



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:05 PM UTC

PDB ID : 1QO5 / pdb_00001qo5
Title : Fructose 1,6-bisphosphate Aldolase from Human Liver Tissue
Authors : Dalby, A.R.; Littlechild, J.A.
Deposited on : 1999-11-03
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

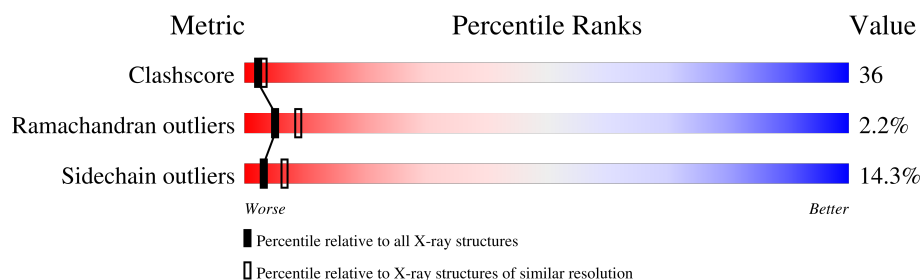
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

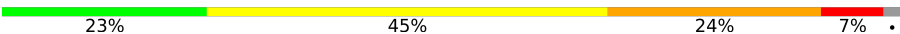
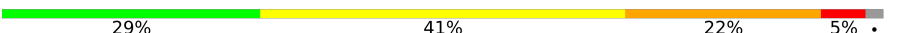
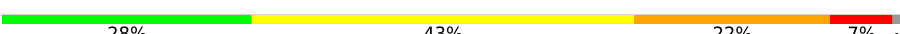
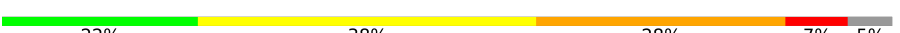
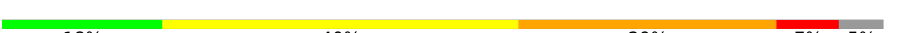
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	
1	F	363	
1	G	363	
1	H	363	

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Mol	Chain	Length	Quality of chain
1	I	363	
1	J	363	
1	K	363	
1	L	363	
1	M	363	
1	N	363	
1	O	363	
1	P	363	
1	Q	363	
1	R	363	

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	SO4	A	401	-	-	X	-
2	SO4	A	402	-	-	X	-
2	SO4	D	400	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49278 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 FRUCTOSE-BISPHOSPHATE ALDOLASE B.

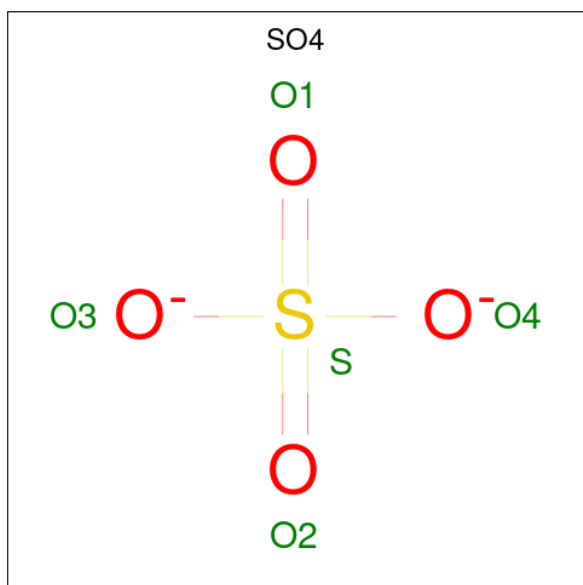
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2730	1708	486	521	15			
1	B	348	Total	C	N	O	S	0	0	0
			2651	1660	473	504	14			
1	C	345	Total	C	N	O	S	0	0	0
			2635	1652	470	499	14			
1	D	356	Total	C	N	O	S	0	0	0
			2701	1689	482	516	14			
1	E	354	Total	C	N	O	S	0	0	0
			2687	1680	480	513	14			
1	F	353	Total	C	N	O	S	0	0	0
			2675	1674	474	513	14			
1	G	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	H	357	Total	C	N	O	S	0	0	0
			2712	1698	483	517	14			
1	I	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	J	356	Total	C	N	O	S	0	0	0
			2701	1689	482	516	14			
1	K	354	Total	C	N	O	S	0	0	0
			2686	1683	475	514	14			
1	L	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	M	360	Total	C	N	O	S	29	0	0
			2730	1708	486	521	15			
1	N	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	O	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	P	360	Total	C	N	O	S	0	0	0
			2730	1708	486	521	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	R	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	M	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		

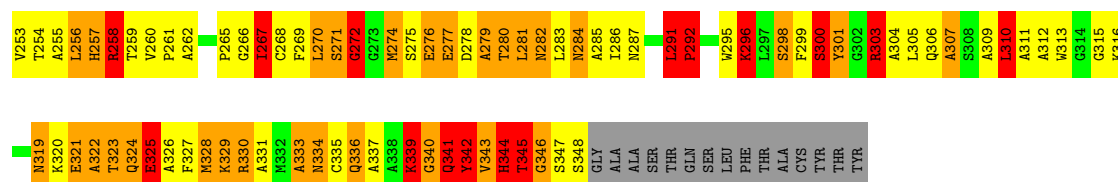
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	34	Total	O	0	0
			34	34		
3	C	44	Total	O	0	0
			44	44		
3	D	82	Total	O	0	0
			82	82		
3	E	75	Total	O	0	0
			75	75		
3	F	80	Total	O	0	0
			80	80		
3	G	75	Total	O	0	0
			75	75		
3	H	70	Total	O	0	0
			70	70		
3	I	45	Total	O	0	0
			45	45		
3	J	78	Total	O	0	0
			78	78		
3	K	71	Total	O	0	0
			71	71		
3	L	28	Total	O	0	0
			28	28		
3	M	81	Total	O	0	0
			81	81		

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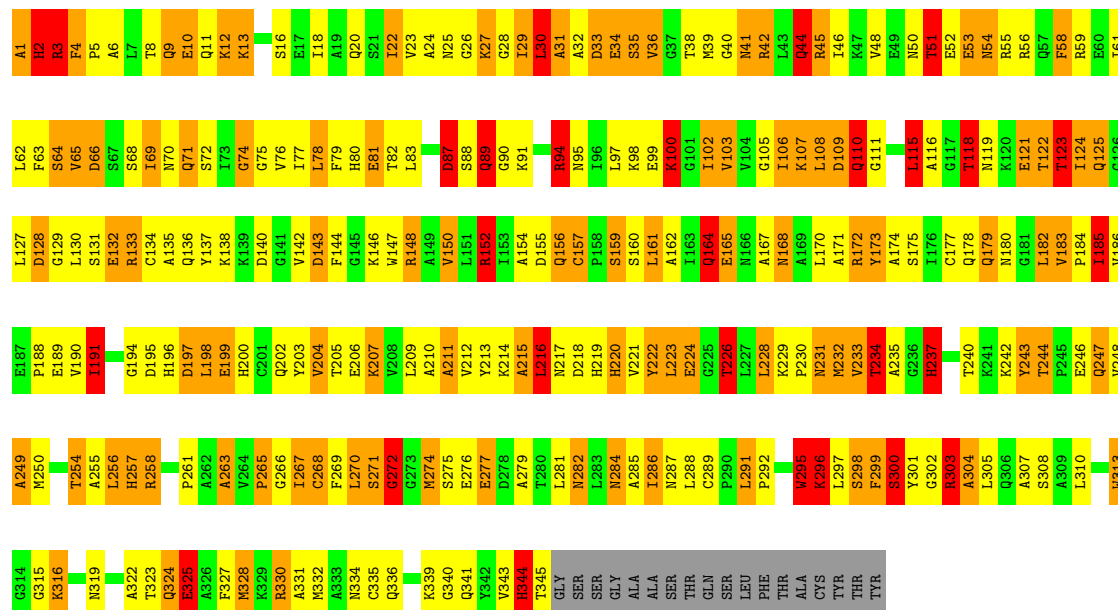
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	53	Total 53	O 53	0	0
3	O	37	Total 37	O 37	0	0
3	P	78	Total 78	O 78	0	0
3	Q	80	Total 80	O 80	0	0
3	R	72	Total 72	O 72	0	0



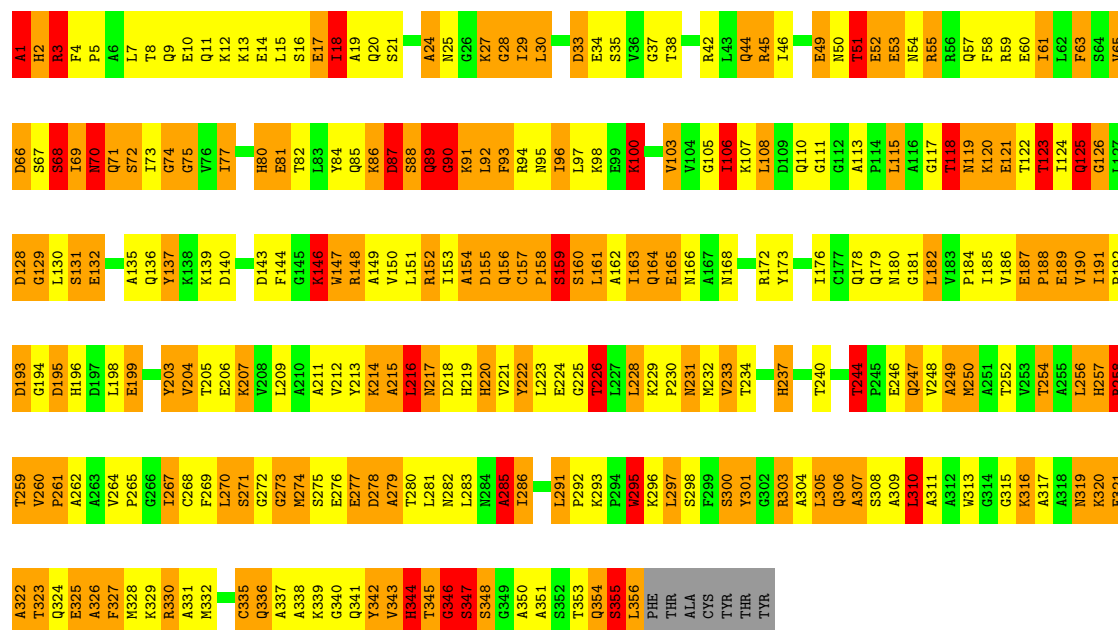
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain C: 22% 38% 27% 8% 5%

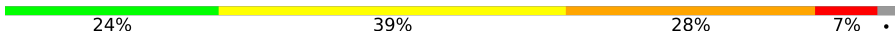


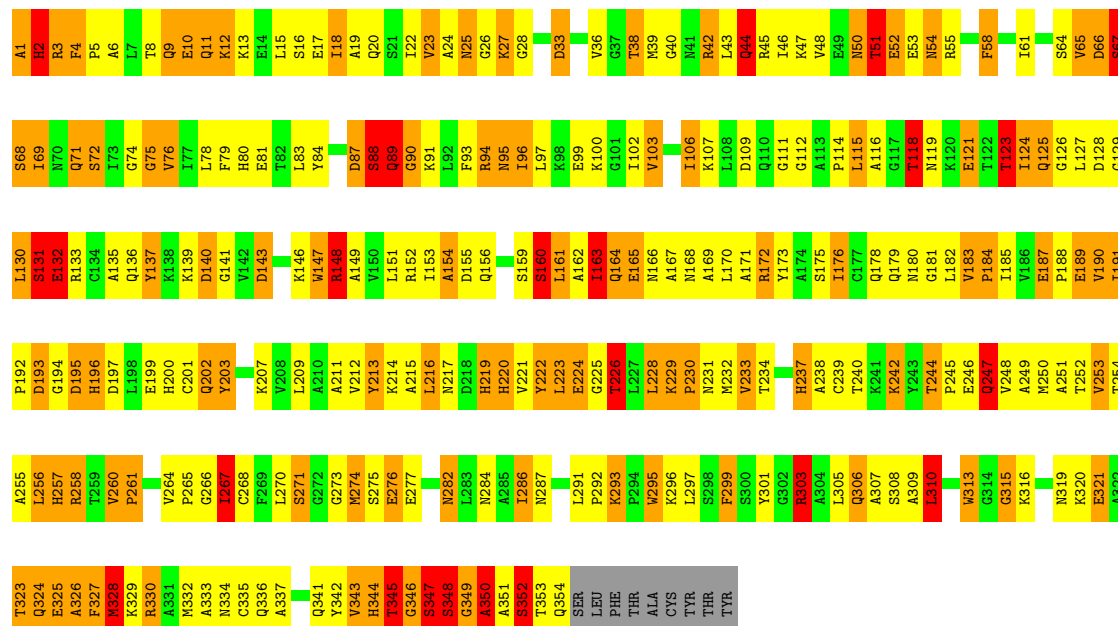
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain D: 21% 36% 34% 7%

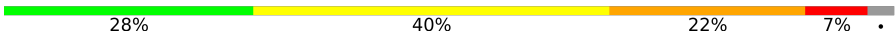


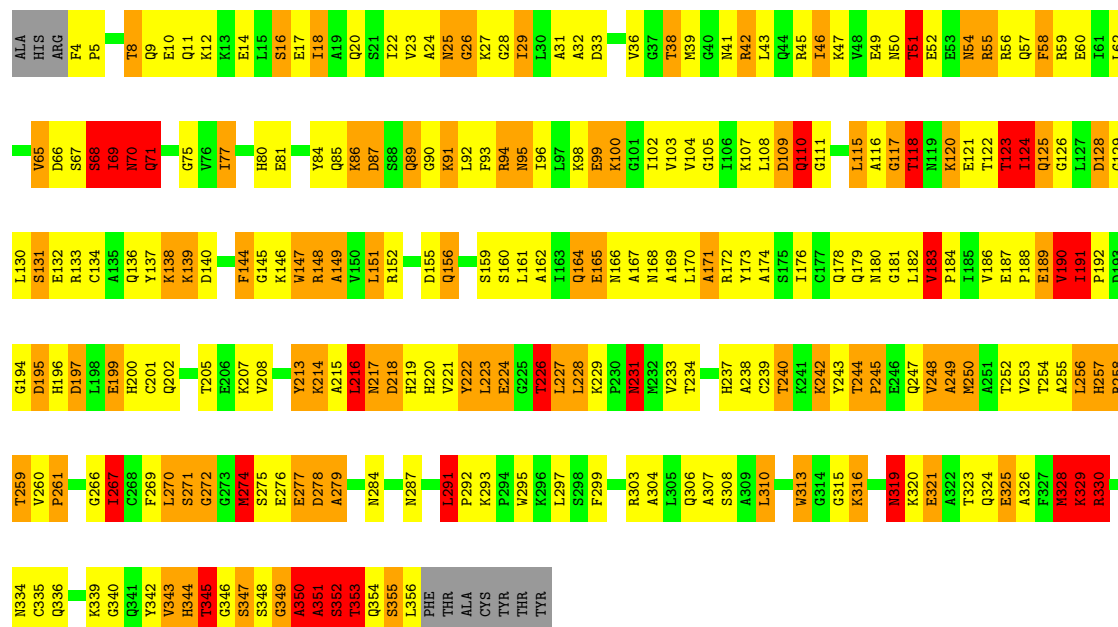
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain E:  24% 39% 28% 7%

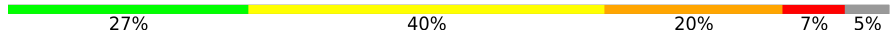


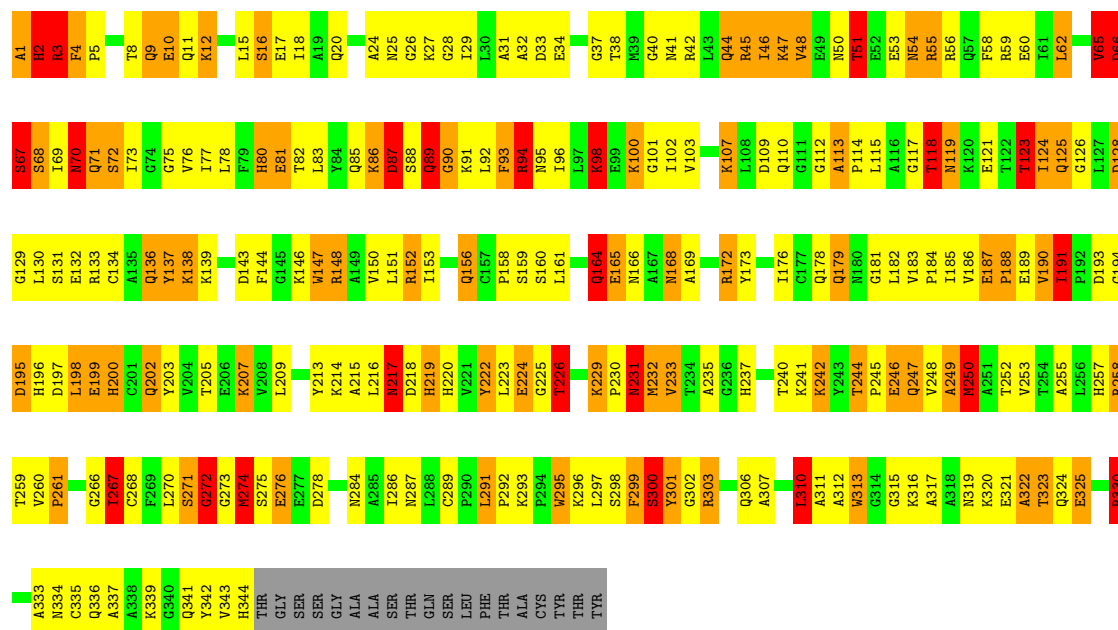
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain F:  28% 40% 22% 7%



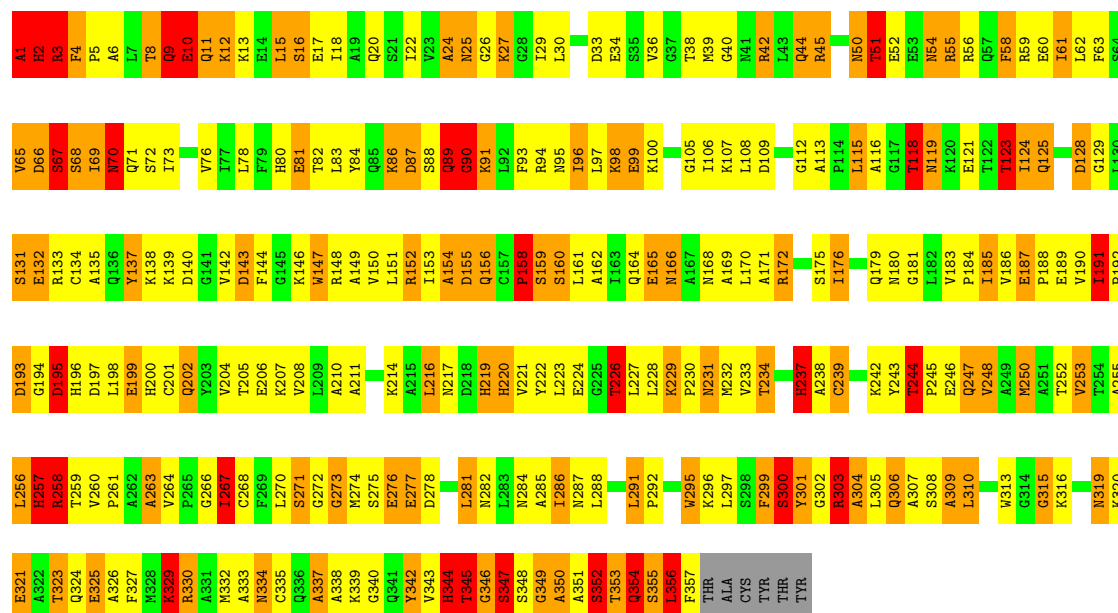
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain G:  27% 40% 20% 7% 5%



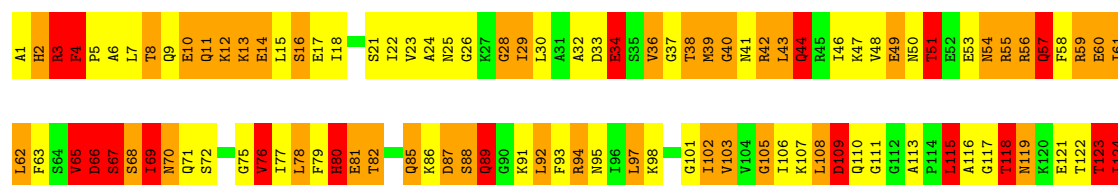
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

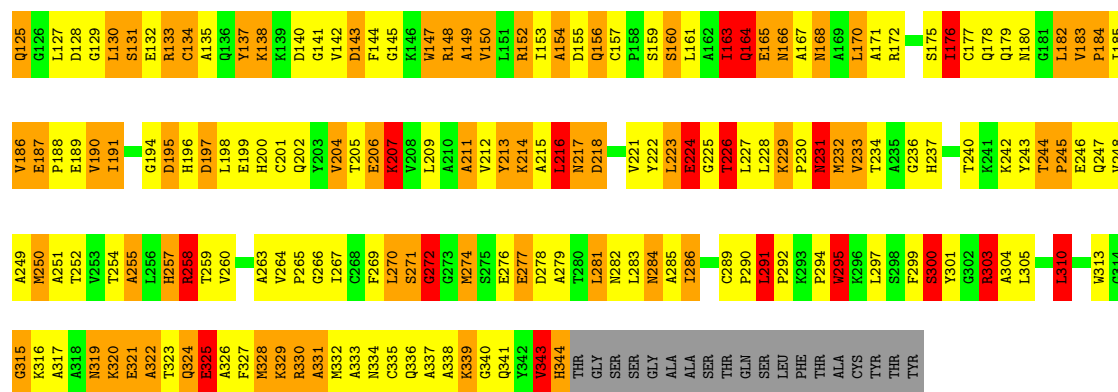
Chain H: 23% 41% 26% 8% .



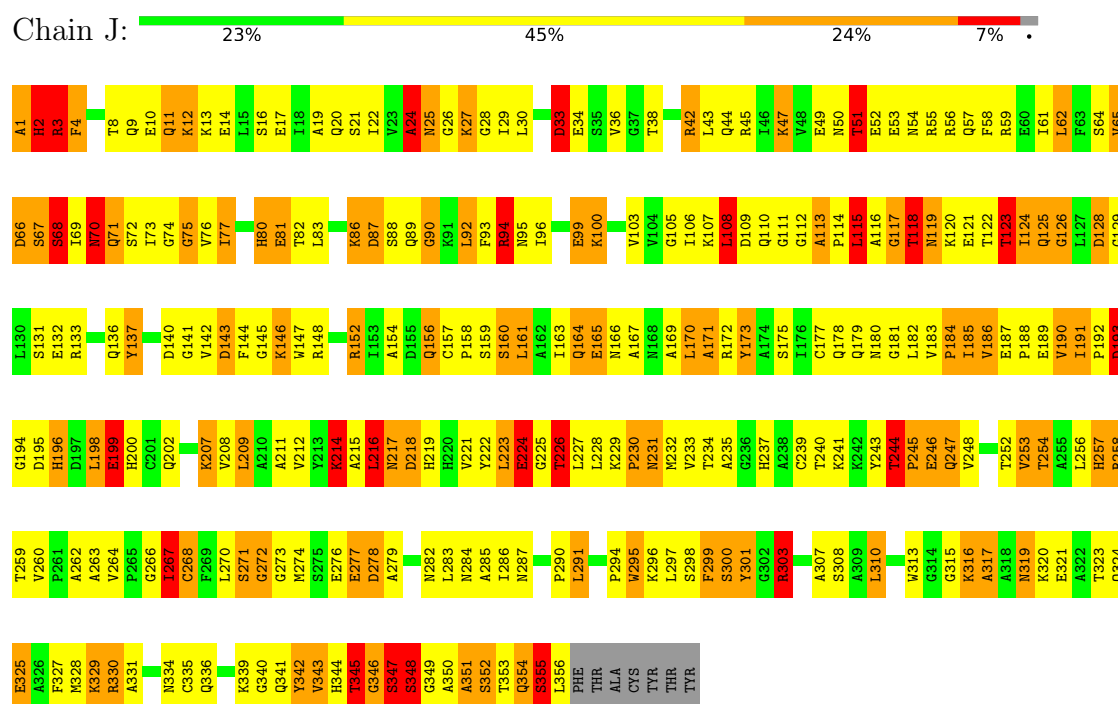
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

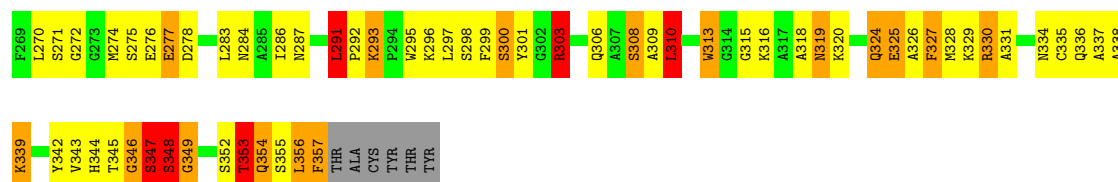
Chain I: 18% 39% 29% 10% 5%





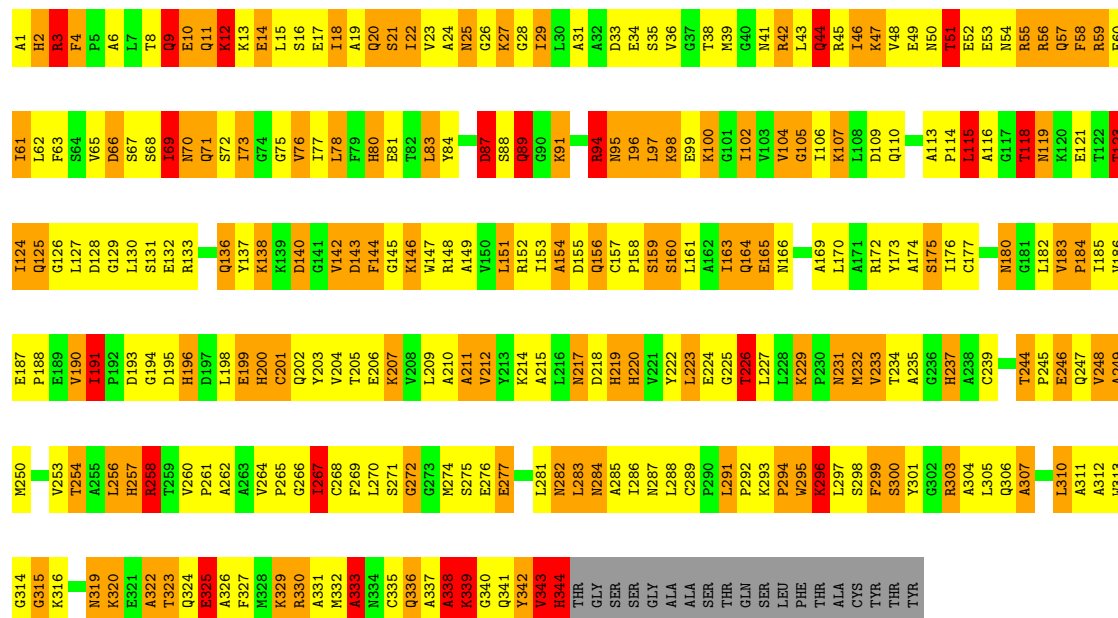
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B





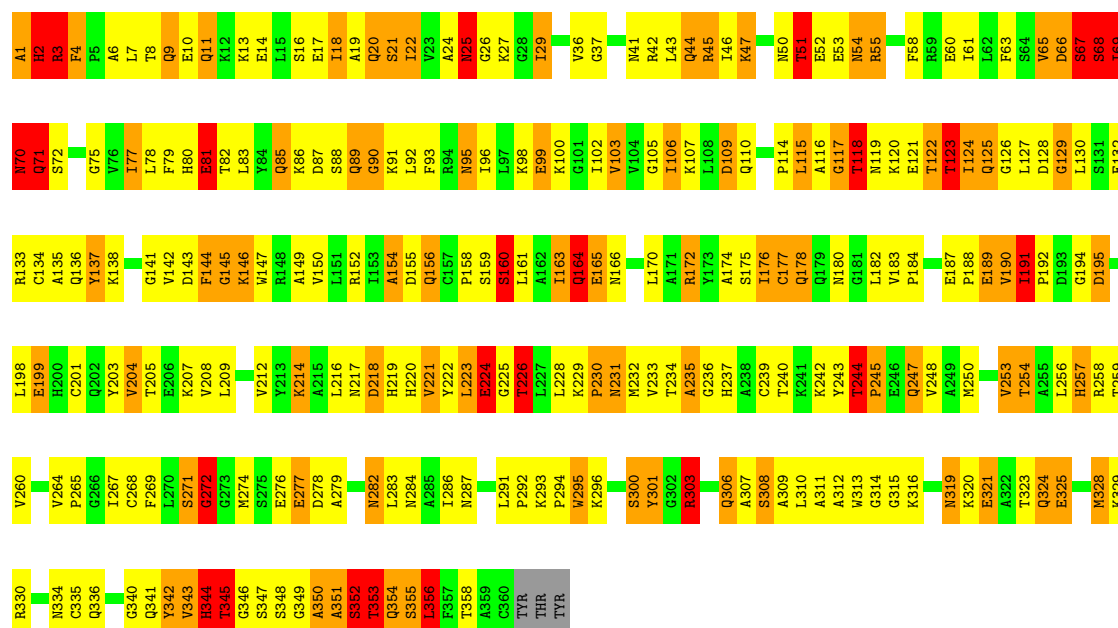
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain L: 19% 40% 29% 6% 5%



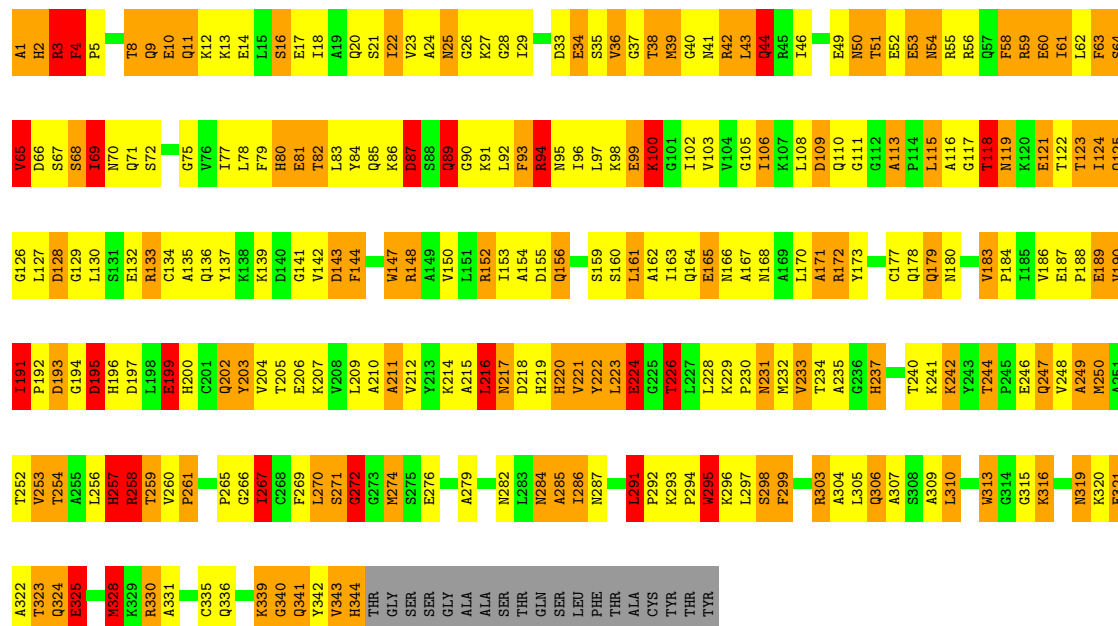
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain M: 28% 43% 22% 7%



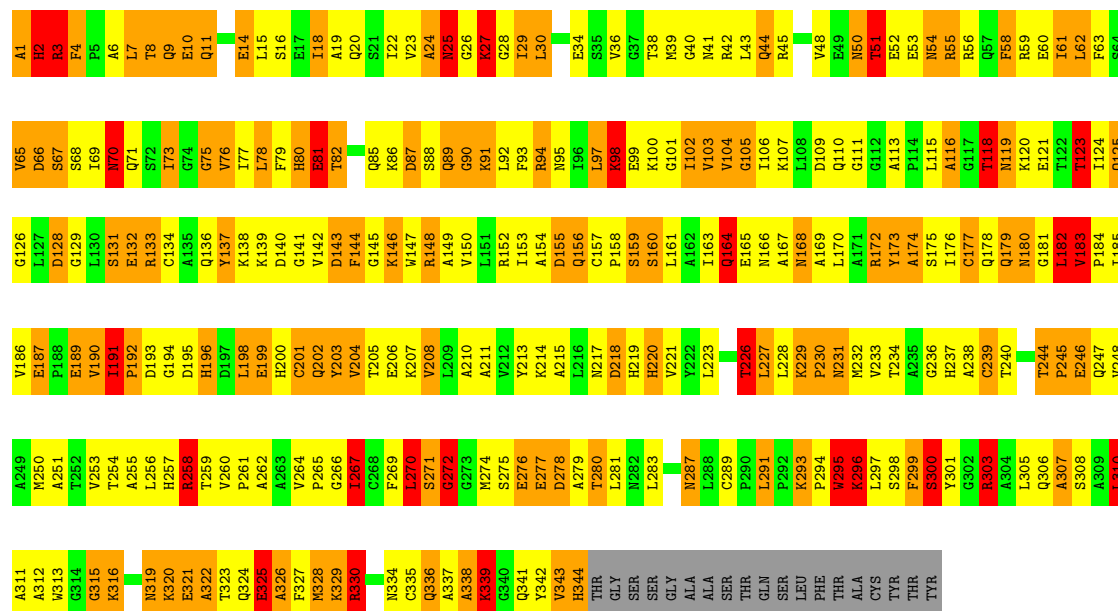
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain N:



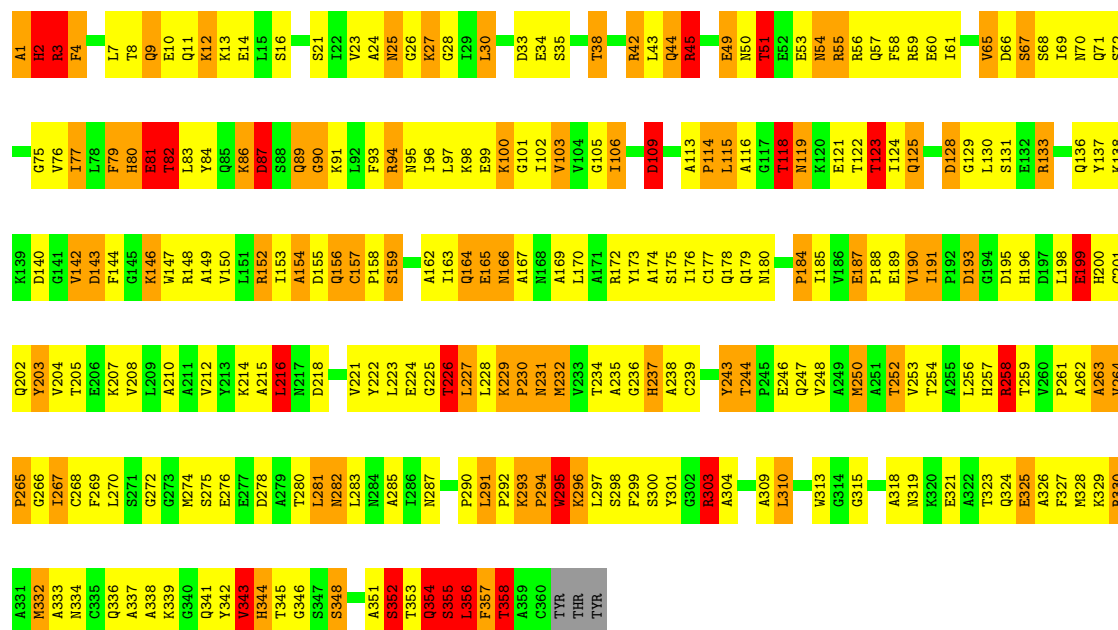
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain O:



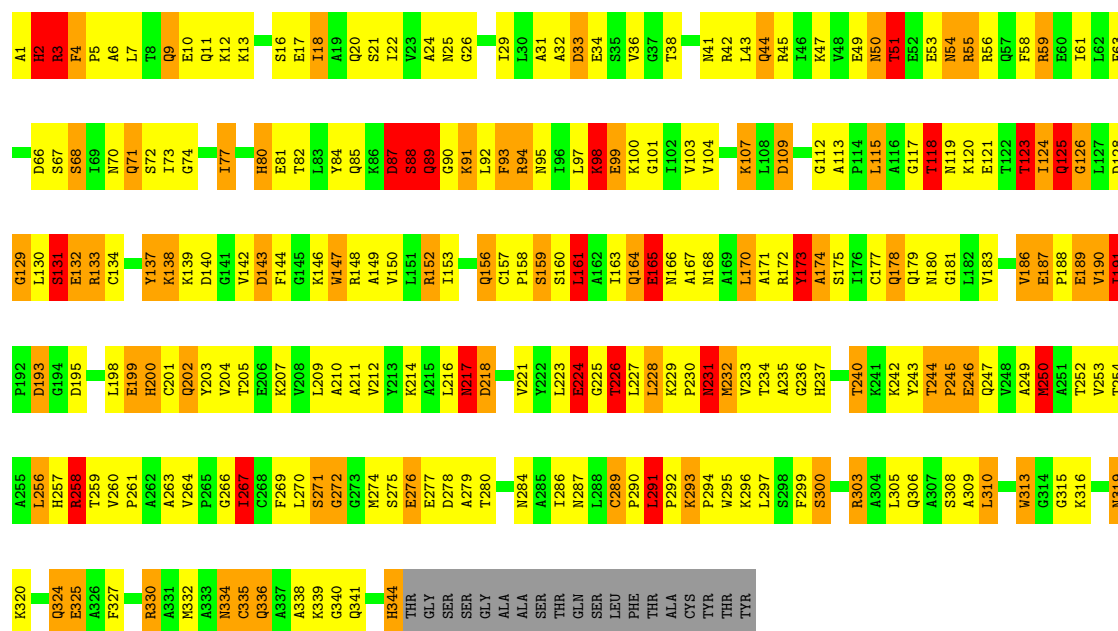
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain P:



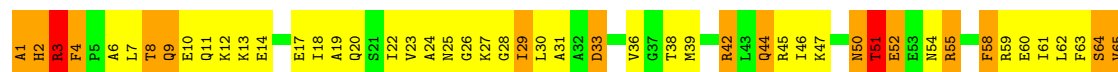
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

