42
1:D:551:HIS:C	1:D:552:ASP:CG	2.86	0.42
1:E:70:HIS:CG	1:E:71:TRP:N	2.87	0.42
1:E:271:ARG:NH2	1:E:377:ASP:OD2	2.52	0.42
1:E:650:VAL:HG12	1:E:651:HIS:H	1.84	0.42
1:F:425:PHE:CD1	1:F:425:PHE:C	2.96	0.42
1:A:140:ILE:C	1:A:141:THR:HG23	2.41	0.42
1:A:338:GLN:HE22	1:E:316:ARG:HH21	1.66	0.42
1:A:624:TYR:HA	1:A:625:PRO:HA	1.77	0.42
1:B:9:GLN:O	1:B:10:LYS:C	2.58	0.42
1:B:291:ILE:O	1:B:292:THR:C	2.62	0.42
1:B:569:LEU:CD2	1:B:570:LEU:HD13	2.46	0.42
1:B:580:PHE:HD2	1:B:649:ILE:HG13	1.82	0.42
1:B:653:LEU:HA	1:B:653:LEU:HD12	1.46	0.42
1:C:65:LEU:HD12	1:C:82:GLU:HG2	2.00	0.42
1:C:178:GLU:O	1:C:178:GLU:HG3	2.18	0.42
1:C:329:GLU:HA	1:C:344:HIS:HB3	2.01	0.42
1:D:192:ILE:HD13	1:D:192:ILE:HA	1.48	0.42
1:D:224:HIS:O	1:D:228:THR:OG1	2.30	0.42
1:D:275:ILE:HG23	1:D:276:HIS:N	2.33	0.42
1:D:285:HIS:HB2	1:D:288:ASP:OD2	2.19	0.42
1:D:324:LEU:HD23	1:D:324:LEU:HA	1.82	0.42
1:D:576:GLU:HG3	1:D:576:GLU:H	1.20	0.42
1:E:367:VAL:HA	1:E:373:THR:CG2	2.49	0.42
1:F:173:THR:O	1:F:176:ASN:HB2	2.18	0.42
1:F:433:LEU:HD23	1:F:433:LEU:HA	1.55	0.42
1:F:623:GLY:O	1:F:626:LEU:N	2.39	0.42
1:A:271:ARG:NH2	1:A:377:ASP:OD2	2.52	0.42
1:B:39:PRO:HB2	1:B:53:VAL:HG12	2.01	0.42
1:B:65:LEU:HD12	1:B:65:LEU:HA	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:HD21	1:B:70:HIS:ND1	2.34	0.42
1:B:285:HIS:HB2	1:B:288:ASP:OD2	2.19	0.42
1:B:372:GLU:H	1:B:372:GLU:HG2	1.02	0.42
1:B:592:ASP:O	1:B:594:GLU:N	2.45	0.42
1:C:185:GLY:HA2	1:C:375:THR:HG23	2.01	0.42
1:C:495:LEU:HD13	1:C:583:TYR:CZ	2.55	0.42
1:C:634:ARG:HE	1:E:64:ARG:CZ	2.31	0.42
1:D:39:PRO:HB2	1:D:53:VAL:HG12	2.01	0.42
1:D:65:LEU:HD12	1:D:82:GLU:HG2	2.00	0.42
1:D:66:LEU:HD21	1:D:70:HIS:ND1	2.34	0.42
1:E:27:TYR:HA	1:E:28:PRO:HD2	1.60	0.42
1:E:43:THR:O	1:E:44:SER:CB	2.63	0.42
1:E:48:ASP:OD2	1:E:52:ALA:N	2.52	0.42
1:F:211:TYR:CE1	1:F:612:HIS:HA	2.53	0.42
1:F:314:ASP:OD1	1:F:316:ARG:N	2.48	0.42
1:A:345:ASN:O	1:A:346:THR:C	2.60	0.42
1:A:486:GLU:HA	1:A:492:THR:H	1.84	0.42
1:B:314:ASP:OD1	1:B:316:ARG:N	2.48	0.42
1:B:486:GLU:HA	1:B:492:THR:H	1.84	0.42
1:B:564:ILE:HG21	1:B:564:ILE:HD13	1.87	0.42
1:C:259:LEU:HD12	1:C:259:LEU:HA	1.80	0.42
1:C:515:GLY:O	1:C:516:PRO:C	2.63	0.42
1:C:650:VAL:HG12	1:C:651:HIS:H	1.84	0.42
1:D:29:ASP:O	1:D:30:LEU:C	2.59	0.42
1:D:296:ILE:HA	1:D:296:ILE:HD13	1.38	0.42
1:D:329:GLU:HA	1:D:344:HIS:HB3	2.01	0.42
1:E:425:PHE:CD1	1:E:425:PHE:C	2.96	0.42
1:F:99:PHE:O	1:F:100:ARG:C	2.59	0.42
1:F:296:ILE:HD12	1:F:296:ILE:HG23	1.42	0.42
1:A:70:HIS:CG	1:A:71:TRP:N	2.87	0.42
1:A:239:TRP:CZ3	1:A:574:LYS:NZ	2.79	0.42
1:A:256:PHE:HA	1:B:361:PHE:CE1	2.54	0.42
1:C:70:HIS:CG	1:C:71:TRP:N	2.87	0.42
1:C:143:HIS:CE1	1:C:151:ILE:HG13	2.55	0.42
1:C:324:LEU:HD23	1:C:324:LEU:HA	1.82	0.42
1:C:624:TYR:HA	1:C:625:PRO:HA	1.77	0.42
1:D:30:LEU:HA	1:D:30:LEU:HD23	1.55	0.42
1:D:105:TYR:O	1:D:109:ARG:NE	2.46	0.42
1:D:239:TRP:HH2	1:D:574:LYS:HE3	1.81	0.42
1:E:132:ILE:CG2	1:E:133:VAL:N	2.83	0.42
1:E:190:MET:HG3	1:E:568:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:495:LEU:HD13	1:E:583:TYR:CZ	2.55	0.42
1:F:185:GLY:HA2	1:F:375:THR:HG23	2.01	0.42
1:F:495:LEU:HD13	1:F:583:TYR:CZ	2.55	0.42
1:F:569:LEU:CD2	1:F:570:LEU:HD13	2.46	0.42
1:A:190:MET:HG3	1:A:568:MET:CE	2.49	0.42
1:A:337:VAL:H	1:A:337:VAL:HG12	1.70	0.42
1:A:495:LEU:HD13	1:A:583:TYR:CZ	2.55	0.42
1:A:569:LEU:CD2	1:A:570:LEU:HD13	2.46	0.42
1:B:48:ASP:OD1	1:B:92:GLN:HG3	2.18	0.42
1:B:57:MET:O	1:B:58:LYS:C	2.62	0.42
1:B:106:PHE:O	1:B:109:ARG:N	2.43	0.42
1:B:185:GLY:HA2	1:B:375:THR:HG23	2.01	0.42
1:B:195:VAL:CG2	1:B:196:THR:N	2.81	0.42
1:B:329:GLU:HA	1:B:344:HIS:HB3	2.01	0.42
1:B:515:GLY:O	1:B:516:PRO:C	2.63	0.42
1:B:632:ASP:C	1:B:634:ARG:N	2.73	0.42
1:D:318:PRO:C	1:D:320:GLY:N	2.74	0.42
1:E:78:ARG:NH1	1:E:82:GLU:OE2	2.52	0.42
1:F:285:HIS:HB2	1:F:288:ASP:OD2	2.19	0.42
1:F:318:PRO:C	1:F:320:GLY:N	2.74	0.42
1:F:329:GLU:HA	1:F:344:HIS:HB3	2.01	0.42
1:A:39:PRO:HB2	1:A:53:VAL:HG12	2.01	0.42
1:A:143:HIS:CE1	1:A:151:ILE:HG13	2.55	0.42
1:A:155:TYR:HD1	1:A:155:TYR:HA	1.74	0.42
1:B:318:PRO:C	1:B:320:GLY:H	2.23	0.42
1:C:12:GLN:NE2	1:C:544:ASP:OD1	2.52	0.42
1:C:190:MET:HG3	1:C:568:MET:CE	2.49	0.42
1:C:367:VAL:HB	1:C:373:THR:HG23	2.02	0.42
1:C:623:GLY:O	1:C:626:LEU:N	2.39	0.42
1:D:65:LEU:HD12	1:D:65:LEU:HA	1.71	0.42
1:D:132:ILE:CG2	1:D:133:VAL:N	2.83	0.42
1:D:162:LYS:HA	1:D:163:PRO:HD3	1.67	0.42
1:D:271:ARG:NH2	1:D:377:ASP:OD2	2.52	0.42
1:D:515:GLY:O	1:D:516:PRO:C	2.63	0.42
1:E:84:LEU:HD11	1:E:204:TRP:CD2	2.54	0.42
1:E:140:ILE:CG2	1:E:141:THR:HG23	2.14	0.42
1:E:318:PRO:C	1:E:320:GLY:H	2.23	0.42
1:E:386:TYR:O	1:E:387:MET:C	2.61	0.42
1:E:433:LEU:HG	1:E:450:ALA:HB2	2.02	0.42
1:F:48:ASP:OD2	1:F:52:ALA:N	2.53	0.42
1:F:65:LEU:HD12	1:F:65:LEU:HA	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:PRO:O	1:F:137:LEU:C	2.61	0.42
1:F:233:PHE:O	1:F:234:GLU:C	2.59	0.42
1:F:399:PRO:HA	1:F:400:PRO:HD3	1.59	0.42
1:F:653:LEU:HA	1:F:653:LEU:HD12	1.47	0.42
1:A:285:HIS:HB2	1:A:288:ASP:OD2	2.19	0.42
1:A:380:PHE:CD1	1:A:380:PHE:C	2.97	0.42
1:A:433:LEU:HG	1:A:450:ALA:HB2	2.02	0.42
1:A:515:GLY:O	1:A:516:PRO:C	2.62	0.42
1:B:43:THR:O	1:B:44:SER:CB	2.63	0.42
1:B:78:ARG:NH1	1:B:82:GLU:OE2	2.52	0.42
1:B:177:ARG:HE	1:B:177:ARG:HB3	1.42	0.42
1:C:486:GLU:HA	1:C:492:THR:H	1.84	0.42
1:E:244:ASP:OD1	1:E:382:ARG:NH1	2.53	0.42
1:E:285:HIS:HB2	1:E:288:ASP:OD2	2.19	0.42
1:F:39:PRO:HB2	1:F:53:VAL:HG12	2.01	0.42
1:F:486:GLU:HA	1:F:492:THR:H	1.84	0.42
1:A:78:ARG:NH1	1:A:82:GLU:OE2	2.52	0.42
1:A:291:ILE:HD12	1:A:291:ILE:HG21	1.77	0.42
1:A:494:THR:O	1:A:495:LEU:C	2.61	0.42
1:B:271:ARG:NH2	1:B:377:ASP:OD2	2.52	0.42
1:B:433:LEU:HG	1:B:450:ALA:HB2	2.02	0.42
1:C:86:LEU:CD2	1:C:86:LEU:C	2.92	0.42
1:C:106:PHE:O	1:C:109:ARG:N	2.43	0.42
1:C:158:LYS:HD3	1:C:158:LYS:HA	1.72	0.42
1:D:419:ASP:HB2	1:D:463:LYS:HZ2	1.83	0.42
1:D:469:ASN:HD22	1:D:469:ASN:HA	1.40	0.42
1:D:513:PRO:HD3	1:D:517:GLU:CD	2.45	0.42
1:E:66:LEU:HD21	1:E:70:HIS:ND1	2.34	0.42
1:E:300:ILE:HG12	1:E:324:LEU:CD1	2.48	0.42
1:F:12:GLN:O	1:F:13:ASP:C	2.63	0.42
1:F:43:THR:O	1:F:44:SER:CB	2.63	0.42
1:F:125:HIS:CE1	1:F:200:ASP:O	2.73	0.42
1:F:300:ILE:HG12	1:F:324:LEU:CD1	2.48	0.42
1:F:380:PHE:CD1	1:F:380:PHE:C	2.97	0.42
1:F:513:PRO:HD3	1:F:517:GLU:CD	2.45	0.42
1:A:367:VAL:HB	1:A:373:THR:HG23	2.02	0.42
1:B:12:GLN:O	1:B:13:ASP:C	2.63	0.42
1:B:190:MET:HG3	1:B:568:MET:CE	2.49	0.42
1:C:84:LEU:HD11	1:C:204:TRP:CD2	2.54	0.42
1:C:271:ARG:NH2	1:C:377:ASP:OD2	2.52	0.42
1:C:300:ILE:HG12	1:C:324:LEU:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ASN:ND2	1:C:457:HIS:H	2.05	0.42
1:D:367:VAL:HA	1:D:373:THR:CG2	2.49	0.42
1:E:12:GLN:O	1:E:13:ASP:C	2.63	0.42
1:E:366:GLY:N	1:E:369:GLU:HG3	2.22	0.42
1:E:551:HIS:CD2	1:E:552:ASP:CA	2.99	0.42
1:F:78:ARG:NH1	1:F:82:GLU:OE2	2.52	0.42
1:F:86:LEU:CD2	1:F:86:LEU:C	2.92	0.42
1:F:329:GLU:HA	1:F:344:HIS:CB	2.50	0.42
1:F:426:PHE:CD1	1:F:455:LEU:HA	2.55	0.42
1:A:329:GLU:HA	1:A:344:HIS:HB3	2.01	0.41
1:A:425:PHE:CD1	1:A:425:PHE:C	2.96	0.41
1:A:470:ASN:HB3	1:A:474:ARG:HD3	2.02	0.41
1:B:256:PHE:CZ	1:B:377:ASP:HA	2.55	0.41
1:B:513:PRO:HD3	1:B:517:GLU:CD	2.45	0.41
1:C:53:VAL:C	1:C:55:THR:N	2.78	0.41
1:C:241:ASP:HA	1:C:242:PRO:HD3	1.93	0.41
1:C:244:ASP:OD1	1:C:382:ARG:NH1	2.53	0.41
1:C:285:HIS:HB2	1:C:288:ASP:OD2	2.19	0.41
1:C:296:ILE:HD13	1:C:296:ILE:HA	1.38	0.41
1:C:329:GLU:HA	1:C:344:HIS:CB	2.50	0.41
1:D:23:GLU:HA	1:D:24:PRO:HD2	1.87	0.41
1:D:158:LYS:HD3	1:D:158:LYS:HA	1.72	0.41
1:D:301:ASP:CB	1:F:295:ARG:NH2	2.83	0.41
1:E:185:GLY:HA2	1:E:375:THR:HG23	2.01	0.41
1:E:296:ILE:HD13	1:E:296:ILE:HA	1.38	0.41
1:E:314:ASP:OD1	1:E:316:ARG:N	2.48	0.41
1:E:553:LEU:HA	1:E:553:LEU:HD23	1.55	0.41
1:F:70:HIS:CG	1:F:71:TRP:N	2.88	0.41
1:F:105:TYR:O	1:F:109:ARG:NE	2.46	0.41
1:F:158:LYS:HA	1:F:158:LYS:HD3	1.72	0.41
1:A:513:PRO:HD3	1:A:517:GLU:CD	2.45	0.41
1:B:495:LEU:HD13	1:B:583:TYR:CZ	2.55	0.41
1:C:45:ILE:HG12	1:C:45:ILE:H	1.49	0.41
1:C:125:HIS:CE1	1:C:200:ASP:O	2.73	0.41
1:C:291:ILE:O	1:C:292:THR:C	2.62	0.41
1:C:526:SER:HB3	1:C:529:THR:HB	2.02	0.41
1:D:57:MET:O	1:D:58:LYS:C	2.62	0.41
1:D:367:VAL:HB	1:D:373:THR:HG23	2.02	0.41
1:D:650:VAL:HG12	1:D:651:HIS:H	1.84	0.41
1:E:99:PHE:CZ	1:E:123:VAL:HG23	2.55	0.41
1:E:515:GLY:O	1:E:516:PRO:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:526:SER:HB3	1:E:529:THR:HB	2.02	0.41
1:E:653:LEU:HD12	1:E:653:LEU:HA	1.46	0.41
1:F:143:HIS:CE1	1:F:151:ILE:HG13	2.55	0.41
1:F:173:THR:O	1:F:174:LYS:C	2.62	0.41
1:F:176:ASN:HD22	1:F:176:ASN:HA	1.74	0.41
1:F:433:LEU:HG	1:F:450:ALA:HB2	2.02	0.41
1:F:650:VAL:HG12	1:F:651:HIS:H	1.84	0.41
1:A:248:TRP:HD1	4:A:753:HOH:O	2.03	0.41
1:A:427:ASP:HB3	1:A:567:ARG:HH12	1.86	0.41
1:A:440:GLY:O	1:A:441:GLU:HG3	2.20	0.41
1:B:53:VAL:C	1:B:55:THR:N	2.78	0.41
1:B:70:HIS:CG	1:B:71:TRP:N	2.88	0.41
1:B:143:HIS:CE1	1:B:151:ILE:HG13	2.55	0.41
1:B:244:ASP:OD1	1:B:382:ARG:NH1	2.53	0.41
1:B:295:ARG:HH11	1:B:295:ARG:HD2	1.31	0.41
1:B:367:VAL:HA	1:B:373:THR:CG2	2.49	0.41
1:B:470:ASN:HB3	1:B:474:ARG:HD3	2.03	0.41
1:C:29:ASP:O	1:C:30:LEU:C	2.59	0.41
1:C:398:PHE:HD1	1:C:398:PHE:HA	1.70	0.41
1:D:70:HIS:CG	1:D:71:TRP:N	2.87	0.41
1:D:143:HIS:CE1	1:D:151:ILE:HG13	2.55	0.41
1:D:256:PHE:CZ	1:D:377:ASP:HA	2.55	0.41
1:D:425:PHE:C	1:D:425:PHE:CD1	2.96	0.41
1:D:634:ARG:HE	1:F:64:ARG:NH2	2.18	0.41
1:E:143:HIS:CE1	1:E:151:ILE:HG13	2.55	0.41
1:E:241:ASP:HA	1:E:242:PRO:HD3	1.93	0.41
1:E:630:ILE:HG21	1:E:630:ILE:HD13	1.71	0.41
1:F:150:VAL:CG1	1:F:433:LEU:HD11	2.50	0.41
1:F:318:PRO:C	1:F:320:GLY:H	2.23	0.41
1:F:427:ASP:HB3	1:F:567:ARG:HH12	1.86	0.41
1:F:456:ASN:ND2	1:F:457:HIS:H	2.05	0.41
1:A:99:PHE:CZ	1:A:123:VAL:HG23	2.55	0.41
1:A:185:GLY:HA2	1:A:375:THR:HG23	2.01	0.41
1:A:222:TRP:O	1:A:223:VAL:C	2.59	0.41
1:B:99:PHE:CZ	1:B:123:VAL:HG23	2.55	0.41
1:B:125:HIS:CE1	1:B:200:ASP:O	2.73	0.41
1:B:132:ILE:CG2	1:B:133:VAL:N	2.83	0.41
1:B:440:GLY:O	1:B:441:GLU:HG3	2.20	0.41
1:C:39:PRO:HB2	1:C:53:VAL:HG12	2.01	0.41
1:D:125:HIS:CE1	1:D:200:ASP:O	2.73	0.41
1:D:314:ASP:OD1	1:D:316:ARG:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:ASP:O	1:E:594:GLU:N	2.45	0.41
1:F:56:LEU:O	1:F:57:MET:C	2.62	0.41
1:F:112:GLU:CD	1:F:112:GLU:H	2.24	0.41
1:F:271:ARG:NH2	1:F:377:ASP:CG	2.79	0.41
1:A:271:ARG:NH2	1:A:377:ASP:CG	2.79	0.41
1:A:355:GLY:N	4:A:707:HOH:O	2.54	0.41
1:A:614:GLU:H	1:A:614:GLU:HG3	1.15	0.41
1:B:105:TYR:CD2	1:B:105:TYR:C	2.98	0.41
1:B:233:PHE:O	1:B:234:GLU:C	2.59	0.41
1:B:367:VAL:HB	1:B:373:THR:HG23	2.02	0.41
1:C:426:PHE:CD1	1:C:455:LEU:HA	2.55	0.41
1:D:433:LEU:HG	1:D:450:ALA:HB2	2.02	0.41
1:D:433:LEU:HD23	1:D:433:LEU:HA	1.55	0.41
1:D:495:LEU:HD13	1:D:583:TYR:CZ	2.55	0.41
1:D:628:ARG:O	1:D:630:ILE:HG13	2.21	0.41
1:E:53:VAL:C	1:E:55:THR:N	2.78	0.41
1:E:86:LEU:CD2	1:E:86:LEU:C	2.92	0.41
1:F:241:ASP:HA	1:F:242:PRO:HD3	1.93	0.41
1:F:324:LEU:HD23	1:F:324:LEU:HA	1.82	0.41
1:A:177:ARG:HE	1:A:177:ARG:HB3	1.42	0.41
1:A:244:ASP:OD1	1:A:382:ARG:NH1	2.53	0.41
1:B:256:PHE:CD1	1:B:256:PHE:O	2.74	0.41
1:B:363:LEU:HA	1:B:363:LEU:HD12	1.79	0.41
1:C:256:PHE:CD1	1:C:256:PHE:O	2.74	0.41
1:C:427:ASP:HB3	1:C:567:ARG:HH12	1.86	0.41
1:C:513:PRO:HD3	1:C:517:GLU:CD	2.45	0.41
1:D:185:GLY:HA2	1:D:375:THR:HG23	2.01	0.41
1:D:244:ASP:OD1	1:D:382:ARG:NH1	2.53	0.41
1:D:329:GLU:HA	1:D:344:HIS:CB	2.50	0.41
1:D:380:PHE:CD1	1:D:380:PHE:C	2.97	0.41
1:D:528:VAL:H	1:D:528:VAL:HG13	1.51	0.41
1:D:626:LEU:HD23	1:D:626:LEU:N	2.36	0.41
1:E:105:TYR:CD2	1:E:105:TYR:C	2.98	0.41
1:E:230:ARG:HH11	1:E:230:ARG:HD2	1.64	0.41
1:E:256:PHE:CD1	1:E:256:PHE:O	2.74	0.41
1:E:329:GLU:HA	1:E:344:HIS:CB	2.50	0.41
1:F:48:ASP:C	1:F:50:GLY:N	2.70	0.41
1:F:244:ASP:OD1	1:F:382:ARG:NH1	2.53	0.41
1:A:256:PHE:CZ	1:A:377:ASP:HA	2.56	0.41
1:A:386:TYR:O	1:A:387:MET:C	2.61	0.41
1:A:426:PHE:CD1	1:A:455:LEU:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLN:NE2	1:B:544:ASP:OD1	2.51	0.41
1:B:300:ILE:HG12	1:B:324:LEU:CD1	2.48	0.41
1:B:329:GLU:HA	1:B:344:HIS:CB	2.50	0.41
1:C:43:THR:O	1:C:44:SER:CB	2.63	0.41
1:C:78:ARG:NH1	1:C:82:GLU:OE2	2.52	0.41
1:C:99:PHE:CZ	1:C:123:VAL:HG23	2.55	0.41
1:C:291:ILE:HD12	1:C:291:ILE:HG21	1.77	0.41
1:C:433:LEU:HG	1:C:450:ALA:HB2	2.02	0.41
1:C:475:LEU:HD23	1:C:475:LEU:HA	1.88	0.41
1:D:177:ARG:HE	1:D:177:ARG:HB3	1.41	0.41
1:D:425:PHE:O	1:D:456:ASN:N	2.54	0.41
1:D:456:ASN:ND2	1:D:457:HIS:H	2.05	0.41
1:D:475:LEU:HB3	1:D:589:GLY:HA3	2.03	0.41
1:D:614:GLU:H	1:D:614:GLU:HG3	1.15	0.41
1:E:39:PRO:HB2	1:E:53:VAL:HG12	2.01	0.41
1:E:291:ILE:O	1:E:292:THR:C	2.62	0.41
1:E:427:ASP:HB3	1:E:567:ARG:HH12	1.85	0.41
1:E:440:GLY:O	1:E:441:GLU:HG3	2.20	0.41
1:F:319:LYS:HD3	1:F:319:LYS:HA	1.85	0.41
1:A:363:LEU:HA	1:A:363:LEU:HD12	1.79	0.41
1:B:426:PHE:CD1	1:B:455:LEU:HA	2.55	0.41
1:C:127:LYS:HZ1	1:C:211:TYR:HE2	1.67	0.41
1:C:132:ILE:CG2	1:C:133:VAL:N	2.83	0.41
1:D:251:ILE:H	1:D:251:ILE:HG12	1.45	0.41
1:D:256:PHE:CD1	1:D:256:PHE:O	2.74	0.41
1:D:426:PHE:CD1	1:D:455:LEU:HA	2.55	0.41
1:D:526:SER:HB3	1:D:529:THR:HB	2.02	0.41
1:E:125:HIS:CE1	1:E:200:ASP:O	2.73	0.41
1:E:139:GLN:NE2	1:E:432:SER:H	2.19	0.41
1:E:256:PHE:CZ	1:E:377:ASP:HA	2.56	0.41
1:E:329:GLU:HA	1:E:344:HIS:HB3	2.01	0.41
1:E:426:PHE:CD1	1:E:455:LEU:HA	2.55	0.41
1:F:38:ASN:O	1:F:40:LEU:N	2.54	0.41
1:F:470:ASN:HB3	1:F:474:ARG:HD3	2.03	0.41
1:F:475:LEU:HB3	1:F:589:GLY:HA3	2.03	0.41
1:F:567:ARG:HH11	1:F:567:ARG:HD3	1.42	0.41
1:F:626:LEU:HD23	1:F:626:LEU:N	2.36	0.41
1:A:23:GLU:HA	1:A:24:PRO:HD2	1.87	0.41
1:A:132:ILE:CG2	1:A:133:VAL:N	2.83	0.41
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.56	0.41
1:A:564:ILE:HD13	1:A:564:ILE:HG21	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ALA:CB	1:B:89:VAL:HG23	2.51	0.41
1:B:87:PHE:CD1	1:B:121:VAL:HG12	2.56	0.41
1:B:173:THR:C	1:B:174:LYS:O	2.62	0.41
1:B:271:ARG:NH2	1:B:377:ASP:CG	2.79	0.41
1:B:425:PHE:O	1:B:456:ASN:N	2.54	0.41
1:B:487:ASP:C	1:B:489:ASN:H	2.26	0.41
1:B:560:ARG:HH12	1:B:606:HIS:N	2.19	0.41
1:C:12:GLN:O	1:C:13:ASP:C	2.63	0.41
1:C:56:LEU:O	1:C:57:MET:C	2.62	0.41
1:C:87:PHE:CD1	1:C:121:VAL:HG12	2.56	0.41
1:C:105:TYR:CD2	1:C:105:TYR:C	2.98	0.41
1:C:162:LYS:HA	1:C:163:PRO:HD3	1.67	0.41
1:C:169:SER:O	1:C:170:PHE:HB2	2.21	0.41
1:C:256:PHE:CZ	1:C:377:ASP:HA	2.56	0.41
1:C:272:PRO:HG2	1:F:272:PRO:CD	2.50	0.41
1:C:528:VAL:O	1:C:528:VAL:HG23	2.21	0.41
1:C:560:ARG:HH12	1:C:606:HIS:N	2.19	0.41
1:C:626:LEU:HD23	1:C:626:LEU:N	2.36	0.41
1:D:12:GLN:O	1:D:13:ASP:C	2.63	0.41
1:D:52:ALA:CB	1:D:89:VAL:HG23	2.51	0.41
1:D:291:ILE:O	1:D:292:THR:C	2.62	0.41
1:D:345:ASN:O	1:D:346:THR:C	2.60	0.41
1:D:635:VAL:C	1:D:637:ASP:N	2.77	0.41
1:E:31:LYS:C	1:E:33:ILE:N	2.77	0.41
1:E:112:GLU:CD	1:E:112:GLU:H	2.24	0.41
1:E:150:VAL:CG1	1:E:433:LEU:HD11	2.50	0.41
1:E:291:ILE:HD12	1:E:291:ILE:HG21	1.77	0.41
1:E:474:ARG:NH1	1:E:474:ARG:HB3	2.36	0.41
1:E:513:PRO:HD3	1:E:517:GLU:CD	2.45	0.41
1:E:591:LYS:HB2	1:E:591:LYS:HZ2	1.84	0.41
1:F:139:GLN:NE2	1:F:432:SER:H	2.19	0.41
1:F:256:PHE:CD1	1:F:256:PHE:O	2.74	0.41
1:F:515:GLY:O	1:F:516:PRO:C	2.62	0.41
1:F:528:VAL:O	1:F:528:VAL:HG23	2.21	0.41
1:F:628:ARG:O	1:F:630:ILE:HG13	2.21	0.41
1:F:630:ILE:HG21	1:F:630:ILE:HD13	1.71	0.41
1:A:84:LEU:HD11	1:A:204:TRP:CD2	2.54	0.41
1:B:62:ASP:O	1:B:63:HIS:CD2	2.70	0.41
1:B:169:SER:O	1:B:170:PHE:HB2	2.21	0.41
1:B:173:THR:O	1:B:174:LYS:C	2.62	0.41
1:B:567:ARG:HH11	1:B:567:ARG:HD3	1.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LEU:HD21	1:C:90:LEU:HD22	1.98	0.41
1:C:316:ARG:HE	1:E:338:GLN:HE22	1.69	0.41
1:C:425:PHE:O	1:C:456:ASN:N	2.54	0.41
1:D:159:MET:CE	1:E:155:TYR:CD1	2.99	0.41
1:D:236:LEU:HD12	1:D:236:LEU:HA	1.83	0.41
1:D:256:PHE:HA	1:E:361:PHE:CZ	2.56	0.41
1:D:271:ARG:NH2	1:D:377:ASP:CG	2.79	0.41
1:F:398:PHE:HD1	1:F:398:PHE:HA	1.70	0.41
1:F:526:SER:HB3	1:F:529:THR:HB	2.02	0.41
1:F:609:CYS:C	1:F:611:VAL:N	2.79	0.41
1:F:624:TYR:HA	1:F:625:PRO:HA	1.77	0.41
1:A:12:GLN:O	1:A:13:ASP:C	2.63	0.40
1:A:39:PRO:O	1:A:53:VAL:HG11	2.22	0.40
1:A:125:HIS:CE1	1:A:200:ASP:O	2.73	0.40
1:A:256:PHE:CD1	1:A:256:PHE:O	2.74	0.40
1:A:329:GLU:HA	1:A:344:HIS:CB	2.50	0.40
1:A:551:HIS:C	1:A:552:ASP:CG	2.86	0.40
1:B:319:LYS:HD3	1:B:319:LYS:HA	1.85	0.40
1:B:629:ARG:HG3	1:B:629:ARG:NH1	2.36	0.40
1:C:39:PRO:O	1:C:53:VAL:HG11	2.22	0.40
1:C:139:GLN:NE2	1:C:432:SER:H	2.19	0.40
1:C:177:ARG:CD	1:F:360:LYS:HB3	2.48	0.40
1:C:609:CYS:C	1:C:611:VAL:N	2.80	0.40
1:D:38:ASN:O	1:D:40:LEU:N	2.54	0.40
1:D:87:PHE:CD1	1:D:121:VAL:HG12	2.56	0.40
1:D:226:GLN:O	1:D:227:LEU:C	2.64	0.40
1:E:38:ASN:O	1:E:40:LEU:N	2.54	0.40
1:E:87:PHE:CD1	1:E:121:VAL:HG12	2.56	0.40
1:E:271:ARG:NH2	1:E:377:ASP:CG	2.79	0.40
1:E:367:VAL:HB	1:E:373:THR:HG23	2.02	0.40
1:E:528:VAL:H	1:E:528:VAL:HG13	1.51	0.40
1:F:132:ILE:CG2	1:F:133:VAL:N	2.83	0.40
1:F:256:PHE:O	1:F:256:PHE:HD1	2.04	0.40
1:F:440:GLY:O	1:F:441:GLU:HG3	2.20	0.40
1:F:566:ASP:O	1:F:567:ARG:C	2.63	0.40
1:A:87:PHE:CD1	1:A:121:VAL:HG12	2.56	0.40
1:B:64:ARG:O	1:B:78:ARG:NH1	2.55	0.40
1:B:157:ALA:HB1	1:B:448:ILE:HG12	2.03	0.40
1:B:275:ILE:HD13	1:B:275:ILE:HG21	1.54	0.40
1:B:427:ASP:HB3	1:B:567:ARG:HH12	1.86	0.40
1:B:528:VAL:H	1:B:528:VAL:HG13	1.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:LEU:HD23	1:B:626:LEU:N	2.36	0.40
1:C:57:MET:O	1:C:58:LYS:C	2.62	0.40
1:D:39:PRO:O	1:D:53:VAL:HG11	2.22	0.40
1:D:64:ARG:O	1:D:78:ARG:NH1	2.55	0.40
1:D:596:HIS:ND1	1:D:596:HIS:N	2.69	0.40
1:D:624:TYR:HA	1:D:625:PRO:HA	1.77	0.40
1:E:402:THR:C	1:E:405:ASN:HB2	2.47	0.40
1:A:31:LYS:C	1:A:33:ILE:N	2.77	0.40
1:A:474:ARG:NH1	1:A:474:ARG:HB3	2.36	0.40
1:A:523:SER:OG	1:A:524:LYS:HG3	2.22	0.40
1:A:631:PRO:HD2	4:A:818:HOH:O	2.20	0.40
1:B:162:LYS:HA	1:B:163:PRO:HD3	1.67	0.40
1:C:271:ARG:NH2	1:C:377:ASP:CG	2.79	0.40
1:C:470:ASN:HB3	1:C:474:ARG:HD3	2.02	0.40
1:C:475:LEU:HB3	1:C:589:GLY:HA3	2.03	0.40
1:C:569:LEU:CD2	1:C:570:LEU:HD13	2.46	0.40
1:D:99:PHE:CZ	1:D:123:VAL:HG23	2.55	0.40
1:D:399:PRO:HA	1:D:400:PRO:HD3	1.59	0.40
1:D:440:GLY:O	1:D:441:GLU:HG3	2.20	0.40
1:E:169:SER:O	1:E:170:PHE:HB2	2.21	0.40
1:E:551:HIS:C	1:E:552:ASP:CG	2.86	0.40
1:F:271:ARG:HA	1:F:272:PRO:HD3	1.69	0.40
1:F:367:VAL:HB	1:F:373:THR:HG23	2.02	0.40
1:A:132:ILE:H	1:A:132:ILE:HG13	1.46	0.40
1:A:157:ALA:HB1	1:A:448:ILE:HG12	2.04	0.40
1:A:411:MET:HE1	1:A:474:ARG:HB2	2.04	0.40
1:B:25:THR:HG22	1:B:26:LYS:H	1.87	0.40
1:B:38:ASN:O	1:B:40:LEU:N	2.54	0.40
1:B:124:ILE:HG21	1:B:124:ILE:HD13	1.73	0.40
1:B:239:TRP:HH2	1:B:574:LYS:HE3	1.81	0.40
1:C:38:ASN:O	1:C:40:LEU:N	2.54	0.40
1:C:173:THR:O	1:C:174:LYS:C	2.62	0.40
1:D:56:LEU:O	1:D:57:MET:C	2.62	0.40
1:D:105:TYR:CD2	1:D:105:TYR:C	2.98	0.40
1:E:569:LEU:CD2	1:E:570:LEU:HD13	2.46	0.40
1:F:99:PHE:CZ	1:F:123:VAL:HG23	2.55	0.40
1:F:192:ILE:HA	1:F:192:ILE:HD13	1.48	0.40
1:F:487:ASP:C	1:F:489:ASN:H	2.26	0.40
1:A:38:ASN:O	1:A:40:LEU:N	2.54	0.40
1:A:159:MET:HB3	1:B:158:LYS:HG3	2.04	0.40
1:A:230:ARG:HH11	1:A:230:ARG:HD2	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:ARG:O	1:A:630:ILE:HG13	2.21	0.40
1:B:72:TYR:CD1	1:B:72:TYR:C	2.99	0.40
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.82	0.40
1:B:316:ARG:HH21	1:D:338:GLN:HE22	1.68	0.40
1:B:526:SER:HB3	1:B:529:THR:HB	2.02	0.40
1:B:609:CYS:C	1:B:611:VAL:N	2.79	0.40
1:B:628:ARG:O	1:B:630:ILE:HG13	2.21	0.40
1:C:64:ARG:O	1:C:78:ARG:NH1	2.54	0.40
1:C:311:HIS:HD2	1:C:311:HIS:HA	1.65	0.40
1:D:17:LEU:HA	1:D:17:LEU:HD23	1.89	0.40
1:D:256:PHE:O	1:D:256:PHE:HD1	2.04	0.40
1:D:474:ARG:HB3	1:D:474:ARG:NH1	2.36	0.40
1:E:162:LYS:HA	1:E:163:PRO:HD3	1.67	0.40
1:E:390:ILE:HD13	1:E:390:ILE:HA	1.92	0.40
1:E:462:TYR:O	1:E:520:GLU:CA	2.62	0.40
1:E:470:ASN:HB3	1:E:474:ARG:HD3	2.02	0.40
1:E:475:LEU:HB3	1:E:589:GLY:HA3	2.03	0.40
1:E:551:HIS:CG	1:E:552:ASP:N	2.89	0.40
1:E:626:LEU:HD23	1:E:626:LEU:N	2.36	0.40
1:F:87:PHE:CD1	1:F:121:VAL:HG12	2.56	0.40
1:F:411:MET:HE1	1:F:474:ARG:HB2	2.04	0.40
1:F:425:PHE:O	1:F:456:ASN:N	2.54	0.40
1:F:523:SER:OG	1:F:524:LYS:HG3	2.22	0.40
1:F:560:ARG:HH12	1:F:606:HIS:N	2.19	0.40