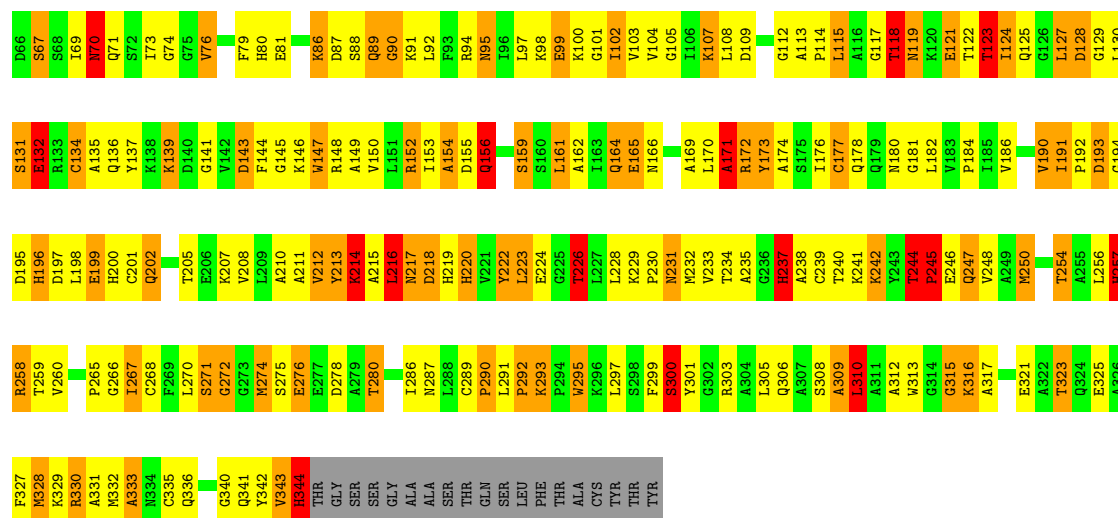
Chain Q: 27% 42% 19% 6% 5%



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain R: 27% 40% 22% 5% 5%





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	291.10Å 489.84Å 103.36Å 90.00° 103.68° 90.00°	Depositor
Resolution (Å)	29.00 – 2.50	Depositor
% Data completeness (in resolution range)	71.0 (29.00-2.50)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	0.12	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	49278	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.51	22/2776 (0.8%)	3.29	395/3754 (10.5%)
1	B	1.79	56/2696 (2.1%)	3.58	525/3645 (14.4%)
1	C	1.34	5/2680 (0.2%)	3.27	404/3624 (11.1%)
1	D	1.69	34/2746 (1.2%)	3.59	488/3713 (13.1%)
1	E	1.44	16/2732 (0.6%)	3.57	434/3694 (11.7%)
1	F	1.36	9/2719 (0.3%)	3.25	380/3677 (10.3%)
1	G	1.40	15/2673 (0.6%)	3.21	380/3614 (10.5%)
1	H	1.36	13/2758 (0.5%)	3.34	405/3729 (10.9%)
1	I	1.45	13/2673 (0.5%)	3.42	449/3614 (12.4%)
1	J	1.43	13/2746 (0.5%)	3.29	384/3713 (10.3%)
1	K	1.42	13/2731 (0.5%)	3.19	377/3693 (10.2%)
1	L	1.39	7/2673 (0.3%)	3.13	368/3614 (10.2%)
1	M	1.43	14/2776 (0.5%)	3.27	380/3754 (10.1%)
1	N	1.41	11/2673 (0.4%)	3.39	431/3614 (11.9%)
1	O	1.41	15/2673 (0.6%)	3.22	431/3614 (11.9%)
1	P	1.37	8/2776 (0.3%)	3.13	347/3754 (9.2%)
1	Q	1.34	7/2673 (0.3%)	3.17	364/3614 (10.1%)
1	R	1.38	9/2673 (0.3%)	3.28	369/3614 (10.2%)
All	All	1.45	280/48847 (0.6%)	3.31	7311/66048 (11.1%)

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	13
1	C	0	6
1	D	0	13
1	E	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	4
1	G	0	8
1	H	0	7
1	I	0	11
1	J	0	4
1	K	0	6
1	L	0	6
1	M	0	8
1	N	0	6
1	O	0	5
1	P	0	6
1	Q	0	6
1	R	0	10
All	All	0	133

All (280) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	TYR	C-O	-15.14	1.06	1.24
1	B	214	LYS	N-CA	-13.19	1.30	1.46
1	D	70	ASN	CA-CB	12.44	1.74	1.53
1	E	89	GLN	CA-C	11.65	1.68	1.52
1	G	4	PHE	CA-CB	10.55	1.61	1.52
1	D	212	VAL	C-O	10.49	1.35	1.24
1	B	215	ALA	N-CA	-10.37	1.33	1.46
1	D	214	LYS	N-CA	10.00	1.59	1.46
1	M	70	ASN	N-CA	-9.94	1.33	1.46
1	I	67	SER	N-CA	-9.42	1.34	1.46
1	B	1	ALA	N-CA	9.33	1.64	1.46
1	I	266	GLY	N-CA	9.28	1.54	1.45
1	B	215	ALA	C-O	9.25	1.34	1.24
1	B	214	LYS	C-O	9.24	1.34	1.24
1	D	211	ALA	C-O	-9.15	1.13	1.24
1	D	215	ALA	C-O	-9.07	1.13	1.24
1	B	25	ASN	N-CA	9.07	1.58	1.47
1	J	25	ASN	CA-CB	-8.77	1.41	1.53
1	B	145	GLY	N-CA	8.72	1.53	1.44
1	I	67	SER	CA-CB	8.47	1.67	1.53
1	E	25	ASN	N-CA	8.34	1.64	1.46
1	B	221	VAL	N-CA	-8.31	1.36	1.46
1	C	266	GLY	N-CA	8.23	1.53	1.45
1	J	25	ASN	N-CA	8.13	1.64	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	70	ASN	CA-CB	8.07	1.68	1.53
1	D	87	ASP	CA-CB	8.01	1.67	1.53
1	R	25	ASN	N-CA	8.01	1.60	1.46
1	E	89	GLN	CB-CG	7.95	1.76	1.52
1	D	18	ILE	C-O	-7.94	1.15	1.24
1	D	17	GLU	C-O	-7.90	1.14	1.24
1	B	282	ASN	N-CA	7.88	1.55	1.46
1	H	24	ALA	C-O	7.88	1.33	1.24
1	B	11	GLN	C-N	7.83	1.43	1.33
1	Q	90	GLY	N-CA	7.80	1.56	1.45
1	K	75	GLY	N-CA	7.72	1.53	1.45
1	K	349	GLY	N-CA	7.69	1.56	1.45
1	N	260	VAL	CA-C	-7.66	1.47	1.53
1	H	25	ASN	N-CA	7.59	1.62	1.46
1	L	16	SER	N-CA	7.51	1.55	1.46
1	B	24	ALA	C-O	7.37	1.32	1.24
1	L	24	ALA	C-O	7.36	1.32	1.24
1	A	119	ASN	N-CA	7.35	1.56	1.46
1	B	333	ALA	N-CA	7.21	1.55	1.46
1	F	183	VAL	N-CA	7.17	1.51	1.46
1	B	15	LEU	N-CA	7.16	1.55	1.46
1	B	212	VAL	C-O	-7.14	1.15	1.24
1	O	16	SER	N-CA	7.11	1.55	1.46
1	B	219	HIS	C-N	7.10	1.43	1.33
1	B	219	HIS	N-CA	7.09	1.55	1.46
1	O	25	ASN	N-CA	7.07	1.56	1.47
1	J	24	ALA	C-O	7.01	1.32	1.24
1	D	187	GLU	CD-OE1	-7.00	1.12	1.25
1	D	212	VAL	C-N	6.97	1.43	1.34
1	F	94	ARG	CD-NE	-6.96	1.36	1.46
1	G	302	GLY	N-CA	6.93	1.55	1.45
1	Q	25	ASN	N-CA	6.92	1.58	1.46
1	A	75	GLY	N-CA	6.91	1.52	1.45
1	D	25	ASN	N-CA	6.82	1.61	1.46
1	G	342	TYR	N-CA	6.81	1.53	1.45
1	B	207	LYS	C-O	6.81	1.32	1.24
1	B	333	ALA	C-N	6.79	1.43	1.34
1	K	260	VAL	CA-C	-6.76	1.48	1.53
1	A	199	GLU	C-O	6.76	1.32	1.24
1	B	210	ALA	C-N	6.76	1.42	1.33
1	N	59	ARG	CD-NE	6.74	1.55	1.46
1	M	69	ILE	N-CA	6.72	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	25	ASN	CA-CB	-6.72	1.44	1.53
1	O	128	ASP	N-CA	6.70	1.54	1.46
1	O	161	LEU	N-CA	6.67	1.54	1.46
1	B	213	TYR	N-CA	6.66	1.54	1.46
1	B	337	ALA	N-CA	6.66	1.54	1.46
1	O	75	GLY	N-CA	6.64	1.52	1.45
1	B	213	TYR	C-N	-6.64	1.25	1.33
1	B	211	ALA	C-N	6.62	1.42	1.33
1	J	181	GLY	C-N	-6.61	1.24	1.33
1	E	94	ARG	CD-NE	-6.58	1.37	1.46
1	D	213	TYR	C-O	6.46	1.32	1.24
1	D	30	LEU	N-CA	6.44	1.54	1.46
1	B	209	LEU	C-O	6.43	1.32	1.24
1	B	23	VAL	N-CA	6.42	1.54	1.46
1	B	214	LYS	C-N	6.42	1.42	1.33
1	G	70	ASN	CA-CB	6.41	1.64	1.53
1	H	94	ARG	NE-CZ	-6.39	1.26	1.33
1	F	267	ILE	CA-CB	-6.37	1.46	1.54
1	D	159	SER	CA-C	6.36	1.61	1.53
1	L	25	ASN	N-CA	6.34	1.58	1.46
1	M	55	ARG	N-CA	-6.33	1.38	1.46
1	R	143	ASP	CA-CB	6.33	1.62	1.54
1	F	222	TYR	N-CA	6.33	1.54	1.46
1	H	219	HIS	ND1-CE1	6.31	1.38	1.32
1	K	348	SER	N-CA	-6.29	1.38	1.46
1	A	118	THR	CA-C	-6.26	1.45	1.52
1	D	273	GLY	N-CA	6.26	1.54	1.45
1	L	201	CYS	C-O	6.23	1.31	1.24
1	N	148	ARG	NE-CZ	-6.20	1.26	1.33
1	Q	104	VAL	N-CA	6.20	1.53	1.46
1	D	212	VAL	N-CA	-6.17	1.39	1.46
1	R	128	ASP	N-CA	6.17	1.53	1.46
1	A	266	GLY	N-CA	6.16	1.52	1.45
1	K	266	GLY	N-CA	6.16	1.51	1.45
1	R	260	VAL	CA-C	-6.15	1.48	1.53
1	G	87	ASP	CA-CB	6.14	1.63	1.53
1	B	18	ILE	C-N	6.10	1.41	1.33
1	M	68	SER	N-CA	-6.10	1.38	1.46
1	P	25	ASN	N-CA	6.10	1.55	1.46
1	G	4	PHE	CA-C	-6.08	1.48	1.53
1	A	258	ARG	CZ-NH2	6.08	1.41	1.33
1	E	260	VAL	N-CA	6.06	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	ASN	C-O	6.05	1.31	1.24
1	N	186	VAL	CA-C	-6.05	1.46	1.52
1	D	211	ALA	C-N	-6.03	1.26	1.33
1	P	229	LYS	N-CA	-6.03	1.39	1.46
1	A	196	HIS	N-CA	6.03	1.54	1.45
1	J	264	VAL	N-CA	6.01	1.53	1.46
1	F	184	PRO	CA-CB	6.00	1.61	1.53
1	E	24	ALA	C-O	6.00	1.31	1.24
1	K	88	SER	C-N	-6.00	1.25	1.33
1	J	128	ASP	N-CA	5.99	1.53	1.46
1	D	150	VAL	N-CA	5.99	1.53	1.46
1	E	159	SER	N-CA	5.98	1.53	1.45
1	M	67	SER	C-O	-5.98	1.16	1.24
1	B	161	LEU	N-CA	5.97	1.53	1.46
1	G	80	HIS	CE1-NE2	5.97	1.38	1.32
1	E	128	ASP	N-CA	5.96	1.53	1.46
1	D	307	ALA	N-CA	5.96	1.53	1.46
1	F	91	LYS	N-CA	5.96	1.53	1.46
1	D	73	ILE	C-O	-5.94	1.17	1.24
1	D	211	ALA	N-CA	5.93	1.53	1.46
1	B	280	THR	N-CA	5.93	1.53	1.46
1	D	75	GLY	C-O	5.92	1.30	1.24
1	H	263	ALA	C-N	-5.91	1.28	1.33
1	D	106	ILE	N-CA	-5.91	1.39	1.46
1	O	24	ALA	C-O	5.90	1.30	1.24
1	D	309	ALA	C-N	-5.90	1.26	1.33
1	B	211	ALA	C-O	5.89	1.30	1.24
1	B	268	CYS	N-CA	-5.89	1.39	1.46
1	B	210	ALA	N-CA	5.88	1.53	1.46
1	I	88	SER	C-N	-5.88	1.26	1.33
1	M	25	ASN	N-CA	5.86	1.59	1.46
1	K	219	HIS	N-CA	5.81	1.53	1.46
1	P	159	SER	CB-OG	5.80	1.53	1.42
1	M	219	HIS	CG-ND1	5.80	1.44	1.38
1	A	87	ASP	CA-CB	5.78	1.63	1.53
1	M	145	GLY	CA-C	5.78	1.58	1.52
1	I	23	VAL	N-CA	5.78	1.51	1.46
1	B	334	ASN	N-CA	5.77	1.53	1.46
1	J	267	ILE	CA-CB	-5.76	1.47	1.54
1	N	269	PHE	C-O	-5.76	1.16	1.23
1	B	199	GLU	CA-CB	-5.75	1.43	1.53
1	D	195	ASP	CA-CB	-5.72	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	187	GLU	CD-OE2	5.72	1.36	1.25
1	F	118	THR	N-CA	5.71	1.53	1.45
1	K	75	GLY	CA-C	5.71	1.57	1.51
1	H	302	GLY	CA-C	5.70	1.55	1.51
1	A	220	HIS	CE1-NE2	-5.69	1.26	1.32
1	P	263	ALA	C-O	5.69	1.31	1.24
1	J	94	ARG	CD-NE	-5.69	1.38	1.46
1	B	206	GLU	N-CA	5.68	1.53	1.46
1	L	16	SER	C-N	5.66	1.41	1.33
1	A	308	SER	CB-OG	-5.65	1.30	1.42
1	A	357	PHE	N-CA	-5.63	1.39	1.46
1	M	219	HIS	N-CA	5.62	1.52	1.46
1	I	113	ALA	C-N	-5.62	1.26	1.33
1	O	329	LYS	N-CA	5.60	1.53	1.46
1	H	354	GLN	N-CA	-5.60	1.39	1.46
1	J	273	GLY	N-CA	5.60	1.53	1.45
1	J	9	GLN	C-O	-5.59	1.17	1.24
1	B	15	LEU	C-N	5.57	1.41	1.33
1	E	137	TYR	N-CA	5.57	1.53	1.46
1	B	215	ALA	CA-CB	-5.56	1.44	1.53
1	J	148	ARG	CD-NE	-5.55	1.38	1.46
1	D	222	TYR	C-N	5.54	1.41	1.34
1	R	148	ARG	NE-CZ	-5.54	1.26	1.33
1	D	172	ARG	N-CA	5.54	1.52	1.46
1	P	195	ASP	CA-CB	-5.54	1.45	1.53
1	Q	232	MET	C-N	-5.54	1.27	1.33
1	N	124	ILE	N-CA	5.53	1.52	1.46
1	B	225	GLY	C-O	5.53	1.31	1.23
1	E	148	ARG	NE-CZ	-5.53	1.26	1.33
1	O	228	LEU	C-N	-5.52	1.28	1.33
1	A	200	HIS	CE1-NE2	5.50	1.38	1.32
1	B	183	VAL	CA-C	5.50	1.57	1.52
1	A	119	ASN	C-N	-5.50	1.26	1.33
1	O	25	ASN	CA-C	-5.49	1.47	1.53
1	D	187	GLU	N-CA	-5.49	1.38	1.46
1	B	267	ILE	CA-CB	-5.48	1.47	1.54
1	N	216	LEU	N-CA	5.48	1.53	1.46
1	M	21	SER	C-N	-5.48	1.27	1.34
1	D	213	TYR	C-N	5.47	1.41	1.33
1	C	102	ILE	CA-CB	-5.46	1.48	1.54
1	R	191	ILE	CA-CB	-5.46	1.47	1.54
1	J	258	ARG	CD-NE	-5.46	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	353	THR	N-CA	-5.45	1.39	1.46
1	N	247	GLN	N-CA	5.45	1.52	1.46
1	Q	163	ILE	N-CA	5.43	1.52	1.46
1	M	219	HIS	CG-CD2	-5.42	1.29	1.35
1	A	128	ASP	N-CA	5.42	1.53	1.46
1	D	25	ASN	CA-CB	-5.42	1.46	1.53
1	A	267	ILE	CA-CB	-5.42	1.47	1.54
1	G	222	TYR	N-CA	5.42	1.53	1.46
1	I	145	GLY	N-CA	5.41	1.50	1.44
1	I	182	LEU	C-O	5.40	1.30	1.23
1	L	220	HIS	CE1-NE2	5.40	1.38	1.32
1	F	25	ASN	N-CA	5.40	1.57	1.46
1	A	219	HIS	N-CA	5.39	1.52	1.46
1	B	298	SER	CA-CB	5.39	1.62	1.53
1	B	68	SER	C-O	5.38	1.30	1.24
1	C	234	THR	N-CA	-5.37	1.38	1.45
1	G	94	ARG	CD-NE	-5.37	1.38	1.46
1	B	11	GLN	N-CA	5.37	1.52	1.46
1	K	258	ARG	CD-NE	-5.37	1.38	1.46
1	B	212	VAL	N-CA	5.36	1.52	1.46
1	B	220	HIS	CA-CB	-5.36	1.44	1.53
1	B	21	SER	CA-CB	5.35	1.62	1.53
1	B	29	ILE	CA-C	-5.34	1.46	1.52
1	C	2	HIS	N-CA	-5.34	1.39	1.46
1	O	278	ASP	N-CA	5.34	1.52	1.46
1	B	87	ASP	CA-C	-5.33	1.47	1.53
1	O	253	VAL	N-CA	5.32	1.53	1.46
1	E	89	GLN	C-N	5.32	1.40	1.33
1	O	111	GLY	N-CA	5.32	1.50	1.45
1	P	133	ARG	NE-CZ	5.31	1.38	1.33
1	A	115	LEU	C-O	5.29	1.30	1.24
1	D	21	SER	C-N	-5.28	1.27	1.33
1	Q	292	PRO	C-N	-5.28	1.25	1.33
1	D	215	ALA	N-CA	5.27	1.52	1.46
1	E	75	GLY	N-CA	5.27	1.50	1.45
1	H	134	CYS	N-CA	5.25	1.52	1.46
1	C	222	TYR	C-O	5.24	1.30	1.24
1	N	291	LEU	C-O	5.24	1.28	1.24
1	I	211	ALA	C-N	5.23	1.40	1.33
1	P	293	LYS	C-O	-5.22	1.18	1.24
1	Q	124	ILE	C-N	-5.21	1.26	1.33
1	G	186	VAL	CA-CB	5.21	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	267	ILE	CA-CB	-5.21	1.47	1.54
1	A	24	ALA	N-CA	-5.20	1.40	1.46
1	B	89	GLN	C-N	-5.19	1.25	1.33
1	A	118	THR	C-O	5.19	1.30	1.23
1	G	292	PRO	C-N	-5.18	1.26	1.33
1	K	122	THR	N-CA	-5.18	1.39	1.45
1	E	260	VAL	CA-C	-5.17	1.49	1.53
1	I	66	ASP	C-O	-5.17	1.17	1.24
1	G	232	MET	SD-CE	-5.15	1.66	1.79
1	K	248	VAL	N-CA	-5.15	1.40	1.46
1	G	124	ILE	C-N	-5.14	1.25	1.33
1	L	294	PRO	N-CA	-5.13	1.41	1.47
1	N	128	ASP	N-CA	5.13	1.52	1.46
1	H	13	LYS	N-CA	5.13	1.52	1.46
1	E	266	GLY	N-CA	5.13	1.50	1.45
1	H	25	ASN	CA-CB	-5.13	1.48	1.53
1	D	161	LEU	N-CA	5.11	1.52	1.46
1	G	26	GLY	CA-C	5.11	1.58	1.51
1	P	297	LEU	C-O	-5.11	1.18	1.24
1	I	24	ALA	N-CA	-5.10	1.40	1.46
1	B	216	LEU	C-O	5.10	1.30	1.24
1	I	254	THR	C-O	5.10	1.30	1.24
1	K	133	ARG	NE-CZ	5.09	1.38	1.33
1	A	349	GLY	N-CA	5.09	1.52	1.45
1	O	271	SER	N-CA	5.09	1.52	1.46
1	B	188	PRO	C-O	-5.08	1.17	1.24
1	O	89	GLN	C-N	-5.07	1.26	1.33
1	E	116	ALA	C-N	-5.07	1.26	1.33
1	F	353	THR	N-CA	-5.07	1.39	1.46
1	R	92	LEU	N-CA	5.07	1.52	1.46
1	H	184	PRO	C-O	-5.07	1.18	1.23
1	R	247	GLN	C-O	-5.06	1.18	1.24
1	M	221	VAL	CA-CB	-5.06	1.48	1.54
1	R	24	ALA	N-CA	-5.06	1.40	1.46
1	H	30	LEU	C-N	-5.05	1.27	1.33
1	B	205	THR	CB-OG1	-5.05	1.35	1.43
1	I	264	VAL	C-N	-5.05	1.29	1.33
1	J	295	TRP	NE1-CE2	-5.05	1.31	1.37
1	O	219	HIS	CE1-NE2	5.04	1.37	1.32
1	G	123	THR	CA-C	5.04	1.59	1.53
1	K	124	ILE	C-O	-5.03	1.19	1.24
1	B	70	ASN	CA-CB	-5.03	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	THR	C-O	5.03	1.30	1.24
1	E	112	GLY	N-CA	5.03	1.50	1.45
1	A	356	LEU	C-O	-5.01	1.17	1.23
1	A	123	THR	C-O	-5.01	1.18	1.24