All (1) 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:419:ASP:OD2	1:E:547:VAL:O[1_556]	1.86	0.34

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	640/657 (97%)	524 (82%)	88 (14%)	28 (4%)	2	15
1	B	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	15
1	C	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	15
1	D	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	15
1	E	640/657 (97%)	524 (82%)	88 (14%)	28 (4%)	2	15
1	F	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	15
All	All	3840/3942 (97%)	3140 (82%)	532 (14%)	168 (4%)	2	15

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	147	ASN
1	A	176	ASN
1	A	473	GLU
1	A	552	ASP
1	B	7	ASN
1	B	147	ASN
1	B	176	ASN
1	B	473	GLU
1	B	552	ASP
1	C	7	ASN
1	C	147	ASN
1	C	176	ASN
1	C	473	GLU
1	C	552	ASP
1	D	7	ASN
1	D	147	ASN
1	D	176	ASN
1	D	473	GLU
1	D	552	ASP
1	E	7	ASN
1	E	147	ASN
1	E	176	ASN
1	E	473	GLU
1	E	552	ASP
1	F	7	ASN
1	F	147	ASN
1	F	176	ASN

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Mol	Chain	Res	Type
1	F	473	GLU
1	F	552	ASP
1	A	8	ALA
1	A	20	LYS
1	A	42	ASP
1	A	44	SER
1	A	90	LEU
1	A	170	PHE
1	A	171	THR
1	A	320	GLY
1	A	427	ASP
1	A	516	PRO
1	A	557	ALA
1	A	561	SER
1	B	8	ALA
1	B	20	LYS
1	B	42	ASP
1	B	44	SER
1	B	90	LEU
1	B	170	PHE
1	B	171	THR
1	B	320	GLY
1	B	427	ASP
1	B	516	PRO
1	B	557	ALA
1	B	561	SER
1	C	8	ALA
1	C	20	LYS
1	C	42	ASP
1	C	44	SER
1	C	90	LEU
1	C	170	PHE
1	C	171	THR
1	C	320	GLY
1	C	427	ASP
1	C	516	PRO
1	C	557	ALA
1	C	561	SER
1	D	8	ALA
1	D	20	LYS
1	D	42	ASP
1	D	44	SER

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Mol	Chain	Res	Type
1	D	90	LEU
1	D	170	PHE
1	D	171	THR
1	D	320	GLY
1	D	427	ASP
1	D	516	PRO
1	D	557	ALA
1	D	561	SER
1	E	8	ALA
1	E	20	LYS
1	E	42	ASP
1	E	44	SER
1	E	90	LEU
1	E	170	PHE
1	E	171	THR
1	E	320	GLY
1	E	427	ASP
1	E	516	PRO
1	E	557	ALA
1	E	561	SER
1	F	8	ALA
1	F	20	LYS
1	F	42	ASP
1	F	44	SER
1	F	90	LEU
1	F	170	PHE
1	F	171	THR
1	F	320	GLY
1	F	427	ASP
1	F	516	PRO
1	F	557	ALA
1	F	561	SER
1	A	5	THR
1	A	104	ALA
1	A	242	PRO
1	A	560	ARG
1	A	569	LEU
1	A	595	GLY
1	B	5	THR
1	B	104	ALA
1	B	242	PRO
1	B	560	ARG

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Mol	Chain	Res	Type
1	B	569	LEU
1	B	595	GLY
1	C	5	THR
1	C	104	ALA
1	C	242	PRO
1	C	560	ARG
1	C	569	LEU
1	C	595	GLY
1	D	5	THR
1	D	104	ALA
1	D	242	PRO
1	D	560	ARG
1	D	569	LEU
1	D	595	GLY
1	E	5	THR
1	E	104	ALA
1	E	242	PRO
1	E	560	ARG
1	E	569	LEU
1	E	595	GLY
1	F	5	THR
1	F	104	ALA
1	F	242	PRO
1	F	560	ARG
1	F	569	LEU
1	F	595	GLY
1	A	63	HIS
1	A	273	ASP
1	B	63	HIS
1	B	273	ASP
1	C	63	HIS
1	C	273	ASP
1	D	63	HIS
1	D	273	ASP
1	E	63	HIS
1	E	273	ASP
1	F	63	HIS
1	F	273	ASP
1	A	496	ASP
1	B	496	ASP
1	C	496	ASP
1	D	496	ASP

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Mol	Chain	Res	Type
1	E	496	ASP
1	F	496	ASP
1	A	549	GLY
1	B	549	GLY
1	C	549	GLY
1	D	549	GLY
1	E	549	GLY
1	F	549	GLY
1	A	24	PRO
1	B	24	PRO
1	C	24	PRO
1	D	24	PRO
1	E	24	PRO
1	F	24	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	B	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	C	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	D	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	E	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	F	570/580 (98%)	393 (69%)	177 (31%)	0	1
All	All	3420/3480 (98%)	2358 (69%)	1062 (31%)	0	1

All (1062) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	12	GLN
1	A	14	ILE
1	A	15	ASN

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Mol	Chain	Res	Type
1	A	18	LEU
1	A	25	THR
1	A	31	LYS
1	A	44	SER
1	A	45	ILE
1	A	48	ASP
1	A	53	VAL
1	A	58	LYS
1	A	60	LEU
1	A	63	HIS
1	A	64	ARG
1	A	66	LEU
1	A	67	GLU
1	A	69	ARG
1	A	72	TYR
1	A	77	THR
1	A	81	LYS
1	A	85	MET
1	A	86	LEU
1	A	94	LYS
1	A	95	GLU
1	A	108	GLU
1	A	110	MET
1	A	111	ASN
1	A	112	GLU
1	A	121	VAL
1	A	123	VAL
1	A	127	LYS
1	A	128	LEU
1	A	137	LEU
1	A	140	ILE
1	A	145	PHE
1	A	148	SER
1	A	151	ILE
1	A	153	LYS
1	A	156	SER
1	A	158	LYS
1	A	165	THR
1	A	175	LYS
1	A	176	ASN
1	A	179	GLN
1	A	180	ARG

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Mol	Chain	Res	Type
1	A	181	VAL
1	A	195	VAL
1	A	199	MET
1	A	212	HIS
1	A	216	LYS
1	A	219	LEU
1	A	233	PHE
1	A	235	ARG
1	A	241	ASP
1	A	242	PRO
1	A	243	VAL
1	A	244	ASP
1	A	246	LEU
1	A	249	ASP
1	A	251	ILE
1	A	252	ILE
1	A	256	PHE
1	A	259	LEU
1	A	270	VAL
1	A	272	PRO
1	A	275	ILE
1	A	280	VAL
1	A	281	ASP
1	A	291	ILE
1	A	292	THR
1	A	294	SER
1	A	295	ARG
1	A	297	HIS
1	A	305	ILE
1	A	306	THR
1	A	313	ILE
1	A	316	ARG
1	A	318	PRO
1	A	319	LYS
1	A	322	GLU
1	A	323	LEU
1	A	329	GLU
1	A	332	LYS
1	A	334	SER
1	A	335	SER
1	A	342	SER
1	A	343	LEU

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Mol	Chain	Res	Type
1	A	349	VAL
1	A	351	LEU
1	A	362	ASN
1	A	363	LEU
1	A	367	VAL
1	A	369	GLU
1	A	372	GLU
1	A	373	THR
1	A	375	THR
1	A	376	ARG
1	A	382	ARG
1	A	389	ASN
1	A	395	THR
1	A	396	ASP
1	A	397	SER
1	A	399	PRO
1	A	402	THR
1	A	405	ASN
1	A	411	MET
1	A	412	VAL
1	A	416	VAL
1	A	418	ILE
1	A	423	ILE
1	A	427	ASP
1	A	435	ASN
1	A	438	ASP
1	A	439	SER
1	A	446	VAL
1	A	452	VAL
1	A	453	HIS
1	A	456	ASN
1	A	461	THR
1	A	466	MET
1	A	467	SER
1	A	473	GLU
1	A	474	ARG
1	A	475	LEU
1	A	482	LEU
1	A	487	ASP
1	A	491	ILE
1	A	493	LEU
1	A	501	PHE

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Mol	Chain	Res	Type
1	A	502	CYS
1	A	503	ILE
1	A	505	LEU
1	A	511	LYS
1	A	519	ILE
1	A	523	SER
1	A	525	ASP
1	A	528	VAL
1	A	529	THR
1	A	530	VAL
1	A	532	ASP
1	A	533	MET
1	A	535	SER
1	A	539	LEU
1	A	547	VAL
1	A	552	ASP
1	A	554	ASP
1	A	555	LEU
1	A	559	GLU
1	A	565	PRO
1	A	567	ARG
1	A	570	LEU
1	A	574	LYS
1	A	578	MET
1	A	579	GLU
1	A	586	VAL
1	A	587	THR
1	A	591	LYS
1	A	596	HIS
1	A	606	HIS
1	A	608	GLN
1	A	609	CYS
1	A	620	ARG
1	A	622	LEU
1	A	625	PRO
1	A	626	LEU
1	A	629	ARG
1	A	634	ARG
1	A	635	VAL
1	A	636	ILE
1	A	639	VAL
1	A	641	ASN

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Mol	Chain	Res	Type
1	A	643	LYS
1	A	645	VAL
1	A	646	VAL
1	A	649	ILE
1	A	650	VAL
1	B	10	LYS
1	B	12	GLN
1	B	14	ILE
1	B	15	ASN
1	B	18	LEU
1	B	25	THR
1	B	31	LYS
1	B	44	SER
1	B	45	ILE
1	B	48	ASP
1	B	53	VAL
1	B	58	LYS
1	B	60	LEU
1	B	63	HIS
1	B	64	ARG
1	B	66	LEU
1	B	67	GLU
1	B	69	ARG
1	B	72	TYR
1	B	77	THR
1	B	81	LYS
1	B	85	MET
1	B	86	LEU
1	B	94	LYS
1	B	95	GLU
1	B	108	GLU
1	B	110	MET
1	B	111	ASN
1	B	112	GLU
1	B	121	VAL
1	B	123	VAL
1	B	127	LYS
1	B	128	LEU
1	B	137	LEU
1	B	140	ILE
1	B	145	PHE
1	B	148	SER

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Mol	Chain	Res	Type
1	B	151	ILE
1	B	153	LYS
1	B	156	SER
1	B	158	LYS
1	B	165	THR
1	B	175	LYS
1	B	176	ASN
1	B	179	GLN
1	B	180	ARG
1	B	181	VAL
1	B	195	VAL
1	B	199	MET
1	B	212	HIS
1	B	216	LYS
1	B	219	LEU
1	B	233	PHE
1	B	235	ARG
1	B	241	ASP
1	B	242	PRO
1	B	243	VAL
1	B	244	ASP
1	B	246	LEU
1	B	249	ASP
1	B	251	ILE
1	B	252	ILE
1	B	256	PHE
1	B	259	LEU
1	B	270	VAL
1	B	272	PRO
1	B	275	ILE
1	B	280	VAL
1	B	281	ASP
1	B	291	ILE
1	B	292	THR
1	B	294	SER
1	B	295	ARG
1	B	297	HIS
1	B	305	ILE
1	B	306	THR
1	B	313	ILE
1	B	316	ARG
1	B	318	PRO

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Mol	Chain	Res	Type
1	B	319	LYS
1	B	322	GLU
1	B	323	LEU
1	B	329	GLU
1	B	332	LYS
1	B	334	SER
1	B	335	SER
1	B	342	SER
1	B	343	LEU
1	B	349	VAL
1	B	351	LEU
1	B	362	ASN
1	B	363	LEU
1	B	367	VAL
1	B	369	GLU
1	B	372	GLU
1	B	373	THR
1	B	375	THR
1	B	376	ARG
1	B	382	ARG
1	B	389	ASN
1	B	395	THR
1	B	396	ASP
1	B	397	SER
1	B	399	PRO
1	B	402	THR
1	B	405	ASN
1	B	411	MET
1	B	412	VAL
1	B	416	VAL
1	B	418	ILE
1	B	423	ILE
1	B	427	ASP
1	B	435	ASN
1	B	438	ASP
1	B	439	SER
1	B	446	VAL
1	B	452	VAL
1	B	453	HIS
1	B	456	ASN
1	B	461	THR
1	B	466	MET

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Mol	Chain	Res	Type
1	B	467	SER
1	B	473	GLU
1	B	474	ARG
1	B	475	LEU
1	B	482	LEU
1	B	487	ASP
1	B	491	ILE
1	B	493	LEU
1	B	501	PHE
1	B	502	CYS
1	B	503	ILE
1	B	505	LEU
1	B	511	LYS
1	B	519	ILE
1	B	523	SER
1	B	525	ASP
1	B	528	VAL
1	B	529	THR
1	B	530	VAL
1	B	532	ASP
1	B	533	MET
1	B	535	SER
1	B	539	LEU
1	B	547	VAL
1	B	552	ASP
1	B	554	ASP
1	B	555	LEU
1	B	559	GLU
1	B	565	PRO
1	B	567	ARG
1	B	570	LEU
1	B	574	LYS
1	B	578	MET
1	B	579	GLU
1	B	586	VAL
1	B	587	THR
1	B	591	LYS
1	B	596	HIS
1	B	606	HIS
1	B	608	GLN
1	B	609	CYS
1	B	620	ARG

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Mol	Chain	Res	Type
1	B	622	LEU
1	B	625	PRO
1	B	626	LEU
1	B	629	ARG
1	B	634	ARG
1	B	635	VAL
1	B	636	ILE
1	B	639	VAL
1	B	641	ASN
1	B	643	LYS
1	B	645	VAL
1	B	646	VAL
1	B	649	ILE
1	B	650	VAL
1	C	10	LYS
1	C	12	GLN
1	C	14	ILE
1	C	15	ASN
1	C	18	LEU
1	C	25	THR
1	C	31	LYS
1	C	44	SER
1	C	45	ILE
1	C	48	ASP
1	C	53	VAL
1	C	58	LYS
1	C	60	LEU
1	C	63	HIS
1	C	64	ARG
1	C	66	LEU
1	C	67	GLU
1	C	69	ARG
1	C	72	TYR
1	C	77	THR
1	C	81	LYS
1	C	85	MET
1	C	86	LEU
1	C	94	LYS
1	C	95	GLU
1	C	108	GLU
1	C	110	MET
1	C	111	ASN

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Mol	Chain	Res	Type
1	C	112	GLU
1	C	121	VAL
1	C	123	VAL
1	C	127	LYS
1	C	128	LEU
1	C	137	LEU
1	C	140	ILE
1	C	145	PHE
1	C	148	SER
1	C	151	ILE
1	C	153	LYS
1	C	156	SER
1	C	158	LYS
1	C	165	THR
1	C	175	LYS
1	C	176	ASN
1	C	179	GLN
1	C	180	ARG
1	C	181	VAL
1	C	195	VAL
1	C	199	MET
1	C	212	HIS
1	C	216	LYS
1	C	219	LEU
1	C	233	PHE
1	C	235	ARG
1	C	241	ASP
1	C	242	PRO
1	C	243	VAL
1	C	244	ASP
1	C	246	LEU
1	C	249	ASP
1	C	251	ILE
1	C	252	ILE
1	C	256	PHE
1	C	259	LEU
1	C	270	VAL
1	C	272	PRO
1	C	275	ILE
1	C	280	VAL
1	C	281	ASP
1	C	291	ILE

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Mol	Chain	Res	Type
1	C	292	THR
1	C	294	SER
1	C	295	ARG
1	C	297	HIS
1	C	305	ILE
1	C	306	THR
1	C	313	ILE
1	C	316	ARG
1	C	318	PRO
1	C	319	LYS
1	C	322	GLU
1	C	323	LEU
1	C	329	GLU
1	C	332	LYS
1	C	334	SER
1	C	335	SER
1	C	342	SER
1	C	343	LEU
1	C	349	VAL
1	C	351	LEU
1	C	362	ASN
1	C	363	LEU
1	C	367	VAL
1	C	369	GLU
1	C	372	GLU
1	C	373	THR
1	C	375	THR
1	C	376	ARG
1	C	382	ARG
1	C	389	ASN
1	C	395	THR
1	C	396	ASP
1	C	397	SER
1	C	399	PRO
1	C	402	THR
1	C	405	ASN
1	C	411	MET
1	C	412	VAL
1	C	416	VAL
1	C	418	ILE
1	C	423	ILE
1	C	427	ASP

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Mol	Chain	Res	Type
1	C	435	ASN
1	C	438	ASP
1	C	439	SER
1	C	446	VAL
1	C	452	VAL
1	C	453	HIS
1	C	456	ASN
1	C	461	THR
1	C	466	MET
1	C	467	SER
1	C	473	GLU
1	C	474	ARG
1	C	475	LEU
1	C	482	LEU
1	C	487	ASP
1	C	491	ILE
1	C	493	LEU
1	C	501	PHE
1	C	502	CYS
1	C	503	ILE
1	C	505	LEU
1	C	511	LYS
1	C	519	ILE
1	C	523	SER
1	C	525	ASP
1	C	528	VAL
1	C	529	THR
1	C	530	VAL
1	C	532	ASP
1	C	533	MET
1	C	535	SER
1	C	539	LEU
1	C	547	VAL
1	C	552	ASP
1	C	554	ASP
1	C	555	LEU
1	C	559	GLU
1	C	565	PRO
1	C	567	ARG
1	C	570	LEU
1	C	574	LYS
1	C	578	MET

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Mol	Chain	Res	Type
1	C	579	GLU
1	C	586	VAL
1	C	587	THR
1	C	591	LYS
1	C	596	HIS
1	C	606	HIS
1	C	608	GLN
1	C	609	CYS
1	C	620	ARG
1	C	622	LEU
1	C	625	PRO
1	C	626	LEU
1	C	629	ARG
1	C	634	ARG
1	C	635	VAL
1	C	636	ILE
1	C	639	VAL
1	C	641	ASN
1	C	643	LYS
1	C	645	VAL
1	C	646	VAL
1	C	649	ILE
1	C	650	VAL
1	D	10	LYS
1	D	12	GLN
1	D	14	ILE
1	D	15	ASN
1	D	18	LEU
1	D	25	THR
1	D	31	LYS
1	D	44	SER
1	D	45	ILE
1	D	48	ASP
1	D	53	VAL
1	D	58	LYS
1	D	60	LEU
1	D	63	HIS
1	D	64	ARG
1	D	66	LEU
1	D	67	GLU
1	D	69	ARG
1	D	72	TYR

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Mol	Chain	Res	Type
1	D	77	THR
1	D	81	LYS
1	D	85	MET
1	D	86	LEU
1	D	94	LYS
1	D	95	GLU
1	D	108	GLU
1	D	110	MET
1	D	111	ASN
1	D	112	GLU
1	D	121	VAL
1	D	123	VAL
1	D	127	LYS
1	D	128	LEU
1	D	137	LEU
1	D	140	ILE
1	D	145	PHE
1	D	148	SER
1	D	151	ILE
1	D	153	LYS
1	D	156	SER
1	D	158	LYS
1	D	165	THR
1	D	175	LYS
1	D	176	ASN
1	D	179	GLN
1	D	180	ARG
1	D	181	VAL
1	D	195	VAL
1	D	199	MET
1	D	212	HIS
1	D	216	LYS
1	D	219	LEU
1	D	233	PHE
1	D	235	ARG
1	D	241	ASP
1	D	242	PRO
1	D	243	VAL
1	D	244	ASP
1	D	246	LEU
1	D	249	ASP
1	D	251	ILE

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Mol	Chain	Res	Type
1	D	252	ILE
1	D	256	PHE
1	D	259	LEU
1	D	270	VAL
1	D	272	PRO
1	D	275	ILE
1	D	280	VAL
1	D	281	ASP
1	D	291	ILE
1	D	292	THR
1	D	294	SER
1	D	295	ARG
1	D	297	HIS
1	D	305	ILE
1	D	306	THR
1	D	313	ILE
1	D	316	ARG
1	D	318	PRO
1	D	319	LYS
1	D	322	GLU
1	D	323	LEU
1	D	329	GLU
1	D	332	LYS
1	D	334	SER
1	D	335	SER
1	D	342	SER
1	D	343	LEU
1	D	349	VAL
1	D	351	LEU
1	D	362	ASN
1	D	363	LEU
1	D	367	VAL
1	D	369	GLU
1	D	372	GLU
1	D	373	THR
1	D	375	THR
1	D	376	ARG
1	D	382	ARG
1	D	389	ASN
1	D	395	THR
1	D	396	ASP
1	D	397	SER

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Mol	Chain	Res	Type
1	D	399	PRO
1	D	402	THR
1	D	405	ASN
1	D	411	MET
1	D	412	VAL
1	D	416	VAL
1	D	418	ILE
1	D	423	ILE
1	D	427	ASP
1	D	435	ASN
1	D	438	ASP
1	D	439	SER
1	D	446	VAL
1	D	452	VAL
1	D	453	HIS
1	D	456	ASN
1	D	461	THR
1	D	466	MET
1	D	467	SER
1	D	473	GLU
1	D	474	ARG
1	D	475	LEU
1	D	482	LEU
1	D	487	ASP
1	D	491	ILE
1	D	493	LEU
1	D	501	PHE
1	D	502	CYS
1	D	503	ILE
1	D	505	LEU
1	D	511	LYS
1	D	519	ILE
1	D	523	SER
1	D	525	ASP
1	D	528	VAL
1	D	529	THR
1	D	530	VAL
1	D	532	ASP
1	D	533	MET
1	D	535	SER
1	D	539	LEU
1	D	547	VAL

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Mol	Chain	Res	Type
1	D	552	ASP
1	D	554	ASP
1	D	555	LEU
1	D	559	GLU
1	D	565	PRO
1	D	567	ARG
1	D	570	LEU
1	D	574	LYS
1	D	578	MET
1	D	579	GLU
1	D	586	VAL
1	D	587	THR
1	D	591	LYS
1	D	596	HIS
1	D	606	HIS
1	D	608	GLN
1	D	609	CYS
1	D	620	ARG
1	D	622	LEU
1	D	625	PRO
1	D	626	LEU
1	D	629	ARG
1	D	634	ARG
1	D	635	VAL
1	D	636	ILE
1	D	639	VAL
1	D	641	ASN
1	D	643	LYS
1	D	645	VAL
1	D	646	VAL
1	D	649	ILE
1	D	650	VAL
1	E	10	LYS
1	E	12	GLN
1	E	14	ILE
1	E	15	ASN
1	E	18	LEU
1	E	25	THR
1	E	31	LYS
1	E	44	SER
1	E	45	ILE
1	E	48	ASP

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Mol	Chain	Res	Type
1	E	53	VAL
1	E	58	LYS
1	E	60	LEU
1	E	63	HIS
1	E	64	ARG
1	E	66	LEU
1	E	67	GLU
1	E	69	ARG
1	E	72	TYR
1	E	77	THR
1	E	81	LYS
1	E	85	MET
1	E	86	LEU
1	E	94	LYS
1	E	95	GLU
1	E	108	GLU
1	E	110	MET
1	E	111	ASN
1	E	112	GLU
1	E	121	VAL
1	E	123	VAL
1	E	127	LYS
1	E	128	LEU
1	E	137	LEU
1	E	140	ILE
1	E	145	PHE
1	E	148	SER
1	E	151	ILE
1	E	153	LYS
1	E	156	SER
1	E	158	LYS
1	E	165	THR
1	E	175	LYS
1	E	176	ASN
1	E	179	GLN
1	E	180	ARG
1	E	181	VAL
1	E	195	VAL
1	E	199	MET
1	E	212	HIS
1	E	216	LYS
1	E	219	LEU

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Mol	Chain	Res	Type
1	E	233	PHE
1	E	235	ARG
1	E	241	ASP
1	E	242	PRO
1	E	243	VAL
1	E	244	ASP
1	E	246	LEU
1	E	249	ASP
1	E	251	ILE
1	E	252	ILE
1	E	256	PHE
1	E	259	LEU
1	E	270	VAL
1	E	272	PRO
1	E	275	ILE
1	E	280	VAL
1	E	281	ASP
1	E	291	ILE
1	E	292	THR
1	E	294	SER
1	E	295	ARG
1	E	297	HIS
1	E	305	ILE
1	E	306	THR
1	E	313	ILE
1	E	316	ARG
1	E	318	PRO
1	E	319	LYS
1	E	322	GLU
1	E	323	LEU
1	E	329	GLU
1	E	332	LYS
1	E	334	SER
1	E	335	SER
1	E	342	SER
1	E	343	LEU
1	E	349	VAL
1	E	351	LEU
1	E	362	ASN
1	E	363	LEU
1	E	367	VAL
1	E	369	GLU

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Mol	Chain	Res	Type
1	E	372	GLU
1	E	373	THR
1	E	375	THR
1	E	376	ARG
1	E	382	ARG
1	E	389	ASN
1	E	395	THR
1	E	396	ASP
1	E	397	SER
1	E	399	PRO
1	E	402	THR
1	E	405	ASN
1	E	411	MET
1	E	412	VAL
1	E	416	VAL
1	E	418	ILE
1	E	423	ILE
1	E	427	ASP
1	E	435	ASN
1	E	438	ASP
1	E	439	SER
1	E	446	VAL
1	E	452	VAL
1	E	453	HIS
1	E	456	ASN
1	E	461	THR
1	E	466	MET
1	E	467	SER
1	E	473	GLU
1	E	474	ARG
1	E	475	LEU
1	E	482	LEU
1	E	487	ASP
1	E	491	ILE
1	E	493	LEU
1	E	501	PHE
1	E	502	CYS
1	E	503	ILE
1	E	505	LEU
1	E	511	LYS
1	E	519	ILE
1	E	523	SER