All (7311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	89	GLN	OE1-CD-NE2	46.95	169.55	122.60
1	J	94	ARG	CD-NE-CZ	38.79	178.70	124.40
1	C	3	ARG	CD-NE-CZ	37.00	176.21	124.40
1	E	94	ARG	CD-NE-CZ	36.10	174.94	124.40
1	D	1	ALA	CA-C-N	35.59	177.08	121.56
1	D	1	ALA	C-N-CA	35.59	177.08	121.56
1	Q	172	ARG	CD-NE-CZ	34.17	172.24	124.40
1	R	2	HIS	CA-CB-CG	34.14	147.94	113.80
1	J	42	ARG	NE-CZ-NH2	33.60	149.44	119.20
1	R	344	HIS	CA-CB-CG	31.63	145.43	113.80
1	E	148	ARG	CD-NE-CZ	31.63	168.68	124.40
1	R	148	ARG	CD-NE-CZ	30.51	167.11	124.40
1	F	94	ARG	CD-NE-CZ	30.11	166.56	124.40
1	H	1	ALA	CA-C-N	29.80	178.46	121.54
1	H	1	ALA	C-N-CA	29.80	178.46	121.54
1	M	352	SER	CA-C-N	29.19	177.29	121.54
1	M	352	SER	C-N-CA	29.19	177.29	121.54
1	F	352	SER	CA-C-N	28.01	175.04	121.54
1	F	352	SER	C-N-CA	28.01	175.04	121.54
1	H	344	HIS	CA-C-N	27.73	174.50	121.54
1	H	344	HIS	C-N-CA	27.73	174.50	121.54
1	M	3	ARG	CD-NE-CZ	26.91	162.07	124.40
1	C	1	ALA	CA-C-N	26.30	166.51	122.33
1	C	1	ALA	C-N-CA	26.30	166.51	122.33
1	A	258	ARG	NE-CZ-NH1	26.11	147.61	121.50
1	E	89	GLN	CA-CB-CG	-26.06	61.98	114.10
1	G	94	ARG	CD-NE-CZ	25.91	160.67	124.40
1	R	258	ARG	CD-NE-CZ	25.44	160.01	124.40
1	A	356	LEU	CA-C-N	25.30	169.85	121.54
1	A	356	LEU	C-N-CA	25.30	169.85	121.54
1	H	94	ARG	CD-NE-CZ	24.15	158.21	124.40
1	M	356	LEU	O-C-N	-23.57	91.79	122.19
1	P	330	ARG	NE-CZ-NH2	23.53	140.38	119.20
1	A	148	ARG	CD-NE-CZ	23.47	157.25	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	ASN	CA-CB-CG	-23.02	89.58	112.60
1	I	2	HIS	CA-CB-CG	22.90	136.70	113.80
1	Q	258	ARG	NE-CZ-NH1	22.90	144.40	121.50
1	E	88	SER	CA-C-O	-22.67	94.30	122.64
1	K	347	SER	CA-C-N	22.60	164.71	121.54
1	K	347	SER	C-N-CA	22.60	164.71	121.54
1	N	258	ARG	CD-NE-CZ	22.57	156.00	124.40
1	M	68	SER	N-CA-CB	22.19	148.00	110.49
1	L	258	ARG	NE-CZ-NH2	-21.99	99.41	119.20
1	P	152	ARG	CB-CG-CD	21.77	161.37	111.30
1	E	89	GLN	N-CA-CB	-21.47	74.21	110.49
1	D	215	ALA	CA-C-O	21.28	142.97	120.42
1	E	88	SER	O-C-N	-20.71	95.42	122.56
1	N	148	ARG	CD-NE-CZ	20.27	152.78	124.40
1	D	258	ARG	NE-CZ-NH1	19.98	141.48	121.50
1	N	125	GLN	OE1-CD-NE2	-19.97	102.63	122.60
1	E	89	GLN	CG-CD-NE2	-19.85	86.63	116.40
1	F	330	ARG	NE-CZ-NH1	-19.63	101.87	121.50
1	H	2	HIS	CA-CB-CG	19.43	133.23	113.80
1	E	89	GLN	CB-CA-C	-19.34	71.92	110.42
1	P	195	ASP	CA-CB-CG	19.24	131.84	112.60
1	B	11	GLN	CA-C-O	19.18	140.75	120.42
1	Q	267	ILE	CA-CB-CG2	19.15	143.06	110.50
1	P	330	ARG	NE-CZ-NH1	-19.01	102.49	121.50
1	F	330	ARG	NE-CZ-NH2	19.00	136.31	119.20
1	A	3	ARG	CD-NE-CZ	18.93	150.91	124.40
1	N	3	ARG	CA-C-O	18.89	147.52	120.51
1	E	1	ALA	CA-C-N	18.86	157.55	121.54
1	E	1	ALA	C-N-CA	18.86	157.55	121.54
1	Q	330	ARG	NE-CZ-NH2	18.62	135.96	119.20
1	D	191	ILE	CA-CB-CG2	18.55	142.03	110.50
1	L	25	ASN	CA-CB-CG	18.47	131.07	112.60
1	G	65	VAL	CA-C-O	-18.47	97.69	120.78
1	J	25	ASN	CA-CB-CG	18.42	131.02	112.60
1	G	267	ILE	CA-CB-CG2	18.39	141.77	110.50
1	D	3	ARG	CD-NE-CZ	18.35	150.09	124.40
1	D	303	ARG	CA-C-O	-18.26	101.90	120.70
1	N	284	ASN	OD1-CG-ND2	-18.24	104.36	122.60
1	N	303	ARG	NE-CZ-NH1	-18.17	103.33	121.50
1	M	68	SER	CA-C-N	-18.12	89.36	121.97
1	M	68	SER	C-N-CA	-18.12	89.36	121.97
1	D	195	ASP	CA-CB-CG	18.11	130.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	94	ARG	CD-NE-CZ	18.09	149.73	124.40
1	J	42	ARG	NE-CZ-NH1	-17.90	103.60	121.50
1	M	69	ILE	CB-CA-C	17.88	140.61	111.29
1	J	113	ALA	O-C-N	17.85	134.55	121.88
1	G	330	ARG	NE-CZ-NH2	17.79	135.21	119.20
1	F	258	ARG	NE-CZ-NH2	-17.77	103.20	119.20
1	D	199	GLU	CA-CB-CG	17.76	149.62	114.10
1	N	191	ILE	CA-CB-CG2	17.75	140.67	110.50
1	E	3	ARG	CD-NE-CZ	17.66	149.13	124.40
1	N	94	ARG	CD-NE-CZ	17.66	149.13	124.40
1	N	330	ARG	NE-CZ-NH2	17.59	135.03	119.20
1	Q	24	ALA	CA-C-N	-17.49	96.96	122.67
1	Q	24	ALA	C-N-CA	-17.49	96.96	122.67
1	I	195	ASP	CA-CB-CG	-17.49	95.11	112.60
1	N	303	ARG	NE-CZ-NH2	17.39	134.85	119.20
1	H	191	ILE	CA-CB-CG2	17.38	140.04	110.50
1	D	66	ASP	CA-CB-CG	17.31	129.91	112.60
1	K	133	ARG	CD-NE-CZ	-17.25	100.25	124.40
1	I	191	ILE	CA-CB-CG2	17.21	139.76	110.50
1	M	70	ASN	CA-CB-CG	-17.12	95.48	112.60
1	A	258	ARG	NE-CZ-NH2	-17.08	103.83	119.20
1	M	69	ILE	N-CA-CB	-17.05	83.09	111.23
1	F	25	ASN	CA-CB-CG	17.00	129.60	112.60
1	B	6	ALA	CA-C-O	-16.91	102.47	121.07
1	K	88	SER	CA-C-O	-16.81	101.37	120.70
1	E	89	GLN	CB-CG-CD	-16.79	84.06	112.60
1	M	199	GLU	CA-CB-CG	16.74	147.58	114.10
1	G	4	PHE	CB-CA-C	-16.67	99.37	111.20
1	O	24	ALA	CA-C-O	-16.53	103.21	120.90
1	B	87	ASP	CA-C-O	-16.52	103.46	122.13
1	D	24	ALA	CA-C-N	-16.50	96.81	123.04
1	D	24	ALA	C-N-CA	-16.50	96.81	123.04
1	K	258	ARG	NE-CZ-NH1	16.33	137.83	121.50
1	M	24	ALA	CA-C-O	-16.28	103.73	120.82
1	C	132	GLU	CB-CG-CD	16.26	140.25	112.60
1	D	87	ASP	CA-CB-CG	-16.22	96.38	112.60
1	B	212	VAL	O-C-N	16.17	137.56	121.87
1	H	171	ALA	CA-C-O	-16.16	103.85	120.82
1	J	258	ARG	NE-CZ-NH2	-16.10	104.71	119.20
1	D	164	GLN	CA-CB-CG	16.02	146.13	114.10
1	D	70	ASN	CB-CA-C	-16.01	78.57	110.42
1	I	24	ALA	CA-C-N	-15.96	99.21	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	24	ALA	C-N-CA	-15.96	99.21	122.67
1	R	24	ALA	CA-C-N	-15.89	99.31	122.67
1	R	24	ALA	C-N-CA	-15.89	99.31	122.67
1	J	2	HIS	CA-CB-CG	15.87	129.67	113.80
1	E	258	ARG	NE-CZ-NH1	15.85	137.35	121.50
1	D	186	VAL	N-CA-CB	-15.71	92.83	111.21
1	D	258	ARG	NE-CZ-NH2	-15.68	105.08	119.20
1	I	152	ARG	NE-CZ-NH2	15.68	133.31	119.20
1	M	67	SER	CA-C-O	15.60	142.82	120.51
1	H	25	ASN	CA-CB-CG	15.50	128.10	112.60
1	G	191	ILE	CA-CB-CG2	15.46	136.79	110.50
1	I	271	SER	CA-C-O	15.44	137.73	118.43
1	B	214	LYS	O-C-N	-15.35	106.26	122.07
1	Q	258	ARG	NE-CZ-NH2	-15.33	105.40	119.20
1	B	87	ASP	O-C-N	-15.31	105.25	122.55
1	Q	303	ARG	CG-CD-NE	15.29	145.65	112.00
1	M	199	GLU	CB-CG-CD	15.28	138.57	112.60
1	R	217	ASN	OD1-CG-ND2	-15.25	107.35	122.60
1	E	344	HIS	CA-C-N	15.25	150.67	121.54
1	E	344	HIS	C-N-CA	15.25	150.67	121.54
1	B	260	VAL	CA-C-O	15.13	127.59	119.12
1	J	258	ARG	NE-CZ-NH1	15.04	136.54	121.50
1	E	352	SER	CA-C-N	15.01	144.95	121.98
1	E	352	SER	C-N-CA	15.01	144.95	121.98
1	J	24	ALA	CA-C-N	-15.00	99.20	123.04
1	J	24	ALA	C-N-CA	-15.00	99.20	123.04
1	O	25	ASN	CA-CB-CG	14.97	127.57	112.60
1	J	148	ARG	CD-NE-CZ	14.95	145.33	124.40
1	A	24	ALA	CA-C-N	-14.94	100.71	122.67
1	A	24	ALA	C-N-CA	-14.94	100.71	122.67
1	P	357	PHE	CA-CB-CG	14.86	128.66	113.80
1	R	303	ARG	CD-NE-CZ	-14.85	103.62	124.40
1	H	353	THR	CA-C-O	14.84	135.22	118.90
1	D	356	LEU	CA-C-O	14.82	145.99	120.80
1	I	70	ASN	OD1-CG-ND2	-14.74	107.86	122.60
1	N	71	GLN	OE1-CD-NE2	14.71	137.31	122.60
1	K	258	ARG	CD-NE-CZ	14.69	144.97	124.40
1	G	65	VAL	O-C-N	-14.63	104.29	122.57
1	N	3	ARG	O-C-N	-14.60	103.17	122.59
1	Q	25	ASN	CA-CB-CG	14.53	127.13	112.60
1	E	89	GLN	CG-CD-OE1	-14.51	91.78	120.80
1	E	3	ARG	CA-C-O	14.50	141.25	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	1	ALA	CB-CA-C	14.45	132.18	110.50
1	Q	267	ILE	CB-CA-C	14.45	127.93	110.73
1	A	358	THR	N-CA-CB	14.43	134.88	110.49
1	P	2	HIS	CA-CB-CG	14.42	128.22	113.80
1	M	1	ALA	CB-CA-C	14.34	132.01	110.50
1	A	358	THR	CA-C-O	14.33	141.00	120.51
1	B	259	THR	CA-C-N	14.32	132.34	122.60
1	B	259	THR	C-N-CA	14.32	132.34	122.60
1	M	352	SER	CA-C-O	14.31	140.97	120.51
1	A	308	SER	CA-CB-OG	14.30	139.70	111.10
1	I	67	SER	CB-CA-C	-14.20	82.16	110.42
1	J	191	ILE	CA-CB-CG2	14.16	134.57	110.50
1	C	24	ALA	CA-C-N	-14.12	100.59	123.04
1	C	24	ALA	C-N-CA	-14.12	100.59	123.04
1	K	66	ASP	CA-CB-CG	14.08	126.68	112.60
1	A	330	ARG	NE-CZ-NH2	14.07	131.87	119.20
1	C	87	ASP	CB-CA-C	-14.06	82.43	110.42
1	Q	10	GLU	CA-C-O	-14.03	106.26	121.00
1	B	94	ARG	CD-NE-CZ	14.01	144.02	124.40
1	J	24	ALA	CA-C-O	-14.01	106.27	120.70
1	J	260	VAL	CA-C-O	14.00	129.42	119.20
1	E	148	ARG	CA-C-N	13.99	143.50	122.65
1	E	148	ARG	C-N-CA	13.99	143.50	122.65
1	H	3	ARG	CA-C-O	13.93	140.42	120.51
1	J	160	SER	O-C-N	13.88	136.83	122.12
1	E	75	GLY	O-C-N	13.85	133.80	123.27
1	E	66	ASP	O-C-N	-13.81	106.23	122.11
1	M	89	GLN	CB-CG-CD	-13.81	89.13	112.60
1	P	179	GLN	OE1-CD-NE2	13.79	136.39	122.60
1	M	191	ILE	CA-CB-CG2	13.78	133.92	110.50
1	I	69	ILE	O-C-N	-13.74	105.40	122.57
1	N	195	ASP	CA-CB-CG	-13.73	98.87	112.60
1	I	67	SER	N-CA-C	13.72	140.03	110.80
1	B	183	VAL	CB-CA-C	-13.72	95.99	110.53
1	K	265	PRO	CA-C-N	-13.70	107.24	121.35
1	K	265	PRO	C-N-CA	-13.70	107.24	121.35
1	C	258	ARG	NE-CZ-NH1	13.57	135.07	121.50
1	M	70	ASN	CB-CA-C	-13.57	83.42	110.42
1	E	25	ASN	CA-CB-CG	13.54	126.14	112.60
1	M	67	SER	CA-C-N	13.54	147.40	121.54
1	M	67	SER	C-N-CA	13.54	147.40	121.54
1	K	330	ARG	NE-CZ-NH2	13.52	131.37	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	223	LEU	O-C-N	13.52	136.45	122.12
1	A	303	ARG	CD-NE-CZ	-13.51	105.48	124.40
1	N	3	ARG	CA-C-N	13.51	154.75	121.80
1	N	3	ARG	C-N-CA	13.51	154.75	121.80
1	M	352	SER	O-C-N	-13.45	104.70	122.59
1	B	191	ILE	CA-CB-CG2	13.44	133.34	110.50
1	H	66	ASP	O-C-N	-13.42	104.74	122.59
1	R	343	VAL	CA-C-O	-13.41	104.02	120.78
1	A	237	HIS	CA-CB-CG	-13.41	100.39	113.80
1	F	191	ILE	CA-CB-CG2	13.39	133.26	110.50
1	L	258	ARG	NE-CZ-NH1	13.37	134.87	121.50
1	D	264	VAL	CA-C-O	-13.34	107.30	119.71
1	C	344	HIS	CA-CB-CG	-13.31	100.49	113.80
1	A	153	ILE	O-C-N	-13.30	108.83	122.93
1	H	96	ILE	O-C-N	13.30	134.94	121.91
1	N	87	ASP	CB-CA-C	-13.29	83.97	110.42
1	C	3	ARG	CA-C-O	-13.29	101.51	120.51
1	N	152	ARG	NE-CZ-NH1	-13.28	108.22	121.50
1	Q	3	ARG	O-C-N	-13.28	104.93	122.59
1	K	330	ARG	NE-CZ-NH1	-13.27	108.23	121.50
1	Q	199	GLU	CB-CG-CD	13.23	135.09	112.60
1	R	343	VAL	N-CA-CB	13.23	133.06	111.23
1	F	110	GLN	OE1-CD-NE2	13.21	135.81	122.60
1	B	215	ALA	N-CA-C	13.19	125.66	111.28
1	G	181	GLY	O-C-N	13.18	138.06	122.38
1	L	87	ASP	CA-CB-CG	-13.18	99.42	112.60
1	B	25	ASN	CA-CB-CG	13.17	125.77	112.60
1	C	258	ARG	CD-NE-CZ	13.17	142.84	124.40
1	P	191	ILE	CA-CB-CG2	13.17	132.88	110.50
1	M	303	ARG	CD-NE-CZ	13.08	142.71	124.40
1	E	256	LEU	CA-C-O	13.07	135.00	119.97
1	K	339	LYS	CG-CD-CE	13.07	141.37	111.30
1	M	89	GLN	OE1-CD-NE2	13.07	135.67	122.60
1	B	267	ILE	CA-CB-CG2	13.06	132.71	110.50
1	R	330	ARG	NE-CZ-NH2	13.06	130.96	119.20
1	I	71	GLN	OE1-CD-NE2	13.06	135.66	122.60
1	N	267	ILE	CA-CB-CG2	13.03	132.64	110.50
1	A	345	THR	N-CA-C	-13.00	89.65	110.32
1	C	191	ILE	CA-CB-CG2	12.98	132.56	110.50
1	D	226	THR	CA-C-O	-12.97	107.00	121.40
1	B	71	GLN	CA-C-N	12.94	141.97	122.56
1	B	71	GLN	C-N-CA	12.94	141.97	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	260	VAL	CA-C-O	12.90	126.35	119.12
1	P	354	GLN	N-CA-C	12.90	129.25	113.38
1	B	25	ASN	O-C-N	12.90	138.24	123.28
1	J	244	THR	N-CA-CB	-12.90	91.57	109.88
1	I	133	ARG	CA-C-N	-12.82	102.82	120.38
1	I	133	ARG	C-N-CA	-12.82	102.82	120.38
1	G	9	GLN	OE1-CD-NE2	-12.81	109.79	122.60
1	R	1	ALA	CA-C-N	12.79	145.97	121.54
1	R	1	ALA	C-N-CA	12.79	145.97	121.54
1	B	24	ALA	CA-C-N	-12.77	98.50	121.87
1	B	24	ALA	C-N-CA	-12.77	98.50	121.87
1	R	1	ALA	CB-CA-C	12.77	129.65	110.50
1	J	260	VAL	O-C-N	-12.76	111.50	121.46
1	A	87	ASP	CB-CA-C	-12.75	85.04	110.42
1	H	303	ARG	CD-NE-CZ	-12.70	106.62	124.40
1	I	51	THR	CA-C-O	-12.69	106.65	120.36
1	F	148	ARG	CD-NE-CZ	12.66	142.12	124.40
1	R	121	GLU	CA-C-O	12.64	136.53	121.87
1	B	319	ASN	CA-CB-CG	-12.62	99.98	112.60
1	E	109	ASP	O-C-N	12.62	137.17	122.79
1	G	24	ALA	CA-C-N	-12.60	103.00	123.04
1	G	24	ALA	C-N-CA	-12.60	103.00	123.04
1	O	24	ALA	CA-C-N	-12.60	98.82	121.87
1	O	24	ALA	C-N-CA	-12.60	98.82	121.87
1	I	70	ASN	CB-CG-OD1	12.56	145.91	120.80
1	F	267	ILE	CA-CB-CG2	12.55	131.84	110.50
1	J	166	ASN	OD1-CG-ND2	-12.51	110.09	122.60
1	N	3	ARG	NE-CZ-NH1	-12.51	108.99	121.50
1	C	217	ASN	OD1-CG-ND2	-12.49	110.11	122.60
1	E	295	TRP	CA-C-O	-12.48	106.86	121.46
1	A	258	ARG	CD-NE-CZ	12.46	141.85	124.40
1	C	237	HIS	CA-CB-CG	-12.46	101.34	113.80
1	K	99	GLU	CA-C-O	-12.44	106.05	120.10
1	D	164	GLN	OE1-CD-NE2	-12.42	110.18	122.60
1	H	66	ASP	CA-C-O	-12.42	102.75	120.51
1	K	89	GLN	OE1-CD-NE2	12.41	135.01	122.60
1	P	148	ARG	CA-C-O	-12.40	106.68	120.32
1	F	94	ARG	NE-CZ-NH1	-12.40	109.10	121.50
1	H	89	GLN	CB-CG-CD	-12.38	91.55	112.60
1	M	68	SER	CB-CA-C	-12.38	85.79	110.42
1	J	70	ASN	CB-CA-C	-12.35	84.27	110.32
1	K	166	ASN	CA-CB-CG	-12.35	100.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	ASP	N-CA-CB	12.32	131.31	110.49
1	E	132	GLU	CB-CG-CD	12.30	133.52	112.60
1	P	133	ARG	CD-NE-CZ	-12.30	107.18	124.40
1	G	148	ARG	NE-CZ-NH1	-12.29	109.21	121.50
1	P	87	ASP	CB-CA-C	-12.26	86.02	110.42
1	I	303	ARG	CD-NE-CZ	12.24	141.53	124.40
1	N	59	ARG	CD-NE-CZ	-12.23	107.28	124.40
1	B	182	LEU	O-C-N	-12.22	109.25	122.94
1	K	123	THR	CB-CA-C	-12.18	93.76	113.37
1	D	25	ASN	CA-CB-CG	12.17	124.77	112.60
1	I	22	ILE	CA-C-O	-12.16	107.11	120.25
1	F	95	ASN	CA-CB-CG	-12.16	100.44	112.60
1	C	136	GLN	OE1-CD-NE2	-12.16	110.44	122.60
1	G	231	ASN	O-C-N	12.15	136.67	123.06
1	C	71	GLN	OE1-CD-NE2	12.14	134.74	122.60
1	L	24	ALA	CA-C-O	-12.13	107.33	120.92
1	I	260	VAL	N-CA-C	12.11	118.58	107.56
1	M	24	ALA	CA-C-N	-12.11	103.79	123.04
1	M	24	ALA	C-N-CA	-12.11	103.79	123.04
1	D	89	GLN	O-C-N	-12.10	106.50	122.59
1	D	226	THR	N-CA-CB	-12.05	91.18	111.31
1	P	258	ARG	NE-CZ-NH2	12.03	130.03	119.20
1	F	10	GLU	CA-CB-CG	12.00	138.11	114.10
1	B	228	LEU	O-C-N	12.00	138.00	123.24
1	B	11	GLN	OE1-CD-NE2	-11.98	110.62	122.60
1	Q	191	ILE	CA-CB-CG2	11.98	130.86	110.50
1	D	152	ARG	O-C-N	11.98	138.72	123.15
1	N	3	ARG	CD-NE-CZ	11.98	141.17	124.40
1	G	123	THR	N-CA-CB	11.97	128.94	110.87
1	H	70	ASN	CA-CB-CG	-11.93	100.67	112.60
1	G	87	ASP	CA-CB-CG	-11.93	100.67	112.60
1	L	23	VAL	N-CA-C	-11.93	101.46	112.43
1	F	110	GLN	CG-CD-NE2	-11.90	98.55	116.40
1	M	69	ILE	CA-CB-CG2	-11.90	90.27	110.50
1	F	110	GLN	CB-CG-CD	11.89	132.82	112.60
1	G	179	GLN	N-CA-C	-11.89	98.80	113.18
1	N	186	VAL	N-CA-CB	-11.88	97.63	110.82
1	E	347	SER	CB-CA-C	-11.86	86.82	110.42
1	G	226	THR	N-CA-CB	-11.85	92.42	111.62
1	R	258	ARG	NE-CZ-NH1	11.85	133.35	121.50
1	K	109	ASP	CA-CB-CG	11.84	124.44	112.60
1	I	69	ILE	CA-C-N	11.84	140.46	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	69	ILE	C-N-CA	11.84	140.46	121.99
1	F	89	GLN	CB-CG-CD	-11.82	92.51	112.60
1	H	353	THR	CA-C-N	11.81	144.10	121.54
1	H	353	THR	C-N-CA	11.81	144.10	121.54
1	O	261	PRO	CA-C-O	11.80	135.25	121.56
1	H	42	ARG	NE-CZ-NH2	11.74	129.76	119.20
1	N	260	VAL	N-CA-C	11.73	118.23	107.56
1	F	329	LYS	CG-CD-CE	11.72	138.27	111.30
1	Q	10	GLU	N-CA-CB	11.72	127.03	109.91
1	A	348	SER	CA-C-O	-11.72	107.36	121.66
1	P	341	GLN	OE1-CD-NE2	-11.72	110.88	122.60
1	G	70	ASN	CB-CA-C	-11.72	87.10	110.42
1	B	154	ALA	CA-C-O	-11.71	108.48	121.25
1	O	319	ASN	CA-CB-CG	-11.70	100.90	112.60
1	J	330	ARG	NE-CZ-NH1	-11.69	109.81	121.50
1	I	237	HIS	CA-CB-CG	-11.68	102.12	113.80
1	A	114	PRO	CA-C-N	11.67	138.01	122.84
1	A	114	PRO	C-N-CA	11.67	138.01	122.84
1	B	213	TYR	CA-C-N	11.67	135.61	120.44
1	B	213	TYR	C-N-CA	11.67	135.61	120.44
1	D	228	LEU	CA-C-O	-11.66	108.10	120.70
1	J	166	ASN	CB-CG-ND2	11.66	133.89	116.40
1	A	292	PRO	O-C-N	-11.64	108.11	122.89
1	L	26	GLY	N-CA-C	-11.64	100.04	115.40
1	L	183	VAL	CA-C-O	11.64	126.02	119.15
1	E	148	ARG	O-C-N	-11.62	110.14	123.27
1	D	224	GLU	CB-CG-CD	11.62	132.35	112.60
1	P	258	ARG	CB-CG-CD	11.59	137.97	111.30
1	D	325	GLU	CB-CG-CD	-11.59	92.89	112.60
1	G	10	GLU	CA-C-O	-11.59	108.50	120.90
1	L	229	LYS	O-C-N	11.59	131.02	121.17
1	O	260	VAL	N-CA-C	11.59	118.11	107.56
1	G	70	ASN	N-CA-CB	-11.55	90.97	110.49
1	L	267	ILE	CA-CB-CG2	11.54	130.12	110.50
1	F	9	GLN	OE1-CD-NE2	-11.53	111.07	122.60
1	K	287	ASN	CA-CB-CG	-11.53	101.08	112.60
1	B	199	GLU	CA-CB-CG	11.52	137.14	114.10
1	H	42	ARG	NE-CZ-NH1	-11.51	109.99	121.50
1	B	183	VAL	N-CA-C	-11.50	94.48	108.05
1	B	212	VAL	CA-C-N	-11.50	104.87	120.28
1	B	212	VAL	C-N-CA	-11.50	104.87	120.28
1	D	191	ILE	CA-CB-CG1	-11.49	90.87	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASN	CA-CB-CG	-11.48	101.12	112.60
1	N	1	ALA	N-CA-CB	11.48	127.62	110.40
1	I	67	SER	N-CA-CB	-11.46	91.11	110.49
1	N	22	ILE	CA-C-O	-11.45	108.10	120.47
1	P	138	LYS	O-C-N	11.45	134.26	122.12
1	B	90	GLY	CA-C-O	-11.45	100.65	120.57
1	A	199	GLU	CB-CG-CD	11.44	132.05	112.60
1	K	309	ALA	CA-C-O	11.44	133.12	119.97
1	H	22	ILE	CA-C-O	-11.43	108.12	120.47
1	J	152	ARG	CB-CA-C	-11.43	90.68	110.45
1	O	148	ARG	NE-CZ-NH2	11.43	129.48	119.20
1	I	215	ALA	CA-C-O	-11.42	108.83	120.82
1	O	154	ALA	CA-C-O	-11.42	109.06	121.05
1	O	94	ARG	CD-NE-CZ	11.40	140.37	124.40
1	B	212	VAL	N-CA-CB	-11.39	95.05	110.54
1	D	348	SER	CA-C-O	11.39	133.30	119.98
1	A	217	ASN	OD1-CG-ND2	-11.38	111.22	122.60
1	K	195	ASP	CA-CB-CG	-11.38	101.22	112.60
1	N	2	HIS	CA-CB-CG	11.37	125.17	113.80
1	E	66	ASP	CA-C-O	-11.37	108.19	120.92
1	D	70	ASN	O-C-N	-11.36	107.48	122.59
1	G	259	THR	CA-C-N	-11.34	112.60	123.04
1	G	259	THR	C-N-CA	-11.34	112.60	123.04
1	N	24	ALA	CA-C-N	-11.34	105.01	123.04
1	N	24	ALA	C-N-CA	-11.34	105.01	123.04
1	A	336	GLN	OE1-CD-NE2	-11.33	111.27	122.60
1	E	258	ARG	NE-CZ-NH2	-11.33	109.00	119.20
1	J	258	ARG	CD-NE-CZ	11.31	140.24	124.40
1	F	226	THR	N-CA-CB	-11.31	93.44	111.43
1	L	80	HIS	CA-CB-CG	-11.30	102.50	113.80
1	E	346	GLY	CA-C-N	11.30	143.12	121.54
1	E	346	GLY	C-N-CA	11.30	143.12	121.54
1	I	66	ASP	CA-C-O	11.30	136.67	120.51
1	G	168	ASN	CA-CB-CG	-11.30	101.30	112.60
1	N	258	ARG	NE-CZ-NH1	11.25	132.75	121.50
1	J	199	GLU	CB-CG-CD	11.24	131.71	112.60
1	A	133	ARG	NH1-CZ-NH2	11.24	133.91	119.30
1	R	94	ARG	NE-CZ-NH1	-11.22	110.28	121.50
1	Q	289	CYS	CA-C-O	11.22	130.30	119.75
1	D	301	TYR	O-C-N	-11.22	110.20	123.10
1	F	330	ARG	CD-NE-CZ	-11.19	108.73	124.40
1	J	114	PRO	CA-C-N	11.20	138.72	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	114	PRO	C-N-CA	11.20	138.72	123.05
1	N	284	ASN	CB-CG-ND2	11.19	133.19	116.40
1	H	344	HIS	CA-C-O	11.18	136.49	120.51
1	I	68	SER	O-C-N	11.17	137.45	122.59
1	I	341	GLN	CA-C-N	-11.17	106.01	122.65
1	I	341	GLN	C-N-CA	-11.17	106.01	122.65
1	K	152	ARG	NE-CZ-NH1	-11.17	110.33	121.50
1	N	79	PHE	CA-C-O	-11.16	108.08	120.92
1	G	125	GLN	OE1-CD-NE2	-11.16	111.44	122.60
1	C	24	ALA	N-CA-C	11.14	123.42	111.28
1	I	330	ARG	NE-CZ-NH2	11.12	129.21	119.20
1	O	89	GLN	CB-CG-CD	-11.12	93.70	112.60
1	R	114	PRO	CA-C-O	-11.11	108.67	121.34
1	F	352	SER	CA-C-O	11.11	136.40	120.51
1	G	41	ASN	CA-C-O	-11.09	108.79	120.55
1	O	257	HIS	O-C-N	11.09	137.77	122.46
1	Q	9	GLN	OE1-CD-NE2	-11.08	111.52	122.60
1	K	133	ARG	NE-CZ-NH1	-11.06	110.44	121.50
1	D	272	GLY	CA-C-N	-11.05	102.05	122.05
1	D	272	GLY	C-N-CA	-11.05	102.05	122.05
1	L	154	ALA	CA-C-O	-11.04	109.46	121.05
1	N	186	VAL	O-C-N	-11.03	109.98	122.66
1	B	214	LYS	CA-C-O	11.02	132.39	120.82
1	C	152	ARG	NE-CZ-NH2	11.01	129.11	119.20
1	R	149	ALA	CA-C-N	-11.00	108.73	123.14
1	R	149	ALA	C-N-CA	-11.00	108.73	123.14
1	L	95	ASN	CA-CB-CG	-11.00	101.60	112.60
1	H	70	ASN	CB-CA-C	-11.00	85.55	110.18
1	M	109	ASP	CA-CB-CG	10.99	123.59	112.60
1	H	67	SER	N-CA-CB	10.99	129.07	110.49
1	O	95	ASN	CA-CB-CG	-10.99	101.61	112.60
1	F	182	LEU	CA-C-N	-10.97	114.69	122.59
1	F	182	LEU	C-N-CA	-10.97	114.69	122.59
1	H	149	ALA	CA-C-N	-10.96	108.45	123.13
1	H	149	ALA	C-N-CA	-10.96	108.45	123.13
1	A	119	ASN	CA-C-O	-10.95	108.85	121.66
1	J	195	ASP	CA-CB-CG	-10.95	101.65	112.60
1	J	267	ILE	CA-CB-CG2	10.93	129.08	110.50
1	A	115	LEU	CA-C-O	10.92	131.90	120.54
1	B	336	GLN	O-C-N	10.92	133.31	122.07
1	B	3	ARG	CD-NE-CZ	10.90	139.66	124.40
1	I	56	ARG	CD-NE-CZ	-10.90	109.14	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	3	ARG	O-C-N	-10.89	108.10	122.59
1	G	325	GLU	CA-C-O	10.89	132.09	120.55
1	D	237	HIS	CA-CB-CG	-10.89	102.91	113.80
1	D	152	ARG	CA-C-O	-10.88	108.71	121.44
1	E	148	ARG	NE-CZ-NH2	-10.88	109.41	119.20
1	J	344	HIS	CA-CB-CG	-10.86	102.94	113.80
1	E	226	THR	CA-CB-CG2	10.86	128.96	110.50
1	I	70	ASN	O-C-N	10.86	134.06	122.23
1	O	82	THR	O-C-N	-10.85	109.53	122.22
1	H	210	ALA	N-CA-C	-10.84	99.47	111.07
1	E	258	ARG	CD-NE-CZ	10.84	139.58	124.40
1	C	195	ASP	CA-CB-CG	-10.84	101.77	112.60
1	F	324	GLN	OE1-CD-NE2	-10.83	111.77	122.60
1	I	26	GLY	N-CA-C	-10.83	100.15	115.43
1	P	89	GLN	OE1-CD-NE2	10.83	133.43	122.60
1	I	164	GLN	CA-C-O	10.82	132.02	120.55
1	B	204	VAL	O-C-N	10.80	132.96	121.83
1	M	25	ASN	CA-CB-CG	10.79	123.39	112.60
1	Q	123	THR	N-CA-CB	10.79	128.27	111.22
1	N	344	HIS	CA-CB-CG	-10.79	103.01	113.80
1	O	219	HIS	CA-C-O	10.78	132.47	119.43
1	N	111	GLY	CA-C-O	10.77	129.66	122.23
1	Q	179	GLN	OE1-CD-NE2	10.76	133.36	122.60
1	R	148	ARG	CA-C-O	10.76	132.16	120.32
1	R	231	ASN	OD1-CG-ND2	10.76	133.35	122.60
1	E	182	LEU	CA-C-O	-10.75	109.01	121.16
1	Q	42	ARG	CD-NE-CZ	10.73	139.43	124.40
1	J	282	ASN	CA-C-O	-10.73	109.05	120.42
1	I	148	ARG	CD-NE-CZ	10.72	139.40	124.40
1	I	67	SER	O-C-N	10.72	136.84	122.59
1	I	191	ILE	N-CA-CB	-10.71	96.21	111.21
1	B	81	GLU	CA-C-O	10.71	132.36	120.90
1	P	90	GLY	CA-C-N	-10.69	107.11	122.19
1	P	90	GLY	C-N-CA	-10.69	107.11	122.19
1	N	237	HIS	CA-CB-CG	-10.69	103.11	113.80
1	M	42	ARG	CD-NE-CZ	10.68	139.35	124.40
1	I	24	ALA	CA-C-O	-10.67	108.97	120.92
1	B	55	ARG	CD-NE-CZ	-10.65	109.49	124.40
1	B	334	ASN	CA-C-O	-10.65	108.07	120.10
1	I	42	ARG	NE-CZ-NH2	10.65	128.78	119.20
1	P	287	ASN	OD1-CG-ND2	10.65	133.25	122.60
1	D	118	THR	N-CA-CB	-10.64	91.73	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	180	ASN	CA-CB-CG	-10.64	101.96	112.60
1	I	179	GLN	OE1-CD-NE2	10.64	133.24	122.60
1	I	68	SER	CA-C-O	-10.63	105.31	120.51
1	G	10	GLU	CA-CB-CG	10.63	135.35	114.10
1	K	191	ILE	N-CA-CB	-10.62	96.34	111.21
1	R	333	ALA	O-C-N	10.62	133.01	122.07
1	E	95	ASN	CA-CB-CG	-10.62	101.98	112.60
1	D	74	GLY	O-C-N	-10.61	108.91	122.70
1	F	260	VAL	CA-C-O	10.61	125.41	119.15
1	N	305	LEU	CA-C-N	-10.61	105.85	122.08
1	N	305	LEU	C-N-CA	-10.61	105.85	122.08
1	J	352	SER	CA-C-O	10.60	135.67	120.51
1	K	191	ILE	CA-CB-CG2	10.60	128.52	110.50
1	J	353	THR	N-CA-C	-10.60	97.67	114.09
1	F	24	ALA	CA-C-N	-10.59	97.74	122.95
1	F	24	ALA	C-N-CA	-10.59	97.74	122.95
1	D	2	HIS	CA-CB-CG	-10.58	103.22	113.80
1	D	303	ARG	O-C-N	10.58	133.52	122.09
1	Q	10	GLU	O-C-N	10.58	133.03	122.03
1	H	118	THR	N-CA-CB	-10.58	94.61	111.43
1	J	152	ARG	CD-NE-CZ	-10.57	109.60	124.40
1	N	65	VAL	CA-C-O	10.57	133.99	120.78
1	M	137	TYR	O-C-N	-10.56	111.10	122.09
1	D	87	ASP	CB-CA-C	-10.56	89.40	110.42
1	I	223	LEU	O-C-N	10.56	132.94	122.07
1	M	66	ASP	CA-C-O	-10.55	109.54	121.15
1	E	94	ARG	NH1-CZ-NH2	10.54	133.01	119.30
1	E	194	GLY	CA-C-O	10.54	130.85	122.52
1	B	267	ILE	CA-C-N	10.54	139.04	123.13
1	B	267	ILE	C-N-CA	10.54	139.04	123.13
1	B	183	VAL	O-C-N	10.53	131.19	121.61
1	A	199	GLU	CB-CA-C	10.53	130.88	110.67
1	B	144	PHE	CA-C-N	-10.53	112.98	121.82
1	B	144	PHE	C-N-CA	-10.53	112.98	121.82
1	L	237	HIS	CA-CB-CG	-10.51	103.29	113.80
1	I	67	SER	CA-CB-OG	-10.50	90.10	111.10
1	N	267	ILE	CB-CA-C	10.50	124.60	110.42
1	D	70	ASN	CB-CG-ND2	-10.49	100.66	116.40
1	C	2	HIS	CA-CB-CG	-10.49	103.31	113.80
1	E	2	HIS	N-CA-C	10.48	133.12	110.80
1	J	217	ASN	CB-CG-OD1	10.48	141.75	120.80
1	F	174	ALA	CA-C-O	10.47	131.86	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	118	THR	N-CA-CB	-10.47	94.10	110.85
1	C	330	ARG	NE-CZ-NH2	10.46	128.62	119.20
1	L	24	ALA	CA-C-N	-10.46	97.93	122.20
1	L	24	ALA	C-N-CA	-10.46	97.93	122.20
1	C	87	ASP	CA-CB-CG	10.46	123.06	112.60
1	O	78	LEU	O-C-N	10.46	136.78	123.19
1	M	345	THR	N-CA-C	10.46	133.07	110.80
1	B	219	HIS	CA-C-O	10.45	132.08	119.43
1	E	68	SER	N-CA-C	-10.45	100.20	113.16
1	E	332	MET	CA-C-O	10.45	131.62	120.55
1	I	42	ARG	CA-C-O	-10.44	108.30	120.10
1	E	165	GLU	OE1-CD-OE2	10.44	147.95	122.90
1	J	160	SER	CA-C-O	-10.42	109.50	120.55
1	A	223	LEU	O-C-N	10.42	133.16	122.12
1	G	147	TRP	O-C-N	10.42	136.68	123.14
1	D	132	GLU	CB-CG-CD	10.41	130.30	112.60
1	K	133	ARG	NH1-CZ-NH2	10.41	132.84	119.30
1	A	148	ARG	CA-C-O	-10.41	109.04	120.38
1	I	207	LYS	CA-CB-CG	10.40	134.90	114.10
1	K	88	SER	O-C-N	-10.40	109.18	123.01
1	K	119	ASN	CA-CB-CG	-10.40	102.20	112.60
1	B	186	VAL	N-CA-CB	-10.39	99.81	111.66
1	P	327	PHE	CA-C-O	10.39	131.73	120.82
1	I	115	LEU	O-C-N	-10.39	110.38	122.84
1	L	87	ASP	CB-CA-C	-10.39	89.75	110.42
1	M	195	ASP	CA-CB-CG	-10.38	102.22	112.60
1	D	199	GLU	CA-C-O	10.38	131.91	119.97
1	G	267	ILE	CB-CA-C	10.38	125.51	110.77
1	R	141	GLY	CA-C-O	-10.36	107.47	118.97
1	C	133	ARG	NE-CZ-NH2	10.35	128.51	119.20
1	B	229	LYS	CA-C-N	10.34	131.93	120.66
1	B	229	LYS	C-N-CA	10.34	131.93	120.66
1	D	178	GLN	OE1-CD-NE2	-10.34	112.26	122.60
1	F	344	HIS	CA-C-O	10.34	132.52	121.15
1	P	336	GLN	OE1-CD-NE2	-10.34	112.26	122.60