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Mol	Chain	Res	Type
1	E	525	ASP
1	E	528	VAL
1	E	529	THR
1	E	530	VAL
1	E	532	ASP
1	E	533	MET
1	E	535	SER
1	E	539	LEU
1	E	547	VAL
1	E	552	ASP
1	E	554	ASP
1	E	555	LEU
1	E	559	GLU
1	E	565	PRO
1	E	567	ARG
1	E	570	LEU
1	E	574	LYS
1	E	578	MET
1	E	579	GLU
1	E	586	VAL
1	E	587	THR
1	E	591	LYS
1	E	596	HIS
1	E	606	HIS
1	E	608	GLN
1	E	609	CYS
1	E	620	ARG
1	E	622	LEU
1	E	625	PRO
1	E	626	LEU
1	E	629	ARG
1	E	634	ARG
1	E	635	VAL
1	E	636	ILE
1	E	639	VAL
1	E	641	ASN
1	E	643	LYS
1	E	645	VAL
1	E	646	VAL
1	E	649	ILE
1	E	650	VAL
1	F	10	LYS

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Mol	Chain	Res	Type
1	F	12	GLN
1	F	14	ILE
1	F	15	ASN
1	F	18	LEU
1	F	25	THR
1	F	31	LYS
1	F	44	SER
1	F	45	ILE
1	F	48	ASP
1	F	53	VAL
1	F	58	LYS
1	F	60	LEU
1	F	63	HIS
1	F	64	ARG
1	F	66	LEU
1	F	67	GLU
1	F	69	ARG
1	F	72	TYR
1	F	77	THR
1	F	81	LYS
1	F	85	MET
1	F	86	LEU
1	F	94	LYS
1	F	95	GLU
1	F	108	GLU
1	F	110	MET
1	F	111	ASN
1	F	112	GLU
1	F	121	VAL
1	F	123	VAL
1	F	127	LYS
1	F	128	LEU
1	F	137	LEU
1	F	140	ILE
1	F	145	PHE
1	F	148	SER
1	F	151	ILE
1	F	153	LYS
1	F	156	SER
1	F	158	LYS
1	F	165	THR
1	F	175	LYS

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Mol	Chain	Res	Type
1	F	176	ASN
1	F	179	GLN
1	F	180	ARG
1	F	181	VAL
1	F	195	VAL
1	F	199	MET
1	F	212	HIS
1	F	216	LYS
1	F	219	LEU
1	F	233	PHE
1	F	235	ARG
1	F	241	ASP
1	F	242	PRO
1	F	243	VAL
1	F	244	ASP
1	F	246	LEU
1	F	249	ASP
1	F	251	ILE
1	F	252	ILE
1	F	256	PHE
1	F	259	LEU
1	F	270	VAL
1	F	272	PRO
1	F	275	ILE
1	F	280	VAL
1	F	281	ASP
1	F	291	ILE
1	F	292	THR
1	F	294	SER
1	F	295	ARG
1	F	297	HIS
1	F	305	ILE
1	F	306	THR
1	F	313	ILE
1	F	316	ARG
1	F	318	PRO
1	F	319	LYS
1	F	322	GLU
1	F	323	LEU
1	F	329	GLU
1	F	332	LYS
1	F	334	SER

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Mol	Chain	Res	Type
1	F	335	SER
1	F	342	SER
1	F	343	LEU
1	F	349	VAL
1	F	351	LEU
1	F	362	ASN
1	F	363	LEU
1	F	367	VAL
1	F	369	GLU
1	F	372	GLU
1	F	373	THR
1	F	375	THR
1	F	376	ARG
1	F	382	ARG
1	F	389	ASN
1	F	395	THR
1	F	396	ASP
1	F	397	SER
1	F	399	PRO
1	F	402	THR
1	F	405	ASN
1	F	411	MET
1	F	412	VAL
1	F	416	VAL
1	F	418	ILE
1	F	423	ILE
1	F	427	ASP
1	F	435	ASN
1	F	438	ASP
1	F	439	SER
1	F	446	VAL
1	F	452	VAL
1	F	453	HIS
1	F	456	ASN
1	F	461	THR
1	F	466	MET
1	F	467	SER
1	F	473	GLU
1	F	474	ARG
1	F	475	LEU
1	F	482	LEU
1	F	487	ASP

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Mol	Chain	Res	Type
1	F	491	ILE
1	F	493	LEU
1	F	501	PHE
1	F	502	CYS
1	F	503	ILE
1	F	505	LEU
1	F	511	LYS
1	F	519	ILE
1	F	523	SER
1	F	525	ASP
1	F	528	VAL
1	F	529	THR
1	F	530	VAL
1	F	532	ASP
1	F	533	MET
1	F	535	SER
1	F	539	LEU
1	F	547	VAL
1	F	552	ASP
1	F	554	ASP
1	F	555	LEU
1	F	559	GLU
1	F	565	PRO
1	F	567	ARG
1	F	570	LEU
1	F	574	LYS
1	F	578	MET
1	F	579	GLU
1	F	586	VAL
1	F	587	THR
1	F	591	LYS
1	F	596	HIS
1	F	606	HIS
1	F	608	GLN
1	F	609	CYS
1	F	620	ARG
1	F	622	LEU
1	F	625	PRO
1	F	626	LEU
1	F	629	ARG
1	F	634	ARG
1	F	635	VAL

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Mol	Chain	Res	Type
1	F	636	ILE
1	F	639	VAL
1	F	641	ASN
1	F	643	LYS
1	F	645	VAL
1	F	646	VAL
1	F	649	ILE
1	F	650	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	ASN
1	A	36	ASN
1	A	38	ASN
1	A	63	HIS
1	A	76	ASN
1	A	91	ASN
1	A	92	GLN
1	A	102	ASN
1	A	161	GLN
1	A	225	HIS
1	A	336	ASN
1	A	338	GLN
1	A	354	GLN
1	A	414	ASN
1	A	449	ASN
1	A	453	HIS
1	A	456	ASN
1	A	469	ASN
1	A	551	HIS
1	A	606	HIS
1	A	608	GLN
1	A	612	HIS
1	A	644	HIS
1	B	11	GLN
1	B	15	ASN
1	B	36	ASN
1	B	38	ASN
1	B	63	HIS
1	B	76	ASN

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Mol	Chain	Res	Type
1	B	91	ASN
1	B	92	GLN
1	B	102	ASN
1	B	143	HIS
1	B	161	GLN
1	B	225	HIS
1	B	226	GLN
1	B	336	ASN
1	B	338	GLN
1	B	354	GLN
1	B	394	HIS
1	B	414	ASN
1	B	449	ASN
1	B	453	HIS
1	B	456	ASN
1	B	469	ASN
1	B	470	ASN
1	B	551	HIS
1	B	606	HIS
1	B	608	GLN
1	B	612	HIS
1	B	644	HIS
1	C	11	GLN
1	C	15	ASN
1	C	16	HIS
1	C	36	ASN
1	C	38	ASN
1	C	63	HIS
1	C	76	ASN
1	C	91	ASN
1	C	92	GLN
1	C	102	ASN
1	C	225	HIS
1	C	336	ASN
1	C	338	GLN
1	C	354	GLN
1	C	414	ASN
1	C	449	ASN
1	C	453	HIS
1	C	456	ASN
1	C	469	ASN
1	C	551	HIS

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Mol	Chain	Res	Type
1	C	606	HIS
1	C	608	GLN
1	C	612	HIS
1	C	644	HIS
1	D	11	GLN
1	D	15	ASN
1	D	16	HIS
1	D	36	ASN
1	D	38	ASN
1	D	63	HIS
1	D	76	ASN
1	D	91	ASN
1	D	92	GLN
1	D	102	ASN
1	D	143	HIS
1	D	225	HIS
1	D	226	GLN
1	D	336	ASN
1	D	338	GLN
1	D	354	GLN
1	D	414	ASN
1	D	449	ASN
1	D	453	HIS
1	D	456	ASN
1	D	469	ASN
1	D	551	HIS
1	D	606	HIS
1	D	608	GLN
1	D	612	HIS
1	D	644	HIS
1	E	11	GLN
1	E	15	ASN
1	E	36	ASN
1	E	38	ASN
1	E	63	HIS
1	E	76	ASN
1	E	91	ASN
1	E	92	GLN
1	E	102	ASN
1	E	225	HIS
1	E	226	GLN
1	E	336	ASN

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Mol	Chain	Res	Type
1	E	338	GLN
1	E	354	GLN
1	E	394	HIS
1	E	414	ASN
1	E	449	ASN
1	E	453	HIS
1	E	456	ASN
1	E	469	ASN
1	E	551	HIS
1	E	606	HIS
1	E	608	GLN
1	E	612	HIS
1	E	644	HIS
1	F	11	GLN
1	F	15	ASN
1	F	16	HIS
1	F	36	ASN
1	F	38	ASN
1	F	63	HIS
1	F	76	ASN
1	F	91	ASN
1	F	92	GLN
1	F	102	ASN
1	F	143	HIS
1	F	225	HIS
1	F	226	GLN
1	F	336	ASN
1	F	338	GLN
1	F	354	GLN
1	F	394	HIS
1	F	414	ASN
1	F	449	ASN
1	F	453	HIS
1	F	456	ASN
1	F	469	ASN
1	F	551	HIS
1	F	606	HIS
1	F	608	GLN
1	F	612	HIS
1	F	644	HIS

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

12 monosaccharides 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	$\#\|Z\| > 2$
2	NAG	G	1	2,1	14,14,15	18.12	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	G	2	2	14,14,15	21.58	4 (28%)	17,19,21	11.25	7 (41%)
2	NAG	H	1	2,1	14,14,15	18.12	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	H	2	2	14,14,15	21.59	4 (28%)	17,19,21	11.25	7 (41%)
2	NAG	I	1	2,1	14,14,15	18.12	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	I	2	2	14,14,15	21.59	4 (28%)	17,19,21	11.25	7 (41%)
2	NAG	J	1	2,1	14,14,15	18.11	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	J	2	2	14,14,15	21.59	4 (28%)	17,19,21	11.25	7 (41%)
2	NAG	K	1	2,1	14,14,15	18.11	4 (28%)	17,19,21	11.29	12 (70%)
2	NAG	K	2	2	14,14,15	21.58	4 (28%)	17,19,21	11.25	7 (41%)
2	NAG	L	1	2,1	14,14,15	18.12	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	L	2	2	14,14,15	21.57	4 (28%)	17,19,21	11.25	7 (41%)

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
2	NAG	G	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	C8-C7	79.03	3.14	1.50
2	H	2	NAG	C8-C7	79.01	3.14	1.50
2	J	2	NAG	C8-C7	79.00	3.14	1.50
2	K	2	NAG	C8-C7	78.99	3.14	1.50
2	G	2	NAG	C8-C7	78.99	3.14	1.50
2	L	2	NAG	C8-C7	78.95	3.14	1.50
2	L	1	NAG	C8-C7	66.70	2.88	1.50
2	I	1	NAG	C8-C7	66.68	2.88	1.50
2	H	1	NAG	C8-C7	66.66	2.88	1.50
2	G	1	NAG	C8-C7	66.66	2.88	1.50
2	K	1	NAG	C8-C7	66.65	2.88	1.50
2	J	1	NAG	C8-C7	66.64	2.88	1.50
2	L	2	NAG	O7-C7	15.94	1.58	1.23
2	G	2	NAG	O7-C7	15.92	1.58	1.23
2	K	2	NAG	O7-C7	15.92	1.58	1.23
2	H	2	NAG	O7-C7	15.91	1.58	1.23
2	I	2	NAG	O7-C7	15.89	1.58	1.23
2	J	2	NAG	O7-C7	15.89	1.58	1.23
2	J	1	NAG	O7-C7	11.28	1.48	1.23
2	K	1	NAG	O7-C7	11.27	1.48	1.23
2	H	1	NAG	O7-C7	11.27	1.48	1.23
2	G	1	NAG	O7-C7	11.27	1.48	1.23
2	I	1	NAG	O7-C7	11.22	1.48	1.23
2	L	1	NAG	O7-C7	11.22	1.48	1.23
2	J	1	NAG	O5-C1	3.24	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O5-C1	3.20	1.49	1.43
2	I	1	NAG	O5-C1	3.20	1.49	1.43
2	L	1	NAG	O5-C1	3.18	1.49	1.43
2	H	1	NAG	O5-C1	3.18	1.49	1.43
2	K	1	NAG	O5-C1	3.17	1.49	1.43
2	K	2	NAG	O5-C5	3.10	1.49	1.43
2	J	2	NAG	O5-C5	3.09	1.49	1.43
2	G	2	NAG	O5-C5	3.08	1.49	1.43
2	H	2	NAG	O5-C5	3.07	1.49	1.43
2	I	2	NAG	O5-C5	3.07	1.49	1.43
2	L	2	NAG	O5-C5	3.07	1.49	1.43
2	L	2	NAG	O5-C1	2.70	1.48	1.43
2	K	2	NAG	O5-C1	2.68	1.48	1.43
2	G	2	NAG	O5-C1	2.67	1.48	1.43
2	I	2	NAG	O5-C1	2.66	1.48	1.43
2	H	2	NAG	O5-C1	2.65	1.48	1.43
2	J	2	NAG	O5-C1	2.63	1.48	1.43
2	K	1	NAG	O5-C5	2.01	1.47	1.43