1	H	334	ASN	CA-CB-CG	-10.34	102.27	112.60
1	D	160	SER	CA-C-N	-10.33	104.61	120.31
1	D	160	SER	C-N-CA	-10.33	104.61	120.31
1	M	195	ASP	N-CA-C	10.33	123.80	111.82
1	C	327	PHE	CA-C-O	10.32	131.77	120.63
1	K	258	ARG	NH1-CZ-NH2	-10.31	105.89	119.30
1	B	95	ASN	CA-CB-CG	-10.31	102.29	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	94	ARG	NE-CZ-NH2	10.31	128.47	119.20
1	D	185	ILE	O-C-N	-10.30	110.37	122.94
1	R	231	ASN	CA-C-O	-10.30	109.62	121.47
1	D	124	ILE	O-C-N	-10.30	112.08	123.10
1	E	133	ARG	NE-CZ-NH1	-10.29	111.21	121.50
1	F	156	GLN	CB-CG-CD	-10.29	95.12	112.60
1	D	216	LEU	N-CA-CB	10.28	126.06	110.22
1	F	344	HIS	CA-C-N	10.28	141.18	121.54
1	F	344	HIS	C-N-CA	10.28	141.18	121.54
1	G	24	ALA	N-CA-C	10.28	123.53	111.71
1	D	95	ASN	CA-CB-CG	10.27	122.87	112.60
1	R	33	ASP	CA-CB-CG	-10.26	102.34	112.60
1	N	11	GLN	O-C-N	10.25	132.99	122.12
1	A	267	ILE	CA-CB-CG2	10.25	127.92	110.50
1	J	89	GLN	OE1-CD-NE2	10.24	132.84	122.60
1	M	166	ASN	CB-CG-ND2	10.24	131.77	116.40
1	D	89	GLN	CB-CG-CD	-10.24	95.20	112.60
1	D	311	ALA	CA-C-O	-10.23	110.16	120.70
1	H	186	VAL	O-C-N	-10.23	111.53	122.68
1	C	133	ARG	CD-NE-CZ	-10.23	110.08	124.40
1	D	70	ASN	OD1-CG-ND2	10.23	132.83	122.60
1	L	138	LYS	N-CA-C	-10.22	100.10	111.14
1	P	172	ARG	NE-CZ-NH2	-10.22	110.00	119.20
1	F	90	GLY	CA-C-N	-10.22	106.81	121.42
1	F	90	GLY	C-N-CA	-10.22	106.81	121.42
1	C	168	ASN	CA-CB-CG	-10.20	102.40	112.60
1	F	70	ASN	CB-CA-C	-10.20	90.12	110.42
1	Q	226	THR	N-CA-CB	-10.20	93.80	111.55
1	G	186	VAL	N-CA-CB	-10.20	100.55	111.46
1	F	348	SER	CA-C-O	10.19	135.08	120.51
1	O	191	ILE	CA-CB-CG2	10.19	127.82	110.50
1	C	188	PRO	N-CA-CB	10.19	110.17	102.73
1	O	267	ILE	CB-CA-C	10.18	122.84	110.73
1	B	240	THR	CA-C-O	-10.18	107.07	119.18
1	N	124	ILE	CA-C-O	-10.17	109.35	120.43
1	C	226	THR	N-CA-CB	-10.16	95.50	111.56
1	B	57	GLN	CA-C-O	-10.15	109.66	120.42
1	I	130	LEU	CA-C-O	10.15	131.48	120.82
1	A	238	ALA	CA-C-N	-10.15	105.42	120.75
1	A	238	ALA	C-N-CA	-10.15	105.42	120.75
1	P	24	ALA	CA-C-O	-10.14	109.56	120.92
1	B	136	GLN	OE1-CD-NE2	10.14	132.74	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	VAL	O-C-N	-10.13	111.01	122.66
1	O	186	VAL	N-CA-CB	-10.13	99.64	111.39
1	G	47	LYS	CA-C-N	10.12	137.43	122.75
1	G	47	LYS	C-N-CA	10.12	137.43	122.75
1	F	258	ARG	NE-CZ-NH1	10.12	131.62	121.50
1	P	343	VAL	CA-C-O	-10.11	108.15	120.78
1	E	24	ALA	CA-C-N	-10.10	98.91	122.95
1	E	24	ALA	C-N-CA	-10.10	98.91	122.95
1	D	237	HIS	CB-CG-ND1	10.10	137.84	122.70
1	B	202	GLN	CA-C-O	10.09	131.41	120.82
1	N	210	ALA	N-CA-C	-10.09	99.52	112.23
1	A	152	ARG	CD-NE-CZ	-10.08	110.29	124.40
1	A	300	SER	CA-C-O	-10.07	108.10	120.89
1	N	1	ALA	CA-C-O	-10.06	103.70	120.80
1	Q	152	ARG	CD-NE-CZ	-10.06	110.32	124.40
1	B	333	ALA	O-C-N	10.06	132.95	122.09
1	F	95	ASN	OD1-CG-ND2	10.06	132.66	122.60
1	H	24	ALA	CA-C-N	-10.06	99.01	122.95
1	H	24	ALA	C-N-CA	-10.06	99.01	122.95
1	L	266	GLY	CA-C-N	-10.04	108.73	122.98
1	L	266	GLY	C-N-CA	-10.04	108.73	122.98
1	O	217	ASN	CA-CB-CG	-10.03	102.57	112.60
1	I	178	GLN	OE1-CD-NE2	10.02	132.62	122.60
1	M	69	ILE	CA-C-N	10.02	140.68	121.54
1	M	69	ILE	C-N-CA	10.02	140.68	121.54
1	H	353	THR	N-CA-C	-10.01	100.20	114.12
1	J	344	HIS	CA-C-N	10.01	140.65	121.54
1	J	344	HIS	C-N-CA	10.01	140.65	121.54
1	O	200	HIS	CA-CB-CG	10.01	123.81	113.80
1	K	42	ARG	NE-CZ-NH2	10.00	128.20	119.20
1	N	118	THR	N-CA-CB	-9.99	95.02	111.20
1	O	133	ARG	NE-CZ-NH1	-9.99	111.51	121.50
1	G	9	GLN	CG-CD-NE2	9.98	131.37	116.40
1	J	209	LEU	O-C-N	9.98	133.53	122.15
1	J	89	GLN	CB-CG-CD	-9.98	95.64	112.60
1	M	286	ILE	N-CA-C	-9.98	100.44	110.62
1	Q	210	ALA	CA-C-O	-9.97	108.83	120.10
1	E	118	THR	N-CA-CB	-9.97	94.34	111.69
1	M	11	GLN	OE1-CD-NE2	-9.97	112.63	122.60
1	N	152	ARG	NE-CZ-NH2	9.97	128.17	119.20
1	C	170	LEU	O-C-N	9.96	132.33	122.07
1	R	3	ARG	CA-C-O	-9.96	106.26	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	287	ASN	OD1-CG-ND2	9.96	132.56	122.60
1	K	60	GLU	O-C-N	9.95	132.67	122.12
1	E	299	PHE	O-C-N	-9.94	111.01	123.24
1	Q	195	ASP	CA-CB-CG	9.94	122.54	112.60
1	I	94	ARG	CD-NE-CZ	9.94	138.31	124.40
1	H	191	ILE	CA-CB-CG1	-9.93	93.52	110.40
1	Q	166	ASN	CA-CB-CG	-9.93	102.67	112.60
1	P	138	LYS	CA-C-O	-9.92	110.04	120.55
1	I	123	THR	CB-CA-C	-9.92	93.49	112.43
1	G	89	GLN	OE1-CD-NE2	9.91	132.51	122.60
1	M	70	ASN	CA-C-O	-9.91	106.34	120.51
1	C	109	ASP	CA-CB-CG	9.90	122.50	112.60
1	P	133	ARG	NE-CZ-NH1	-9.90	111.60	121.50
1	O	237	HIS	CA-CB-CG	-9.89	103.91	113.80
1	A	23	VAL	CA-C-N	9.88	133.29	120.44
1	A	23	VAL	C-N-CA	9.88	133.29	120.44
1	A	89	GLN	OE1-CD-NE2	9.89	132.49	122.60
1	I	3	ARG	CA-CB-CG	9.88	133.87	114.10
1	I	168	ASN	CA-CB-CG	-9.88	102.72	112.60
1	O	36	VAL	O-C-N	9.88	132.63	121.96
1	Q	41	ASN	CA-C-O	-9.88	110.07	120.55
1	Q	341	GLN	OE1-CD-NE2	9.88	132.48	122.60
1	R	333	ALA	CA-C-O	-9.88	110.45	120.82
1	B	267	ILE	CA-CB-CG1	-9.87	93.61	110.40
1	L	3	ARG	NE-CZ-NH2	9.87	128.08	119.20
1	N	330	ARG	CD-NE-CZ	-9.87	110.58	124.40
1	L	186	VAL	CA-C-O	-9.87	109.11	120.65
1	G	258	ARG	CB-CG-CD	9.86	133.98	111.30
1	F	125	GLN	OE1-CD-NE2	-9.86	112.74	122.60
1	M	309	ALA	CA-C-O	9.86	130.85	120.70
1	Q	10	GLU	CB-CA-C	-9.86	95.78	110.96
1	I	11	GLN	O-C-N	9.86	132.57	122.12
1	G	95	ASN	OD1-CG-ND2	9.85	132.45	122.60
1	Q	109	ASP	CA-CB-CG	-9.84	102.76	112.60
1	L	89	GLN	CB-CG-CD	-9.83	95.88	112.60
1	H	303	ARG	NE-CZ-NH1	-9.82	111.68	121.50
1	M	69	ILE	CA-C-O	9.82	133.05	120.78
1	R	123	THR	CA-CB-OG1	9.81	124.32	109.60
1	R	143	ASP	CA-CB-CG	-9.81	102.78	112.60
1	D	212	VAL	CA-C-O	9.81	131.57	121.17
1	N	11	GLN	CA-C-N	-9.81	107.69	120.44
1	N	11	GLN	C-N-CA	-9.81	107.69	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	100	LYS	CA-CB-CG	9.81	133.72	114.10
1	C	42	ARG	CA-C-O	-9.80	110.16	120.55
1	J	111	GLY	N-CA-C	9.80	124.19	112.33
1	R	156	GLN	OE1-CD-NE2	9.80	132.41	122.60
1	B	104	VAL	CB-CA-C	-9.80	97.16	110.98
1	C	108	LEU	CA-C-O	9.79	129.44	118.97
1	B	217	ASN	OD1-CG-ND2	-9.79	112.81	122.60
1	G	179	GLN	OE1-CD-NE2	9.79	132.39	122.60
1	Q	87	ASP	CA-CB-CG	-9.79	102.81	112.60
1	A	169	ALA	O-C-N	9.78	133.30	122.15
1	B	68	SER	N-CA-CB	-9.78	93.96	110.49
1	R	327	PHE	CA-C-O	9.78	130.78	120.42
1	I	289	CYS	CA-C-O	9.78	128.94	119.75
1	B	282	ASN	O-C-N	-9.77	111.93	122.09
1	C	124	ILE	CA-C-O	-9.77	110.14	120.39
1	D	271	SER	CA-C-O	9.77	129.88	119.14
1	J	9	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	R	42	ARG	O-C-N	9.76	133.27	122.15
1	M	219	HIS	CA-CB-CG	9.76	123.56	113.80
1	I	87	ASP	N-CA-CB	9.75	123.83	110.38
1	D	71	GLN	CA-C-O	-9.74	108.05	119.15
1	H	185	ILE	O-C-N	-9.73	112.07	122.68
1	D	21	SER	CA-C-O	-9.73	108.31	119.79
1	Q	330	ARG	NH1-CZ-NH2	-9.73	106.65	119.30
1	I	11	GLN	CA-C-N	-9.73	107.21	120.44
1	I	11	GLN	C-N-CA	-9.73	107.21	120.44
1	N	282	ASN	OD1-CG-ND2	-9.72	112.88	122.60
1	H	42	ARG	O-C-N	9.71	132.42	122.12
1	F	89	GLN	OE1-CD-NE2	9.71	132.31	122.60
1	B	303	ARG	CD-NE-CZ	9.70	137.99	124.40
1	D	180	ASN	CA-CB-CG	-9.69	102.91	112.60
1	D	190	VAL	CA-C-N	9.69	140.06	122.13
1	D	190	VAL	C-N-CA	9.69	140.06	122.13
1	L	58	PHE	CA-CB-CG	-9.69	104.11	113.80
1	K	257	HIS	CA-CB-CG	9.69	123.49	113.80
1	N	81	GLU	CB-CG-CD	9.69	129.07	112.60
1	G	118	THR	CA-C-N	-9.69	106.84	122.34
1	G	118	THR	C-N-CA	-9.69	106.84	122.34
1	D	260	VAL	N-CA-C	9.68	116.37	107.56
1	D	226	THR	CA-CB-CG2	9.68	126.95	110.50
1	O	89	GLN	O-C-N	-9.68	114.16	123.26
1	C	244	THR	N-CA-CB	-9.67	98.33	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	172	ARG	NE-CZ-NH1	9.67	131.17	121.50
1	M	71	GLN	CA-CB-CG	9.66	133.42	114.10
1	L	340	GLY	CA-C-N	-9.66	107.32	122.49
1	L	340	GLY	C-N-CA	-9.66	107.32	122.49
1	L	306	GLN	OE1-CD-NE2	9.66	132.26	122.60
1	C	119	ASN	OD1-CG-ND2	9.66	132.26	122.60
1	D	38	THR	O-C-N	9.65	133.15	122.15
1	R	162	ALA	O-C-N	9.65	133.15	122.15
1	G	89	GLN	CB-CG-CD	-9.65	96.20	112.60
1	I	215	ALA	O-C-N	9.65	132.01	122.07
1	I	260	VAL	N-CA-CB	-9.64	100.50	111.20
1	N	168	ASN	CA-CB-CG	-9.64	102.96	112.60
1	G	41	ASN	O-C-N	9.63	132.33	122.12
1	G	187	GLU	CB-CA-C	-9.63	100.63	110.65
1	H	10	GLU	CA-CB-CG	9.63	133.36	114.10
1	B	21	SER	O-C-N	9.62	134.10	122.27
1	L	262	ALA	N-CA-CB	-9.62	94.25	110.41
1	O	271	SER	N-CA-C	-9.61	102.64	114.75
1	B	336	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	I	150	VAL	O-C-N	-9.61	112.88	123.26
1	K	261	PRO	CA-C-N	9.60	134.10	120.28
1	K	261	PRO	C-N-CA	9.60	134.10	120.28
1	E	67	SER	N-CA-CB	9.60	126.71	110.49
1	A	202	GLN	CA-C-O	9.60	130.72	120.55
1	K	258	ARG	CA-C-O	-9.60	108.04	119.27
1	M	137	TYR	CA-C-O	9.59	131.16	120.90
1	R	25	ASN	CA-CB-CG	9.59	122.19	112.60
1	A	354	GLN	CA-C-O	-9.58	110.41	121.72
1	F	344	HIS	N-CA-CB	9.58	124.93	109.69
1	B	21	SER	CA-C-O	-9.58	108.95	119.97
1	K	9	GLN	CA-C-N	-9.58	107.99	120.44
1	K	9	GLN	C-N-CA	-9.58	107.99	120.44
1	B	241	LYS	N-CA-CB	9.57	123.50	110.38
1	F	190	VAL	CA-C-N	9.57	139.84	122.13
1	F	190	VAL	C-N-CA	9.57	139.84	122.13
1	B	207	LYS	CG-CD-CE	9.57	133.31	111.30
1	D	42	ARG	NE-CZ-NH2	9.57	127.81	119.20
1	O	295	TRP	CA-C-O	-9.57	110.27	121.46
1	C	177	CYS	O-C-N	-9.56	112.15	122.09
1	P	330	ARG	CD-NE-CZ	-9.56	111.02	124.40
1	B	164	GLN	CB-CG-CD	9.55	128.84	112.60
1	G	133	ARG	NH1-CZ-NH2	9.56	131.72	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	150	VAL	CA-C-N	9.55	137.27	122.94
1	I	150	VAL	C-N-CA	9.55	137.27	122.94
1	L	125	GLN	OE1-CD-NE2	-9.55	113.05	122.60
1	L	184	PRO	CB-CA-C	-9.55	102.70	111.40
1	R	148	ARG	O-C-N	-9.55	112.00	123.27
1	C	94	ARG	CB-CG-CD	9.55	133.27	111.30
1	P	248	VAL	CA-C-O	9.54	130.88	120.95
1	E	24	ALA	CA-C-O	-9.54	110.31	120.42
1	N	24	ALA	CA-C-O	-9.53	110.71	120.90
1	R	9	GLN	OE1-CD-NE2	-9.52	113.08	122.60
1	F	303	ARG	CD-NE-CZ	-9.52	111.07	124.40
1	C	265	PRO	CA-C-N	-9.52	108.71	121.27
1	C	265	PRO	C-N-CA	-9.52	108.71	121.27
1	H	24	ALA	N-CA-C	9.52	122.65	111.71
1	D	71	GLN	N-CA-C	-9.51	101.68	113.38
1	E	71	GLN	CA-C-N	9.51	139.72	122.79
1	E	71	GLN	C-N-CA	9.51	139.72	122.79
1	F	258	ARG	CD-NE-CZ	9.51	137.71	124.40
1	A	304	ALA	CA-C-O	-9.50	109.36	120.10
1	D	20	GLN	CA-CB-CG	-9.50	95.10	114.10
1	H	172	ARG	CA-C-N	9.50	134.00	120.79
1	H	172	ARG	C-N-CA	9.50	134.00	120.79
1	P	26	GLY	N-CA-C	-9.50	101.78	115.64
1	J	42	ARG	NH1-CZ-NH2	-9.49	106.96	119.30
1	O	227	LEU	CA-C-O	-9.49	111.08	121.33
1	P	318	ALA	CA-C-O	-9.49	109.38	120.10
1	E	348	SER	CA-C-O	9.48	131.85	121.05
1	Q	68	SER	N-CA-CB	-9.48	93.12	110.18
1	H	95	ASN	CA-CB-CG	-9.47	103.13	112.60
1	J	92	LEU	O-C-N	-9.46	111.23	122.87
1	B	9	GLN	OE1-CD-NE2	9.46	132.06	122.60
1	H	207	LYS	CA-CB-CG	9.46	133.03	114.10
1	H	260	VAL	CA-C-O	9.45	126.10	119.20
1	M	102	ILE	N-CA-CB	-9.45	99.65	110.99
1	P	353	THR	N-CA-C	-9.45	101.44	113.72
1	I	186	VAL	N-CA-CB	-9.45	100.42	110.72
1	L	214	LYS	CA-C-O	9.44	130.43	120.42
1	Q	334	ASN	CA-CB-CG	-9.44	103.16	112.60
1	Q	133	ARG	NH1-CZ-NH2	9.43	131.56	119.30
1	L	73	ILE	O-C-N	-9.42	112.35	122.81
1	R	344	HIS	N-CA-CB	9.41	126.50	110.50
1	A	207	LYS	CG-CD-CE	9.40	132.93	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	LEU	N-CA-C	-9.40	95.98	110.17
1	B	335	CYS	CA-C-O	9.40	130.38	120.42
1	P	89	GLN	CB-CG-CD	-9.40	96.62	112.60
1	K	152	ARG	CA-CB-CG	9.40	132.90	114.10
1	P	325	GLU	CB-CG-CD	-9.40	96.62	112.60
1	C	218	ASP	CA-CB-CG	-9.39	103.21	112.60
1	D	348	SER	CA-C-N	9.39	138.42	121.05
1	D	348	SER	C-N-CA	9.39	138.42	121.05
1	D	237	HIS	CB-CG-CD2	-9.39	119.00	131.20
1	H	302	GLY	O-C-N	-9.39	116.59	121.85
1	O	168	ASN	CA-CB-CG	-9.39	103.21	112.60
1	D	91	LYS	CA-C-O	-9.38	109.94	120.54
1	F	26	GLY	N-CA-C	-9.37	102.89	115.36
1	B	211	ALA	CA-C-N	-9.37	107.62	120.46
1	B	211	ALA	C-N-CA	-9.37	107.62	120.46
1	M	14	GLU	CA-C-N	-9.37	106.79	120.28
1	M	14	GLU	C-N-CA	-9.37	106.79	120.28
1	B	220	HIS	CA-C-O	-9.36	110.68	121.54
1	H	3	ARG	CD-NE-CZ	9.36	137.50	124.40
1	H	195	ASP	N-CA-C	9.36	122.68	111.82
1	B	267	ILE	CB-CG1-CD1	-9.36	94.15	113.80
1	D	87	ASP	N-CA-CB	-9.36	94.68	110.49
1	F	248	VAL	CA-C-O	9.36	131.09	121.17
1	A	203	TYR	CA-C-O	-9.35	111.18	121.00
1	B	61	ILE	CA-C-O	-9.35	111.29	121.29
1	H	8	THR	OG1-CB-CG2	-9.35	90.61	109.30
1	D	24	ALA	N-CA-CB	9.35	123.62	110.07
1	L	55	ARG	CD-NE-CZ	-9.34	111.32	124.40
1	O	166	ASN	CA-CB-CG	-9.34	103.26	112.60
1	I	67	SER	CA-C-N	-9.34	103.71	121.54
1	I	67	SER	C-N-CA	-9.34	103.71	121.54
1	I	89	GLN	N-CA-CB	-9.34	96.26	110.73
1	I	232	MET	N-CA-C	-9.34	98.49	110.53
1	N	3	ARG	NE-CZ-NH2	9.33	127.59	119.20
1	B	166	ASN	OD1-CG-ND2	-9.33	113.27	122.60
1	D	28	GLY	CA-C-O	9.32	136.79	120.57
1	G	20	GLN	O-C-N	-9.32	111.31	122.22
1	C	27	LYS	CG-CD-CE	9.32	132.74	111.30
1	H	143	ASP	CA-CB-CG	-9.32	103.28	112.60
1	A	25	ASN	CA-CB-CG	9.31	121.91	112.60
1	L	94	ARG	CD-NE-CZ	9.31	137.43	124.40
1	C	199	GLU	CB-CG-CD	9.31	128.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	VAL	O-C-N	-9.30	113.34	123.20
1	F	334	ASN	CA-CB-CG	-9.29	103.31	112.60
1	R	95	ASN	OD1-CG-ND2	-9.29	113.31	122.60
1	R	223	LEU	N-CA-C	9.29	121.41	111.28
1	O	61	ILE	CA-C-O	-9.29	110.74	121.05
1	C	81	GLU	CB-CG-CD	9.28	128.38	112.60
1	O	80	HIS	CA-CB-CG	-9.28	104.52	113.80
1	Q	266	GLY	CA-C-O	9.28	129.41	121.06
1	O	233	VAL	CA-C-O	-9.27	109.36	120.76
1	L	87	ASP	N-CA-CB	-9.27	94.82	110.49
1	R	103	VAL	CA-C-O	-9.27	110.08	121.11
1	R	171	ALA	CA-C-O	-9.27	111.15	120.70
1	Q	70	ASN	CA-CB-CG	9.27	121.87	112.60
1	L	319	ASN	CA-CB-CG	-9.27	103.33	112.60
1	I	79	PHE	CA-C-O	-9.26	110.07	120.54
1	I	226	THR	N-CA-CB	-9.26	96.93	111.56
1	M	134	CYS	O-C-N	-9.26	112.31	122.12
1	N	103	VAL	CA-C-N	-9.26	111.16	123.10
1	N	103	VAL	C-N-CA	-9.26	111.16	123.10
1	L	311	ALA	O-C-N	9.26	131.60	122.07
1	B	207	LYS	N-CA-CB	-9.25	95.94	110.28
1	J	217	ASN	CB-CG-ND2	-9.24	102.54	116.40
1	B	226	THR	CA-CB-OG1	-9.23	95.75	109.60
1	N	71	GLN	CA-C-N	9.23	136.41	122.56
1	N	71	GLN	C-N-CA	9.23	136.41	122.56
1	H	237	HIS	CB-CA-C	-9.23	94.99	110.68
1	Q	150	VAL	O-C-N	9.23	132.78	123.18
1	B	85	GLN	CA-C-O	9.23	132.61	121.72
1	I	265	PRO	CA-C-N	-9.23	109.09	121.27
1	I	265	PRO	C-N-CA	-9.23	109.09	121.27
1	L	186	VAL	N-CA-CB	-9.22	100.49	111.00
1	A	343	VAL	N-CA-CB	9.22	126.44	111.23
1	A	357	PHE	N-CA-C	9.21	130.43	110.80
1	R	166	ASN	CA-CB-CG	-9.21	103.39	112.60
1	O	183	VAL	N-CA-C	-9.21	97.85	107.89
1	I	291	LEU	CA-C-O	-9.20	107.55	120.16
1	B	11	GLN	CG-CD-OE1	9.20	139.20	120.80
1	B	227	LEU	N-CA-CB	-9.20	96.61	111.24
1	O	97	LEU	O-C-N	-9.20	112.59	122.07
1	D	21	SER	O-C-N	9.19	134.65	122.33
1	C	182	LEU	O-C-N	-9.19	112.65	122.94
1	D	344	HIS	CA-C-N	9.19	139.09	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	344	HIS	C-N-CA	9.19	139.09	121.54
1	I	109	ASP	CA-C-O	-9.18	112.37	122.01
1	D	135	ALA	O-C-N	9.18	132.61	122.15
1	I	68	SER	CA-C-N	-9.17	105.46	121.97
1	I	68	SER	C-N-CA	-9.17	105.46	121.97
1	G	60	GLU	O-C-N	9.17	133.55	122.27
1	L	151	LEU	CD1-CG-CD2	-9.16	90.65	110.80
1	F	10	GLU	CA-C-O	-9.15	110.85	120.55
1	G	10	GLU	CB-CG-CD	-9.14	97.07	112.60
1	N	147	TRP	CA-C-N	-9.14	110.26	123.05
1	N	147	TRP	C-N-CA	-9.14	110.26	123.05
1	O	90	GLY	CA-C-N	-9.13	108.47	121.72
1	O	90	GLY	C-N-CA	-9.13	108.47	121.72
1	J	336	GLN	O-C-N	9.13	131.80	122.12
1	B	27	LYS	CG-CD-CE	-9.13	90.30	111.30
1	A	168	ASN	O-C-N	9.13	132.56	122.15
1	R	256	LEU	CA-C-O	9.13	130.56	119.79
1	F	91	LYS	CA-C-O	-9.12	110.65	121.05
1	K	183	VAL	CA-C-O	-9.12	113.77	119.15
1	Q	74	GLY	CA-C-N	-9.12	109.23	121.27
1	Q	74	GLY	C-N-CA	-9.12	109.23	121.27
1	F	116	ALA	CA-C-N	9.12	137.90	120.66
1	F	116	ALA	C-N-CA	9.12	137.90	120.66
1	E	226	THR	CA-CB-OG1	-9.12	95.93	109.60
1	L	246	GLU	O-C-N	9.11	131.77	122.12
1	D	218	ASP	CA-CB-CG	9.10	121.70	112.60
1	P	176	ILE	CA-C-O	-9.10	111.48	120.95
1	I	271	SER	O-C-N	-9.10	112.28	121.93
1	J	219	HIS	CA-CB-CG	9.10	122.89	113.80
1	C	304	ALA	CA-C-O	-9.09	110.02	120.20
1	A	87	ASP	CA-CB-CG	-9.08	103.52	112.60
1	A	218	ASP	CA-C-N	-9.08	107.58	122.65
1	A	218	ASP	C-N-CA	-9.08	107.58	122.65
1	J	51	THR	N-CA-CB	-9.08	94.85	111.37
1	L	166	ASN	CA-CB-CG	-9.08	103.52	112.60
1	F	118	THR	N-CA-CB	-9.07	94.86	111.37
1	D	160	SER	O-C-N	9.07	131.73	122.12
1	A	357	PHE	CA-C-N	9.06	138.84	121.54
1	A	357	PHE	C-N-CA	9.06	138.84	121.54
1	Q	87	ASP	CB-CG-OD2	-9.05	97.57	118.40
1	R	309	ALA	N-CA-CB	9.05	123.56	110.16
1	A	133	ARG	CD-NE-CZ	-9.05	111.73	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	VAL	N-CA-CB	-9.05	100.78	110.82
1	Q	139	LYS	CA-C-O	-9.05	109.88	120.10
1	J	266	GLY	CA-C-N	-9.04	111.07	123.10
1	J	266	GLY	C-N-CA	-9.04	111.07	123.10
1	J	17	GLU	CB-CG-CD	9.04	127.97	112.60
1	K	310	LEU	N-CA-C	-9.04	100.99	111.03
1	C	24	ALA	CA-C-O	-9.04	110.97	120.55
1	D	45	ARG	NE-CZ-NH2	-9.04	111.06	119.20
1	L	284	ASN	CA-C-O	9.03	130.00	120.70
1	N	115	LEU	CA-C-O	9.03	131.00	120.70
1	L	56	ARG	NE-CZ-NH2	-9.03	111.07	119.20
1	Q	249	ALA	O-C-N	-9.03	112.55	122.12
1	K	325	GLU	CB-CG-CD	-9.03	97.26	112.60
1	O	118	THR	N-CA-CB	-9.03	97.00	111.62
1	R	199	GLU	CA-CB-CG	9.03	132.15	114.10
1	R	180	ASN	OD1-CG-ND2	9.02	131.62	122.60
1	D	164	GLN	CB-CG-CD	9.02	127.93	112.60
1	G	66	ASP	O-C-N	9.02	134.59	122.59
1	F	164	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	I	168	ASN	O-C-N	9.01	132.43	122.15
1	J	237	HIS	CA-C-N	-9.01	107.69	122.65
1	J	237	HIS	C-N-CA	-9.01	107.69	122.65
1	A	118	THR	CA-C-N	-9.01	106.46	122.32
1	A	118	THR	C-N-CA	-9.01	106.46	122.32
1	B	33	ASP	CA-C-O	-9.01	108.51	119.59
1	M	282	ASN	OD1-CG-ND2	9.01	131.61	122.60
1	A	118	THR	OG1-CB-CG2	9.01	127.31	109.30
1	A	196	HIS	N-CA-CB	-9.00	98.05	110.29
1	F	244	THR	N-CA-CB	-9.00	95.16	110.10
1	A	2	HIS	CA-CB-CG	9.00	122.80	113.80
1	O	303	ARG	CD-NE-CZ	8.99	136.99	124.40
1	G	303	ARG	CD-NE-CZ	-8.99	111.81	124.40
1	B	1	ALA	O-C-N	-8.99	108.62	123.00
1	K	199	GLU	CA-CB-CG	8.98	132.07	114.10
1	O	159	SER	CA-C-O	8.98	132.41	121.81
1	G	247	GLN	OE1-CD-NE2	-8.98	113.62	122.60
1	A	22	ILE	CA-C-O	-8.98	110.96	120.57
1	H	128	ASP	CA-CB-CG	8.98	121.58	112.60
1	P	185	ILE	CA-C-O	-8.98	110.62	120.85
1	F	123	THR	N-CA-CB	8.97	126.30	111.31
1	P	24	ALA	CA-C-N	-8.97	107.99	122.62
1	P	24	ALA	C-N-CA	-8.97	107.99	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	232	MET	N-CA-C	-8.97	98.96	110.53
1	D	151	LEU	CD1-CG-CD2	-8.96	91.08	110.80
1	B	166	ASN	CA-CB-CG	-8.96	103.64	112.60
1	E	152	ARG	CD-NE-CZ	-8.96	111.86	124.40
1	D	214	LYS	N-CA-CB	-8.95	96.51	110.30
1	M	189	GLU	O-C-N	8.95	133.54	123.16
1	J	195	ASP	N-CA-C	8.95	121.11	111.36
1	G	25	ASN	CA-CB-CG	8.94	121.54	112.60
1	O	266	GLY	CA-C-N	-8.94	110.77	123.11
1	O	266	GLY	C-N-CA	-8.94	110.77	123.11
1	B	300	SER	N-CA-C	-8.94	91.76	110.80
1	E	353	THR	N-CA-C	-8.94	101.43	114.39
1	I	195	ASP	N-CA-C	8.94	122.19	111.82
1	P	94	ARG	NH1-CZ-NH2	8.94	130.92	119.30
1	A	202	GLN	CB-CG-CD	-8.94	97.41	112.60
1	N	123	THR	CA-C-N	-8.93	109.80	122.75
1	N	123	THR	C-N-CA	-8.93	109.80	122.75
1	F	42	ARG	NE-CZ-NH2	8.93	127.24	119.20
1	C	107	LYS	O-C-N	-8.93	111.88	122.95
1	G	334	ASN	CA-CB-CG	-8.93	103.67	112.60
1	A	226	THR	N-CA-CB	-8.92	97.46	111.56
1	F	89	GLN	CB-CA-C	-8.92	96.10	111.45
1	H	171	ALA	N-CA-CB	8.92	122.94	110.01
1	I	336	GLN	O-C-N	8.91	131.25	122.07
1	F	352	SER	O-C-N	-8.91	110.74	122.59
1	A	344	HIS	CB-CA-C	-8.90	92.70	110.42
1	I	188	PRO	N-CA-CB	8.90	109.23	102.73
1	N	87	ASP	OD1-CG-OD2	8.90	144.27	122.90
1	C	11	GLN	CA-C-N	-8.90	108.33	120.44
1	C	11	GLN	C-N-CA	-8.90	108.33	120.44
1	M	107	LYS	CA-C-O	-8.90	110.17	120.49
1	N	330	ARG	NE-CZ-NH1	-8.90	112.60	121.50
1	C	111	GLY	CA-C-O	8.89	133.45	122.78
1	C	133	ARG	CA-C-O	8.89	129.98	120.55
1	B	280	THR	CA-C-N	-8.89	108.88	120.44
1	B	280	THR	C-N-CA	-8.89	108.88	120.44
1	N	125	GLN	CG-CD-OE1	8.89	138.57	120.80
1	K	152	ARG	NE-CZ-NH2	8.88	127.20	119.20
1	L	256	LEU	CA-C-N	-8.88	106.39	120.60
1	L	256	LEU	C-N-CA	-8.88	106.39	120.60
1	D	86	LYS	CA-C-N	8.88	138.50	121.54
1	D	86	LYS	C-N-CA	8.88	138.50	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	3	ARG	CG-CD-NE	8.88	131.53	112.00
1	C	59	ARG	NE-CZ-NH1	-8.87	112.63	121.50
1	A	118	THR	N-CA-CB	-8.87	95.03	111.53
1	L	136	GLN	OE1-CD-NE2	8.87	131.47	122.60
1	J	22	ILE	CA-C-O	-8.87	110.89	120.47
1	I	43	LEU	CA-C-O	8.87	130.25	119.79
1	L	226	THR	N-CA-CB	-8.86	96.51	111.31
1	K	218	ASP	CA-C-O	8.85	129.94	120.55
1	O	168	ASN	OD1-CG-ND2	8.85	131.45	122.60
1	A	70	ASN	CA-CB-CG	8.85	121.45	112.60
1	G	341	GLN	CA-C-N	-8.85	107.59	122.64
1	G	341	GLN	C-N-CA	-8.85	107.59	122.64
1	I	305	LEU	CA-C-N	-8.85	108.44	121.98
1	I	305	LEU	C-N-CA	-8.85	108.44	121.98
1	I	111	GLY	CA-C-O	8.85	130.71	122.57
1	N	167	ALA	CA-C-N	-8.85	108.42	120.28
1	N	167	ALA	C-N-CA	-8.85	108.42	120.28
1	N	2	HIS	CA-C-N	8.84	138.43	121.54
1	N	2	HIS	C-N-CA	8.84	138.43	121.54
1	N	11	GLN	CG-CD-NE2	-8.84	103.14	116.40
1	H	267	ILE	CA-C-O	-8.84	111.20	120.39
1	F	218	ASP	CA-C-O	-8.84	109.81	119.97
1	J	136	GLN	OE1-CD-NE2	8.84	131.44	122.60
1	B	76	VAL	CA-C-O	-8.83	110.80	120.43
1	G	81	GLU	CB-CG-CD	8.83	127.61	112.60
1	I	191	ILE	CA-CB-CG1	-8.83	95.39	110.40
1	P	189	GLU	CA-C-O	-8.83	110.62	120.69
1	C	330	ARG	NE-CZ-NH1	-8.82	112.68	121.50
1	N	123	THR	CB-CA-C	-8.81	95.60	112.43
1	R	55	ARG	NE-CZ-NH2	-8.81	111.27	119.20
1	I	62	LEU	CA-C-O	-8.81	111.21	120.55
1	B	42	ARG	NE-CZ-NH2	8.81	127.13	119.20
1	J	254	THR	CA-C-O	-8.81	111.57	120.82
1	P	49	GLU	CA-CB-CG	8.81	131.72	114.10
1	B	118	THR	N-CA-CB	-8.80	97.43	111.43
1	B	336	GLN	CA-C-O	-8.80	111.58	120.82
1	C	118	THR	N-CA-CB	-8.80	96.94	111.20
1	C	233	VAL	O-C-N	-8.80	112.20	122.94
1	P	234	THR	CA-C-O	-8.80	111.65	121.51
1	I	167	ALA	CA-C-N	-8.80	107.79	120.29
1	I	167	ALA	C-N-CA	-8.80	107.79	120.29
1	B	344	HIS	O-C-N	8.80	132.42	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	ASP	CA-C-O	-8.80	108.01	119.80
1	M	67	SER	N-CA-CB	8.80	125.36	110.49
1	O	168	ASN	N-CA-CB	8.80	123.92	110.28
1	C	328	MET	N-CA-CB	-8.80	97.14	110.16
1	G	330	ARG	CA-C-N	-8.79	106.94	120.31
1	G	330	ARG	C-N-CA	-8.79	106.94	120.31
1	H	267	ILE	CA-CB-CG2	8.79	125.45	110.50
1	N	221	VAL	CA-C-O	-8.79	110.65	121.11
1	O	199	GLU	CA-CB-CG	8.79	131.68	114.10
1	O	229	LYS	O-C-N	8.79	127.38	121.23
1	M	343	VAL	CA-C-O	8.79	127.64	119.20
1	N	164	GLN	CB-CG-CD	8.79	127.54	112.60
1	F	344	HIS	CA-CB-CG	-8.79	105.01	113.80
1	D	161	LEU	N-CA-C	-8.78	101.63	111.82
1	K	152	ARG	N-CA-CB	8.78	126.83	111.55
1	G	246	GLU	O-C-N	-8.78	112.81	122.12
1	P	214	LYS	O-C-N	8.78	131.42	122.12
1	E	89	GLN	CA-C-N	8.77	136.78	121.07
1	E	89	GLN	C-N-CA	8.77	136.78	121.07
1	M	294	PRO	CA-C-O	-8.77	106.72	119.00
1	N	207	LYS	CG-CD-CE	8.77	131.48	111.30
1	H	248	VAL	O-C-N	8.77	130.73	121.87
1	A	133	ARG	NE-CZ-NH2	-8.77	111.31	119.20
1	D	9	GLN	OE1-CD-NE2	-8.77	113.83	122.60
1	K	191	ILE	CA-CB-CG1	-8.77	95.49	110.40
1	D	16	SER	N-CA-C	-8.77	101.18	112.23
1	O	133	ARG	CD-NE-CZ	-8.77	112.13	124.40
1	B	89	GLN	CB-CG-CD	-8.76	97.70	112.60
1	P	291	LEU	O-C-N	8.76	128.05	121.65
1	E	256	LEU	O-C-N	-8.76	111.50	122.27
1	G	89	GLN	CB-CA-C	-8.76	97.51	111.18
1	M	330	ARG	NE-CZ-NH1	-8.76	112.74	121.50
1	I	250	MET	O-C-N	8.76	132.13	122.15
1	A	87	ASP	N-CA-CB	-8.76	95.69	110.49
1	B	160	SER	CB-CA-C	-8.76	95.97	110.85
1	B	203	TYR	CB-CG-CD1	-8.76	107.67	120.80
1	R	70	ASN	CB-CA-C	-8.76	90.57	110.18
1	K	24	ALA	CA-C-N	-8.75	105.38	122.62
1	K	24	ALA	C-N-CA	-8.75	105.38	122.62
1	I	11	GLN	OE1-CD-NE2	-8.75	113.85	122.60
1	B	237	HIS	CA-CB-CG	-8.75	105.05	113.80
1	K	183	VAL	O-C-N	8.75	129.18	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	283	LEU	CA-C-N	8.74	132.71	120.29
1	M	283	LEU	C-N-CA	8.74	132.71	120.29
1	O	42	ARG	CA-C-O	-8.74	111.64	120.82
1	A	163	ILE	CA-C-O	8.74	130.75	121.05
1	H	9	GLN	O-C-N	8.74	131.38	122.12
1	N	50	ASN	CA-CB-CG	-8.73	103.86	112.60
1	O	259	THR	CA-C-N	-8.73	116.66	122.60
1	O	259	THR	C-N-CA	-8.73	116.66	122.60
1	C	5	PRO	CB-CA-C	-8.73	100.47	111.56
1	M	109	ASP	CA-C-O	-8.73	111.75	121.87
1	G	87	ASP	CB-CG-OD2	8.73	138.47	118.40
1	B	195	ASP	CA-CB-CG	8.72	121.33	112.60
1	H	199	GLU	O-C-N	-8.72	111.54	122.27
1	J	160	SER	CA-C-N	-8.71	107.92	120.29
1	J	160	SER	C-N-CA	-8.71	107.92	120.29
1	J	191	ILE	CA-CB-CG1	-8.72	95.58	110.40
1	M	172	ARG	NE-CZ-NH2	-8.71	111.36	119.20
1	O	164	GLN	CB-CG-CD	8.71	127.41	112.60
1	B	26	GLY	CA-C-N	-8.71	104.53	122.03
1	B	26	GLY	C-N-CA	-8.71	104.53	122.03
1	K	220	HIS	N-CA-C	8.70	123.39	111.90
1	K	303	ARG	N-CA-C	8.70	121.55	111.11
1	G	152	ARG	CB-CA-C	-8.70	92.79	109.66
1	M	166	ASN	OD1-CG-ND2	-8.70	113.90	122.60
1	I	217	ASN	O-C-N	8.70	131.03	122.07
1	R	222	TYR	CA-C-O	-8.69	111.59	120.98
1	K	172	ARG	CD-NE-CZ	-8.69	112.24	124.40
1	A	119	ASN	CA-C-N	8.68	134.99	122.40
1	A	119	ASN	C-N-CA	8.68	134.99	122.40
1	M	344	HIS	N-CA-C	-8.68	92.30	110.80
1	P	90	GLY	O-C-N	8.68	133.09	122.32
1	J	253	VAL	CA-C-O	8.68	129.62	120.25
1	Q	125	GLN	CG-CD-NE2	8.68	129.42	116.40
1	R	89	GLN	OE1-CD-NE2	8.68	131.28	122.60
1	J	348	SER	N-CA-CB	8.68	125.15	110.49
1	M	340	GLY	N-CA-C	-8.68	101.54	114.90
1	O	283	LEU	CA-C-O	8.67	129.91	120.20
1	G	237	HIS	CA-CB-CG	-8.67	105.13	113.80
1	E	15	LEU	O-C-N	-8.67	113.14	122.07
1	M	93	PHE	CA-C-O	8.67	130.17	120.90
1	P	9	GLN	CA-C-N	-8.67	107.98	120.29
1	P	9	GLN	C-N-CA	-8.67	107.98	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ARG	N-CA-CB	8.66	126.63	111.55
1	H	147	TRP	CA-C-O	-8.66	109.34	120.25
1	M	189	GLU	CA-C-O	-8.66	110.96	120.92
1	A	296	LYS	CA-C-O	-8.65	112.38	121.55
1	P	54	ASN	CA-C-O	-8.65	111.25	120.42
1	N	341	GLN	CA-C-N	-8.65	107.94	122.64
1	N	341	GLN	C-N-CA	-8.65	107.94	122.64
1	P	60	GLU	O-C-N	8.65	131.28	122.12
1	K	4	PHE	CA-CB-CG	-8.64	105.16	113.80
1	P	87	ASP	N-CA-CB	-8.64	95.89	110.49
1	B	227	LEU	CA-C-N	-8.62	109.17	122.62
1	B	227	LEU	C-N-CA	-8.62	109.17	122.62
1	O	18	ILE	CA-C-N	-8.62	109.23	120.44
1	O	18	ILE	C-N-CA	-8.62	109.23	120.44
1	N	194	GLY	CA-C-N	8.62	135.12	120.72
1	N	194	GLY	C-N-CA	8.62	135.12	120.72
1	R	19	ALA	CB-CA-C	-8.62	97.35	110.88
1	G	4	PHE	CA-CB-CG	-8.62	105.18	113.80
1	E	94	ARG	NE-CZ-NH1	-8.62	112.88	121.50
1	H	172	ARG	CA-C-O	8.62	130.12	120.90
1	J	195	ASP	CB-CA-C	-8.61	96.21	110.85
1	C	164	GLN	CB-CG-CD	8.61	127.24	112.60
1	K	184	PRO	CA-C-O	-8.61	110.17	120.85
1	N	13	LYS	CA-C-N	-8.61	108.75	120.28
1	N	13	LYS	C-N-CA	-8.61	108.75	120.28
1	J	26	GLY	CA-C-O	-8.61	109.72	119.10
1	K	25	ASN	N-CA-CB	8.61	125.68	110.79
1	Q	51	THR	N-CA-CB	-8.61	95.52	111.53
1	E	50	ASN	OD1-CG-ND2	-8.60	114.00	122.60
1	C	170	LEU	CA-C-O	-8.60	111.79	120.82
1	J	14	GLU	CA-C-O	-8.60	111.31	120.42
1	O	168	ASN	CA-C-O	-8.60	110.08	119.97
1	G	148	ARG	NH1-CZ-NH2	8.60	130.47	119.30
1	K	18	ILE	CA-C-O	8.60	130.35	121.41
1	O	257	HIS	CA-C-O	-8.60	107.87	119.05
1	D	143	ASP	CA-C-O	-8.59	109.32	119.03
1	K	297	LEU	O-C-N	-8.59	112.31	123.13
1	P	113	ALA	CA-C-O	8.59	127.98	119.22
1	N	133	ARG	CD-NE-CZ	-8.59	112.38	124.40
1	Q	26	GLY	N-CA-C	-8.59	103.47	115.32
1	L	118	THR	N-CA-CB	-8.58	97.91	110.70
1	K	296	LYS	O-C-N	8.58	132.98	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	LEU	N-CA-C	-8.57	102.01	111.36
1	D	322	ALA	N-CA-CB	-8.57	97.52	110.12
1	H	162	ALA	CA-C-N	-8.56	108.26	120.42
1	H	162	ALA	C-N-CA	-8.56	108.26	120.42
1	K	287	ASN	CB-CG-ND2	-8.56	103.56	116.40
1	L	10	GLU	CB-CA-C	-8.56	96.58	110.79
1	N	179	GLN	CG-CD-NE2	-8.56	103.56	116.40
1	J	24	ALA	O-C-N	-8.56	112.85	122.09
1	H	108	LEU	CA-C-O	8.55	128.46	119.05
1	F	267	ILE	CB-CA-C	8.55	122.91	110.77
1	I	68	SER	CA-CB-OG	-8.55	94.00	111.10
1	I	282	ASN	OD1-CG-ND2	-8.55	114.05	122.60
1	F	350	ALA	CA-C-N	8.54	137.85	121.54
1	F	350	ALA	C-N-CA	8.54	137.85	121.54
1	H	70	ASN	N-CA-CB	-8.54	94.81	110.18
1	R	132	GLU	N-CA-CB	8.54	122.87	110.06
1	H	190	VAL	CA-C-N	8.54	136.88	119.72
1	H	190	VAL	C-N-CA	8.54	136.88	119.72
1	R	293	LYS	CB-CG-CD	-8.54	91.67	111.30
1	B	168	ASN	OD1-CG-ND2	8.53	131.13	122.60
1	K	94	ARG	NE-CZ-NH2	-8.53	111.52	119.20
1	Q	89	GLN	CA-C-N	-8.53	104.69	121.41
1	Q	89	GLN	C-N-CA	-8.53	104.69	121.41
1	Q	168	ASN	CB-CG-ND2	-8.53	103.61	116.40
1	K	9	GLN	N-CA-CB	8.53	122.65	110.12
1	E	233	VAL	CA-C-N	8.52	136.48	121.75
1	E	233	VAL	C-N-CA	8.52	136.48	121.75
1	F	237	HIS	CA-CB-CG	-8.52	105.28	113.80
1	N	10	GLU	CB-CA-C	-8.52	96.65	110.79
1	P	51	THR	N-CA-CB	-8.52	97.27	110.56
1	N	26	GLY	N-CA-C	-8.52	103.04	115.30
1	L	248	VAL	CA-C-N	-8.51	108.87	120.28
1	L	248	VAL	C-N-CA	-8.51	108.87	120.28
1	I	216	LEU	CA-C-O	8.51	129.73	120.20
1	H	135	ALA	CA-C-O	8.50	129.81	120.63
1	Q	2	HIS	CA-CB-CG	8.50	122.30	113.80
1	A	354	GLN	N-CA-C	8.49	123.09	110.52
1	F	68	SER	CA-CB-OG	8.49	128.08	111.10
1	P	357	PHE	N-CA-C	8.49	122.62	110.14
1	L	39	MET	O-C-N	8.49	131.88	122.20
1	M	277	GLU	CA-C-N	-8.49	107.41	120.31
1	M	277	GLU	C-N-CA	-8.49	107.41	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	147	TRP	CA-C-O	-8.49	110.90	120.32
1	F	248	VAL	O-C-N	-8.48	113.60	121.91
1	E	267	ILE	CA-CB-CG2	8.48	124.91	110.50
1	P	166	ASN	CA-CB-CG	-8.48	104.12	112.60
1	P	143	ASP	CA-CB-CG	-8.47	104.13	112.60
1	R	193	ASP	CA-CB-CG	-8.46	104.14	112.60
1	D	38	THR	CA-C-O	-8.46	111.45	120.42
1	D	282	ASN	OD1-CG-ND2	8.46	131.06	122.60
1	I	191	ILE	O-C-N	-8.46	111.46	121.10
1	L	258	ARG	CD-NE-CZ	8.46	136.24	124.40
1	G	178	GLN	OE1-CD-NE2	-8.46	114.14	122.60
1	Q	36	VAL	CA-C-O	8.46	129.74	120.95
1	J	254	THR	O-C-N	8.45	130.78	122.07
1	B	105	GLY	CA-C-N	-8.45	111.40	123.06
1	B	105	GLY	C-N-CA	-8.45	111.40	123.06
1	K	258	ARG	N-CA-CB	8.44	123.61	110.44
1	D	188	PRO	O-C-N	8.44	134.04	122.64
1	F	103	VAL	CA-C-N	-8.44	112.72	123.19
1	F	103	VAL	C-N-CA	-8.44	112.72	123.19
1	B	102	ILE	N-CA-C	8.44	119.92	108.11
1	D	324	GLN	CA-C-O	8.44	129.49	120.55
1	E	3	ARG	CG-CD-NE	8.43	130.55	112.00
1	G	123	THR	CB-CA-C	-8.42	94.21	111.22
1	E	282	ASN	OD1-CG-ND2	8.42	131.02	122.60
1	P	177	CYS	CA-C-O	8.42	129.47	120.55
1	E	143	ASP	CA-CB-CG	-8.42	104.18	112.60
1	E	306	GLN	CA-C-O	8.42	128.31	119.05
1	O	109	ASP	CA-C-O	8.42	131.59	121.99
1	M	91	LYS	CA-C-O	-8.41	111.24	120.92
1	I	257	HIS	CA-C-N	-8.41	108.66	122.54
1	I	257	HIS	C-N-CA	-8.41	108.66	122.54
1	J	260	VAL	N-CA-C	8.41	117.19	107.77
1	H	194	GLY	N-CA-C	8.41	120.62	112.04
1	H	303	ARG	NE-CZ-NH2	8.41	126.77	119.20
1	M	129	GLY	CA-C-O	8.41	127.27	118.95
1	I	319	ASN	CA-CB-CG	-8.40	104.20	112.60
1	Q	138	LYS	N-CA-C	-8.40	102.08	111.07
1	I	330	ARG	NE-CZ-NH1	-8.40	113.10	121.50
1	R	124	ILE	CB-CG1-CD1	8.39	131.43	113.80
1	E	229	LYS	O-C-N	8.39	128.92	121.37
1	H	58	PHE	CA-CB-CG	-8.39	105.41	113.80
1	M	283	LEU	O-C-N	-8.39	113.23	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	35	SER	O-C-N	8.39	132.73	121.74
1	B	220	HIS	O-C-N	8.38	133.38	122.40
1	D	89	GLN	N-CA-CB	-8.38	96.33	110.49
1	O	220	HIS	CA-C-O	-8.38	111.31	121.28
1	D	72	SER	CA-C-O	8.37	129.30	119.67
1	E	327	PHE	O-C-N	-8.37	113.44	122.07
1	B	277	GLU	CA-C-N	-8.37	109.06	120.44
1	B	277	GLU	C-N-CA	-8.37	109.06	120.44
1	E	295	TRP	O-C-N	8.37	134.33	123.11
1	M	123	THR	N-CA-CB	8.37	124.45	111.22
1	H	8	THR	CA-CB-OG1	-8.37	97.05	109.60
1	D	51	THR	N-CA-CB	-8.37	97.47	110.85
1	E	228	LEU	CA-C-O	-8.36	111.84	120.71
1	R	193	ASP	CA-C-O	-8.36	111.95	121.15
1	C	128	ASP	CA-CB-CG	8.36	120.96	112.60
1	C	292	PRO	O-C-N	-8.36	113.40	123.01
1	I	277	GLU	O-C-N	8.36	131.12	122.09
1	A	264	VAL	CA-C-N	8.36	128.05	119.19
1	A	264	VAL	C-N-CA	8.36	128.05	119.19
1	O	179	GLN	OE1-CD-NE2	8.36	130.96	122.60
1	C	66	ASP	CA-CB-CG	8.36	120.95	112.60
1	I	9	GLN	OE1-CD-NE2	-8.36	114.25	122.60
1	I	14	GLU	CA-C-N	-8.36	107.61	120.31
1	I	14	GLU	C-N-CA	-8.36	107.61	120.31
1	I	152	ARG	NE-CZ-NH1	-8.36	113.14	121.50
1	O	327	PHE	CA-C-O	8.35	129.40	120.55
1	D	225	GLY	O-C-N	8.34	133.54	122.70
1	J	123	THR	N-CA-CB	8.34	124.58	110.49
1	D	343	VAL	N-CA-CB	8.34	122.92	111.41
1	J	226	THR	N-CA-CB	-8.34	97.74	111.66
1	B	25	ASN	CA-C-O	-8.33	110.31	120.89
1	Q	133	ARG	NE-CZ-NH2	-8.33	111.70	119.20
1	F	36	VAL	CA-C-O	8.32	129.61	120.95
1	O	54	ASN	OD1-CG-ND2	8.32	130.93	122.60
1	J	237	HIS	CA-CB-CG	-8.32	105.48	113.80
1	O	94	ARG	NE-CZ-NH1	-8.32	113.18	121.50
1	R	24	ALA	N-CA-C	8.32	121.09	111.11
1	A	334	ASN	CA-CB-CG	-8.31	104.29	112.60
1	B	29	ILE	CA-C-O	8.31	129.12	120.39
1	J	264	VAL	N-CA-C	-8.31	101.48	108.63
1	K	157	CYS	N-CA-CB	-8.31	94.63	110.42
1	I	223	LEU	CA-C-O	-8.31	112.10	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	SER	O-C-N	8.31	133.23	122.10
1	H	42	ARG	CA-C-O	-8.30	111.75	120.55
1	L	180	ASN	CA-CB-CG	-8.30	104.30	112.60
1	A	127	LEU	CA-C-N	-8.30	109.11	120.82
1	A	127	LEU	C-N-CA	-8.30	109.11	120.82
1	N	143	ASP	CA-C-O	-8.30	109.39	119.18
1	M	36	VAL	CA-C-N	-8.30	110.77	119.98
1	M	36	VAL	C-N-CA	-8.30	110.77	119.98
1	F	172	ARG	NE-CZ-NH1	-8.30	113.20	121.50
1	D	88	SER	N-CA-CB	-8.29	96.76	110.53
1	Q	303	ARG	CD-NE-CZ	8.29	136.01	124.40
1	N	68	SER	O-C-N	-8.29	112.07	122.27
1	R	132	GLU	CB-CG-CD	8.29	126.70	112.60
1	N	156	GLN	CA-CB-CG	-8.29	97.52	114.10
1	A	356	LEU	N-CA-C	8.29	122.07	109.23
1	B	13	LYS	CA-C-N	-8.28	109.28	120.79
1	B	13	LYS	C-N-CA	-8.28	109.28	120.79
1	G	195	ASP	N-CA-CB	-8.28	97.52	110.44
1	E	347	SER	N-CA-CB	8.28	124.48	110.49
1	P	152	ARG	CD-NE-CZ	-8.28	112.81	124.40
1	D	68	SER	N-CA-CB	-8.28	96.50	110.49
1	K	26	GLY	N-CA-C	-8.27	103.61	115.27
1	H	172	ARG	O-C-N	-8.27	113.49	122.09
1	M	343	VAL	CB-CA-C	-8.27	98.72	110.95
1	O	98	LYS	CA-C-O	8.27	129.31	120.55
1	L	38	THR	O-C-N	8.26	130.58	122.07
1	O	26	GLY	N-CA-C	-8.26	104.49	115.40
1	Q	13	LYS	CA-C-N	-8.26	109.70	120.44
1	Q	13	LYS	C-N-CA	-8.26	109.70	120.44
1	B	215	ALA	O-C-N	8.26	130.88	122.12
1	P	54	ASN	O-C-N	8.26	131.57	122.15
1	H	125	GLN	CG-CD-NE2	8.26	128.79	116.40
1	P	166	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	N	328	MET	CA-C-O	8.26	129.31	120.55
1	R	191	ILE	CB-CG1-CD1	-8.26	96.45	113.80
1	F	195	ASP	CA-CB-CG	8.26	120.86	112.60
1	A	258	ARG	NH1-CZ-NH2	-8.26	108.57	119.30
1	F	171	ALA	CA-C-O	-8.26	112.20	120.70
1	A	164	GLN	CA-CB-CG	8.25	130.61	114.10
1	F	54	ASN	CA-CB-CG	-8.25	104.35	112.60
1	N	100	LYS	CB-CA-C	-8.25	101.08	111.22
1	N	178	GLN	CA-C-O	-8.25	111.72	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1	ALA	N-CA-CB	-8.25	98.03	110.40
1	R	22	ILE	CA-C-O	-8.25	111.75	120.57
1	B	231	ASN	N-CA-C	-8.24	98.32	110.52
1	L	144	PHE	CA-C-N	-8.24	114.89	121.82
1	F	207	LYS	O-C-N	8.24	130.56	122.07
1	G	71	GLN	O-C-N	8.24	133.54	122.49
1	L	144	PHE	C-N-CA	-8.24	114.89	121.82
1	I	230	PRO	CB-CA-C	-8.24	97.96	111.56
1	B	260	VAL	N-CA-C	8.24	115.06	107.56
1	P	262	ALA	O-C-N	-8.24	112.58	122.22
1	D	152	ARG	CB-CG-CD	8.24	130.25	111.30
1	H	278	ASP	CA-C-O	8.24	129.41	120.10
1	R	141	GLY	O-C-N	8.23	131.97	122.33
1	K	272	GLY	N-CA-C	8.23	125.50	113.48
1	Q	82	THR	CA-C-O	-8.23	110.80	120.10
1	H	113	ALA	CA-C-O	8.23	128.08	120.26
1	J	133	ARG	NE-CZ-NH1	-8.23	113.27	121.50
1	L	201	CYS	CA-C-O	8.23	129.27	120.55
1	M	265	PRO	CA-C-N	-8.23	111.34	121.38
1	M	265	PRO	C-N-CA	-8.23	111.34	121.38
1	P	226	THR	N-CA-CB	-8.23	98.28	111.62
1	L	59	ARG	O-C-N	8.22	130.84	122.12
1	B	211	ALA	CA-C-O	8.22	129.16	120.70
1	M	9	GLN	OE1-CD-NE2	-8.22	114.38	122.60
1	C	152	ARG	NE-CZ-NH1	-8.21	113.29	121.50
1	G	88	SER	N-CA-C	-8.21	103.77	113.21
1	H	244	THR	OG1-CB-CG2	-8.21	92.88	109.30
1	E	171	ALA	CA-C-O	-8.21	111.72	120.42
1	H	199	GLU	CB-CG-CD	8.21	126.55	112.60
1	H	210	ALA	O-C-N	-8.21	113.62	122.07
1	B	214	LYS	N-CA-C	-8.20	102.29	111.07
1	R	67	SER	O-C-N	-8.20	111.52	122.43
1	G	87	ASP	CB-CG-OD1	-8.20	99.54	118.40
1	P	228	LEU	CA-C-O	-8.20	111.23	120.66
1	P	334	ASN	CA-C-O	8.20	129.46	119.79
1	Q	267	ILE	O-C-N	-8.19	115.08	123.03
1	B	287	ASN	OD1-CG-ND2	8.19	130.79	122.60
1	E	343	VAL	CA-C-O	-8.19	110.54	120.78
1	D	296	LYS	CB-CA-C	-8.19	97.56	109.84
1	A	165	GLU	N-CA-CB	-8.19	98.04	110.16
1	Q	24	ALA	N-CA-C	8.19	121.13	111.71
1	B	229	LYS	O-C-N	8.18	128.12	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	343	VAL	N-CA-CB	8.18	124.73	111.23
1	G	80	HIS	CA-CB-CG	-8.18	105.62	113.80
1	H	107	LYS	CG-CD-CE	8.18	130.12	111.30
1	O	73	ILE	O-C-N	-8.18	114.59	123.18
1	O	248	VAL	CA-C-N	-8.18	109.80	120.44
1	O	248	VAL	C-N-CA	-8.18	109.80	120.44
1	A	99	GLU	CA-C-O	-8.18	110.56	119.97
1	D	85	GLN	OE1-CD-NE2	-8.18	114.42	122.60
1	L	336	GLN	OE1-CD-NE2	-8.18	114.42	122.60
1	I	165	GLU	CB-CA-C	8.18	124.75	110.85
1	M	149	ALA	N-CA-CB	8.18	123.94	110.85
1	M	319	ASN	CA-CB-CG	-8.18	104.42	112.60
1	K	114	PRO	O-C-N	8.18	132.91	123.10
1	L	164	GLN	CB-CG-CD	8.18	126.50	112.60
1	Q	11	GLN	CA-C-O	-8.18	111.88	120.55
1	R	123	THR	N-CA-C	-8.17	93.39	110.80
1	D	152	ARG	CD-NE-CZ	-8.17	112.96	124.40
1	I	335	CYS	CA-C-O	8.17	129.31	120.24
1	J	1	ALA	N-CA-CB	-8.17	98.14	110.40
1	K	51	THR	N-CA-CB	-8.17	97.11	110.43
1	R	200	HIS	CA-CB-CG	8.17	121.97	113.80
1	J	117	GLY	O-C-N	8.17	131.23	122.41
1	D	155	ASP	CA-C-O	8.17	132.19	120.51
1	E	119	ASN	CA-CB-CG	-8.17	104.43	112.60
1	J	307	ALA	O-C-N	8.17	130.48	122.07
1	O	14	GLU	O-C-N	8.16	130.48	122.07
1	Q	190	VAL	CA-C-N	8.16	137.23	122.13
1	Q	190	VAL	C-N-CA	8.16	137.23	122.13
1	K	28	GLY	CA-C-N	-8.16	111.80	123.06
1	K	28	GLY	C-N-CA	-8.16	111.80	123.06
1	M	180	ASN	CA-CB-CG	-8.16	104.44	112.60
1	N	220	HIS	CA-CB-CG	-8.16	105.64	113.80
1	Q	175	SER	CA-C-N	8.16	130.84	120.56
1	Q	175	SER	C-N-CA	8.16	130.84	120.56
1	F	218	ASP	CA-CB-CG	8.15	120.75	112.60
1	M	160	SER	CA-C-N	-8.15	108.71	120.29
1	M	160	SER	C-N-CA	-8.15	108.71	120.29
1	B	97	LEU	O-C-N	-8.15	113.28	122.09
1	D	268	CYS	N-CA-CB	-8.15	96.94	110.39
1	G	325	GLU	O-C-N	-8.15	113.48	122.12
1	C	26	GLY	N-CA-C	-8.15	103.97	115.30
1	I	343	VAL	CA-C-O	-8.15	110.59	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	256	LEU	CA-C-O	8.15	129.06	120.42
1	J	267	ILE	CA-C-O	-8.15	111.92	120.39
1	A	156	GLN	N-CA-C	8.14	122.67	112.24
1	K	132	GLU	O-C-N	8.14	131.44	122.15
1	K	258	ARG	CA-CB-CG	8.14	130.39	114.10
1	E	160	SER	O-C-N	-8.14	112.87	122.15
1	P	123	THR	CB-CA-C	-8.14	94.21	110.42
1	B	90	GLY	CA-C-N	-8.14	109.55	120.95
1	B	90	GLY	C-N-CA	-8.14	109.55	120.95
1	C	341	GLN	CA-C-N	-8.14	110.52	122.65
1	C	341	GLN	C-N-CA	-8.14	110.52	122.65
1	G	90	GLY	CA-C-O	-8.14	108.83	119.25
1	K	324	GLN	CA-C-N	8.13	131.50	120.44
1	K	324	GLN	C-N-CA	8.13	131.50	120.44
1	G	299	PHE	O-C-N	-8.13	112.58	123.15
1	H	97	LEU	CA-C-N	-8.13	108.58	120.28
1	H	97	LEU	C-N-CA	-8.13	108.58	120.28
1	B	220	HIS	ND1-CE1-NE2	-8.12	100.28	108.40
1	N	124	ILE	O-C-N	8.12	131.84	123.07
1	E	3	ARG	O-C-N	-8.12	111.79	122.59
1	F	5	PRO	CA-C-N	-8.12	107.97	120.31
1	F	5	PRO	C-N-CA	-8.12	107.97	120.31
1	J	89	GLN	CB-CA-C	-8.12	96.68	110.64
1	F	22	ILE	CA-C-O	-8.11	111.31	120.96
1	A	128	ASP	O-C-N	-8.11	112.90	122.95
1	M	123	THR	CB-CA-C	-8.11	94.08	111.11
1	M	184	PRO	CA-C-N	8.11	133.55	122.93
1	M	184	PRO	C-N-CA	8.11	133.55	122.93
1	R	265	PRO	CA-C-O	8.10	129.64	118.86
1	F	138	LYS	N-CA-C	-8.10	102.53	111.36
1	P	94	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	C	95	ASN	CA-CB-CG	-8.10	104.50	112.60
1	H	24	ALA	CA-C-O	-8.10	110.95	120.10
1	L	219	HIS	CA-C-O	8.10	129.23	119.43
1	Q	237	HIS	CA-CB-CG	-8.10	105.70	113.80
1	O	270	LEU	CA-C-N	-8.10	107.44	121.52
1	O	270	LEU	C-N-CA	-8.10	107.44	121.52
1	I	226	THR	CA-CB-CG2	8.09	124.25	110.50
1	P	296	LYS	CA-C-O	-8.09	112.75	121.56
1	A	2	HIS	CA-C-O	8.09	132.07	120.51
1	D	9	GLN	CA-C-O	8.09	128.99	120.42
1	J	11	GLN	OE1-CD-NE2	-8.09	114.52	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	87	ASP	CB-CA-C	-8.08	94.33	110.42
1	H	160	SER	O-C-N	8.08	131.37	122.15
1	H	171	ALA	O-C-N	8.08	130.40	122.07
1	L	2	HIS	N-CA-CB	8.08	124.15	110.49
1	A	67	SER	N-CA-CB	-8.08	96.84	110.49
1	D	194	GLY	CA-C-N	-8.08	109.83	122.67
1	D	194	GLY	C-N-CA	-8.08	109.83	122.67
1	N	291	LEU	CA-C-O	-8.08	112.78	120.94
1	O	19	ALA	CA-C-O	8.08	129.30	120.82
1	E	153	ILE	CA-CB-CG2	8.07	124.22	110.50
1	K	232	MET	O-C-N	8.07	132.08	122.96
1	L	246	GLU	CA-C-O	-8.07	111.99	120.55
1	B	210	ALA	CA-C-O	8.07	129.25	119.97
1	Q	150	VAL	CA-C-O	-8.07	112.12	120.27
1	D	337	ALA	N-CA-C	-8.07	102.48	111.28
1	A	66	ASP	CA-C-N	8.07	136.95	121.54
1	A	66	ASP	C-N-CA	8.07	136.95	121.54
1	E	39	MET	CA-C-O	8.07	128.97	120.42
1	O	6	ALA	CA-C-O	-8.07	111.87	120.42
1	F	94	ARG	NH1-CZ-NH2	8.06	129.78	119.30
1	E	133	ARG	NH1-CZ-NH2	8.06	129.78	119.30
1	I	157	CYS	O-C-N	8.06	129.39	121.57
1	E	50	ASN	CB-CG-ND2	8.06	128.48	116.40
1	O	3	ARG	CA-CB-CG	8.06	130.21	114.10
1	R	121	GLU	O-C-N	-8.06	113.61	122.79
1	A	351	ALA	O-C-N	8.05	130.66	122.12
1	B	71	GLN	CG-CD-NE2	-8.05	104.32	116.40
1	E	299	PHE	CA-C-O	8.05	130.53	121.11
1	K	232	MET	CA-C-O	-8.05	112.21	121.47
1	P	263	ALA	O-C-N	-8.05	111.92	122.39
1	C	277	GLU	O-C-N	8.05	130.78	122.09
1	F	123	THR	N-CA-C	-8.05	97.51	108.86
1	J	24	ALA	N-CA-CB	8.05	121.74	110.07
1	P	343	VAL	CB-CA-C	-8.04	98.10	111.29
1	Q	336	GLN	CA-C-O	8.04	129.08	120.55
1	A	51	THR	N-CA-CB	-8.04	97.92	110.06
1	F	133	ARG	NE-CZ-NH1	-8.04	113.46	121.50
1	I	231	ASN	CA-CB-CG	-8.04	104.56	112.60
1	C	217	ASN	CA-CB-CG	8.03	120.63	112.60
1	R	67	SER	CA-C-O	8.03	129.22	119.10
1	H	330	ARG	NH1-CZ-NH2	-8.03	108.86	119.30
1	K	118	THR	N-CA-CB	-8.03	97.72	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	353	THR	N-CA-CB	-8.03	98.84	110.80
1	P	296	LYS	O-C-N	8.03	132.34	122.86
1	P	352	SER	N-CA-CB	8.03	126.01	111.96
1	P	357	PHE	CA-C-N	8.03	134.51	122.95
1	P	357	PHE	C-N-CA	8.03	134.51	122.95
1	F	227	LEU	CA-C-O	-8.03	111.72	121.11
1	N	89	GLN	CB-CA-C	-8.03	97.70	110.94
1	N	224	GLU	CA-C-O	-8.02	111.21	120.20
1	F	231	ASN	CB-CA-C	-8.02	95.79	109.83
1	G	330	ARG	NH1-CZ-NH2	-8.02	108.87	119.30
1	N	194	GLY	CA-C-O	8.02	130.20	122.26
1	P	157	CYS	O-C-N	-8.02	113.86	121.72
1	C	95	ASN	OD1-CG-ND2	8.02	130.62	122.60
1	K	348	SER	CA-C-O	-8.02	109.05	120.51
1	R	20	GLN	O-C-N	8.01	130.61	122.12
1	B	281	LEU	N-CA-CB	-8.01	98.39	110.01
1	R	276	GLU	N-CA-CB	8.01	121.87	109.94
1	E	166	ASN	OD1-CG-ND2	8.01	130.61	122.60
1	P	102	ILE	CA-C-O	-8.01	111.86	120.59
1	B	116	ALA	O-C-N	8.01	132.74	122.97
1	F	51	THR	N-CA-CB	-8.01	96.63	111.52
1	M	272	GLY	CA-C-N	-8.01	110.74	123.31
1	M	272	GLY	C-N-CA	-8.01	110.74	123.31
1	P	56	ARG	NE-CZ-NH2	8.01	126.41	119.20
1	Q	87	ASP	N-CA-CB	-8.01	96.96	110.49
1	R	51	THR	N-CA-CB	-8.01	96.51	111.00
1	F	149	ALA	CA-C-O	8.00	130.72	121.28
1	R	89	GLN	N-CA-CB	-8.00	96.97	110.49
1	L	175	SER	O-C-N	8.00	130.41	122.09
1	G	181	GLY	CA-C-N	-7.99	110.00	122.87
1	G	181	GLY	C-N-CA	-7.99	110.00	122.87
1	C	214	LYS	CA-C-O	7.99	129.02	120.55
1	O	94	ARG	N-CA-C	-7.99	102.55	111.82
1	A	128	ASP	CA-CB-CG	7.99	120.59	112.60
1	D	49	GLU	CA-C-O	7.99	129.99	120.81
1	D	212	VAL	O-C-N	-7.99	114.08	121.91
1	H	306	GLN	N-CA-CB	-7.99	98.91	110.65
1	J	94	ARG	CA-CB-CG	7.99	130.07	114.10
1	R	109	ASP	CA-CB-CG	7.98	120.58	112.60
1	N	93	PHE	CA-CB-CG	7.98	121.78	113.80
1	P	282	ASN	CA-CB-CG	-7.98	104.62	112.60
1	D	129	GLY	CA-C-O	7.98	129.82	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	300	SER	N-CA-C	-7.98	98.65	110.06
1	O	91	LYS	CA-CB-CG	-7.98	98.14	114.10
1	D	9	GLN	CG-CD-NE2	7.98	128.37	116.40
1	I	160	SER	CA-C-N	-7.98	109.77	120.54
1	I	160	SER	C-N-CA	-7.98	109.77	120.54
1	J	339	LYS	CA-CB-CG	7.98	130.06	114.10
1	L	198	LEU	O-C-N	-7.98	113.73	122.03
1	O	126	GLY	CA-C-N	-7.98	107.40	120.72
1	O	126	GLY	C-N-CA	-7.98	107.40	120.72
1	F	259	THR	CA-C-N	-7.97	116.85	122.59
1	F	259	THR	C-N-CA	-7.97	116.85	122.59
1	I	134	CYS	O-C-N	-7.97	113.67	122.12
1	J	172	ARG	CA-C-O	7.97	128.91	120.70
1	L	18	ILE	CA-C-N	-7.97	110.07	120.44
1	L	18	ILE	C-N-CA	-7.97	110.07	120.44
1	A	220	HIS	CA-CB-CG	-7.97	105.83	113.80
1	H	82	THR	CA-CB-OG1	-7.97	97.64	109.60
1	Q	41	ASN	O-C-N	7.97	130.57	122.12
1	P	280	THR	CA-C-O	-7.97	112.43	120.80
1	I	185	ILE	CA-C-O	-7.97	111.33	120.65
1	K	66	ASP	N-CA-CB	-7.97	98.69	110.17
1	H	267	ILE	O-C-N	7.97	131.64	123.20
1	I	59	ARG	CD-NE-CZ	-7.97	113.25	124.40
1	N	56	ARG	CD-NE-CZ	-7.97	113.25	124.40
1	E	27	LYS	CD-CE-NZ	7.96	137.39	111.90
1	H	27	LYS	O-C-N	-7.96	113.43	122.75
1	B	333	ALA	N-CA-C	-7.96	102.54	111.14
1	M	17	GLU	CB-CG-CD	7.96	126.13	112.60
1	D	228	LEU	O-C-N	7.96	133.57	123.23
1	E	327	PHE	CA-C-O	7.96	129.17	120.82
1	J	221	VAL	CA-CB-CG2	-7.96	96.88	110.40
1	A	26	GLY	N-CA-C	-7.95	104.22	115.43
1	G	10	GLU	O-C-N	7.95	130.36	122.09
1	F	29	ILE	O-C-N	-7.95	114.59	123.18
1	Q	132	GLU	CB-CG-CD	7.95	126.11	112.60
1	J	66	ASP	CA-CB-CG	7.95	120.55	112.60
1	K	218	ASP	CA-C-N	-7.95	109.45	122.65
1	K	218	ASP	C-N-CA	-7.95	109.45	122.65
1	H	217	ASN	OD1-CG-ND2	-7.95	114.65	122.60
1	J	191	ILE	N-CA-CB	-7.95	100.08	111.21
1	B	305	LEU	CA-C-O	-7.95	110.22	119.59
1	I	71	GLN	N-CA-C	-7.95	103.38	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	127	LEU	CA-C-N	-7.95	109.62	120.82
1	R	127	LEU	C-N-CA	-7.95	109.62	120.82
1	H	96	ILE	CA-C-O	-7.94	112.75	121.17
1	L	232	MET	CA-C-O	-7.94	111.83	121.36
1	R	101	GLY	O-C-N	-7.94	112.47	122.32
1	O	109	ASP	O-C-N	-7.94	112.96	122.65
1	B	168	ASN	CA-C-N	-7.94	109.01	120.29
1	B	168	ASN	C-N-CA	-7.94	109.01	120.29
1	G	179	GLN	CG-CD-NE2	-7.94	104.49	116.40
1	B	218	ASP	N-CA-C	7.94	120.84	111.71
1	E	109	ASP	N-CA-CB	7.94	121.71	110.36
1	O	71	GLN	CA-C-N	7.93	139.00	122.58
1	O	71	GLN	C-N-CA	7.93	139.00	122.58
1	Q	103	VAL	CA-C-N	-7.93	112.86	123.10
1	Q	103	VAL	C-N-CA	-7.93	112.86	123.10
1	H	211	ALA	CA-C-O	7.93	129.09	119.97
1	I	148	ARG	N-CA-C	7.93	121.76	108.20
1	G	110	GLN	CG-CD-NE2	-7.93	104.51	116.40
1	J	239	CYS	CA-C-O	-7.93	112.28	121.16
1	B	292	PRO	CB-CA-C	-7.92	101.87	111.46
1	C	258	ARG	NH1-CZ-NH2	-7.92	109.00	119.30
1	I	25	ASN	O-C-N	7.92	136.21	121.63
1	P	267	ILE	N-CA-CB	-7.92	101.05	111.82
1	P	352	SER	CA-C-N	7.92	134.85	122.26
1	P	352	SER	C-N-CA	7.92	134.85	122.26
1	K	260	VAL	N-CA-C	7.92	114.76	107.56
1	O	23	VAL	CA-C-O	7.92	129.44	120.42
1	L	332	MET	CA-C-O	7.92	129.66	120.00
1	E	4	PHE	N-CA-CB	-7.91	101.28	111.09
1	G	186	VAL	O-C-N	-7.91	113.78	122.64
1	H	191	ILE	CA-C-O	7.91	126.72	119.76
1	M	294	PRO	O-C-N	7.91	133.06	122.30
1	A	258	ARG	CA-CB-CG	7.91	129.91	114.10
1	D	143	ASP	CA-CB-CG	-7.91	104.69	112.60
1	H	333	ALA	O-C-N	7.91	130.63	122.09
1	N	9	GLN	CA-C-N	-7.91	109.69	120.28
1	N	9	GLN	C-N-CA	-7.91	109.69	120.28
1	A	345	THR	CB-CA-C	7.90	123.02	109.51
1	D	148	ARG	NE-CZ-NH1	-7.90	113.60	121.50
1	N	223	LEU	O-C-N	7.90	130.49	122.12
1	E	265	PRO	CA-C-N	-7.90	110.85	121.27
1	E	265	PRO	C-N-CA	-7.90	110.85	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	9	GLN	N-CA-C	-7.90	102.75	111.36
1	R	30	LEU	CB-CA-C	-7.90	97.03	110.22
1	N	71	GLN	CB-CG-CD	-7.90	99.18	112.60
1	Q	334	ASN	CA-C-O	7.90	129.02	120.10
1	L	73	ILE	N-CA-C	7.89	119.31	108.89
1	E	58	PHE	CA-CB-CG	-7.89	105.91	113.80
1	C	195	ASP	N-CA-CB	-7.89	96.59	110.39
1	E	350	ALA	CA-C-O	7.89	131.79	120.51
1	J	68	SER	CB-CA-C	-7.89	94.73	110.42
1	J	345	THR	N-CA-C	7.89	127.60	110.80
1	O	341	GLN	CA-C-N	-7.89	111.66	122.86
1	O	341	GLN	C-N-CA	-7.89	111.66	122.86
1	I	297	LEU	CA-C-O	7.88	128.60	120.24
1	N	127	LEU	CA-C-N	-7.88	109.91	120.95
1	N	127	LEU	C-N-CA	-7.88	109.91	120.95
1	P	9	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	C	152	ARG	CD-NE-CZ	-7.88	113.37	124.40
1	I	272	GLY	CA-C-N	-7.88	110.94	123.31
1	I	272	GLY	C-N-CA	-7.88	110.94	123.31
1	J	334	ASN	CA-CB-CG	-7.88	104.72	112.60
1	C	256	LEU	CA-C-O	-7.88	112.10	120.92
1	D	29	ILE	CB-CG1-CD1	-7.87	97.27	113.80
1	B	203	TYR	CB-CG-CD2	7.87	132.61	120.80
1	F	54	ASN	OD1-CG-ND2	7.87	130.47	122.60
1	I	186	VAL	O-C-N	-7.87	113.98	122.95
1	J	345	THR	CA-C-O	7.87	131.77	120.51
1	B	178	GLN	CA-CB-CG	-7.87	98.36	114.10
1	I	44	GLN	O-C-N	7.86	130.27	122.09
1	R	124	ILE	N-CA-CB	-7.86	98.54	111.44
1	D	301	TYR	CA-C-O	7.86	130.55	121.28
1	I	70	ASN	N-CA-C	-7.86	101.48	113.89
1	E	170	LEU	CA-C-O	7.85	128.87	120.55
1	Q	267	ILE	CA-CB-CG1	-7.85	97.05	110.40
1	I	236	GLY	N-CA-C	-7.85	102.49	112.54
1	F	219	HIS	O-C-N	-7.85	109.78	122.42
1	H	256	LEU	CA-C-O	7.85	128.74	120.42
1	H	277	GLU	CA-C-O	-7.85	112.23	120.55
1	I	59	ARG	CG-CD-NE	7.85	129.27	112.00
1	Q	81	GLU	CB-CG-CD	7.85	125.94	112.60
1	N	270	LEU	CA-C-O	-7.85	112.46	121.72
1	N	59	ARG	CB-CG-CD	7.84	129.34	111.30
1	N	128	ASP	CA-CB-CG	7.84	120.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	85	GLN	OE1-CD-NE2	-7.84	114.76	122.60
1	G	296	LYS	CB-CA-C	-7.84	97.34	109.89
1	N	336	GLN	OE1-CD-NE2	-7.84	114.76	122.60
1	L	329	LYS	CG-CD-CE	7.84	129.34	111.30
1	M	19	ALA	CA-C-O	-7.84	112.24	120.55
1	R	31	ALA	CA-C-O	-7.84	112.80	121.58
1	E	149	ALA	CA-C-N	-7.84	112.67	123.10
1	E	149	ALA	C-N-CA	-7.84	112.67	123.10
1	F	347	SER	CA-CB-OG	7.84	126.78	111.10
1	B	204	VAL	CA-C-O	-7.83	112.55	120.85
1	N	244	THR	CA-C-O	-7.83	110.91	120.54
1	B	260	VAL	O-C-N	-7.83	115.99	121.55
1	P	118	THR	CA-C-N	-7.83	110.42	122.16
1	P	118	THR	C-N-CA	-7.83	110.42	122.16
1	A	165	GLU	O-C-N	-7.83	113.23	122.15
1	F	303	ARG	CG-CD-NE	7.83	129.22	112.00
1	O	328	MET	CB-CA-C	7.82	126.13	110.17
1	B	38	THR	O-C-N	7.82	130.16	122.03
1	O	160	SER	CA-C-N	-7.82	109.19	120.29
1	O	160	SER	C-N-CA	-7.82	109.19	120.29
1	F	59	ARG	NE-CZ-NH2	7.82	126.24	119.20
1	A	109	ASP	CA-C-O	-7.82	112.48	121.47
1	C	87	ASP	N-CA-CB	-7.82	97.28	110.49
1	R	76	VAL	O-C-N	-7.82	115.05	123.18
1	H	208	VAL	CA-C-O	-7.82	113.14	121.27
1	L	212	VAL	N-CA-CB	-7.82	101.83	110.51
1	H	132	GLU	N-CA-CB	7.81	121.58	109.94
1	I	68	SER	N-CA-C	-7.81	94.16	110.80
1	H	13	LYS	CB-CA-C	7.81	123.75	110.79
1	N	271	SER	CA-C-O	7.81	127.49	118.90
1	K	357	PHE	N-CA-CB	7.81	123.77	110.50
1	J	298	SER	N-CA-C	7.81	118.84	108.07
1	N	222	TYR	CA-C-N	-7.81	109.82	120.28