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	C8-C7-N2	-39.08	51.30	116.12
2	J	2	NAG	C8-C7-N2	-39.07	51.33	116.12
2	G	2	NAG	C8-C7-N2	-39.07	51.33	116.12
2	L	2	NAG	C8-C7-N2	-39.06	51.34	116.12
2	K	2	NAG	C8-C7-N2	-39.06	51.34	116.12
2	H	2	NAG	C8-C7-N2	-39.06	51.35	116.12
2	H	1	NAG	C8-C7-N2	-32.47	62.27	116.12
2	I	1	NAG	C8-C7-N2	-32.46	62.28	116.12
2	L	1	NAG	C8-C7-N2	-32.46	62.29	116.12
2	G	1	NAG	C8-C7-N2	-32.44	62.31	116.12
2	J	1	NAG	C8-C7-N2	-32.44	62.31	116.12
2	K	1	NAG	C8-C7-N2	-32.43	62.34	116.12
2	I	1	NAG	O7-C7-C8	30.35	176.10	122.05
2	K	1	NAG	O7-C7-C8	30.35	176.10	122.05
2	L	1	NAG	O7-C7-C8	30.35	176.09	122.05
2	G	1	NAG	O7-C7-C8	30.34	176.08	122.05
2	H	1	NAG	O7-C7-C8	30.34	176.08	122.05
2	J	1	NAG	O7-C7-C8	30.34	176.07	122.05
2	K	2	NAG	O7-C7-C8	21.97	161.17	122.05
2	L	2	NAG	O7-C7-C8	21.97	161.17	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	2	NAG	O7-C7-C8	21.96	161.16	122.05
2	I	2	NAG	O7-C7-C8	21.96	161.16	122.05
2	J	2	NAG	O7-C7-C8	21.95	161.15	122.05
2	G	2	NAG	O7-C7-C8	21.95	161.14	122.05
2	H	1	NAG	C1-C2-N2	8.81	124.31	110.43
2	I	1	NAG	C1-C2-N2	8.81	124.31	110.43
2	L	1	NAG	C1-C2-N2	8.80	124.30	110.43
2	G	1	NAG	C1-C2-N2	8.79	124.29	110.43
2	J	1	NAG	C1-C2-N2	8.79	124.28	110.43
2	K	1	NAG	C1-C2-N2	8.78	124.26	110.43
2	G	2	NAG	O7-C7-N2	-6.86	109.86	121.98
2	H	2	NAG	O7-C7-N2	-6.86	109.86	121.98
2	J	2	NAG	O7-C7-N2	-6.85	109.87	121.98
2	K	2	NAG	O7-C7-N2	-6.85	109.88	121.98
2	L	2	NAG	O7-C7-N2	-6.84	109.89	121.98
2	I	2	NAG	O7-C7-N2	-6.83	109.91	121.98
2	H	2	NAG	C1-C2-N2	5.65	119.34	110.43
2	J	2	NAG	C1-C2-N2	5.64	119.33	110.43
2	G	2	NAG	C1-C2-N2	5.62	119.30	110.43
2	I	2	NAG	C1-C2-N2	5.62	119.29	110.43
2	K	2	NAG	C1-C2-N2	5.60	119.25	110.43
2	L	2	NAG	C1-C2-N2	5.59	119.24	110.43
2	J	1	NAG	O5-C1-C2	-5.57	102.67	111.29
2	G	1	NAG	O5-C1-C2	-5.54	102.72	111.29
2	H	1	NAG	O5-C1-C2	-5.53	102.73	111.29
2	K	1	NAG	O5-C1-C2	-5.53	102.73	111.29
2	L	1	NAG	O5-C1-C2	-5.53	102.74	111.29
2	I	1	NAG	O5-C1-C2	-5.52	102.75	111.29
2	K	2	NAG	C1-O5-C5	-5.12	105.33	112.19
2	H	2	NAG	C1-O5-C5	-5.11	105.34	112.19
2	G	2	NAG	C1-O5-C5	-5.11	105.34	112.19
2	I	2	NAG	C1-O5-C5	-5.10	105.36	112.19
2	L	2	NAG	C1-O5-C5	-5.08	105.38	112.19
2	J	2	NAG	C1-O5-C5	-5.08	105.38	112.19
2	L	1	NAG	C3-C4-C5	4.39	118.19	110.23
2	I	2	NAG	O5-C1-C2	-4.39	104.50	111.29
2	I	1	NAG	C3-C4-C5	4.39	118.18	110.23
2	L	2	NAG	O5-C1-C2	-4.39	104.51	111.29
2	G	1	NAG	C3-C4-C5	4.37	118.16	110.23
2	K	2	NAG	O5-C1-C2	-4.37	104.53	111.29
2	K	1	NAG	C3-C4-C5	4.37	118.16	110.23
2	J	1	NAG	C3-C4-C5	4.37	118.15	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	NAG	O5-C1-C2	-4.37	104.54	111.29
2	H	1	NAG	C3-C4-C5	4.37	118.15	110.23
2	G	2	NAG	O5-C1-C2	-4.36	104.55	111.29
2	H	2	NAG	O5-C1-C2	-4.33	104.58	111.29
2	K	1	NAG	C1-O5-C5	-3.50	107.50	112.19
2	H	1	NAG	C1-O5-C5	-3.49	107.51	112.19
2	G	1	NAG	C1-O5-C5	-3.48	107.52	112.19
2	J	1	NAG	C1-O5-C5	-3.48	107.53	112.19
2	L	1	NAG	C1-O5-C5	-3.46	107.55	112.19
2	I	1	NAG	C1-O5-C5	-3.45	107.56	112.19
2	J	1	NAG	O7-C7-N2	-3.19	116.34	121.98
2	K	1	NAG	O7-C7-N2	-3.19	116.34	121.98
2	G	1	NAG	O7-C7-N2	-3.18	116.36	121.98
2	L	1	NAG	O7-C7-N2	-3.17	116.38	121.98
2	H	1	NAG	O7-C7-N2	-3.16	116.40	121.98
2	I	1	NAG	O7-C7-N2	-3.15	116.41	121.98
2	K	1	NAG	C2-N2-C7	2.99	126.91	122.90
2	J	1	NAG	C2-N2-C7	2.98	126.89	122.90
2	G	1	NAG	C2-N2-C7	2.96	126.87	122.90
2	L	1	NAG	C2-N2-C7	2.94	126.84	122.90
2	H	1	NAG	C2-N2-C7	2.92	126.81	122.90
2	I	1	NAG	C2-N2-C7	2.92	126.81	122.90
2	J	2	NAG	O3-C3-C4	-2.91	103.51	110.38
2	G	2	NAG	O3-C3-C4	-2.91	103.51	110.38
2	K	2	NAG	O3-C3-C4	-2.91	103.52	110.38
2	I	2	NAG	O3-C3-C4	-2.91	103.52	110.38
2	K	1	NAG	O4-C4-C3	-2.91	103.52	110.38
2	L	2	NAG	O3-C3-C4	-2.91	103.53	110.38
2	H	2	NAG	O3-C3-C4	-2.90	103.53	110.38
2	I	1	NAG	O4-C4-C3	-2.90	103.53	110.38
2	L	1	NAG	O4-C4-C3	-2.90	103.53	110.38
2	J	1	NAG	O4-C4-C3	-2.90	103.55	110.38
2	G	1	NAG	O4-C4-C3	-2.90	103.55	110.38
2	H	1	NAG	O4-C4-C3	-2.89	103.57	110.38
2	I	1	NAG	O6-C6-C5	-2.82	101.74	111.33
2	H	1	NAG	O6-C6-C5	-2.81	101.75	111.33
2	G	1	NAG	O6-C6-C5	-2.81	101.76	111.33
2	J	1	NAG	O6-C6-C5	-2.81	101.76	111.33
2	L	1	NAG	O6-C6-C5	-2.81	101.76	111.33
2	K	1	NAG	O6-C6-C5	-2.80	101.79	111.33
2	K	1	NAG	C4-C3-C2	2.78	115.09	111.02
2	H	1	NAG	C4-C3-C2	2.77	115.08	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	1	NAG	C4-C3-C2	2.76	115.06	111.02
2	G	1	NAG	C4-C3-C2	2.75	115.06	111.02
2	J	1	NAG	C4-C3-C2	2.75	115.04	111.02
2	I	1	NAG	C4-C3-C2	2.74	115.04	111.02
2	K	1	NAG	C6-C5-C4	2.47	119.09	113.02
2	H	1	NAG	C6-C5-C4	2.47	119.08	113.02
2	J	1	NAG	C6-C5-C4	2.46	119.06	113.02
2	L	1	NAG	C6-C5-C4	2.46	119.06	113.02
2	G	1	NAG	C6-C5-C4	2.46	119.05	113.02
2	I	1	NAG	C6-C5-C4	2.45	119.03	113.02

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1
2	H	1	NAG	C1
2	I	1	NAG	C1
2	J	1	NAG	C1
2	K	1	NAG	C1
2	L	1	NAG	C1

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7
2	K	1	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7

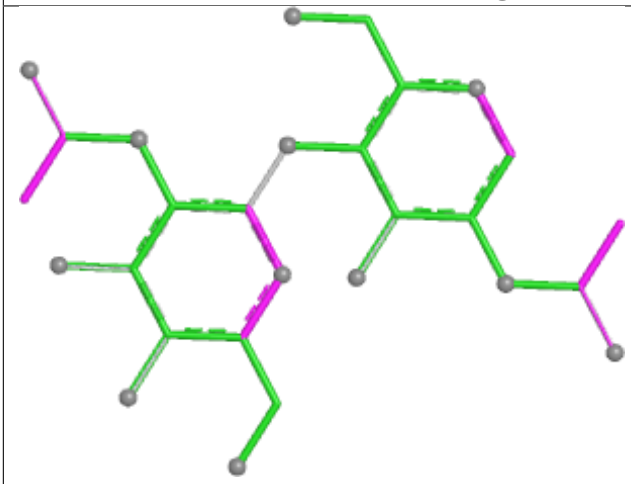
There are no ring outliers.

12 monomers are involved in 36 short contacts:

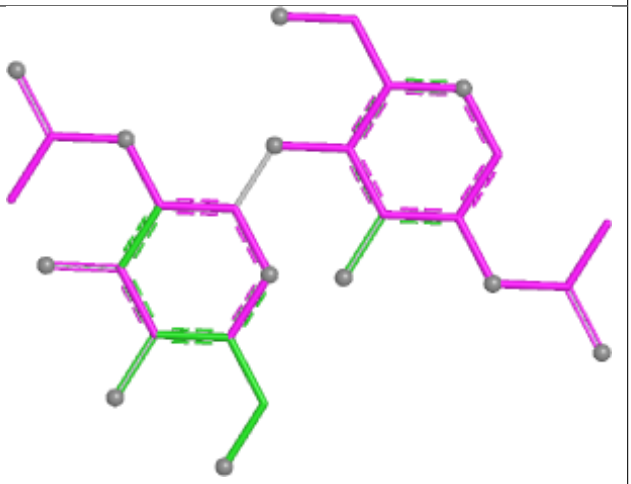
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	4	0
2	H	1	NAG	4	0
2	H	2	NAG	2	0
2	J	2	NAG	2	0
2	G	1	NAG	4	0
2	L	2	NAG	2	0
2	I	1	NAG	4	0
2	G	2	NAG	2	0
2	I	2	NAG	2	0
2	K	2	NAG	2	0
2	L	1	NAG	4	0
2	K	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

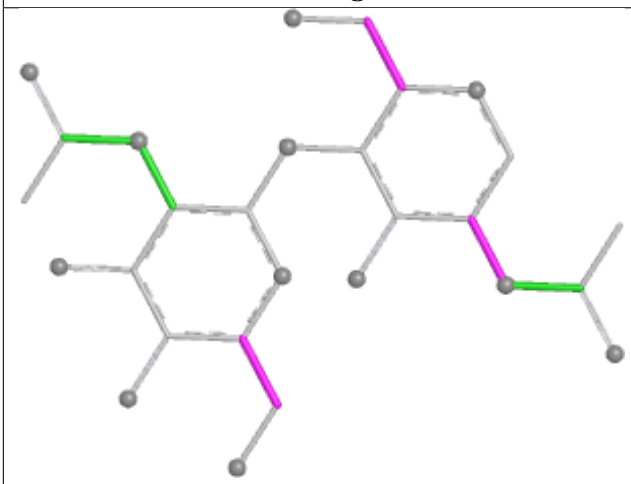
Oligosaccharide Chain G



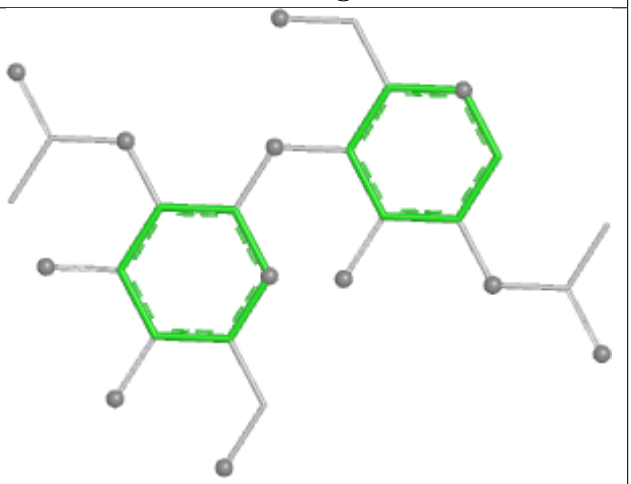
Bond lengths



Bond angles

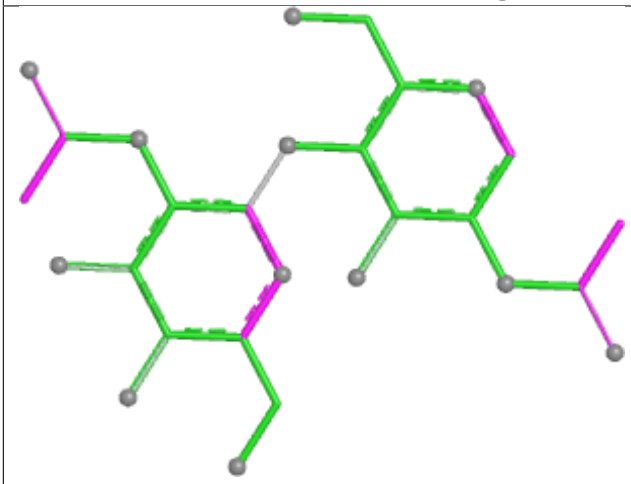


Torsions

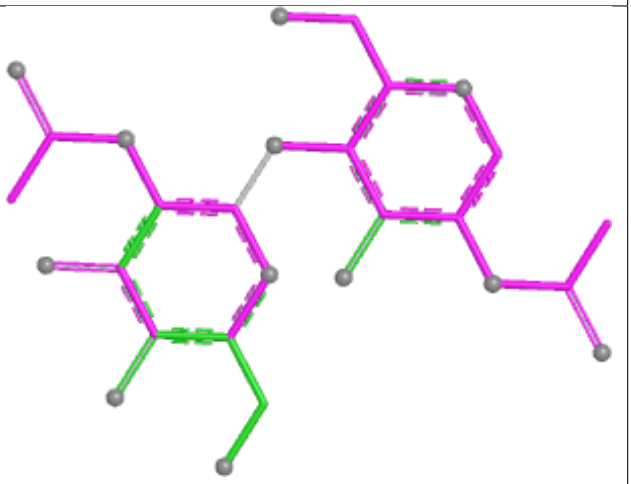


Rings

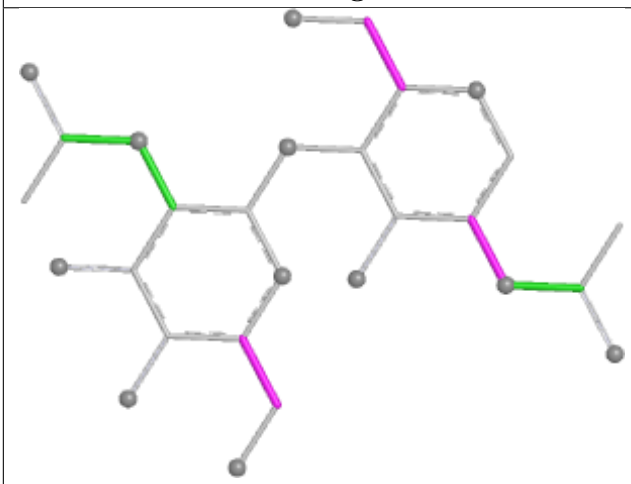
Oligosaccharide Chain H



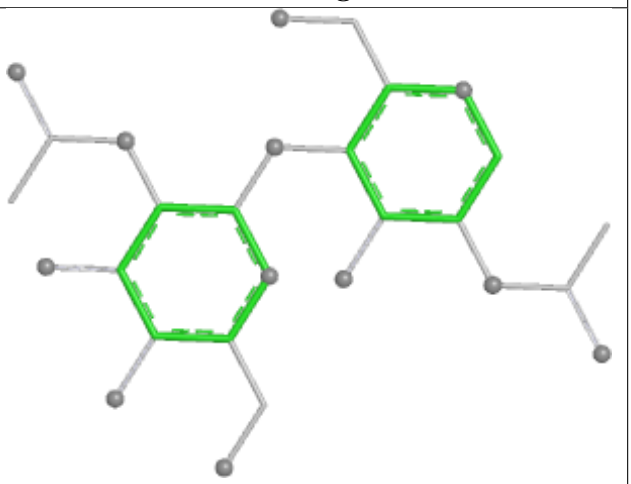
Bond lengths



Bond angles

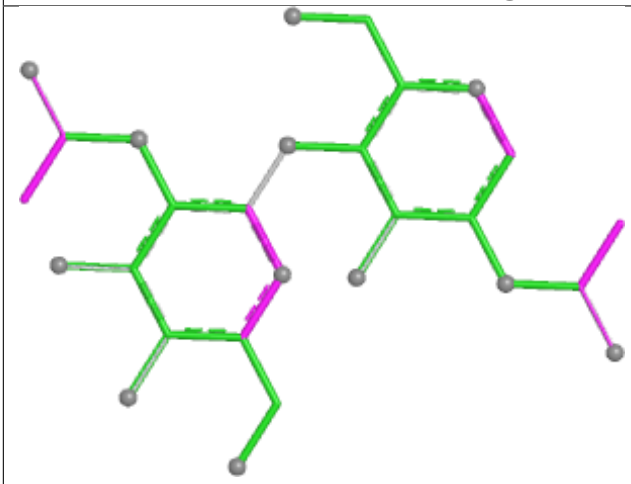


Torsions

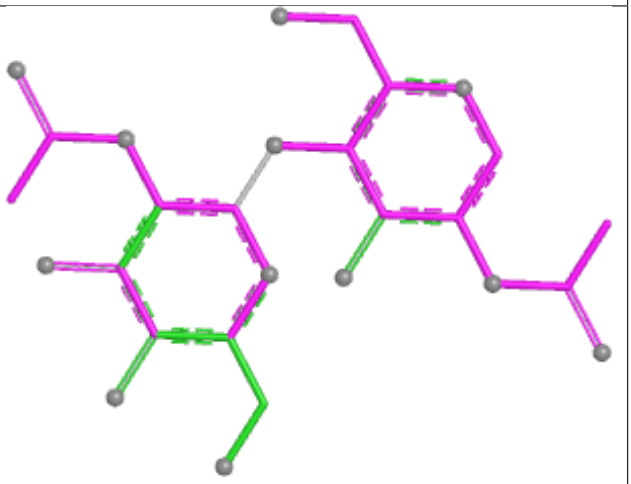


Rings

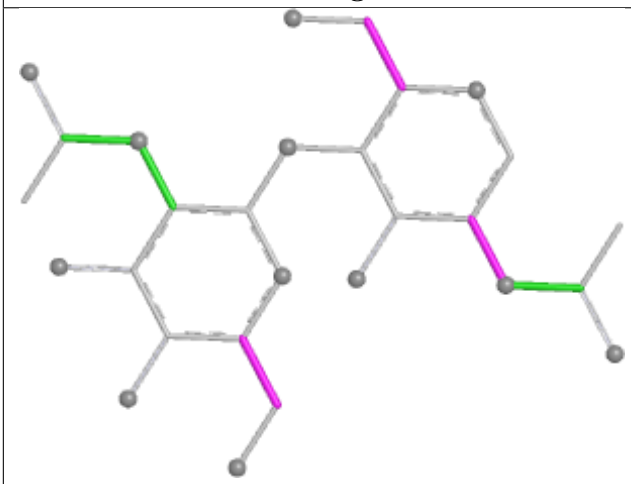
Oligosaccharide Chain I



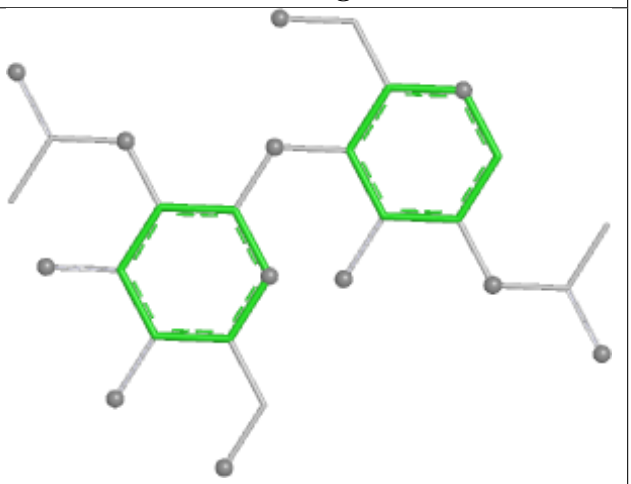
Bond lengths



Bond angles

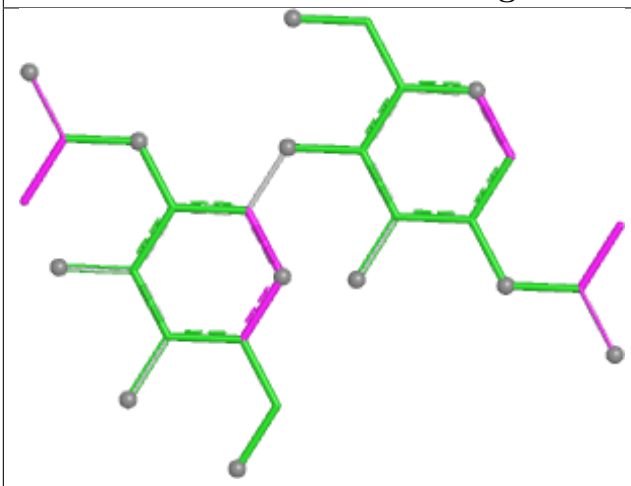


Torsions

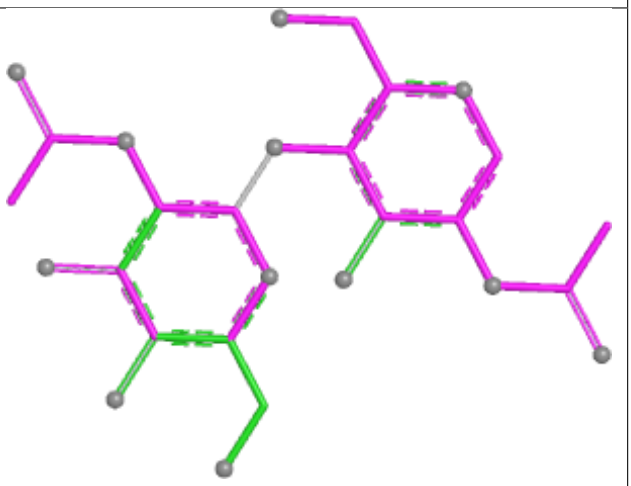


Rings

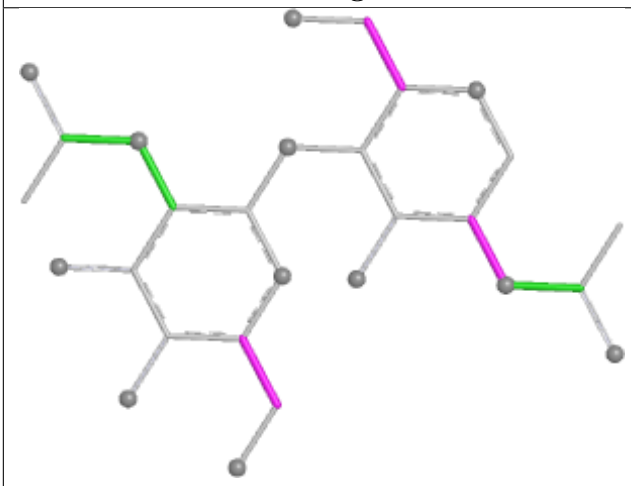
Oligosaccharide Chain J



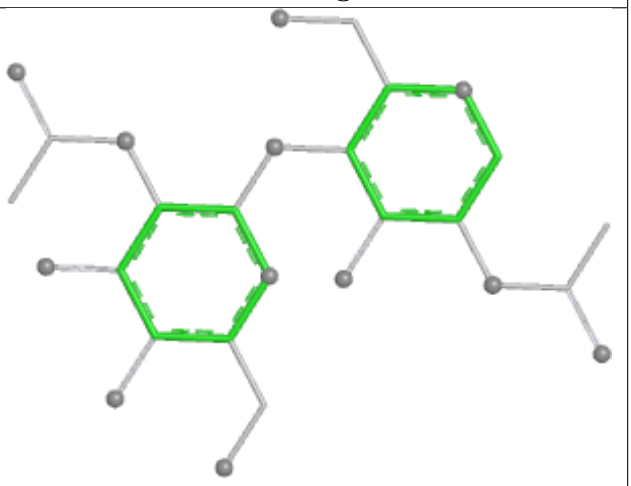
Bond lengths



Bond angles

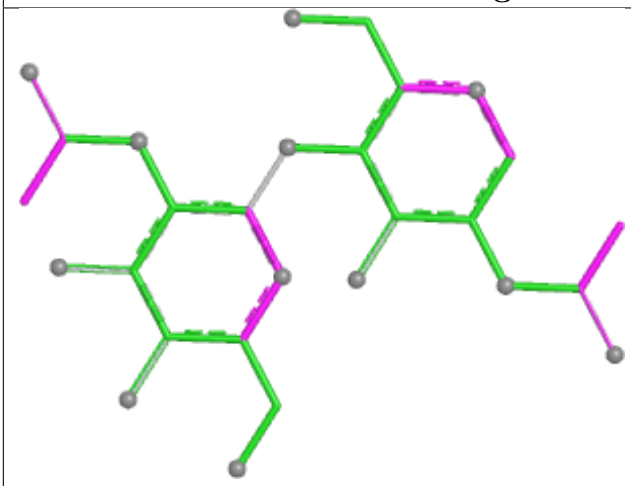


Torsions

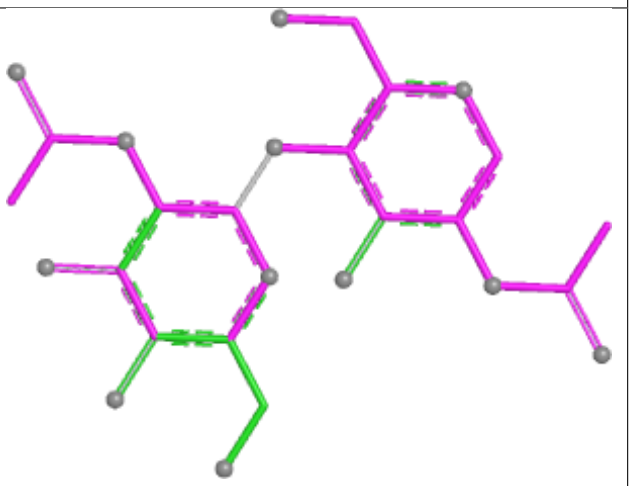


Rings

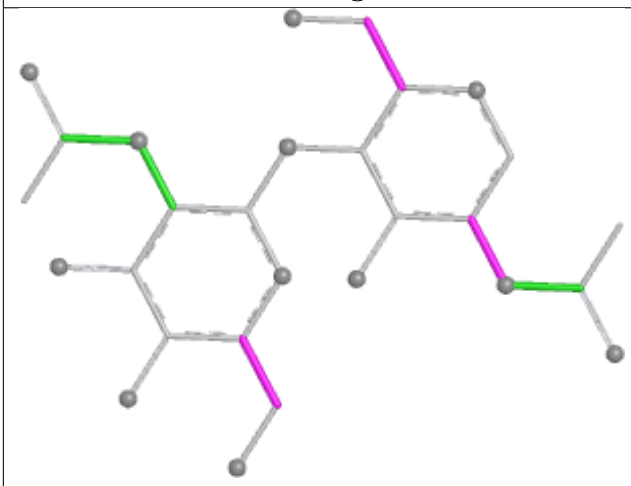
Oligosaccharide Chain K



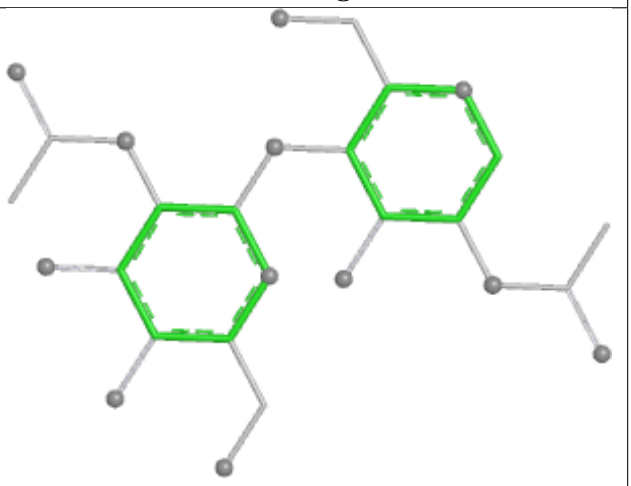
Bond lengths



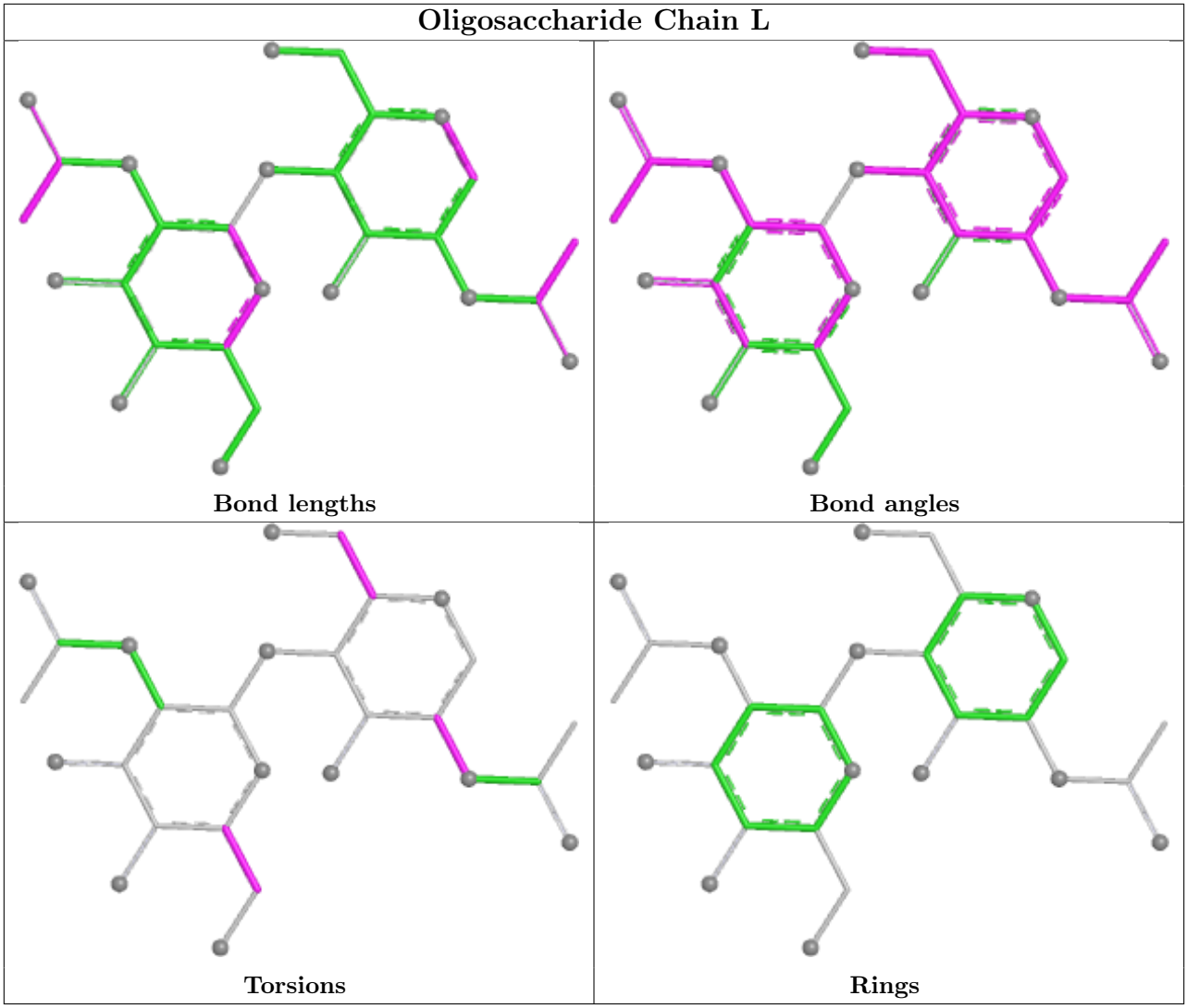
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	644/657 (98%)	-0.33	3 (0%)	87	76	2, 11, 53, 85	0
1	B	644/657 (98%)	-0.23	7 (1%)	78	61	2, 11, 53, 85	0
1	C	644/657 (98%)	-0.17	8 (1%)	76	58	2, 11, 53, 85	0
1	D	644/657 (98%)	-0.19	10 (1%)	70	51	2, 11, 53, 85	0
1	E	644/657 (98%)	-0.23	5 (0%)	82	67	2, 11, 53, 85	0
1	F	644/657 (98%)	-0.23	9 (1%)	73	54	2, 11, 53, 85	0
All	All	3864/3942 (98%)	-0.23	42 (1%)	78	61	2, 11, 54, 85	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	548	ASN	4.7
1	A	3	LEU	4.0
1	C	1	ASP	4.0
1	F	2	ALA	4.0
1	C	640	SER	3.9
1	A	2	ALA	3.5
1	B	2	ALA	3.2
1	D	549	GLY	2.9
1	D	551	HIS	2.8
1	D	2	ALA	2.8
1	B	3	LEU	2.6
1	E	551	HIS	2.5
1	D	546	ALA	2.5
1	B	548	ASN	2.5
1	E	1	ASP	2.5
1	D	548	ASN	2.5
1	F	551	HIS	2.5
1	B	554	ASP	2.4
1	D	442	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	551	HIS	2.4
1	F	472	GLY	2.4
1	F	607	ALA	2.4
1	F	520	GLU	2.4
1	C	471	ASP	2.3
1	C	554	ASP	2.3
1	E	172	GLY	2.3
1	C	608	GLN	2.3
1	C	518	THR	2.2
1	D	513	PRO	2.2
1	C	2	ALA	2.2
1	A	172	GLY	2.2
1	D	1	ASP	2.2
1	D	559	GLU	2.1
1	F	594	GLU	2.1
1	B	561	SER	2.1
1	B	590	ASP	2.1
1	E	471	ASP	2.1
1	B	442	ASN	2.0
1	D	554	ASP	2.0
1	F	1	ASP	2.0
1	F	38	ASN	2.0
1	E	173	THR	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	J	2	14/15	0.47	0.20	73,82,87,89	0
2	NAG	L	2	14/15	0.60	0.18	73,82,87,89	0
2	NAG	J	1	14/15	0.63	0.18	52,57,68,70	0
2	NAG	I	2	14/15	0.65	0.23	73,82,87,89	0
2	NAG	G	2	14/15	0.66	0.15	73,82,87,89	0