1	N	222	TYR	C-N-CA	-7.81	109.82	120.28
1	K	22	ILE	CA-C-O	-7.80	110.17	119.85
1	M	70	ASN	N-CA-C	-7.80	94.18	110.80
1	O	147	TRP	CA-C-N	-7.80	112.00	123.00
1	O	147	TRP	C-N-CA	-7.80	112.00	123.00
1	J	211	ALA	O-C-N	-7.80	113.98	122.09
1	N	63	PHE	CA-CB-CG	7.80	121.60	113.80
1	E	349	GLY	N-CA-C	-7.80	94.69	113.18
1	K	165	GLU	N-CA-CB	-7.80	98.59	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	195	ASP	CA-CB-CG	-7.80	104.80	112.60
1	G	147	TRP	CA-C-O	-7.80	110.42	120.25
1	J	161	LEU	N-CA-C	-7.79	102.86	111.36
1	I	334	ASN	CB-CG-ND2	7.79	128.09	116.40
1	O	80	HIS	CB-CA-C	-7.79	97.90	110.84
1	F	345	THR	CB-CA-C	7.79	125.92	110.42
1	H	260	VAL	O-C-N	-7.79	115.38	121.46
1	P	227	LEU	CA-C-N	-7.79	110.11	122.73
1	P	227	LEU	C-N-CA	-7.79	110.11	122.73
1	R	89	GLN	CB-CG-CD	-7.79	99.36	112.60
1	D	213	TYR	CA-C-N	-7.79	107.45	120.68
1	D	213	TYR	C-N-CA	-7.79	107.45	120.68
1	P	339	LYS	CA-C-O	-7.79	110.40	119.59
1	C	148	ARG	N-CA-C	7.78	120.94	108.41
1	K	226	THR	N-CA-CB	-7.78	98.66	111.66
1	C	32	ALA	N-CA-CB	-7.78	99.89	111.25
1	H	258	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	G	26	GLY	N-CA-C	-7.78	105.01	115.36
1	H	156	GLN	CB-CG-CD	-7.78	99.38	112.60
1	I	282	ASN	CB-CG-ND2	7.78	128.07	116.40
1	A	169	ALA	CA-C-O	-7.78	112.18	120.42
1	K	148	ARG	NE-CZ-NH1	7.78	129.28	121.50
1	M	350	ALA	CA-C-N	7.78	133.55	121.19
1	M	350	ALA	C-N-CA	7.78	133.55	121.19
1	M	90	GLY	CA-C-O	-7.77	109.47	119.58
1	A	94	ARG	CD-NE-CZ	7.77	135.28	124.40
1	B	237	HIS	CA-C-O	7.77	128.88	120.10
1	H	238	ALA	CA-C-N	-7.77	110.59	122.09
1	H	238	ALA	C-N-CA	-7.77	110.59	122.09
1	I	165	GLU	CB-CG-CD	-7.77	99.39	112.60
1	K	205	THR	CA-C-N	-7.77	108.50	120.31
1	K	205	THR	C-N-CA	-7.77	108.50	120.31
1	O	160	SER	CB-CA-C	-7.77	97.89	110.79
1	C	339	LYS	N-CA-CB	7.77	122.77	110.73
1	C	188	PRO	CA-C-N	-7.77	110.31	121.42
1	C	188	PRO	C-N-CA	-7.77	110.31	121.42
1	M	124	ILE	N-CA-CB	-7.77	97.88	111.39
1	D	91	LYS	N-CA-C	-7.76	96.57	109.46
1	H	205	THR	CA-C-N	-7.76	110.35	120.44
1	H	205	THR	C-N-CA	-7.76	110.35	120.44
1	J	226	THR	CA-CB-CG2	7.76	123.69	110.50
1	N	9	GLN	CA-C-O	-7.76	112.25	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	VAL	CA-CB-CG1	7.76	123.59	110.40
1	B	22	ILE	N-CA-C	-7.76	103.88	112.80
1	B	333	ALA	CA-C-N	-7.76	109.11	120.28
1	B	333	ALA	C-N-CA	-7.76	109.11	120.28
1	R	210	ALA	N-CA-C	-7.76	102.77	111.07
1	E	180	ASN	CA-CB-CG	-7.76	104.84	112.60
1	J	9	GLN	O-C-N	7.76	130.99	122.15
1	G	258	ARG	NH1-CZ-NH2	-7.75	109.22	119.30
1	N	232	MET	N-CA-C	-7.75	100.08	110.55
1	G	266	GLY	CA-C-N	-7.75	112.79	123.10
1	G	266	GLY	C-N-CA	-7.75	112.79	123.10
1	A	184	PRO	CA-C-O	-7.74	112.21	121.03
1	I	152	ARG	CA-C-N	-7.74	112.99	122.90
1	I	152	ARG	C-N-CA	-7.74	112.99	122.90
1	R	237	HIS	CB-CA-C	-7.74	97.52	110.68
1	O	338	ALA	CA-C-N	-7.74	110.53	122.60
1	O	338	ALA	C-N-CA	-7.74	110.53	122.60
1	D	151	LEU	CA-C-O	-7.74	112.37	121.11
1	K	132	GLU	CA-C-O	-7.74	112.22	120.42
1	B	201	CYS	N-CA-CB	-7.74	98.29	110.28
1	C	11	GLN	O-C-N	7.74	131.27	122.22
1	G	123	THR	N-CA-C	-7.74	98.55	109.69
1	M	26	GLY	CA-C-O	-7.74	110.84	119.04
1	G	181	GLY	CA-C-O	-7.73	109.76	119.19
1	N	316	LYS	CB-CG-CD	7.73	129.08	111.30
1	M	22	ILE	O-C-N	-7.73	114.06	121.87
1	D	155	ASP	CA-CB-CG	7.73	120.33	112.60
1	N	209	LEU	CA-C-N	-7.73	107.54	120.68
1	N	209	LEU	C-N-CA	-7.73	107.54	120.68
1	O	144	PHE	CA-C-O	-7.73	112.98	121.33
1	C	87	ASP	CB-CG-OD2	-7.72	100.63	118.40
1	G	46	ILE	CB-CG1-CD1	7.72	130.02	113.80
1	L	105	GLY	CA-C-N	-7.72	112.20	122.94
1	L	105	GLY	C-N-CA	-7.72	112.20	122.94
1	H	190	VAL	O-C-N	-7.72	113.58	122.62
1	A	359	ALA	CA-C-N	7.72	135.59	121.70
1	A	359	ALA	C-N-CA	7.72	135.59	121.70
1	J	143	ASP	CA-C-O	-7.72	109.81	118.69
1	Q	118	THR	CA-C-O	-7.72	112.41	121.44
1	B	116	ALA	CA-C-O	-7.72	112.66	121.15
1	C	282	ASN	OD1-CG-ND2	-7.72	114.88	122.60
1	R	186	VAL	N-CA-CB	-7.72	103.57	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	132	GLU	CB-CG-CD	7.71	125.72	112.60
1	D	124	ILE	CA-C-O	7.71	129.31	120.67
1	L	77	ILE	CB-CA-C	-7.71	101.35	110.91
1	R	118	THR	N-CA-CB	-7.71	99.13	111.62
1	C	164	GLN	OE1-CD-NE2	-7.71	114.89	122.60
1	E	277	GLU	CA-C-O	-7.71	112.25	120.42
1	K	25	ASN	CA-CB-CG	7.71	120.31	112.60
1	E	219	HIS	CA-CB-CG	-7.71	106.09	113.80
1	R	118	THR	CA-C-O	-7.71	112.88	121.51
1	F	219	HIS	CA-CB-CG	-7.70	106.10	113.80
1	N	12	LYS	CA-C-O	7.70	128.91	120.82
1	B	14	GLU	CA-C-N	-7.70	109.19	120.28
1	B	14	GLU	C-N-CA	-7.70	109.19	120.28
1	F	156	GLN	OE1-CD-NE2	7.70	130.30	122.60
1	K	14	GLU	CB-CG-CD	7.70	125.68	112.60
1	P	202	GLN	CB-CG-CD	-7.70	99.52	112.60
1	Q	327	PHE	CA-CB-CG	-7.70	106.11	113.80
1	B	248	VAL	O-C-N	-7.69	114.41	121.87
1	D	225	GLY	CA-C-N	-7.69	110.15	122.53
1	D	225	GLY	C-N-CA	-7.69	110.15	122.53
1	I	164	GLN	CB-CG-CD	7.69	125.67	112.60
1	C	2	HIS	CA-C-O	-7.69	110.82	120.28
1	L	61	ILE	CA-C-O	-7.69	113.28	121.27
1	A	330	ARG	NE-CZ-NH1	-7.68	113.81	121.50
1	E	191	ILE	CB-CG1-CD1	-7.68	97.67	113.80
1	G	194	GLY	CA-C-O	7.68	130.53	122.24
1	H	332	MET	CA-C-O	7.68	128.80	119.97
1	H	160	SER	CA-C-O	-7.67	112.29	120.42
1	P	1	ALA	CB-CA-C	7.67	122.01	110.50
1	E	75	GLY	N-CA-C	-7.67	99.06	110.87
1	G	178	GLN	O-C-N	-7.67	112.42	122.39
1	A	47	LYS	CA-C-N	7.67	133.19	123.14
1	A	47	LYS	C-N-CA	7.67	133.19	123.14
1	F	199	GLU	CB-CG-CD	7.67	125.64	112.60
1	I	344	HIS	CA-CB-CG	-7.67	106.13	113.80
1	A	81	GLU	CA-C-O	7.67	129.05	121.00
1	N	123	THR	CA-CB-OG1	-7.67	98.10	109.60
1	N	168	ASN	CA-C-O	-7.67	112.42	120.55
1	M	129	GLY	N-CA-C	7.66	125.71	115.59
1	K	101	GLY	CA-C-O	-7.66	109.48	119.44
1	N	295	TRP	CA-C-O	-7.66	112.14	121.11
1	B	298	SER	CA-C-O	-7.66	109.56	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	131	SER	O-C-N	7.66	129.96	122.07
1	K	293	LYS	N-CA-CB	-7.66	98.89	110.99
1	Q	80	HIS	CA-CB-CG	-7.66	106.14	113.80
1	Q	94	ARG	NE-CZ-NH2	7.66	126.09	119.20
1	G	341	GLN	CA-C-O	-7.66	110.92	119.95
1	K	99	GLU	O-C-N	7.66	131.18	122.22
1	N	42	ARG	CA-C-O	-7.65	112.44	120.55
1	R	214	LYS	CB-CA-C	-7.65	98.03	110.74
1	B	76	VAL	O-C-N	7.65	131.33	123.07
1	E	199	GLU	CB-CG-CD	7.65	125.61	112.60
1	L	195	ASP	N-CA-CB	-7.65	98.45	110.46
1	C	196	HIS	CA-CB-CG	-7.65	106.15	113.80
1	L	300	SER	N-CA-C	-7.65	92.81	108.18
1	D	166	ASN	OD1-CG-ND2	-7.65	114.95	122.60
1	P	258	ARG	N-CA-CB	7.65	122.47	110.46
1	R	297	LEU	CA-C-O	7.65	130.21	120.57
1	D	70	ASN	CA-C-O	-7.64	109.58	120.51
1	I	258	ARG	CA-C-O	-7.64	110.41	119.35
1	P	106	ILE	CB-CG1-CD1	-7.64	97.76	113.80
1	E	167	ALA	O-C-N	7.64	130.86	122.15
1	F	164	GLN	O-C-N	-7.64	114.03	122.12
1	H	9	GLN	CA-C-O	-7.64	112.46	120.55
1	N	56	ARG	NE-CZ-NH2	-7.64	112.33	119.20
1	G	133	ARG	NE-CZ-NH1	-7.63	113.86	121.50
1	H	270	LEU	CA-C-O	-7.63	112.80	121.81
1	Q	56	ARG	NE-CZ-NH1	7.63	129.13	121.50
1	B	346	GLY	CA-C-N	7.63	136.12	121.54
1	B	346	GLY	C-N-CA	7.63	136.12	121.54
1	D	92	LEU	O-C-N	-7.63	113.48	122.87
1	H	226	THR	N-CA-CB	-7.63	98.41	111.69
1	Q	235	ALA	CA-C-O	-7.63	113.24	121.56
1	G	109	ASP	CA-C-O	-7.63	113.02	121.87
1	O	193	ASP	CA-CB-CG	7.63	120.23	112.60
1	O	194	GLY	CA-C-O	7.62	129.81	122.26
1	G	287	ASN	CB-CG-ND2	7.62	127.83	116.40
1	G	247	GLN	CG-CD-NE2	7.62	127.83	116.40
1	H	20	GLN	O-C-N	7.62	131.65	122.27
1	L	66	ASP	CA-C-O	7.62	129.27	120.96
1	O	265	PRO	CA-C-N	-7.62	112.08	121.38
1	O	265	PRO	C-N-CA	-7.62	112.08	121.38
1	R	231	ASN	CB-CG-ND2	-7.62	104.97	116.40
1	H	61	ILE	O-C-N	7.62	129.82	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	136	GLN	O-C-N	-7.62	113.86	122.09
1	Q	284	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	K	35	SER	N-CA-C	-7.62	101.04	110.41
1	G	313	TRP	CA-C-O	7.61	129.00	121.00
1	R	171	ALA	N-CA-CB	7.61	121.11	110.07
1	K	16	SER	CA-C-N	-7.61	110.54	120.44
1	K	16	SER	C-N-CA	-7.61	110.54	120.44
1	N	172	ARG	CA-C-O	7.61	128.62	120.55
1	O	97	LEU	CA-C-O	7.61	128.81	120.82
1	A	76	VAL	CA-C-N	-7.61	113.34	122.93
1	A	76	VAL	C-N-CA	-7.61	113.34	122.93
1	C	64	SER	CA-C-O	7.61	128.48	119.28
1	O	105	GLY	CA-C-N	-7.61	112.37	122.94
1	O	105	GLY	C-N-CA	-7.61	112.37	122.94
1	Q	89	GLN	CA-C-O	-7.61	109.63	120.51
1	E	156	GLN	CB-CG-CD	-7.60	99.67	112.60
1	L	109	ASP	N-CA-CB	7.60	120.80	110.38
1	A	217	ASN	CB-CG-OD1	7.60	136.00	120.80
1	M	89	GLN	CG-CD-NE2	-7.60	105.00	116.40
1	N	211	ALA	CA-C-N	-7.60	110.80	120.60
1	N	211	ALA	C-N-CA	-7.60	110.80	120.60
1	H	332	MET	O-C-N	-7.60	112.93	122.27
1	C	125	GLN	CG-CD-NE2	7.59	127.79	116.40
1	F	229	LYS	O-C-N	7.59	128.21	121.37
1	D	119	ASN	O-C-N	-7.59	112.49	122.59
1	K	94	ARG	CD-NE-CZ	7.59	135.03	124.40
1	L	91	LYS	O-C-N	7.59	132.07	123.19
1	B	168	ASN	CA-CB-CG	-7.59	105.01	112.60
1	C	284	ASN	OD1-CG-ND2	-7.59	115.01	122.60
1	N	14	GLU	CA-C-N	-7.59	110.11	120.28
1	N	14	GLU	C-N-CA	-7.59	110.11	120.28
1	K	129	GLY	CA-C-O	7.59	129.33	119.69
1	N	259	THR	O-C-N	-7.59	113.14	122.25
1	C	203	TYR	CA-C-O	7.59	128.74	119.79
1	O	192	PRO	CB-CA-C	-7.59	100.18	110.88
1	H	345	THR	CA-C-N	7.58	136.27	121.41
1	H	345	THR	C-N-CA	7.58	136.27	121.41
1	G	182	LEU	CA-C-N	-7.58	116.06	123.04
1	G	182	LEU	C-N-CA	-7.58	116.06	123.04
1	R	194	GLY	CA-C-O	7.58	130.37	122.56
1	P	133	ARG	NH1-CZ-NH2	7.58	129.15	119.30
1	R	162	ALA	CA-C-N	-7.58	110.86	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	162	ALA	C-N-CA	-7.58	110.86	120.56
1	E	187	GLU	CA-C-O	7.58	126.58	119.99
1	L	66	ASP	O-C-N	-7.58	113.97	123.06
1	A	140	ASP	CB-CG-OD2	7.58	135.82	118.40
1	E	201	CYS	CA-C-O	7.58	128.58	120.55
1	R	218	ASP	O-C-N	-7.58	113.36	122.22
1	L	58	PHE	CA-C-O	7.57	128.50	120.70
1	M	3	ARG	NE-CZ-NH2	7.57	126.02	119.20
1	M	118	THR	N-CA-CB	-7.57	97.59	111.37
1	I	22	ILE	N-CA-C	-7.57	101.30	111.44
1	P	235	ALA	CA-C-O	-7.57	112.88	121.81
1	G	302	GLY	O-C-N	-7.57	112.86	122.70
1	F	220	HIS	CA-CB-CG	-7.57	106.23	113.80
1	P	237	HIS	O-C-N	-7.57	113.41	122.11
1	A	31	ALA	O-C-N	7.56	131.86	122.63
1	R	91	LYS	CA-C-O	-7.56	112.22	120.92
1	R	278	ASP	CA-C-O	7.56	128.64	120.10
1	D	98	LYS	CA-CB-CG	-7.56	98.98	114.10
1	E	342	TYR	N-CA-CB	7.56	121.11	109.85
1	I	132	GLU	CB-CG-CD	7.56	125.45	112.60
1	M	239	CYS	O-C-N	7.56	131.84	123.22
1	P	237	HIS	CA-CB-CG	-7.56	106.24	113.80
1	H	186	VAL	N-CA-CB	-7.56	102.62	111.39
1	J	180	ASN	CA-CB-CG	-7.56	105.04	112.60
1	H	232	MET	N-CA-C	-7.55	100.78	110.53
1	Q	258	ARG	CD-NE-CZ	7.55	134.98	124.40
1	D	90	GLY	O-C-N	7.55	132.52	122.70
1	E	75	GLY	CA-C-O	-7.55	114.26	121.06
1	O	257	HIS	CA-CB-CG	7.55	121.35	113.80
1	L	6	ALA	CA-C-O	-7.55	112.55	120.55
1	P	234	THR	O-C-N	7.55	132.47	122.96
1	F	353	THR	N-CA-C	-7.54	94.73	110.80
1	K	195	ASP	N-CA-CB	-7.54	99.02	110.33
1	E	13	LYS	O-C-N	-7.54	114.25	122.09
1	E	119	ASN	CA-C-O	7.54	132.07	122.64
1	A	348	SER	N-CA-C	-7.54	98.73	110.42
1	B	205	THR	CA-C-N	-7.54	108.85	120.31
1	B	205	THR	C-N-CA	-7.54	108.85	120.31
1	I	81	GLU	CB-CG-CD	7.54	125.42	112.60
1	B	154	ALA	O-C-N	7.54	130.88	123.04
1	I	317	ALA	O-C-N	7.54	131.54	122.27
1	L	44	GLN	O-C-N	7.53	129.93	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	148	ARG	CA-C-O	7.53	128.36	120.30
1	E	72	SER	CB-CA-C	-7.53	97.67	109.34
1	E	295	TRP	CB-CG-CD2	7.53	137.34	126.80
1	I	168	ASN	CA-C-O	-7.53	112.44	120.42
1	B	22	ILE	CA-C-N	-7.53	108.42	121.97
1	B	22	ILE	C-N-CA	-7.53	108.42	121.97
1	H	266	GLY	CA-C-N	-7.53	113.09	123.10
1	H	266	GLY	C-N-CA	-7.53	113.09	123.10
1	M	81	GLU	CA-C-N	7.53	131.12	120.28
1	M	81	GLU	C-N-CA	7.53	131.12	120.28
1	N	250	MET	O-C-N	7.53	130.73	122.15
1	D	120	LYS	CA-C-O	-7.52	112.33	121.28
1	G	267	ILE	CA-C-N	7.52	134.49	123.13
1	G	267	ILE	C-N-CA	7.52	134.49	123.13
1	C	270	LEU	N-CA-C	-7.52	100.83	110.53
1	L	116	ALA	CA-C-O	-7.52	112.88	121.15
1	O	23	VAL	N-CA-C	-7.52	103.91	111.88
1	O	202	GLN	CA-C-O	7.52	128.75	120.63
1	K	318	ALA	CA-C-O	-7.52	110.39	119.49
1	M	95	ASN	CA-CB-CG	7.51	120.11	112.60
1	Q	332	MET	CA-C-O	7.51	128.59	120.10
1	B	104	VAL	CA-C-N	-7.51	115.51	121.82
1	B	104	VAL	C-N-CA	-7.51	115.51	121.82
1	F	70	ASN	N-CA-CB	-7.51	97.79	110.49
1	F	347	SER	CA-C-N	7.51	135.89	121.54
1	F	347	SER	C-N-CA	7.51	135.89	121.54
1	G	98	LYS	CB-CA-C	-7.51	98.79	110.81
1	B	136	GLN	CG-CD-NE2	-7.51	105.14	116.40
1	P	163	ILE	N-CA-C	-7.51	103.47	110.53
1	P	191	ILE	N-CA-CB	-7.51	101.83	110.17
1	K	175	SER	CA-C-O	7.51	128.74	120.63
1	J	80	HIS	CA-C-O	7.51	128.51	120.55
1	C	334	ASN	CA-CB-CG	-7.50	105.10	112.60
1	K	134	CYS	O-C-N	-7.50	114.34	122.07
1	P	152	ARG	NE-CZ-NH1	-7.50	114.00	121.50
1	J	59	ARG	NE-CZ-NH1	7.50	129.00	121.50
1	K	244	THR	N-CA-CB	-7.50	100.95	110.03
1	M	142	VAL	CA-C-O	-7.50	112.18	121.11
1	C	54	ASN	CA-CB-CG	-7.50	105.10	112.60
1	I	24	ALA	CB-CA-C	-7.50	98.29	110.74
1	K	166	ASN	OD1-CG-ND2	7.50	130.10	122.60
1	E	119	ASN	O-C-N	-7.50	112.74	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	232	MET	N-CA-C	-7.50	99.39	110.48
1	B	56	ARG	CD-NE-CZ	-7.49	113.91	124.40
1	B	311	ALA	O-C-N	7.49	129.79	122.07
1	F	172	ARG	CB-CA-C	-7.49	99.01	110.92
1	I	315	GLY	CA-C-O	-7.49	110.61	119.00
1	Q	89	GLN	O-C-N	-7.49	112.62	122.59
1	D	24	ALA	CA-C-O	-7.49	112.98	120.70
1	E	222	TYR	CA-C-O	-7.49	113.13	120.92
1	I	69	ILE	N-CA-CB	-7.49	98.87	111.23
1	I	87	ASP	CA-CB-CG	7.49	120.09	112.60
1	M	188	PRO	CA-C-N	-7.49	111.00	122.09
1	M	188	PRO	C-N-CA	-7.49	111.00	122.09
1	Q	6	ALA	CA-C-O	-7.49	111.36	119.97
1	H	4	PHE	N-CA-CB	-7.49	101.81	111.09
1	R	24	ALA	CB-CA-C	-7.49	98.83	110.81
1	G	186	VAL	CA-CB-CG2	-7.48	97.68	110.40
1	G	200	HIS	CA-CB-CG	7.48	121.28	113.80
1	M	90	GLY	O-C-N	7.48	131.47	122.34
1	I	60	GLU	O-C-N	-7.48	114.19	122.12
1	K	168	ASN	CA-C-N	-7.48	109.67	120.29
1	K	168	ASN	C-N-CA	-7.48	109.67	120.29
1	Q	303	ARG	N-CA-C	7.48	119.22	111.14
1	M	232	MET	N-CA-C	-7.48	100.45	110.55
1	R	102	ILE	CA-CB-CG1	-7.48	97.69	110.40
1	B	24	ALA	CA-C-O	-7.47	112.56	120.63
1	N	71	GLN	CG-CD-NE2	-7.47	105.19	116.40
1	N	190	VAL	O-C-N	-7.47	113.87	122.62
1	P	319	ASN	N-CA-C	7.47	121.81	113.21
1	B	164	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	H	72	SER	CA-C-N	-7.47	113.14	122.93
1	H	72	SER	C-N-CA	-7.47	113.14	122.93
1	B	6	ALA	CB-CA-C	-7.47	99.04	110.92
1	B	18	ILE	O-C-N	7.47	129.41	121.94
1	D	3	ARG	CA-CB-CG	7.47	129.04	114.10
1	I	77	ILE	O-C-N	7.47	132.05	122.94
1	F	219	HIS	CA-C-O	7.46	130.72	119.23
1	B	191	ILE	CB-CG1-CD1	-7.46	98.13	113.80
1	M	132	GLU	CB-CG-CD	7.46	125.29	112.60
1	E	253	VAL	CA-C-N	-7.46	110.29	120.44
1	E	253	VAL	C-N-CA	-7.46	110.29	120.44
1	A	172	ARG	NE-CZ-NH2	7.46	125.91	119.20
1	A	168	ASN	CA-C-O	-7.46	112.51	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ASP	CA-CB-CG	7.46	120.06	112.60
1	F	20	GLN	CG-CD-NE2	7.46	127.58	116.40
1	A	27	LYS	N-CA-CB	-7.45	99.78	110.44
1	G	194	GLY	O-C-N	-7.45	115.27	123.10
1	N	34	GLU	CA-C-O	7.45	129.39	121.19
1	C	44	GLN	O-C-N	7.45	129.84	122.09
1	D	207	LYS	CA-CB-CG	7.45	129.00	114.10
1	B	132	GLU	CA-C-O	7.45	128.64	120.82
1	D	161	LEU	CA-C-O	7.45	128.53	119.97
1	H	132	GLU	CB-CG-CD	7.45	125.26	112.60
1	O	180	ASN	O-C-N	-7.45	112.67	122.20
1	A	203	TYR	O-C-N	7.45	129.78	122.03
1	L	29	ILE	CA-C-O	7.45	129.01	120.67
1	L	289	CYS	CB-CA-C	-7.45	97.93	109.62
1	C	82	THR	CA-C-O	-7.44	112.66	120.55
1	G	67	SER	N-CA-CB	-7.44	97.91	110.49
1	B	7	LEU	CD1-CG-CD2	-7.44	94.44	110.80
1	C	2	HIS	CB-CA-C	-7.44	96.63	109.65
1	E	226	THR	N-CA-CB	-7.44	99.57	111.62
1	I	110	GLN	N-CA-CB	-7.44	101.24	111.65
1	C	30	LEU	O-C-N	7.43	131.68	123.13
1	A	200	HIS	ND1-CE1-NE2	-7.43	100.97	108.40
1	L	261	PRO	CA-C-O	7.43	129.75	121.43
1	Q	113	ALA	CB-CA-C	7.43	119.31	109.65
1	H	8	THR	CA-CB-CG2	7.43	123.13	110.50
1	I	341	GLN	CA-CB-CG	-7.43	99.24	114.10
1	Q	98	LYS	CB-CA-C	-7.43	98.92	110.81
1	A	287	ASN	O-C-N	-7.43	112.48	122.43
1	H	234	THR	CA-CB-CG2	7.43	123.13	110.50
1	D	256	LEU	CA-C-O	7.43	128.42	120.55
1	F	279	ALA	O-C-N	-7.43	114.31	122.03
1	L	119	ASN	CA-C-O	-7.43	113.83	122.37
1	P	128	ASP	CA-CB-CG	7.43	120.03	112.60
1	R	169	ALA	O-C-N	7.42	129.99	122.12
1	C	307	ALA	CA-C-O	7.42	128.61	120.82
1	M	54	ASN	CA-C-N	7.42	130.09	120.44
1	M	54	ASN	C-N-CA	7.42	130.09	120.44
1	G	5	PRO	CB-CA-C	-7.42	101.89	111.39
1	I	66	ASP	CA-CB-CG	7.42	120.02	112.60
1	O	6	ALA	O-C-N	7.42	130.61	122.15
1	B	191	ILE	N-CA-CB	-7.42	100.83	111.21
1	I	213	TYR	CA-C-N	-7.42	107.90	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	213	TYR	C-N-CA	-7.42	107.90	120.58
1	O	22	ILE	CA-C-O	-7.42	112.46	120.47
1	M	184	PRO	O-C-N	-7.41	113.79	123.13
1	N	132	GLU	N-CA-C	-7.41	103.28	111.36
1	R	309	ALA	CB-CA-C	-7.41	98.25	110.85
1	D	14	GLU	CA-C-O	-7.41	113.06	120.70
1	D	216	LEU	CB-CA-C	-7.41	96.92	110.63
1	F	95	ASN	CA-C-O	7.41	128.53	119.79
1	N	270	LEU	N-CA-C	-7.41	99.56	110.52
1	Q	6	ALA	O-C-N	7.41	131.38	122.27
1	P	261	PRO	O-C-N	-7.41	113.83	123.01
1	C	51	THR	CA-C-O	-7.40	112.14	120.66
1	H	22	ILE	O-C-N	7.40	130.17	121.80
1	P	42	ARG	NE-CZ-NH2	7.40	125.86	119.20
1	P	348	SER	CA-C-N	7.40	128.08	120.60
1	P	348	SER	C-N-CA	7.40	128.08	120.60
1	E	194	GLY	CA-C-N	7.40	131.56	120.31
1	E	194	GLY	C-N-CA	7.40	131.56	120.31
1	R	330	ARG	NH1-CZ-NH2	-7.40	109.68	119.30
1	C	235	ALA	CA-C-O	-7.40	113.67	122.03
1	G	148	ARG	N-CA-C	7.40	120.79	108.73
1	M	224	GLU	CA-CB-CG	7.39	128.89	114.10
1	O	191	ILE	N-CA-CB	-7.39	100.86	111.21
1	F	71	GLN	O-C-N	7.39	132.59	122.46
1	Q	89	GLN	CB-CA-C	-7.39	95.71	110.42
1	J	271	SER	CA-C-O	7.39	127.59	119.24
1	P	66	ASP	CA-CB-CG	7.39	119.99	112.60
1	A	75	GLY	O-C-N	-7.39	115.01	123.51
1	G	166	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	B	343	VAL	CA-C-N	-7.38	112.26	123.04
1	B	343	VAL	C-N-CA	-7.38	112.26	123.04
1	M	258	ARG	CD-NE-CZ	7.38	134.74	124.40
1	Q	68	SER	CA-C-O	7.38	128.32	119.61
1	H	128	ASP	O-C-N	-7.38	113.80	122.95
1	M	69	ILE	CA-CB-CG1	7.38	122.95	110.40
1	A	201	CYS	CA-C-N	-7.38	110.39	120.28
1	A	201	CYS	C-N-CA	-7.38	110.39	120.28
1	B	34	GLU	CA-C-O	7.38	129.41	121.44
1	I	332	MET	O-C-N	7.38	132.97	122.20
1	L	2	HIS	CA-CB-CG	7.38	121.18	113.80
1	C	177	CYS	CA-C-O	7.38	128.79	120.90
1	N	5	PRO	CB-CA-C	-7.38	102.19	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	206	GLU	N-CA-C	-7.38	103.54	112.54
1	K	75	GLY	CA-C-N	7.38	133.44	122.75
1	K	75	GLY	C-N-CA	7.38	133.44	122.75
1	K	238	ALA	CA-C-N	-7.38	110.40	120.87
1	K	238	ALA	C-N-CA	-7.38	110.40	120.87
1	O	203	TYR	CA-CB-CG	-7.38	100.62	113.90
1	I	328	MET	N-CA-CB	-7.38	98.85	110.28
1	B	25	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	J	300	SER	CA-C-N	-7.37	109.32	122.74
1	J	300	SER	C-N-CA	-7.37	109.32	122.74
1	Q	179	GLN	N-CA-C	-7.37	104.26	113.18
1	E	180	ASN	OD1-CG-ND2	7.37	129.97	122.60
1	N	24	ALA	N-CA-C	7.37	119.96	111.11
1	B	212	VAL	CA-CB-CG1	-7.37	97.87	110.40
1	O	226	THR	N-CA-CB	-7.37	99.00	111.31
1	R	309	ALA	CA-C-N	-7.37	110.59	120.54
1	R	309	ALA	C-N-CA	-7.37	110.59	120.54
1	F	46	ILE	CA-C-O	7.37	127.51	120.14
1	L	104	VAL	O-C-N	7.37	131.21	123.03
1	A	156	GLN	CA-C-O	7.37	129.94	120.81
1	B	15	LEU	CA-C-O	7.37	128.42	120.10
1	E	168	ASN	OD1-CG-ND2	-7.36	115.24	122.60
1	E	286	ILE	O-C-N	-7.36	114.67	121.89
1	I	329	LYS	CA-CB-CG	7.36	128.82	114.10
1	Q	164	GLN	CA-C-O	7.36	128.55	120.82
1	I	34	GLU	CA-C-O	7.36	129.44	121.05
1	I	143	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	152	ARG	NE-CZ-NH1	-7.36	114.14	121.50
1	L	218	ASP	O-C-N	7.36	130.83	122.22
1	R	2	HIS	CA-C-O	-7.36	109.99	120.51
1	H	250	MET	CG-SD-CE	-7.36	84.72	100.90
1	G	81	GLU	CA-C-O	7.35	128.34	120.55
1	A	168	ASN	CA-C-N	-7.35	109.85	120.29
1	A	168	ASN	C-N-CA	-7.35	109.85	120.29
1	B	268	CYS	CA-C-O	-7.35	111.31	120.57
1	E	125	GLN	O-C-N	7.35	131.36	122.84
1	K	10	GLU	O-C-N	7.34	129.63	122.07
1	I	196	HIS	N-CA-C	7.34	119.78	110.24
1	P	356	LEU	N-CA-C	7.34	123.02	107.67
1	Q	218	ASP	O-C-N	-7.34	113.24	122.27
1	Q	202	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	C	10	GLU	CB-CA-C	-7.34	98.61	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	284	ASN	CA-C-O	7.34	128.41	119.97
1	H	344	HIS	CB-CA-C	-7.33	95.82	110.42
1	O	267	ILE	CA-CB-CG2	7.33	122.97	110.50
1	P	101	GLY	O-C-N	7.33	130.33	122.41
1	J	209	LEU	CA-C-O	-7.33	112.65	120.42
1	N	89	GLN	CB-CG-CD	-7.33	100.13	112.60
1	N	336	GLN	CA-CB-CG	7.33	128.77	114.10
1	E	353	THR	CA-C-O	7.33	127.12	118.69
1	K	23	VAL	CA-C-N	7.33	135.54	121.54
1	K	23	VAL	C-N-CA	7.33	135.54	121.54
1	L	269	PHE	CA-CB-CG	-7.33	106.47	113.80
1	P	263	ALA	CA-C-O	7.33	128.36	119.49
1	A	34	GLU	CB-CG-CD	7.33	125.06	112.60
1	B	5	PRO	O-C-N	7.33	131.90	123.03
1	M	164	GLN	OE1-CD-NE2	-7.33	115.27	122.60
1	A	55	ARG	NE-CZ-NH2	7.33	125.79	119.20
1	G	164	GLN	CB-CG-CD	7.33	125.05	112.60
1	F	330	ARG	CG-CD-NE	7.32	128.11	112.00
1	Q	211	ALA	CA-C-N	-7.32	111.33	120.56
1	Q	211	ALA	C-N-CA	-7.32	111.33	120.56
1	I	329	LYS	CG-CD-CE	7.32	128.14	111.30
1	R	39	MET	CA-C-O	7.32	128.54	120.63
1	N	2	HIS	N-CA-C	7.32	119.87	110.65
1	Q	3	ARG	N-CA-C	-7.32	95.21	110.80
1	Q	313	TRP	CA-C-O	7.32	128.24	120.70
1	G	107	LYS	CA-C-O	-7.32	112.33	120.60
1	H	68	SER	N-CA-C	-7.32	104.23	113.01
1	R	276	GLU	CA-C-O	-7.31	113.08	120.90
1	D	66	ASP	CA-C-O	7.31	128.93	120.96
1	H	70	ASN	CB-CG-ND2	-7.31	105.43	116.40
1	H	342	TYR	CA-C-O	-7.31	112.36	120.69
1	O	14	GLU	CA-C-O	-7.31	113.14	120.82
1	P	125	GLN	CB-CG-CD	7.31	125.03	112.60
1	I	11	GLN	CG-CD-OE1	7.30	135.41	120.80
1	M	11	GLN	CG-CD-OE1	7.30	135.41	120.80
1	L	194	GLY	CA-C-O	7.30	129.49	122.26
1	Q	138	LYS	CA-C-O	-7.30	113.15	120.82
1	P	24	ALA	O-C-N	-7.30	113.71	122.11
1	C	11	GLN	CG-CD-NE2	-7.30	105.45	116.40
1	D	74	GLY	CA-C-N	7.30	133.29	121.17
1	D	74	GLY	C-N-CA	7.30	133.29	121.17
1	K	61	ILE	O-C-N	7.30	129.06	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	ILE	CA-CB-CG1	-7.30	97.99	110.40
1	C	282	ASN	CA-CB-CG	7.30	119.90	112.60
1	J	21	SER	CA-C-O	-7.30	112.81	120.55
1	M	29	ILE	CB-CG1-CD1	-7.30	98.48	113.80
1	P	97	LEU	CA-C-O	7.30	128.28	120.55
1	Q	87	ASP	CB-CG-OD1	7.30	135.18	118.40
1	C	6	ALA	CA-C-O	-7.29	112.69	120.42
1	E	333	ALA	O-C-N	7.29	129.58	122.07
1	J	125	GLN	CA-C-O	-7.29	113.36	121.89
1	N	282	ASN	CA-C-N	-7.29	109.22	120.31
1	N	282	ASN	C-N-CA	-7.29	109.22	120.31
1	J	179	GLN	N-CA-C	-7.29	103.65	112.54
1	G	205	THR	CA-CB-OG1	-7.29	98.67	109.60
1	O	56	ARG	CD-NE-CZ	-7.29	114.20	124.40
1	A	350	ALA	CA-C-N	7.28	130.36	120.38
1	A	350	ALA	C-N-CA	7.28	130.36	120.38
1	C	286	ILE	CA-C-O	-7.28	113.69	121.27
1	I	29	ILE	CA-C-O	-7.28	112.51	120.67
1	K	296	LYS	CA-C-O	-7.28	113.62	121.56
1	A	221	VAL	CA-CB-CG2	-7.28	98.02	110.40
1	B	232	MET	CA-CB-CG	7.28	128.66	114.10
1	F	350	ALA	CA-C-O	7.28	130.92	120.51
1	R	207	LYS	CG-CD-CE	7.28	128.05	111.30
1	E	237	HIS	CA-CB-CG	-7.28	106.52	113.80
1	G	188	PRO	N-CA-C	-7.28	97.48	112.47
1	I	332	MET	N-CA-C	-7.28	104.03	113.12
1	M	342	TYR	CA-C-O	-7.28	112.32	120.54
1	L	257	HIS	CA-C-N	-7.27	110.54	122.54
1	L	257	HIS	C-N-CA	-7.27	110.54	122.54
1	C	254	THR	O-C-N	7.27	129.56	122.07
1	H	165	GLU	OE1-CD-OE2	7.27	140.34	122.90
1	H	1	ALA	N-CA-C	7.26	131.33	111.00
1	H	301	TYR	CA-C-O	7.26	129.27	120.92
1	P	95	ASN	CA-CB-CG	-7.26	105.34	112.60
1	A	354	GLN	CB-CG-CD	-7.26	100.26	112.60
1	D	153	ILE	O-C-N	-7.26	115.56	123.18
1	C	178	GLN	OE1-CD-NE2	7.26	129.86	122.60
1	C	266	GLY	CA-C-N	-7.25	112.91	122.99
1	C	266	GLY	C-N-CA	-7.25	112.91	122.99
1	Q	259	THR	CA-C-N	-7.25	115.47	123.02
1	Q	259	THR	C-N-CA	-7.25	115.47	123.02
1	A	244	THR	N-CA-CB	-7.25	100.50	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	65	VAL	CA-C-O	7.25	129.85	120.78
1	N	37	GLY	CA-C-N	-7.25	110.58	120.44
1	N	37	GLY	C-N-CA	-7.25	110.58	120.44
1	F	240	THR	O-C-N	7.25	132.39	122.46
1	G	325	GLU	CB-CG-CD	-7.25	100.27	112.60
1	I	59	ARG	NE-CZ-NH1	-7.25	114.25	121.50
1	I	251	ALA	O-C-N	7.25	129.81	122.12
1	K	61	ILE	CA-C-O	-7.25	113.48	121.17
1	P	218	ASP	CA-C-N	-7.25	110.09	122.56
1	P	218	ASP	C-N-CA	-7.25	110.09	122.56
1	D	307	ALA	O-C-N	-7.25	114.20	122.03
1	I	252	THR	CA-C-O	-7.25	113.39	121.00
1	J	329	LYS	CA-C-O	-7.25	113.24	120.70
1	P	77	ILE	N-CA-CB	7.25	118.62	110.72
1	H	69	ILE	CA-C-O	7.24	128.79	120.03
1	L	81	GLU	N-CA-CB	7.24	120.73	109.94
1	R	4	PHE	CA-C-N	7.24	127.17	119.85
1	R	4	PHE	C-N-CA	7.24	127.17	119.85
1	H	190	VAL	CA-CB-CG2	7.24	122.71	110.40
1	I	67	SER	CA-C-O	-7.24	110.16	120.51
1	J	116	ALA	CA-C-O	-7.24	113.14	121.47
1	K	92	LEU	CA-C-O	-7.24	113.05	121.16
1	H	306	GLN	CA-C-O	7.24	127.01	119.05
1	O	24	ALA	N-CA-CB	7.24	120.73	109.94
1	E	67	SER	CA-C-N	-7.24	109.28	122.38
1	E	67	SER	C-N-CA	-7.24	109.28	122.38
1	F	345	THR	N-CA-C	-7.24	95.39	110.80
1	G	53	GLU	CA-C-O	-7.24	112.81	120.63
1	R	342	TYR	O-C-N	7.24	131.55	123.01
1	E	50	ASN	O-C-N	7.24	131.93	122.38
1	G	17	GLU	O-C-N	7.24	130.40	122.15
1	G	103	VAL	CA-C-N	-7.24	112.56	122.91
1	G	103	VAL	C-N-CA	-7.24	112.56	122.91
1	K	234	THR	CA-C-O	-7.23	113.41	121.51