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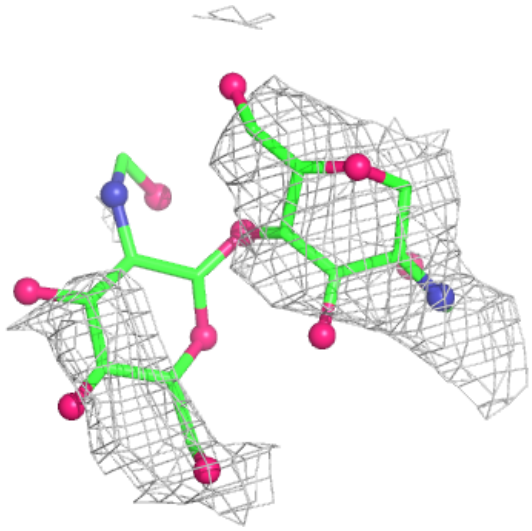
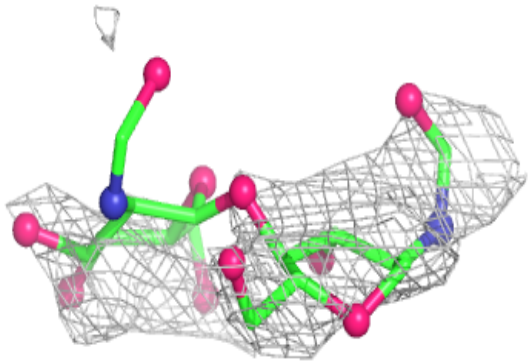
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	H	2	14/15	0.66	0.18	73,82,87,89	0
2	NAG	K	2	14/15	0.68	0.18	73,82,87,89	0
2	NAG	H	1	14/15	0.71	0.13	52,57,68,70	0
2	NAG	L	1	14/15	0.77	0.13	52,57,68,70	0
2	NAG	K	1	14/15	0.78	0.15	52,57,68,70	0
2	NAG	G	1	14/15	0.78	0.12	52,57,68,70	0
2	NAG	I	1	14/15	0.80	0.12	52,57,68,70	0

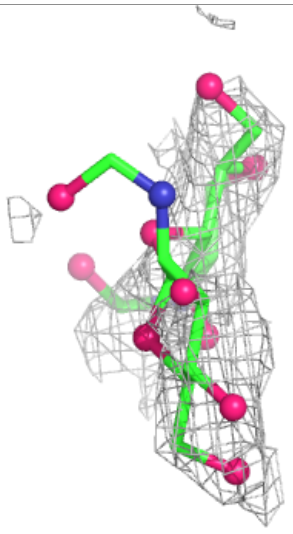
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

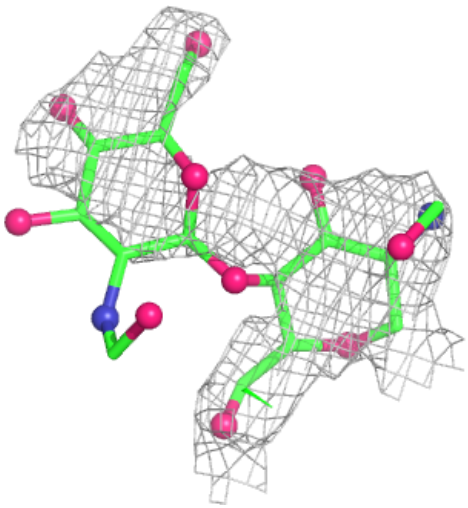


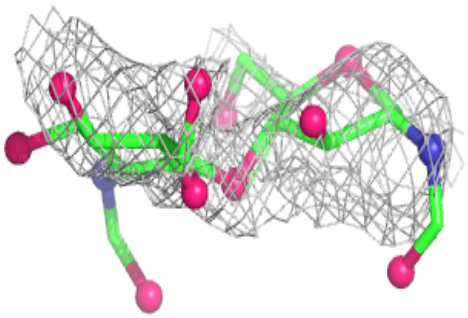


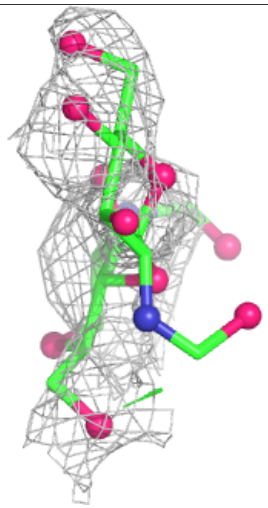


Electron density around Chain H:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

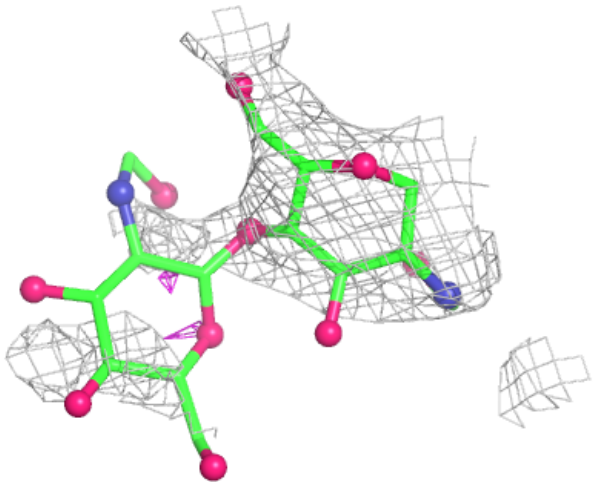


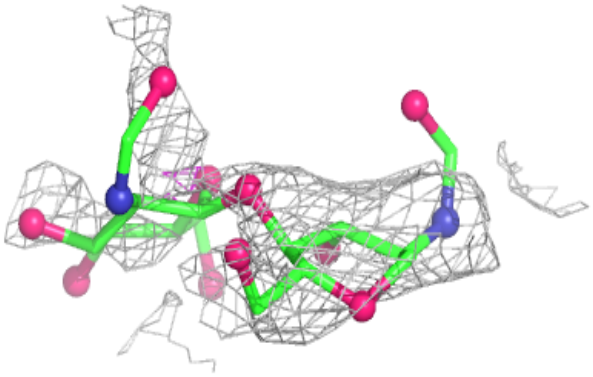


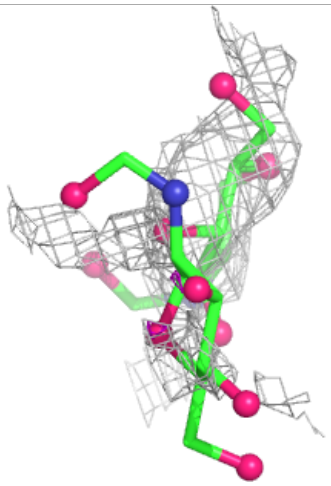


Electron density around Chain I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

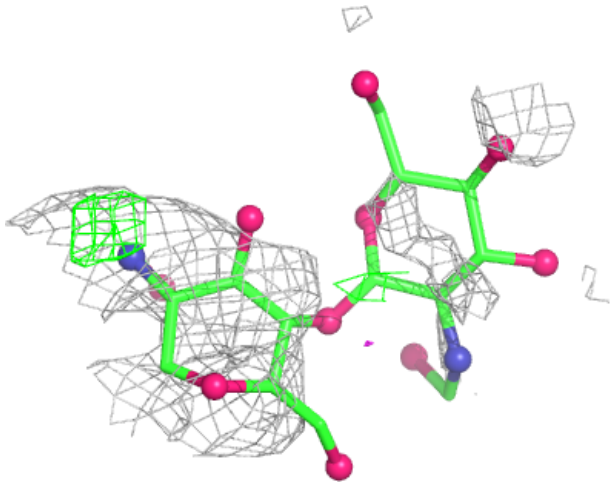


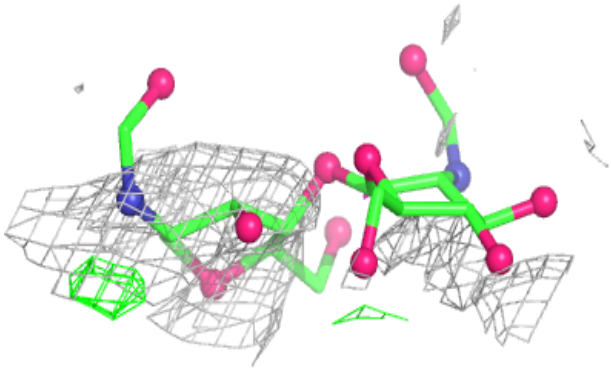


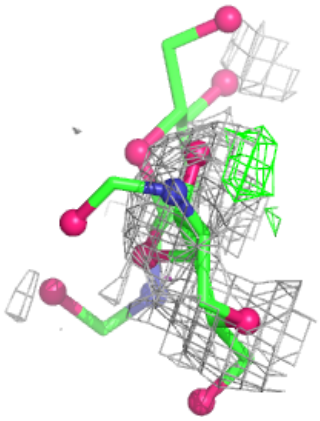


Electron density around Chain J:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

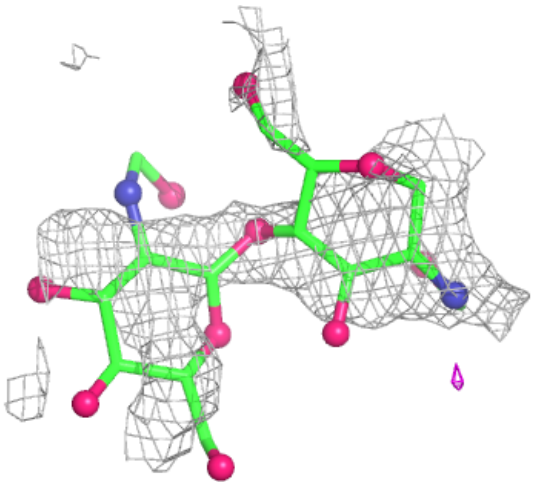


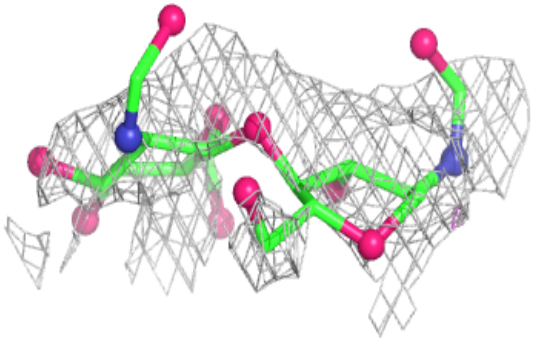


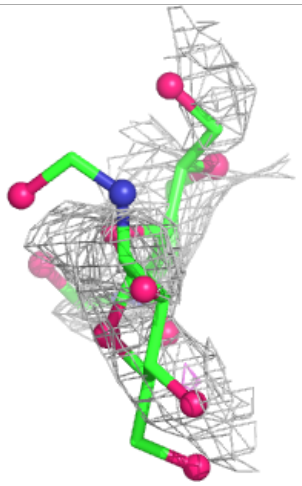


Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

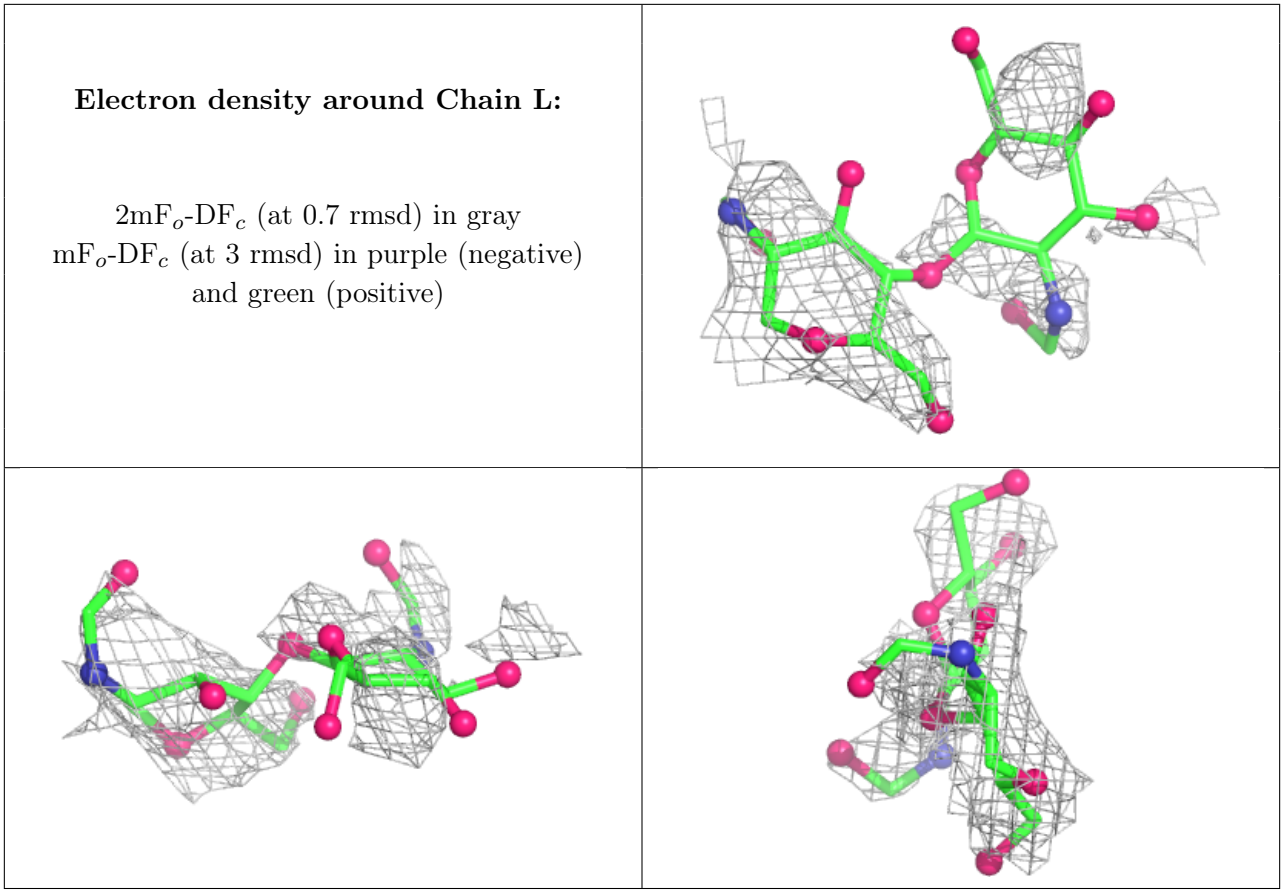






Electron density around Chain L:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CU	A	666	1/1	0.96	0.03	10,10,10,10	0
3	CU	A	665	1/1	0.98	0.03	9,9,9,9	0

6.5 Other polymers

There are no such residues in this entry.