1	N	64	SER	O-C-N	-7.23	111.87	122.43
1	C	106	ILE	N-CA-C	7.23	118.23	108.11
1	K	93	PHE	CA-CB-CG	7.23	121.03	113.80
1	A	343	VAL	CB-CA-C	-7.23	99.43	111.29
1	A	259	THR	O-C-N	-7.22	112.98	122.59
1	D	51	THR	CA-CB-CG2	7.22	122.78	110.50
1	C	327	PHE	O-C-N	-7.22	114.46	122.12
1	I	5	PRO	CB-CA-C	-7.22	102.54	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	75	GLY	CA-C-N	-7.22	112.31	122.71
1	L	75	GLY	C-N-CA	-7.22	112.31	122.71
1	P	4	PHE	CA-C-N	7.22	127.20	119.76
1	P	4	PHE	C-N-CA	7.22	127.20	119.76
1	I	206	GLU	CA-C-O	-7.22	110.50	119.38
1	K	73	ILE	N-CA-CB	-7.22	102.36	111.46
1	Q	99	GLU	CA-C-O	-7.22	111.94	120.10
1	F	5	PRO	CB-CA-C	-7.22	102.47	111.64
1	C	12	LYS	CA-C-O	7.21	128.13	120.70
1	N	328	MET	N-CA-CB	-7.21	99.51	110.12
1	P	164	GLN	CA-CB-CG	7.21	128.53	114.10
1	B	197	ASP	CA-CB-CG	-7.21	105.39	112.60
1	C	330	ARG	CA-C-N	-7.21	109.35	120.31
1	C	330	ARG	C-N-CA	-7.21	109.35	120.31
1	E	251	ALA	O-C-N	7.21	130.66	122.22
1	R	248	VAL	O-C-N	7.21	128.86	121.87
1	R	186	VAL	O-C-N	-7.21	114.74	122.45
1	H	278	ASP	CA-CB-CG	-7.21	105.39	112.60
1	B	93	PHE	CE1-CZ-CE2	-7.20	107.03	120.00
1	J	191	ILE	CB-CG1-CD1	-7.20	98.67	113.80
1	R	132	GLU	CG-CD-OE1	7.20	134.97	118.40
1	C	295	TRP	N-CA-C	7.20	121.40	109.95
1	H	56	ARG	NE-CZ-NH2	-7.20	112.72	119.20
1	G	344	HIS	CA-C-O	7.20	133.04	120.80
1	M	164	GLN	CA-CB-CG	7.20	128.50	114.10
1	H	51	THR	N-CA-CB	-7.20	98.31	110.83
1	B	7	LEU	N-CA-CB	7.20	124.07	111.55
1	B	344	HIS	N-CA-C	-7.20	96.65	108.67
1	F	164	GLN	CB-CG-CD	7.20	124.83	112.60
1	I	25	ASN	CA-C-N	-7.20	109.19	121.85
1	I	25	ASN	C-N-CA	-7.20	109.19	121.85
1	E	237	HIS	CB-CA-C	-7.19	98.45	110.68
1	E	251	ALA	CA-C-O	-7.19	111.97	120.10
1	N	81	GLU	O-C-N	7.19	129.57	122.09
1	C	295	TRP	CA-C-O	-7.19	113.03	121.16
1	L	166	ASN	CA-C-N	-7.19	109.93	120.28
1	L	166	ASN	C-N-CA	-7.19	109.93	120.28
1	I	66	ASP	CA-C-N	7.19	135.27	121.54
1	I	66	ASP	C-N-CA	7.19	135.27	121.54
1	D	286	ILE	N-CA-C	-7.19	103.52	110.42
1	F	69	ILE	CA-CB-CG1	7.19	122.62	110.40
1	O	136	GLN	CB-CA-C	7.19	122.26	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	156	GLN	OE1-CD-NE2	7.18	129.78	122.60
1	L	25	ASN	O-C-N	7.18	136.37	122.22
1	N	265	PRO	CA-C-N	-7.18	112.61	121.38
1	N	265	PRO	C-N-CA	-7.18	112.61	121.38
1	N	303	ARG	CD-NE-CZ	-7.18	114.35	124.40
1	E	248	VAL	CA-C-O	7.18	128.25	120.57
1	K	308	SER	CA-C-O	-7.18	111.71	119.97
1	P	184	PRO	CA-C-O	-7.18	111.95	120.85
1	B	212	VAL	CA-C-O	-7.18	113.49	120.95
1	C	222	TYR	CA-C-O	7.18	128.26	120.58
1	H	99	GLU	O-C-N	7.18	129.73	122.12
1	R	132	GLU	CA-C-O	-7.18	112.88	120.63
1	C	261	PRO	N-CA-CB	7.17	109.69	103.31
1	E	212	VAL	CA-C-O	-7.17	113.57	121.17
1	E	345	THR	N-CA-CB	7.17	122.61	110.49
1	J	10	GLU	CA-CB-CG	7.17	128.45	114.10
1	R	134	CYS	O-C-N	-7.17	113.98	122.15
1	J	257	HIS	CA-CB-CG	7.17	120.97	113.80
1	O	198	LEU	CA-C-O	7.17	128.35	120.82
1	D	295	TRP	N-CA-CB	-7.17	99.81	110.85
1	R	306	GLN	OE1-CD-NE2	-7.17	115.43	122.60
1	K	167	ALA	CA-C-O	7.17	128.52	121.00
1	D	326	ALA	CA-C-N	-7.16	110.12	120.29
1	D	326	ALA	C-N-CA	-7.16	110.12	120.29
1	B	282	ASN	OD1-CG-ND2	7.16	129.76	122.60
1	I	26	GLY	CA-C-N	-7.16	106.13	121.45
1	I	26	GLY	C-N-CA	-7.16	106.13	121.45
1	E	220	HIS	CA-CB-CG	-7.16	106.64	113.80
1	P	334	ASN	CA-CB-CG	-7.16	105.44	112.60
1	E	342	TYR	O-C-N	7.16	131.73	122.93
1	M	311	ALA	CA-C-N	7.16	132.05	120.60
1	M	311	ALA	C-N-CA	7.16	132.05	120.60
1	O	52	GLU	O-C-N	7.15	129.70	122.12
1	F	217	ASN	CB-CG-ND2	7.15	127.13	116.40
1	R	287	ASN	CA-CB-CG	-7.15	105.45	112.60
1	B	14	GLU	O-C-N	7.15	129.73	122.08
1	I	166	ASN	CB-CG-ND2	7.15	127.12	116.40
1	N	170	LEU	CA-C-O	-7.15	112.97	120.55
1	P	343	VAL	N-CA-CB	7.15	123.02	111.23
1	A	221	VAL	CA-C-O	-7.15	112.82	121.54
1	C	180	ASN	OD1-CG-ND2	7.14	129.75	122.60
1	O	3	ARG	CD-NE-CZ	7.14	134.40	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	190	VAL	O-C-N	-7.14	114.89	122.68
1	R	235	ALA	CA-C-O	-7.14	113.84	121.99
1	B	266	GLY	CA-C-N	-7.14	113.06	122.99
1	B	266	GLY	C-N-CA	-7.14	113.06	122.99
1	J	3	ARG	NE-CZ-NH2	7.14	125.63	119.20
1	M	19	ALA	O-C-N	7.14	129.69	122.12
1	E	135	ALA	O-C-N	-7.14	113.09	122.59
1	L	42	ARG	NE-CZ-NH2	7.14	125.63	119.20
1	M	218	ASP	CA-CB-CG	7.14	119.74	112.60
1	O	146	LYS	CA-C-O	-7.14	111.76	120.54
1	C	56	ARG	NE-CZ-NH2	-7.13	112.78	119.20
1	H	42	ARG	CD-NE-CZ	-7.13	114.41	124.40
1	I	260	VAL	CB-CA-C	-7.13	102.67	110.95
1	A	325	GLU	CB-CG-CD	-7.13	100.48	112.60
1	C	109	ASP	N-CA-CB	7.13	120.15	110.38
1	B	160	SER	CA-C-N	-7.13	110.75	120.44
1	B	160	SER	C-N-CA	-7.13	110.75	120.44
1	C	94	ARG	NH1-CZ-NH2	-7.13	110.03	119.30
1	G	34	GLU	CA-C-O	-7.12	112.80	120.92
1	H	160	SER	N-CA-CB	7.12	120.70	110.16
1	C	175	SER	O-C-N	7.12	129.41	122.07
1	H	40	GLY	N-CA-C	-7.12	104.02	112.64
1	D	325	GLU	CA-C-O	7.12	127.97	120.42
1	E	273	GLY	O-C-N	-7.12	113.35	122.39
1	E	301	TYR	CA-C-O	7.12	128.19	120.43
1	J	71	GLN	CA-CB-CG	7.12	128.34	114.10
1	J	118	THR	N-CA-CB	-7.12	98.38	111.13
1	Q	59	ARG	CD-NE-CZ	7.12	134.37	124.40
1	E	38	THR	CA-C-O	7.12	128.19	119.79
1	O	289	CYS	CB-CA-C	-7.12	98.27	109.52
1	F	189	GLU	CA-C-N	-7.12	114.76	122.59
1	F	189	GLU	C-N-CA	-7.12	114.76	122.59
1	A	118	THR	O-C-N	-7.12	115.01	123.27
1	E	258	ARG	CA-CB-CG	7.12	128.33	114.10
1	H	4	PHE	N-CA-C	-7.12	94.33	108.71
1	I	144	PHE	CA-C-N	-7.12	116.14	122.47
1	I	144	PHE	C-N-CA	-7.12	116.14	122.47
1	K	217	ASN	CB-CG-ND2	-7.12	105.73	116.40
1	C	3	ARG	NH1-CZ-NH2	-7.11	110.05	119.30
1	F	123	THR	CA-CB-OG1	7.11	120.27	109.60
1	O	293	LYS	N-CA-CB	-7.11	102.27	111.09
1	Q	123	THR	CB-CA-C	-7.11	96.17	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	248	VAL	CA-CB-CG2	-7.11	98.31	110.40
1	P	337	ALA	CA-C-O	-7.11	112.88	120.42
1	M	283	LEU	CA-C-O	7.11	128.09	120.55
1	H	166	ASN	CB-CG-ND2	-7.11	105.74	116.40
1	O	269	PHE	CA-CB-CG	-7.11	106.69	113.80
1	B	211	ALA	O-C-N	7.10	129.76	122.09
1	C	304	ALA	O-C-N	7.10	130.30	122.20
1	E	3	ARG	CA-C-N	-7.10	115.21	122.74
1	E	3	ARG	C-N-CA	-7.10	115.21	122.74
1	P	148	ARG	O-C-N	7.10	131.65	123.27
1	B	255	ALA	N-CA-CB	-7.10	99.71	110.01
1	N	237	HIS	CB-CA-C	-7.10	97.49	110.63
1	O	159	SER	O-C-N	-7.10	114.76	122.85
1	D	186	VAL	N-CA-C	-7.10	97.63	107.99
1	F	68	SER	N-CA-CB	-7.10	97.41	110.18
1	M	163	ILE	O-C-N	7.10	128.87	121.91
1	E	267	ILE	CB-CA-C	7.10	120.00	110.42
1	R	237	HIS	CA-CB-CG	-7.10	106.70	113.80
1	K	143	ASP	CA-CB-CG	-7.09	105.50	112.60
1	O	29	ILE	CA-C-N	-7.09	112.93	122.72
1	O	29	ILE	C-N-CA	-7.09	112.93	122.72
1	C	335	CYS	O-C-N	7.09	130.24	122.15
1	D	205	THR	CA-C-O	-7.09	113.37	120.82
1	G	94	ARG	NE-CZ-NH1	-7.09	114.41	121.50
1	O	183	VAL	O-C-N	7.09	127.79	121.41
1	F	25	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	F	166	ASN	CA-CB-CG	-7.09	105.51	112.60
1	L	249	ALA	N-CA-C	7.09	119.01	111.28
1	D	217	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	J	175	SER	CA-C-O	7.09	128.06	120.55
1	M	36	VAL	O-C-N	7.09	129.03	121.94
1	N	36	VAL	CA-C-O	-7.09	112.99	120.57
1	D	237	HIS	CA-C-N	-7.08	111.31	122.65
1	D	237	HIS	C-N-CA	-7.08	111.31	122.65
1	P	30	LEU	O-C-N	7.08	131.63	123.27
1	E	130	LEU	CA-C-O	7.08	128.13	120.20
1	G	86	LYS	CA-C-O	7.08	129.80	121.58
1	I	172	ARG	NE-CZ-NH1	-7.08	114.42	121.50
1	K	336	GLN	OE1-CD-NE2	-7.08	115.52	122.60
1	K	68	SER	CB-CA-C	-7.08	96.72	110.46
1	D	321	GLU	CB-CG-CD	-7.08	100.56	112.60
1	L	322	ALA	CB-CA-C	-7.08	99.48	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	95	ASN	CA-CB-CG	-7.08	105.52	112.60
1	B	175	SER	CB-CA-C	-7.08	99.49	110.81
1	B	216	LEU	O-C-N	7.08	129.62	122.12
1	E	154	ALA	N-CA-C	7.08	117.86	107.88
1	G	215	ALA	O-C-N	7.08	129.36	122.07
1	I	107	LYS	O-C-N	-7.08	114.18	122.95
1	C	33	ASP	CA-C-N	-7.07	110.83	120.87
1	C	33	ASP	C-N-CA	-7.07	110.83	120.87
1	L	22	ILE	CA-C-N	-7.07	110.43	122.88
1	L	22	ILE	C-N-CA	-7.07	110.43	122.88
1	M	45	ARG	NE-CZ-NH2	-7.07	112.84	119.20
1	E	274	MET	N-CA-C	-7.07	101.01	110.55
1	L	80	HIS	CB-CA-C	-7.07	96.35	110.42
1	A	260	VAL	CB-CA-C	-7.07	103.15	110.71
1	F	351	ALA	N-CA-CB	-7.07	98.55	110.49
1	E	175	SER	CB-CA-C	-7.07	99.51	110.81
1	L	127	LEU	CA-C-N	-7.07	111.06	120.95
1	L	127	LEU	C-N-CA	-7.07	111.06	120.95
1	N	13	LYS	O-C-N	7.07	129.44	122.09
1	B	252	THR	N-CA-C	7.06	118.87	111.03
1	K	284	ASN	N-CA-C	-7.06	103.27	110.97
1	G	198	LEU	CD1-CG-CD2	-7.06	95.26	110.80
1	H	109	ASP	CA-CB-CG	7.06	119.66	112.60
1	D	59	ARG	CA-CB-CG	-7.06	99.98	114.10
1	G	38	THR	CA-CB-OG1	-7.06	99.01	109.60
1	I	115	LEU	CB-CA-C	7.06	123.41	111.41
1	M	99	GLU	O-C-N	7.06	129.60	122.12
1	A	216	LEU	CA-C-O	7.06	128.08	120.10
1	H	267	ILE	N-CA-CB	7.06	120.81	111.64
1	J	211	ALA	N-CA-C	7.06	119.58	111.11
1	Q	129	GLY	CA-C-O	7.06	128.75	119.58
1	G	202	GLN	OE1-CD-NE2	-7.05	115.55	122.60
1	G	295	TRP	N-CA-C	7.05	120.90	110.46
1	I	55	ARG	N-CA-C	-7.05	103.20	111.03
1	I	206	GLU	CA-C-N	-7.05	108.52	120.58
1	I	206	GLU	C-N-CA	-7.05	108.52	120.58
1	K	327	PHE	O-C-N	7.05	129.43	122.09
1	R	42	ARG	NE-CZ-NH1	-7.05	114.45	121.50
1	G	137	TYR	CA-C-N	-7.05	110.12	120.28
1	G	137	TYR	C-N-CA	-7.05	110.12	120.28
1	J	232	MET	CA-C-O	-7.05	113.69	121.87
1	O	143	ASP	CA-CB-CG	-7.05	105.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	ALA	O-C-N	-7.05	111.72	123.00
1	I	51	THR	N-CA-CB	-7.05	98.83	110.68
1	J	254	THR	N-CA-C	-7.05	103.53	111.07
1	C	204	VAL	N-CA-C	-7.05	103.32	111.00
1	N	23	VAL	CB-CA-C	-7.05	102.70	112.36
1	F	190	VAL	O-C-N	-7.04	113.44	122.32
1	M	226	THR	N-CA-CB	-7.04	99.43	111.69
1	K	221	VAL	CB-CA-C	-7.04	101.56	111.28
1	P	14	GLU	CA-C-O	-7.04	113.09	120.55
1	J	124	ILE	N-CA-CB	-7.04	101.24	111.52
1	K	248	VAL	CA-CB-CG2	-7.04	98.43	110.40
1	O	27	LYS	CA-C-O	7.04	130.04	121.94
1	D	1	ALA	O-C-N	-7.04	111.74	123.00
1	P	318	ALA	O-C-N	7.04	130.46	122.22
1	I	236	GLY	CA-C-N	7.04	129.71	120.28
1	I	236	GLY	C-N-CA	7.04	129.71	120.28
1	Q	59	ARG	CG-CD-NE	7.04	127.48	112.00
1	F	172	ARG	N-CA-CB	7.03	120.51	109.82
1	M	143	ASP	CA-C-O	-7.03	111.08	119.03
1	D	331	ALA	O-C-N	-7.03	114.83	122.07
1	J	258	ARG	CB-CA-C	-7.03	97.35	110.01
1	L	264	VAL	N-CA-C	-7.03	102.06	108.95
1	P	10	GLU	O-C-N	7.03	130.16	122.15
1	N	39	MET	CA-C-O	7.03	128.22	120.63
1	C	10	GLU	N-CA-CB	7.03	120.45	110.12
1	G	72	SER	CA-C-O	7.03	128.00	119.64
1	J	185	ILE	CA-C-O	-7.03	112.44	120.66
1	N	260	VAL	N-CA-CB	-7.03	103.40	111.20
1	P	156	GLN	CA-CB-CG	-7.03	100.05	114.10
1	P	16	SER	CA-C-N	-7.02	110.31	120.29
1	P	16	SER	C-N-CA	-7.02	110.31	120.29
1	Q	258	ARG	NH1-CZ-NH2	-7.02	110.17	119.30
1	R	191	ILE	CA-C-O	7.02	129.36	119.95
1	L	104	VAL	CA-C-O	-7.02	113.06	120.57
1	M	51	THR	N-CA-CB	-7.02	99.07	111.08
1	D	168	ASN	CA-C-O	-7.02	111.90	119.97
1	P	352	SER	N-CA-C	7.02	122.29	108.18
1	C	305	LEU	CA-C-N	-7.02	111.24	121.98
1	C	305	LEU	C-N-CA	-7.02	111.24	121.98
1	L	217	ASN	CA-CB-CG	-7.02	105.58	112.60
1	N	132	GLU	CB-CG-CD	7.02	124.53	112.60
1	B	209	LEU	CA-C-O	7.02	128.07	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	123	THR	CB-CA-C	-7.02	94.81	111.65
1	J	16	SER	N-CA-C	-7.02	103.71	111.36
1	E	90	GLY	N-CA-C	-7.01	104.28	115.08
1	I	55	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	J	264	VAL	CA-C-O	-7.01	113.72	119.47
1	A	245	PRO	CA-C-N	-7.01	110.33	120.29
1	A	245	PRO	C-N-CA	-7.01	110.33	120.29
1	J	286	ILE	O-C-N	-7.01	115.07	121.87
1	C	178	GLN	CG-CD-NE2	-7.01	105.89	116.40
1	P	72	SER	CA-C-N	-7.00	114.01	123.12
1	P	72	SER	C-N-CA	-7.00	114.01	123.12
1	B	218	ASP	CA-CB-CG	-7.00	105.60	112.60
1	P	199	GLU	CA-CB-CG	7.00	128.11	114.10
1	C	289	CYS	O-C-N	7.00	127.53	121.30
1	D	73	ILE	N-CA-C	7.00	117.94	107.51
1	L	190	VAL	CB-CA-C	-7.00	104.70	112.68
1	O	195	ASP	N-CA-CB	-7.00	99.83	110.33
1	G	152	ARG	CD-NE-CZ	-7.00	114.61	124.40
1	N	307	ALA	N-CA-C	7.00	118.91	111.28
1	Q	170	LEU	O-C-N	-7.00	114.22	122.20
1	E	221	VAL	N-CA-C	6.99	118.60	109.58
1	N	62	LEU	CA-C-N	-6.99	109.05	122.06
1	N	62	LEU	C-N-CA	-6.99	109.05	122.06
1	Q	205	THR	CA-C-O	-6.99	113.08	120.63
1	R	287	ASN	CB-CG-ND2	-6.99	105.91	116.40
1	O	298	SER	N-CA-C	6.99	117.72	108.07
1	M	77	ILE	CB-CA-C	-6.99	101.40	110.98
1	P	184	PRO	CA-C-N	-6.99	112.02	121.66
1	P	184	PRO	C-N-CA	-6.99	112.02	121.66
1	J	177	CYS	O-C-N	-6.99	114.72	122.12
1	F	239	CYS	O-C-N	-6.98	114.37	122.89
1	E	24	ALA	N-CA-CB	6.98	120.49	110.16
1	M	330	ARG	NE-CZ-NH2	6.98	125.48	119.20
1	A	42	ARG	NH1-CZ-NH2	-6.98	110.22	119.30
1	A	89	GLN	CB-CG-CD	-6.98	100.73	112.60
1	C	284	ASN	CA-CB-CG	-6.98	105.62	112.60
1	M	2	HIS	CA-C-O	-6.98	110.53	120.51
1	N	296	LYS	N-CA-CB	6.98	120.30	110.04
1	D	42	ARG	CD-NE-CZ	6.98	134.17	124.40
1	E	163	ILE	O-C-N	-6.97	113.85	122.57
1	G	267	ILE	O-C-N	-6.97	115.81	123.20
1	I	5	PRO	CA-C-O	-6.97	113.77	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	232	MET	N-CA-C	-6.97	101.33	110.53
1	R	244	THR	O-C-N	-6.97	114.92	121.20
1	D	75	GLY	O-C-N	6.97	130.04	123.56
1	B	51	THR	N-CA-CB	-6.97	98.56	111.52
1	K	42	ARG	CD-NE-CZ	6.97	134.16	124.40
1	N	10	GLU	CB-CG-CD	-6.97	100.75	112.60
1	N	58	PHE	CA-CB-CG	-6.97	106.83	113.80
1	O	125	GLN	CB-CG-CD	-6.97	100.75	112.60
1	C	65	VAL	N-CA-CB	-6.97	99.73	111.23
1	E	207	LYS	O-C-N	-6.97	114.89	122.07
1	K	51	THR	CA-CB-OG1	-6.97	99.15	109.60
1	C	94	ARG	NE-CZ-NH1	6.97	128.47	121.50
1	G	24	ALA	CA-C-O	-6.97	112.23	120.10
1	K	72	SER	CA-C-N	-6.97	114.06	123.12
1	K	72	SER	C-N-CA	-6.97	114.06	123.12
1	N	252	THR	CA-C-O	-6.97	113.72	120.90
1	R	94	ARG	CA-C-O	-6.97	113.17	120.55
1	R	267	ILE	N-CA-CB	-6.96	102.69	111.46
1	F	26	GLY	CA-C-N	-6.96	108.30	120.97
1	F	26	GLY	C-N-CA	-6.96	108.30	120.97
1	H	8	THR	CA-C-N	-6.96	110.95	120.28
1	H	8	THR	C-N-CA	-6.96	110.95	120.28
1	H	260	VAL	N-CA-CB	-6.96	102.67	111.23
1	B	305	LEU	N-CA-C	-6.96	103.90	112.88
1	C	88	SER	CA-CB-OG	-6.96	97.18	111.10
1	F	59	ARG	CA-CB-CG	-6.96	100.18	114.10
1	K	24	ALA	CA-C-O	-6.96	110.56	120.51
1	I	119	ASN	OD1-CG-ND2	6.96	129.56	122.60
1	O	137	TYR	O-C-N	-6.95	114.75	122.12
1	D	68	SER	CB-CA-C	-6.95	96.59	110.42
1	L	323	THR	O-C-N	-6.95	114.64	122.08
1	C	210	ALA	N-CA-C	-6.95	103.76	111.82
1	E	260	VAL	N-CA-CB	-6.95	103.48	111.20
1	H	281	LEU	CA-C-N	-6.95	110.99	120.44
1	H	281	LEU	C-N-CA	-6.95	110.99	120.44
1	N	110	GLN	OE1-CD-NE2	6.95	129.55	122.60
1	Q	72	SER	N-CA-CB	-6.95	101.34	110.59
1	F	343	VAL	O-C-N	6.95	130.41	123.18
1	P	190	VAL	CA-C-N	6.95	133.59	120.11
1	P	190	VAL	C-N-CA	6.95	133.59	120.11
1	P	264	VAL	CA-C-N	6.95	126.20	118.97
1	P	264	VAL	C-N-CA	6.95	126.20	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	LYS	CA-C-O	6.95	128.33	120.90
1	G	124	ILE	O-C-N	-6.95	115.57	123.00
1	Q	118	THR	CA-C-N	-6.94	111.74	122.16
1	Q	118	THR	C-N-CA	-6.94	111.74	122.16
1	B	17	GLU	CB-CA-C	6.94	121.78	110.88
1	B	54	ASN	CA-C-O	6.94	128.33	120.90
1	B	142	VAL	CA-CB-CG2	-6.94	98.60	110.40
1	M	225	GLY	O-C-N	6.94	131.72	122.70
1	H	344	HIS	N-CA-C	6.94	125.58	110.80
1	B	279	ALA	CA-C-N	-6.94	109.13	120.71
1	B	279	ALA	C-N-CA	-6.94	109.13	120.71
1	H	65	VAL	CA-C-O	6.94	129.45	120.78
1	Q	3	ARG	NE-CZ-NH2	6.94	125.44	119.20
1	B	180	ASN	CA-CB-CG	-6.93	105.67	112.60
1	J	90	GLY	O-C-N	6.93	129.21	122.41
1	L	51	THR	N-CA-CB	-6.93	99.22	111.08
1	B	219	HIS	CA-C-N	-6.93	112.16	122.07
1	B	219	HIS	C-N-CA	-6.93	112.16	122.07
1	G	287	ASN	CA-CB-CG	6.93	119.53	112.60
1	P	125	GLN	O-C-N	6.93	130.78	122.68
1	E	216	LEU	CA-C-O	6.92	127.76	120.42
1	F	239	CYS	CA-C-O	6.92	128.92	121.16
1	G	194	GLY	N-CA-C	6.92	121.66	111.76
1	L	89	GLN	OE1-CD-NE2	6.92	129.53	122.60
1	G	172	ARG	CD-NE-CZ	6.92	134.09	124.40
1	H	334	ASN	O-C-N	-6.92	114.26	122.15
1	J	59	ARG	NH1-CZ-NH2	-6.92	110.30	119.30
1	L	199	GLU	CA-CB-CG	6.92	127.94	114.10
1	Q	271	SER	N-CA-C	-6.92	104.97	113.41
1	F	266	GLY	CA-C-N	-6.92	113.90	123.10
1	F	266	GLY	C-N-CA	-6.92	113.90	123.10
1	K	184	PRO	CB-CA-C	-6.92	105.10	111.40
1	D	340	GLY	N-CA-C	-6.92	103.65	114.10
1	R	195	ASP	N-CA-C	6.92	121.47	112.89
1	G	124	ILE	CA-C-N	6.92	135.33	122.74
1	G	124	ILE	C-N-CA	6.92	135.33	122.74
1	H	345	THR	CA-C-O	6.92	130.40	120.51
1	D	88	SER	CA-C-O	6.91	129.13	121.39
1	F	56	ARG	CD-NE-CZ	6.91	134.08	124.40
1	G	164	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	H	61	ILE	CA-CB-CG1	-6.91	98.65	110.40
1	K	156	GLN	N-CA-C	6.91	121.09	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	91	LYS	CA-C-N	-6.91	111.07	120.82
1	O	91	LYS	C-N-CA	-6.91	111.07	120.82
1	B	196	HIS	CA-C-O	-6.91	114.22	122.03
1	M	199	GLU	CB-CA-C	6.91	124.44	109.99
1	R	178	GLN	OE1-CD-NE2	6.91	129.51	122.60
1	A	232	MET	N-CA-C	-6.91	101.41	110.53
1	E	149	ALA	O-C-N	6.91	131.28	123.19
1	G	144	PHE	CA-CB-CG	6.91	120.71	113.80
1	H	12	LYS	O-C-N	6.91	130.03	122.15
1	H	181	GLY	O-C-N	6.91	129.18	122.41
1	I	70	ASN	CB-CG-ND2	-6.91	106.03	116.40
1	B	183	VAL	CA-C-O	-6.91	114.70	119.19
1	G	3	ARG	O-C-N	-6.91	113.41	122.59
1	G	65	VAL	N-CA-C	6.91	123.70	109.34
1	L	170	LEU	CA-C-N	-6.91	110.48	120.29
1	L	170	LEU	C-N-CA	-6.91	110.48	120.29
1	L	277	GLU	CA-C-N	-6.91	111.03	120.28
1	L	277	GLU	C-N-CA	-6.91	111.03	120.28
1	O	258	ARG	NE-CZ-NH1	-6.90	114.60	121.50
1	R	7	LEU	CA-C-O	-6.90	113.05	121.06
1	A	296	LYS	O-C-N	6.90	131.30	122.81
1	A	166	ASN	OD1-CG-ND2	6.90	129.50	122.60
1	D	131	SER	O-C-N	6.90	129.18	122.07
1	J	217	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	Q	231	ASN	CA-C-O	-6.90	113.08	121.36
1	N	214	LYS	CA-C-O	6.90	127.90	120.24
1	R	293	LYS	CG-CD-CE	6.90	127.16	111.30
1	D	152	ARG	CB-CA-C	-6.90	95.65	109.79
1	P	228	LEU	O-C-N	6.89	131.68	123.27
1	Q	341	GLN	CA-CB-CG	-6.89	100.31	114.10
1	L	235	ALA	CA-C-O	-6.89	113.68	121.81
1	N	161	LEU	O-C-N	-6.89	114.70	122.08
1	O	325	GLU	CA-C-O	6.89	127.80	120.70
1	A	123	THR	CB-CA-C	-6.89	97.30	114.11
1	C	87	ASP	OD1-CG-OD2	6.89	139.44	122.90
1	E	211	ALA	CA-C-O	6.89	127.72	120.42
1	H	82	THR	OG1-CB-CG2	6.89	123.08	109.30
1	K	303	ARG	CD-NE-CZ	-6.89	114.75	124.40
1	Q	293	LYS	O-C-N	-6.89	115.17	121.37
1	A	109	ASP	CA-CB-CG	6.89	119.49	112.60
1	G	172	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	C	4	PHE	CA-C-N	6.88	126.92	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	PHE	C-N-CA	6.88	126.92	119.90
1	J	24	ALA	CB-CA-C	-6.88	100.02	110.90
1	O	58	PHE	CA-CB-CG	-6.88	106.92	113.80
1	C	237	HIS	CA-C-N	-6.88	111.65	122.73
1	C	237	HIS	C-N-CA	-6.88	111.65	122.73
1	N	340	GLY	N-CA-C	-6.88	104.30	114.90
1	I	195	ASP	CB-CA-C	-6.88	97.46	110.67
1	M	125	GLN	OE1-CD-NE2	6.88	129.48	122.60
1	A	67	SER	CA-C-O	6.88	130.35	120.51
1	D	123	THR	CB-CA-C	-6.88	96.73	110.42
1	N	29	ILE	N-CA-C	6.88	118.39	108.48
1	Q	89	GLN	N-CA-C	-6.88	96.15	110.80
1	C	133	ARG	NH1-CZ-NH2	-6.88	110.36	119.30
1	F	179	GLN	N-CA-C	-6.88	104.76	113.01
1	L	98	LYS	N-CA-C	-6.87	103.79	111.28
1	C	29	ILE	N-CA-C	6.87	117.73	108.11
1	P	357	PHE	CA-C-O	6.87	130.58	121.78
1	Q	29	ILE	N-CA-CB	-6.87	98.50	111.21
1	D	343	VAL	CA-C-O	-6.87	113.18	120.39
1	D	51	THR	O-C-N	-6.87	114.50	123.16
1	H	15	LEU	CA-C-O	6.87	127.83	120.55
1	I	34	GLU	CB-CG-CD	6.87	124.27	112.60
1	C	167	ALA	CA-C-N	-6.87	110.54	120.29
1	C	167	ALA	C-N-CA	-6.87	110.54	120.29
1	H	315	GLY	N-CA-C	-6.87	105.75	115.43
1	I	15	LEU	CA-C-O	-6.87	112.07	119.97
1	N	144	PHE	CA-CB-CG	6.87	120.67	113.80
1	C	123	THR	N-CA-CB	6.86	121.23	110.87
1	A	152	ARG	CB-CG-CD	6.86	127.08	111.30
1	E	139	LYS	N-CA-C	-6.86	103.86	111.82
1	D	66	ASP	OD1-CG-OD2	-6.86	106.44	122.90
1	D	80	HIS	N-CA-C	6.86	119.39	111.02
1	C	291	LEU	CA-C-O	-6.86	114.19	120.50
1	D	179	GLN	N-CA-C	-6.86	104.78	113.01
1	P	179	GLN	CA-CB-CG	6.86	127.81	114.10
1	A	95	ASN	CA-C-N	-6.85	110.69	120.42
1	A	95	ASN	C-N-CA	-6.85	110.69	120.42
1	A	193	ASP	CA-CB-CG	-6.85	105.75	112.60
1	A	267	ILE	CB-CG1-CD1	-6.85	99.41	113.80
1	D	323	THR	N-CA-C	-6.85	103.74	111.07
1	G	90	GLY	CA-C-N	-6.85	111.70	121.50
1	G	90	GLY	C-N-CA	-6.85	111.70	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	334	ASN	CA-CB-CG	-6.85	105.75	112.60
1	K	353	THR	CA-CB-CG2	6.85	122.15	110.50
1	O	180	ASN	CA-CB-CG	-6.85	105.75	112.60
1	P	35	SER	CA-CB-OG	-6.85	97.40	111.10
1	I	71	GLN	CG-CD-NE2	-6.85	106.13	116.40
1	K	257	HIS	CA-C-O	-6.85	110.15	119.05
1	Q	171	ALA	N-CA-C	-6.85	103.27	111.69
1	N	195	ASP	N-CA-CB	-6.85	99.02	110.39
1	O	89	GLN	OE1-CD-NE2	6.85	129.45	122.60
1	I	105	GLY	CA-C-N	-6.84	112.85	122.71
1	I	105	GLY	C-N-CA	-6.84	112.85	122.71
1	N	9	GLN	O-C-N	6.84	129.38	122.12
1	P	152	ARG	NH1-CZ-NH2	6.84	128.20	119.30
1	M	152	ARG	NE-CZ-NH2	6.84	125.36	119.20
1	A	338	ALA	CA-C-O	-6.84	110.16	119.05
1	E	323	THR	N-CA-C	-6.84	103.91	111.36
1	J	27	LYS	O-C-N	6.84	130.59	122.79
1	N	223	LEU	CA-C-O	-6.84	113.30	120.55
1	O	99	GLU	CA-C-O	-6.84	110.97	119.38
1	A	353	THR	CA-CB-OG1	6.84	119.85	109.60
1	D	117	GLY	O-C-N	6.84	130.34	122.34
1	K	5	PRO	CA-C-O	6.84	129.09	121.36
1	I	165	GLU	OE1-CD-OE2	6.83	139.30	122.90
1	B	258	ARG	CD-NE-CZ	6.83	133.97	124.40
1	E	18	ILE	CB-CG1-CD1	6.83	128.15	113.80
1	G	325	GLU	N-CA-C	6.83	118.73	111.28
1	O	66	ASP	CA-C-O	6.83	128.67	121.15
1	O	201	CYS	CA-C-O	6.83	127.67	120.42
1	C	324	GLN	CA-C-O	6.83	127.79	120.55
1	D	156	GLN	N-CA-CB	-6.83	101.63	112.63
1	F	120	LYS	CA-CB-CG	-6.83	100.44	114.10
1	L	78	LEU	O-C-N	6.83	132.07	123.19
1	B	5	PRO	CA-C-N	-6.83	111.30	120.79
1	B	5	PRO	C-N-CA	-6.83	111.30	120.79
1	I	85	GLN	OE1-CD-NE2	-6.83	115.77	122.60
1	L	180	ASN	O-C-N	-6.83	113.38	122.19
1	P	178	GLN	OE1-CD-NE2	6.83	129.43	122.60
1	E	51	THR	N-CA-CB	-6.83	99.70	110.69
1	L	11	GLN	O-C-N	6.83	129.19	122.09
1	C	298	SER	CA-C-N	-6.83	111.34	122.81
1	C	298	SER	C-N-CA	-6.83	111.34	122.81
1	D	274	MET	N-CA-C	-6.82	100.38	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	PHE	CA-C-N	-6.82	111.04	120.38
1	A	79	PHE	C-N-CA	-6.82	111.04	120.38
1	H	175	SER	CB-CA-C	-6.82	100.17	110.88
1	H	309	ALA	O-C-N	6.82	130.66	122.27
1	E	228	LEU	O-C-N	6.82	131.87	123.21
1	M	164	GLN	CB-CG-CD	6.82	124.19	112.60
1	O	299	PHE	CA-CB-CG	-6.82	106.98	113.80
1	G	132	GLU	O-C-N	6.82	129.18	122.09
1	G	333	ALA	N-CA-C	-6.82	103.78	111.14
1	I	33	ASP	CA-C-N	-6.82	111.67	121.42
1	I	33	ASP	C-N-CA	-6.82	111.67	121.42
1	D	189	GLU	CB-CG-CD	6.81	124.18	112.60
1	F	89	GLN	CA-C-O	-6.81	113.42	121.32
1	F	171	ALA	O-C-N	6.81	129.45	122.09
1	H	165	GLU	CB-CA-C	6.81	121.58	110.88
1	I	23	VAL	CA-C-N	6.81	131.04	120.82
1	I	23	VAL	C-N-CA	6.81	131.04	120.82
1	R	178	GLN	N-CA-CB	6.81	120.13	110.12
1	E	271	SER	N-CA-C	-6.81	105.25	113.97
1	I	123	THR	N-CA-CB	6.81	121.85	110.14
1	R	89	GLN	CA-C-O	-6.81	110.77	120.51
1	B	300	SER	N-CA-CB	6.81	121.99	110.49
1	D	332	MET	O-C-N	-6.81	115.06	122.07
1	N	148	ARG	O-C-N	6.81	131.30	123.27
1	N	305	LEU	N-CA-CB	6.81	121.28	110.73
1	E	175	SER	CA-C-O	-6.81	113.62	120.90
1	B	89	GLN	N-CA-C	-6.80	96.31	110.80
1	E	352	SER	CA-C-O	6.80	130.24	120.51
1	G	334	ASN	CB-CG-ND2	6.80	126.60	116.40
1	R	23	VAL	CA-C-N	6.80	129.72	120.54
1	R	23	VAL	C-N-CA	6.80	129.72	120.54
1	R	31	ALA	O-C-N	6.80	131.27	122.43
1	B	89	GLN	CA-CB-CG	-6.80	100.50	114.10
1	I	179	GLN	CG-CD-NE2	-6.80	106.20	116.40
1	C	30	LEU	CA-C-N	-6.80	112.71	122.77
1	C	30	LEU	C-N-CA	-6.80	112.71	122.77
1	O	226	THR	OG1-CB-CG2	6.80	122.90	109.30
1	R	172	ARG	N-CA-CB	6.80	120.07	109.94
1	K	258	ARG	O-C-N	6.80	131.77	122.46
1	L	315	GLY	N-CA-C	-6.80	105.85	115.30
1	O	20	GLN	CA-C-O	6.80	127.79	119.97
1	P	252	THR	O-C-N	6.80	129.43	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	305	LEU	N-CA-C	-6.80	104.89	113.72
1	Q	291	LEU	N-CA-C	-6.79	100.37	108.25
1	R	136	GLN	O-C-N	6.79	129.90	122.15
1	E	169	ALA	O-C-N	6.79	129.32	122.12
1	I	141	GLY	N-CA-C	6.79	124.04	115.21
1	H	329	LYS	CA-CB-CG	6.79	127.68	114.10
1	O	10	GLU	CB-CA-C	-6.79	98.07	110.63
1	J	27	LYS	CA-CB-CG	-6.79	100.53	114.10
1	O	51	THR	N-CA-CB	-6.79	98.98	111.13
1	J	294	PRO	O-C-N	6.79	131.85	122.35
1	A	73	ILE	N-CA-CB	-6.79	102.93	111.41
1	D	296	LYS	N-CA-CB	6.79	120.00	109.48
1	N	115	LEU	O-C-N	-6.79	114.19	123.01
1	Q	256	LEU	CA-C-N	-6.79	110.10	122.38
1	Q	256	LEU	C-N-CA	-6.79	110.10	122.38
1	A	324	GLN	O-C-N	-6.78	113.93	122.27
1	E	124	ILE	CB-CG1-CD1	6.78	128.04	113.80
1	H	200	HIS	CA-CB-CG	6.78	120.58	113.80
1	C	69	ILE	N-CA-C	-6.78	104.18	113.00
1	I	28	GLY	CA-C-O	6.78	132.37	120.57
1	N	69	ILE	N-CA-CB	-6.78	100.04	111.23
1	D	128	ASP	CA-CB-CG	6.78	119.38	112.60
1	N	217	ASN	CA-C-N	-6.78	111.20	120.28
1	N	217	ASN	C-N-CA	-6.78	111.20	120.28
1	Q	263	ALA	CA-C-O	-6.78	111.04	119.38
1	K	308	SER	CA-CB-OG	6.78	124.66	111.10
1	N	36	VAL	CA-C-N	-6.78	111.80	120.34
1	N	36	VAL	C-N-CA	-6.78	111.80	120.34
1	C	89	GLN	CA-C-O	-6.78	111.92	119.78
1	G	109	ASP	CA-CB-CG	6.78	119.38	112.60
1	J	66	ASP	CA-C-N	6.78	129.66	120.38
1	J	66	ASP	C-N-CA	6.78	129.66	120.38
1	Q	224	GLU	CB-CG-CD	6.78	124.12	112.60
1	E	123	THR	CA-CB-OG1	6.77	119.76	109.60
1	G	156	GLN	CA-C-O	-6.77	112.41	120.81
1	M	237	HIS	CA-C-N	-6.77	111.83	122.73
1	M	237	HIS	C-N-CA	-6.77	111.83	122.73
1	B	87	ASP	CA-CB-CG	6.77	119.37	112.60
1	O	70	ASN	CB-CA-C	-6.77	98.74	110.72
1	C	258	ARG	CA-C-O	-6.77	111.81	119.79
1	H	323	THR	CA-C-O	6.77	127.67	120.70
1	L	253	VAL	CG1-CB-CG2	-6.77	95.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	271	SER	CA-CB-OG	-6.76	97.57	111.10
1	E	88	SER	CA-C-N	6.76	134.46	121.54
1	E	88	SER	C-N-CA	6.76	134.46	121.54
1	Q	44	GLN	OE1-CD-NE2	-6.76	115.83	122.60
1	R	90	GLY	CA-C-N	-6.76	112.08	122.09
1	R	90	GLY	C-N-CA	-6.76	112.08	122.09
1	D	69	ILE	CA-C-O	-6.76	113.27	120.64
1	K	102	ILE	N-CA-C	6.76	117.61	107.80
1	A	141	GLY	CA-C-O	6.76	126.26	118.96
1	Q	165	GLU	OE1-CD-OE2	6.76	139.13	122.90
1	A	284	ASN	CB-CG-ND2	-6.76	106.26	116.40
1	J	45	ARG	NH1-CZ-NH2	6.76	128.09	119.30
1	K	261	PRO	O-C-N	-6.76	114.41	122.99
1	Q	24	ALA	CA-C-O	-6.76	112.47	120.10
1	B	201	CYS	O-C-N	-6.75	113.96	122.27
1	M	65	VAL	N-CA-CB	-6.75	100.09	111.23
1	A	38	THR	O-C-N	6.75	129.02	122.07
1	C	191	ILE	N-CA-CB	-6.75	101.76	111.21
1	K	144	PHE	O-C-N	6.75	130.64	123.42
1	R	242	LYS	CA-C-N	-6.75	110.63	123.32
1	R	242	LYS	C-N-CA	-6.75	110.63	123.32
1	F	284	ASN	CB-CG-OD1	6.75	134.30	120.80
1	I	38	THR	CA-CB-CG2	-6.75	99.03	110.50
1	N	54	ASN	OD1-CG-ND2	6.75	129.34	122.60
1	D	77	ILE	CB-CA-C	-6.74	102.55	110.91
1	D	261	PRO	CA-C-O	6.74	132.87	120.60
1	K	95	ASN	N-CA-CB	6.74	120.44	110.33
1	E	71	GLN	CG-CD-NE2	-6.74	106.29	116.40
1	I	49	GLU	CA-C-O	6.74	128.45	120.70
1	G	156	GLN	CG-CD-NE2	6.73	126.50	116.40
1	L	123	THR	CB-CA-C	-6.73	98.50	112.44
1	J	10	GLU	CA-C-O	-6.73	113.42	120.55
1	Q	217	ASN	CA-C-O	-6.73	113.29	120.42
1	A	133	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	I	134	CYS	CA-C-O	6.73	127.90	120.63
1	D	190	VAL	CB-CA-C	-6.73	102.59	111.81
1	O	2	HIS	CA-CB-CG	6.73	120.53	113.80
1	Q	205	THR	CB-CA-C	-6.73	99.24	110.68
1	C	286	ILE	N-CA-C	-6.73	103.30	110.36
1	F	219	HIS	CA-C-N	6.73	131.67	122.19
1	F	219	HIS	C-N-CA	6.73	131.67	122.19
1	H	27	LYS	CD-CE-NZ	6.73	133.43	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	124	ILE	N-CA-CB	-6.72	100.41	111.44
1	G	26	GLY	CA-C-N	-6.72	108.73	120.97
1	G	26	GLY	C-N-CA	-6.72	108.73	120.97
1	O	276	GLU	CA-C-N	-6.72	111.70	120.44
1	O	276	GLU	C-N-CA	-6.72	111.70	120.44
1	A	199	GLU	CA-CB-CG	6.72	127.54	114.10
1	E	159	SER	CA-C-O	6.72	129.75	121.89
1	D	52	GLU	N-CA-CB	6.72	120.03	109.82
1	L	56	ARG	CD-NE-CZ	-6.72	115.00	124.40
1	L	98	LYS	CB-CA-C	-6.72	99.64	110.79
1	L	258	ARG	O-C-N	6.72	130.74	122.34
1	P	179	GLN	CG-CD-OE1	-6.72	107.36	120.80
1	D	100	LYS	O-C-N	-6.71	112.45	122.39
1	E	10	GLU	CB-CA-C	6.71	122.27	110.85
1	M	156	GLN	CA-C-O	-6.71	112.60	119.78
1	Q	41	ASN	N-CA-CB	6.71	119.99	110.12
1	R	211	ALA	CA-C-O	6.71	127.67	120.55
1	B	194	GLY	CA-C-N	-6.71	111.95	122.49
1	B	194	GLY	C-N-CA	-6.71	111.95	122.49
1	F	195	ASP	CB-CG-OD1	-6.71	102.96	118.40
1	A	131	SER	N-CA-C	6.71	118.59	111.28
1	C	328	MET	CA-C-O	6.71	127.53	120.42
1	M	156	GLN	CG-CD-NE2	6.71	126.47	116.40
1	D	71	GLN	O-C-N	6.71	131.21	122.42
1	N	165	GLU	N-CA-CB	-6.71	100.28	110.01
1	O	62	LEU	N-CA-CB	6.71	119.74	110.01
1	B	71	GLN	CA-CB-CG	6.71	127.52	114.10
1	H	96	ILE	N-CA-C	-6.71	103.98	110.42
1	J	199	GLU	CA-CB-CG	6.71	127.51	114.10
1	F	218	ASP	O-C-N	6.70	130.51	122.27
1	J	317	ALA	CA-C-O	6.70	127.87	120.63
1	M	103	VAL	N-CA-CB	6.70	117.84	110.53
1	O	110	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	G	222	TYR	N-CA-CB	-6.70	99.22	109.94
1	A	290	PRO	O-C-N	-6.70	113.59	122.64
1	C	258	ARG	CG-CD-NE	-6.70	97.26	112.00
1	E	22	ILE	CA-C-O	-6.70	113.23	120.47
1	H	133	ARG	CD-NE-CZ	6.70	133.78	124.40
1	L	254	THR	O-C-N	6.70	128.97	122.07
1	O	203	TYR	CA-C-O	6.70	127.86	120.82
1	P	9	GLN	CG-CD-NE2	6.70	126.45	116.40
1	O	118	THR	CA-C-O	-6.70	114.01	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	PHE	O-C-N	-6.69	115.39	123.16
1	Q	38	THR	N-CA-CB	-6.69	99.91	110.28
1	B	345	THR	N-CA-C	-6.69	96.54	110.80
1	D	297	LEU	CA-C-N	6.69	130.99	122.16
1	D	297	LEU	C-N-CA	6.69	130.99	122.16
1	B	6	ALA	O-C-N	6.69	129.24	122.08
1	F	145	GLY	O-C-N	-6.69	117.47	123.29
1	I	147	TRP	O-C-N	6.69	132.51	123.34
1	O	30	LEU	O-C-N	6.69	130.83	123.27
1	Q	231	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	B	199	GLU	CA-C-N	-6.69	110.79	120.29
1	B	199	GLU	C-N-CA	-6.69	110.79	120.29
1	K	136	GLN	N-CA-C	-6.69	103.92	111.14
1	R	257	HIS	N-CA-C	-6.69	104.59	112.89
1	A	67	SER	CB-CA-C	-6.69	97.11	110.42
1	C	287	ASN	OD1-CG-ND2	6.69	129.29	122.60
1	J	17	GLU	N-CA-CB	6.69	119.71	110.01
1	J	353	THR	O-C-N	6.69	129.38	122.09
1	B	115	LEU	O-C-N	-6.69	115.09	123.05
1	E	23	VAL	CA-C-O	6.68	129.13	120.78
1	F	16	SER	CA-C-O	6.68	128.05	120.90
1	J	90	GLY	CA-C-O	-6.68	111.72	119.80
1	H	247	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	M	71	GLN	CG-CD-NE2	-6.68	106.38	116.40
1	O	15	LEU	CA-C-N	-6.68	110.16	120.31
1	O	15	LEU	C-N-CA	-6.68	110.16	120.31
1	B	259	THR	CA-CB-OG1	-6.68	99.58	109.60
1	D	92	LEU	N-CA-CB	-6.68	99.75	109.83
1	G	17	GLU	CA-C-N	-6.68	111.31	120.46
1	G	17	GLU	C-N-CA	-6.68	111.31	120.46
1	E	9	GLN	CA-C-N	-6.68	110.81	120.29
1	E	9	GLN	C-N-CA	-6.68	110.81	120.29
1	G	17	GLU	CA-C-O	-6.68	113.34	120.42
1	J	336	GLN	CA-C-O	-6.68	113.47	120.55
1	L	97	LEU	O-C-N	-6.68	115.19	122.07
1	N	259	THR	CA-C-N	-6.68	118.06	122.60
1	N	259	THR	C-N-CA	-6.68	118.06	122.60
1	O	3	ARG	CA-C-O	-6.68	109.85	119.80
1	O	326	ALA	CA-C-N	6.68	129.23	120.28
1	O	326	ALA	C-N-CA	6.68	129.23	120.28
1	L	131	SER	CB-CA-C	-6.67	100.68	110.96
1	D	172	ARG	CA-C-O	6.67	127.83	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	188	PRO	N-CA-CB	6.67	107.09	102.35
1	B	268	CYS	O-C-N	6.67	133.10	122.96
1	F	39	MET	CA-C-O	6.67	127.58	119.38
1	K	175	SER	N-CA-C	6.67	119.40	111.33
1	M	85	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	L	24	ALA	CB-CA-C	-6.67	99.67	110.74
1	P	344	HIS	N-CA-CB	6.67	121.75	110.49
1	I	95	ASN	O-C-N	6.66	129.75	122.15
1	E	137	TYR	CA-C-O	6.66	127.61	120.55
1	M	123	THR	CA-C-N	-6.66	113.87	123.06
1	M	123	THR	C-N-CA	-6.66	113.87	123.06
1	B	281	LEU	CA-C-O	-6.66	113.83	120.82
1	D	270	LEU	N-CA-C	-6.66	99.73	110.32
1	D	311	ALA	N-CA-C	-6.66	103.95	111.14
1	E	140	ASP	CA-CB-CG	-6.66	105.94	112.60
1	L	116	ALA	O-C-N	6.66	131.09	122.97
1	O	103	VAL	CA-C-N	-6.66	113.39	122.91
1	O	103	VAL	C-N-CA	-6.66	113.39	122.91
1	B	267	ILE	CB-CA-C	6.66	120.05	110.33
1	G	27	LYS	CG-CD-CE	6.66	126.61	111.30
1	N	303	ARG	CB-CG-CD	6.66	126.61	111.30
1	O	189	GLU	CA-C-O	6.66	128.21	120.49
1	D	182	LEU	O-C-N	-6.65	115.41	123.19
1	L	232	MET	CA-C-N	-6.65	112.49	121.80
1	L	232	MET	C-N-CA	-6.65	112.49	121.80
1	B	24	ALA	N-CA-CB	6.65	120.04	110.06
1	H	119	ASN	CA-CB-CG	-6.65	105.95	112.60
1	M	106	ILE	O-C-N	6.65	130.58	123.00
1	M	116	ALA	CA-C-O	-6.65	114.56	121.87
1	D	152	ARG	NE-CZ-NH2	6.65	125.18	119.20
1	D	163	ILE	O-C-N	-6.65	115.42	121.87
1	D	283	LEU	CA-C-N	6.65	129.48	120.44
1	D	283	LEU	C-N-CA	6.65	129.48	120.44
1	O	278	ASP	CA-CB-CG	-6.65	105.95	112.60
1	A	358	THR	N-CA-C	-6.65	96.64	110.80
1	D	90	GLY	CA-C-N	-6.65	112.82	122.19
1	D	90	GLY	C-N-CA	-6.65	112.82	122.19
1	A	234	THR	N-CA-C	6.65	119.04	109.14
1	R	144	PHE	CA-C-N	6.64	127.40	121.82
1	R	144	PHE	C-N-CA	6.64	127.40	121.82
1	I	93	PHE	O-C-N	-6.64	114.47	122.11
1	I	117	GLY	CA-C-O	6.64	127.23	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	168	ASN	CA-C-N	-6.64	110.86	120.29
1	O	168	ASN	C-N-CA	-6.64	110.86	120.29
1	A	265	PRO	CA-C-N	-6.64	111.83	121.26
1	A	265	PRO	C-N-CA	-6.64	111.83	121.26
1	C	70	ASN	CB-CG-ND2	-6.64	106.44	116.40
1	C	132	GLU	OE1-CD-OE2	-6.64	106.97	122.90
1	C	138	LYS	CA-C-N	6.64	130.40	120.31
1	C	138	LYS	C-N-CA	6.64	130.40	120.31
1	F	109	ASP	O-C-N	6.64	130.42	122.85
1	L	22	ILE	CA-C-O	-6.64	111.55	119.58
1	Q	207	LYS	CG-CD-CE	6.64	126.57	111.30
1	J	209	LEU	CA-C-N	-6.64	111.58	120.54
1	J	209	LEU	C-N-CA	-6.64	111.58	120.54
1	P	38	THR	O-C-N	6.64	128.91	122.07
1	L	14	GLU	O-C-N	6.63	128.90	122.07
1	M	135	ALA	O-C-N	6.63	130.43	122.27
1	R	152	ARG	NE-CZ-NH1	-6.63	114.86	121.50
1	B	86	LYS	CA-C-N	-6.63	113.06	122.41
1	B	86	LYS	C-N-CA	-6.63	113.06	122.41
1	L	12	LYS	CA-C-N	-6.63	111.40	120.28
1	L	12	LYS	C-N-CA	-6.63	111.40	120.28
1	R	58	PHE	CA-CB-CG	-6.63	107.17	113.80
1	P	180	ASN	CA-CB-CG	-6.63	105.97	112.60
1	R	267	ILE	CA-C-N	6.63	132.75	123.07
1	R	267	ILE	C-N-CA	6.63	132.75	123.07
1	H	123	THR	N-CA-C	-6.63	98.92	108.07
1	J	109	ASP	CA-CB-CG	6.63	119.23	112.60
1	K	223	LEU	CA-C-O	-6.63	113.47	120.63
1	J	166	ASN	CA-CB-CG	-6.62	105.97	112.60
1	L	182	LEU	O-C-N	-6.62	115.48	123.16
1	L	232	MET	N-CA-C	-6.62	99.79	110.32
1	M	102	ILE	O-C-N	-6.62	115.68	123.03
1	P	65	VAL	CA-CB-CG2	6.62	121.66	110.40
1	P	304	ALA	CA-C-O	-6.62	111.24	119.38
1	Q	261	PRO	CB-CA-C	6.62	119.66	111.12
1	R	70	ASN	N-CA-CB	-6.62	98.26	110.18
1	L	198	LEU	CA-C-O	6.62	127.95	121.00
1	N	284	ASN	CA-C-N	-6.62	111.83	120.44
1	N	284	ASN	C-N-CA	-6.62	111.83	120.44
1	P	144	PHE	CA-CB-CG	6.62	120.42	113.80
1	H	68	SER	CA-CB-OG	6.62	124.34	111.10
1	H	156	GLN	OE1-CD-NE2	6.62	129.22	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	186	VAL	N-CA-CB	-6.62	103.14	111.41
1	N	80	HIS	CA-CB-CG	6.62	120.42	113.80
1	P	165	GLU	CB-CA-C	6.62	121.36	110.90
1	I	259	THR	O-C-N	-6.62	114.44	122.25
1	C	277	GLU	CA-C-N	-6.62	111.42	120.28
1	C	277	GLU	C-N-CA	-6.62	111.42	120.28
1	H	89	GLN	N-CA-CB	-6.62	99.31	110.49
1	H	305	LEU	CA-C-O	6.62	126.33	119.05
1	N	336	GLN	O-C-N	6.62	129.17	122.03
1	B	73	ILE	O-C-N	-6.61	115.47	122.81
1	I	56	ARG	NE-CZ-NH1	-6.61	114.89	121.50
1	M	96	ILE	O-C-N	6.61	128.64	121.83
1	N	85	GLN	CB-CG-CD	6.61	123.84	112.60
1	P	332	MET	CA-C-O	-6.61	113.41	120.42
1	P	60	GLU	CA-C-O	-6.61	113.54	120.55
1	P	82	THR	CA-C-N	6.61	131.76	120.72
1	P	82	THR	C-N-CA	6.61	131.76	120.72
1	R	114	PRO	O-C-N	6.61	131.03	123.03
1	J	123	THR	CB-CA-C	-6.61	97.27	110.42
1	N	179	GLN	CB-CG-CD	6.61	123.83	112.60
1	E	127	LEU	CA-C-N	-6.61	111.73	121.24
1	E	127	LEU	C-N-CA	-6.61	111.73	121.24
1	M	72	SER	CA-C-O	6.61	127.50	119.64
1	D	278	ASP	CA-C-O	-6.60	113.90	120.70
1	J	285	ALA	CA-C-O	6.60	127.56	119.97
1	A	217	ASN	CA-CB-CG	6.60	119.20	112.60
1	H	1	ALA	N-CA-CB	-6.60	100.50	110.40
1	J	284	ASN	CA-CB-CG	-6.60	106.00	112.60
1	F	339	LYS	CA-CB-CG	6.60	127.30	114.10
1	O	220	HIS	CB-CA-C	-6.60	102.36	111.73
1	R	26	GLY	N-CA-C	-6.60	106.58	115.36
1	H	193	ASP	CA-CB-CG	-6.60	106.00	112.60
1	M	126	GLY	O-C-N	6.60	131.28	122.70
1	B	203	TYR	O-C-N	-6.60	115.28	122.07
1	C	235	ALA	O-C-N	6.60	130.46	122.68
1	M	195	ASP	N-CA-CB	-6.60	100.06	110.28
1	R	65	VAL	O-C-N	-6.59	114.33	122.57
1	A	42	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	K	123	THR	N-CA-CB	6.59	120.77	109.10
1	L	191	ILE	CA-CB-CG2	6.59	121.70	110.50
1	N	258	ARG	NE-CZ-NH2	-6.59	113.27	119.20
1	O	128	ASP	CA-C-O	-6.59	113.23	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	191	ILE	CA-C-N	6.59	127.52	120.47
1	F	191	ILE	C-N-CA	6.59	127.52	120.47
1	H	194	GLY	CA-C-N	6.59	130.33	120.31
1	H	194	GLY	C-N-CA	6.59	130.33	120.31
1	I	34	GLU	CA-CB-CG	6.59	127.28	114.10
1	I	336	GLN	CA-C-O	-6.59	113.90	120.82
1	N	188	PRO	CA-C-O	-6.59	111.95	122.82
1	P	250	MET	N-CA-CB	6.59	119.91	110.16
1	R	200	HIS	N-CA-C	-6.59	103.93	112.23
1	A	266	GLY	CA-C-N	-6.59	113.63	122.98
1	A	266	GLY	C-N-CA	-6.59	113.63	122.98
1	D	232	MET	O-C-N	6.59	130.69	122.65
1	E	305	LEU	N-CA-C	-6.59	104.97	114.12
1	L	130	LEU	CA-C-O	-6.59	112.82	120.20
1	P	328	MET	CA-C-O	-6.59	113.57	120.55
1	K	34	GLU	CA-C-O	6.58	128.38	120.81
1	E	159	SER	CA-C-N	-6.58	110.94	120.29
1	E	159	SER	C-N-CA	-6.58	110.94	120.29
1	N	328	MET	O-C-N	-6.58	115.14	122.12
1	A	218	ASP	N-CA-C	-6.58	104.14	111.71
1	D	211	ALA	CA-C-N	6.58	128.85	120.56
1	D	211	ALA	C-N-CA	6.58	128.85	120.56
1	M	301	TYR	O-C-N	-6.58	115.69	123.06
1	K	134	CYS	CA-C-O	6.58	127.73	120.82
1	L	76	VAL	CA-C-O	-6.58	113.53	120.76
1	L	291	LEU	N-CA-CB	-6.58	100.35	109.82
1	F	343	VAL	CB-CA-C	-6.58	101.54	110.42
1	J	4	PHE	CA-CB-CG	-6.58	107.22	113.80
1	K	184	PRO	CA-C-N	-6.58	113.89	122.37
1	K	184	PRO	C-N-CA	-6.58	113.89	122.37
1	I	10	GLU	N-CA-CB	6.58	120.35	110.22
1	L	234	THR	CA-CB-CG2	6.58	121.68	110.50
1	A	218	ASP	O-C-N	6.57	129.91	122.22
1	C	1	ALA	CA-C-O	6.57	131.98	120.80
1	C	184	PRO	CB-CA-C	-6.57	105.42	111.40
1	G	44	GLN	CA-C-O	6.57	127.93	120.90
1	I	172	ARG	CA-CB-CG	-6.57	100.95	114.10
1	K	90	GLY	CA-C-N	-6.57	112.86	122.65
1	K	90	GLY	C-N-CA	-6.57	112.86	122.65
1	L	289	CYS	CA-C-O	-6.57	113.57	119.75
1	B	136	GLN	CA-CB-CG	6.57	127.24	114.10
1	I	61	ILE	CA-C-O	-6.57	113.75	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ARG	NH1-CZ-NH2	-6.57	110.76	119.30
1	O	11	GLN	N-CA-C	-6.57	104.04	111.07
1	A	95	ASN	O-C-N	6.57	130.35	122.27
1	D	131	SER	N-CA-CB	6.57	119.54	110.01
1	E	114	PRO	O-C-N	6.57	130.56	123.01
1	F	52	GLU	CA-C-O	-6.57	113.84	121.07
1	I	206	GLU	OE1-CD-OE2	-6.57	107.13	122.90
1	D	152	ARG	N-CA-C	-6.57	99.34	109.52
1	G	136	GLN	CA-C-N	-6.57	110.33	120.31
1	G	136	GLN	C-N-CA	-6.57	110.33	120.31
1	H	119	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	J	71	GLN	CB-CG-CD	-6.56	101.44	112.60
1	J	219	HIS	CA-C-O	6.56	127.59	119.78
1	P	169	ALA	CA-C-O	-6.56	112.42	119.97
1	A	195	ASP	CA-C-N	-6.56	109.27	120.95
1	A	195	ASP	C-N-CA	-6.56	109.27	120.95
1	I	227	LEU	N-CA-C	-6.56	98.69	108.99
1	J	12	LYS	CA-C-O	6.56	127.92	120.90
1	N	266	GLY	CA-C-N	-6.56	113.66	122.98
1	N	266	GLY	C-N-CA	-6.56	113.66	122.98
1	O	123	THR	CB-CA-C	-6.56	98.86	112.44
1	E	74	GLY	CA-C-N	-6.56	112.61	121.27
1	E	74	GLY	C-N-CA	-6.56	112.61	121.27
1	G	100	LYS	CB-CA-C	-6.56	98.22	110.36
1	K	259	THR	CA-CB-OG1	-6.56	99.76	109.60
1	B	85	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	D	310	LEU	CA-C-O	6.56	127.71	120.82
1	N	313	TRP	O-C-N	6.56	129.10	122.08
1	D	264	VAL	N-CA-CB	-6.56	103.98	110.08
1	F	352	SER	N-CA-C	6.56	124.77	110.80
1	H	27	LYS	CA-C-N	6.56	134.26	121.41
1	H	27	LYS	C-N-CA	6.56	134.26	121.41
1	M	277	GLU	CB-CG-CD	6.56	123.75	112.60
1	N	5	PRO	CA-C-O	-6.56	113.95	121.36
1	Q	118	THR	N-CA-CB	-6.56	100.14	111.55
1	C	89	GLN	CB-CA-C	-6.56	100.10	110.85
1	E	221	VAL	CA-CB-CG2	-6.56	99.25	110.40
1	R	312	ALA	O-C-N	-6.56	114.21	122.27
1	E	214	LYS	O-C-N	-6.55	115.17	122.12
1	I	324	GLN	CA-C-O	6.55	127.51	119.97
1	J	2	HIS	CA-C-O	-6.55	111.14	120.51
1	Q	3	ARG	CB-CG-CD	6.55	126.37	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	308	SER	CA-C-O	-6.55	113.55	120.63
1	B	97	LEU	CA-C-O	6.55	127.45	120.70
1	J	12	LYS	CA-CB-CG	-6.55	101.00	114.10
1	R	154	ALA	CA-C-N	-6.55	111.58	120.82
1	R	154	ALA	C-N-CA	-6.55	111.58	120.82
1	B	62	LEU	CA-C-N	-6.55	109.88	122.06
1	B	62	LEU	C-N-CA	-6.55	109.88	122.06
1	D	27	LYS	CG-CD-CE	6.55	126.37	111.30
1	G	249	ALA	O-C-N	-6.55	114.68	122.15
1	M	325	GLU	CB-CG-CD	-6.55	101.46	112.60
1	B	298	SER	CA-C-N	-6.55	111.82	122.82
1	B	298	SER	C-N-CA	-6.55	111.82	122.82
1	J	114	PRO	O-C-N	-6.55	114.88	123.13
1	B	198	LEU	CA-C-O	6.55	127.51	120.24
1	E	213	TYR	CA-CB-CG	-6.55	102.11	113.90
1	R	308	SER	CA-CB-OG	6.55	124.19	111.10
1	E	81	GLU	CB-CG-CD	6.55	123.73	112.60
1	R	335	CYS	CA-C-N	-6.55	111.93	120.44
1	R	335	CYS	C-N-CA	-6.55	111.93	120.44
1	D	115	LEU	N-CA-CB	-6.54	100.31	110.65
1	H	305	LEU	O-C-N	-6.54	114.30	122.35
1	I	26	GLY	O-C-N	6.54	130.11	122.45
1	K	55	ARG	O-C-N	-6.54	115.22	122.03
1	H	257	HIS	CA-CB-CG	6.54	120.34	113.80
1	M	127	LEU	O-C-N	6.54	131.10	122.33
1	R	244	THR	N-CA-CB	-6.54	97.80	110.10
1	F	38	THR	CA-CB-OG1	-6.54	99.79	109.60
1	C	136	GLN	CG-CD-OE1	6.54	133.88	120.80
1	F	277	GLU	CA-C-O	6.54	127.25	119.60
1	J	77	ILE	CB-CA-C	-6.54	102.02	110.98
1	Q	67	SER	CA-C-O	6.54	127.33	119.61
1	D	3	ARG	CB-CA-C	6.54	123.43	110.42
1	G	123	THR	CA-CB-OG1	6.54	119.41	109.60
1	M	70	ASN	O-C-N	6.54	131.29	122.59
1	O	232	MET	CA-C-N	-6.54	112.72	122.01
1	O	232	MET	C-N-CA	-6.54	112.72	122.01
1	L	77	ILE	CA-C-N	-6.54	112.55	122.81
1	L	77	ILE	C-N-CA	-6.54	112.55	122.81
1	B	215	ALA	CB-CA-C	-6.54	99.94	110.79
1	K	10	GLU	CB-CA-C	-6.54	100.62	110.88
1	M	44	GLN	O-C-N	-6.54	115.19	122.12
1	A	152	ARG	O-C-N	6.53	131.64	123.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	322	ALA	O-C-N	6.53	128.88	122.09
1	M	247	GLN	N-CA-C	-6.53	103.43	111.40
1	O	155	ASP	CA-C-O	6.53	129.85	120.51
1	F	24	ALA	O-C-N	-6.53	114.58	122.22
1	P	99	GLU	O-C-N	6.53	129.04	122.12
1	B	161	LEU	N-CA-C	-6.53	104.09	111.14
1	B	261	PRO	CA-C-O	6.53	129.13	121.56
1	F	323	THR	O-C-N	6.53	128.88	122.09
1	N	102	ILE	N-CA-C	6.53	117.98	108.58
1	D	166	ASN	CB-CG-ND2	6.53	126.19	116.40
1	Q	17	GLU	CA-C-N	-6.53	112.20	120.56
1	Q	17	GLU	C-N-CA	-6.53	112.20	120.56
1	I	320	LYS	CD-CE-NZ	6.53	132.78	111.90
1	P	281	LEU	CA-C-O	6.53	128.23	120.92
1	J	160	SER	CB-CA-C	-6.52	99.96	110.79
1	R	6	ALA	O-C-N	6.52	130.71	122.23
1	N	110	GLN	O-C-N	6.52	130.30	122.21
1	A	87	ASP	OD1-CG-OD2	6.52	138.54	122.90
1	A	185	ILE	CA-C-O	-6.52	113.02	120.65
1	D	152	ARG	N-CA-CB	6.52	122.89	111.55
1	L	342	TYR	CA-C-N	-6.52	110.24	121.97
1	L	342	TYR	C-N-CA	-6.52	110.24	121.97
1	N	94	ARG	CA-CB-CG	6.52	127.14	114.10
1	A	222	TYR	CA-C-O	6.52	127.88	120.84
1	A	248	VAL	CA-CB-CG2	-6.52	99.32	110.40
1	B	12	LYS	CA-C-N	-6.52	111.97	120.44
1	B	12	LYS	C-N-CA	-6.52	111.97	120.44
1	D	232	MET	CA-C-N	-6.52	114.39	122.93
1	D	232	MET	C-N-CA	-6.52	114.39	122.93
1	D	330	ARG	NE-CZ-NH1	-6.52	114.98	121.50
1	M	257	HIS	ND1-CE1-NE2	6.52	114.92	108.40
1	G	144	PHE	CA-C-N	-6.52	116.35	121.82
1	G	144	PHE	C-N-CA	-6.52	116.35	121.82
1	M	237	HIS	CA-CB-CG	-6.52	107.28	113.80
1	A	90	GLY	CA-C-N	-6.51	113.73	122.72
1	A	90	GLY	C-N-CA	-6.51	113.73	122.72
1	D	196	HIS	O-C-N	6.51	130.22	122.79
1	Q	260	VAL	CA-C-O	6.51	123.95	119.20
1	R	231	ASN	CA-C-N	-6.51	109.95	121.29
1	R	231	ASN	C-N-CA	-6.51	109.95	121.29
1	O	40	GLY	CA-C-N	-6.51	111.04	120.29
1	O	40	GLY	C-N-CA	-6.51	111.04	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	207	LYS	CG-CD-CE	6.51	126.27	111.30
1	Q	38	THR	CA-CB-OG1	-6.51	99.84	109.60
1	A	160	SER	N-CA-CB	-6.51	100.53	110.16
1	R	14	GLU	CB-CG-CD	6.51	123.66	112.60
1	R	219	HIS	ND1-CE1-NE2	6.51	114.91	108.40
1	A	156	GLN	CA-CB-CG	-6.51	101.09	114.10
1	C	34	GLU	CA-C-O	6.51	128.45	121.16
1	I	87	ASP	OD1-CG-OD2	6.51	138.51	122.90
1	E	139	LYS	N-CA-CB	6.50	120.36	110.28
1	I	214	LYS	CA-C-O	6.50	127.46	120.24
1	K	83	LEU	O-C-N	6.50	131.15	122.43
1	Q	305	LEU	CA-C-O	6.50	126.57	119.15
1	E	4	PHE	N-CA-C	-6.50	95.57	108.71
1	J	179	GLN	CA-C-N	-6.50	112.33	122.67
1	J	179	GLN	C-N-CA	-6.50	112.33	122.67
1	L	258	ARG	CA-C-O	-6.50	111.74	119.35
1	N	191	ILE	CA-CB-CG1	-6.50	99.35	110.40
1	H	8	THR	N-CA-CB	-6.50	101.06	110.36
1	Q	325	GLU	CB-CG-CD	-6.50	101.55	112.60
1	B	304	ALA	CA-C-N	-6.50	112.46	122.60
1	B	304	ALA	C-N-CA	-6.50	112.46	122.60
1	H	87	ASP	CA-CB-CG	6.50	119.10	112.60
1	M	205	THR	N-CA-CB	6.50	119.67	110.12
1	N	297	LEU	N-CA-CB	6.50	120.72	110.84
1	Q	80	HIS	O-C-N	6.50	129.58	122.11
1	I	39	MET	CA-C-O	6.50	127.65	120.63
1	Q	277	GLU	CA-C-O	6.50	127.45	120.24
1	H	172	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	H	352	SER	CA-C-O	6.50	129.80	120.51
1	C	233	VAL	CA-C-N	6.49	132.75	122.36
1	C	233	VAL	C-N-CA	6.49	132.75	122.36
1	O	60	GLU	CA-C-N	-6.49	112.25	120.56
1	O	60	GLU	C-N-CA	-6.49	112.25	120.56
1	A	241	LYS	CA-CB-CG	-6.49	101.12	114.10
1	A	333	ALA	O-C-N	6.49	129.00	122.12
1	H	176	ILE	CB-CG1-CD1	6.49	127.43	113.80
1	O	344	HIS	CA-C-O	-6.49	109.77	120.80
1	K	327	PHE	CA-CB-CG	6.49	120.29	113.80
1	L	147	TRP	CA-C-N	-6.49	113.77	122.72
1	L	147	TRP	C-N-CA	-6.49	113.77	122.72
1	M	191	ILE	N-CA-CB	-6.49	102.13	111.21
1	P	195	ASP	CB-CG-OD2	6.49	133.32	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	ASN	O-C-N	6.49	136.66	121.74
1	G	172	ARG	N-CA-CB	6.49	119.47	110.07
1	H	89	GLN	N-CA-C	-6.49	96.99	110.80
1	J	346	GLY	N-CA-C	-6.49	97.81	113.18
1	N	46	ILE	O-C-N	6.49	130.68	122.57
1	P	140	ASP	CA-C-N	-6.49	111.61	122.25
1	P	140	ASP	C-N-CA	-6.49	111.61	122.25
1	I	54	ASN	O-C-N	-6.48	115.25	122.12
1	A	48	VAL	O-C-N	-6.48	116.26	123.26
1	D	149	ALA	O-C-N	6.48	130.35	123.03
1	E	52	GLU	N-CA-CB	6.48	119.60	109.94
1	H	50	ASN	CB-CG-ND2	6.48	126.12	116.40
1	K	60	GLU	CA-C-O	-6.48	113.68	120.55
1	N	205	THR	CA-C-N	-6.48	110.45	120.31
1	N	205	THR	C-N-CA	-6.48	110.45	120.31
1	K	275	SER	CA-C-N	-6.48	111.59	120.28
1	K	275	SER	C-N-CA	-6.48	111.59	120.28
1	L	262	ALA	CB-CA-C	6.48	122.85	109.95
1	Q	269	PHE	N-CA-C	6.48	119.16	110.35
1	F	216	LEU	CA-C-O	6.48	127.83	120.90
1	P	200	HIS	ND1-CG-CD2	-6.48	99.62	106.10
1	C	216	LEU	CA-C-O	6.48	127.42	120.10
1	G	56	ARG	N-CA-C	-6.48	104.07	112.23
1	G	117	GLY	CA-C-O	6.48	128.00	119.58
1	N	154	ALA	O-C-N	6.48	131.21	122.59
1	E	148	ARG	CA-C-O	6.48	127.49	120.43
1	N	113	ALA	CB-CA-C	6.48	118.07	109.65
1	E	264	VAL	N-CA-CB	-6.47	102.14	111.21
1	N	82	THR	CA-CB-CG2	6.47	121.51	110.50
1	D	335	CYS	CA-C-O	6.47	127.41	119.97
1	H	287	ASN	CA-CB-CG	-6.47	106.13	112.60
1	P	328	MET	CA-CB-CG	6.47	127.03	114.10
1	B	141	GLY	CA-C-O	6.46	127.61	119.72
1	B	203	TYR	N-CA-CB	-6.46	100.64	110.01
1	D	264	VAL	CA-C-N	6.46	127.92	119.84
1	D	264	VAL	C-N-CA	6.46	127.92	119.84
1	G	66	ASP	N-CA-C	-6.46	97.03	110.80
1	Q	171	ALA	CA-C-N	-6.46	112.04	120.44
1	Q	171	ALA	C-N-CA	-6.46	112.04	120.44
1	Q	180	ASN	CA-CB-CG	-6.46	106.14	112.60
1	B	70	ASN	OD1-CG-ND2	6.46	129.06	122.60
1	E	313	TRP	CA-C-O	6.46	127.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	98	LYS	CB-CA-C	-6.46	100.06	110.79
1	E	166	ASN	N-CA-CB	6.46	120.29	110.28
1	G	156	GLN	CB-CG-CD	-6.46	101.62	112.60
1	A	133	ARG	N-CA-C	6.46	118.32	111.28
1	B	86	LYS	CA-C-O	6.46	129.30	121.68
1	B	198	LEU	CA-C-N	-6.46	110.49	120.31
1	B	198	LEU	C-N-CA	-6.46	110.49	120.31
1	E	175	SER	O-C-N	6.46	128.81	122.09
1	O	258	ARG	NH1-CZ-NH2	6.46	127.69	119.30
1	P	94	ARG	CD-NE-CZ	6.46	133.44	124.40
1	B	218	ASP	N-CA-CB	-6.46	100.28	110.22
1	F	120	LYS	N-CA-C	6.46	120.74	112.86
1	G	316	LYS	CD-CE-NZ	6.46	132.56	111.90
1	C	27	LYS	N-CA-CB	-6.46	101.21	110.44
1	B	174	ALA	N-CA-CB	6.45	119.43	110.07
1	E	221	VAL	CA-C-O	-6.45	114.33	121.23
1	L	258	ARG	CG-CD-NE	-6.45	97.80	112.00
1	J	267	ILE	CA-C-N	6.45	132.27	123.11
1	J	267	ILE	C-N-CA	6.45	132.27	123.11
1	K	199	GLU	CB-CG-CD	6.45	123.57	112.60
1	K	319	ASN	CA-CB-CG	-6.45	106.15	112.60
1	L	343	VAL	CA-C-O	-6.45	112.72	120.78
1	M	10	GLU	CA-CB-CG	6.45	127.00	114.10
1	O	4	PHE	CA-C-N	6.45	126.41	119.76
1	O	4	PHE	C-N-CA	6.45	126.41	119.76
1	J	36	VAL	O-C-N	6.45	128.12	121.87
1	M	286	ILE	CA-C-O	-6.45	114.24	120.95
1	P	1	ALA	CA-C-O	6.45	131.76	120.80
1	B	225	GLY	O-C-N	6.45	131.08	122.70
1	H	125	GLN	O-C-N	6.45	130.31	123.03
1	K	348	SER	N-CA-C	6.45	124.53	110.80
1	A	170	LEU	CA-C-N	6.44	129.40	120.63
1	A	170	LEU	C-N-CA	6.44	129.40	120.63
1	P	319	ASN	CA-C-N	6.44	129.75	120.79
1	P	319	ASN	C-N-CA	6.44	129.75	120.79
1	A	129	GLY	CA-C-O	6.44	126.17	119.02
1	I	10	GLU	CB-CG-CD	-6.44	101.65	112.60
1	L	69	ILE	N-CA-C	-6.44	102.61	111.89
1	N	241	LYS	CG-CD-CE	6.44	126.11	111.30
1	N	247	GLN	CA-C-O	6.44	127.33	120.70
1	E	258	ARG	CB-CG-CD	6.44	126.11	111.30
1	I	122	THR	OG1-CB-CG2	-6.44	96.42	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	220	HIS	CA-CB-CG	-6.44	107.36	113.80
1	F	148	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	J	42	ARG	CD-NE-CZ	6.43	133.41	124.40
1	N	38	THR	CA-CB-CG2	-6.43	99.56	110.50
1	Q	93	PHE	CA-C-O	6.43	127.78	120.90
1	R	27	LYS	N-CA-CB	-6.43	101.16	110.36
1	R	61	ILE	O-C-N	6.43	130.33	121.84
1	L	163	ILE	CA-C-O	6.43	128.19	121.05
1	E	334	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	A	203	TYR	CA-C-N	-6.43	111.47	120.53
1	A	203	TYR	C-N-CA	-6.43	111.47	120.53
1	P	295	TRP	CA-C-O	-6.43	113.55	121.78
1	R	159	SER	CA-C-N	-6.43	110.31	120.60
1	R	159	SER	C-N-CA	-6.43	110.31	120.60
1	B	218	ASP	CA-C-O	6.43	127.36	120.10
1	D	150	VAL	N-CA-CB	-6.43	102.48	111.99
1	L	163	ILE	O-C-N	-6.43	115.22	121.90
1	C	63	PHE	CA-CB-CG	6.42	120.22	113.80
1	E	187	GLU	O-C-N	-6.42	114.02	120.83
1	Q	263	ALA	O-C-N	6.42	131.04	122.43
1	G	166	ASN	CB-CG-ND2	6.42	126.03	116.40
1	G	245	PRO	O-C-N	6.42	129.94	122.23
1	M	223	LEU	N-CA-C	6.42	119.10	111.33
1	O	218	ASP	CA-C-N	-6.42	111.52	122.56
1	O	218	ASP	C-N-CA	-6.42	111.52	122.56
1	R	194	GLY	CA-C-N	6.42	132.38	121.14
1	R	194	GLY	C-N-CA	6.42	132.38	121.14
1	G	8	THR	O-C-N	6.42	130.17	122.85
1	J	163	ILE	N-CA-C	6.42	116.56	110.53
1	D	303	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	E	109	ASP	CA-C-N	-6.42	112.33	122.79
1	E	109	ASP	C-N-CA	-6.42	112.33	122.79
1	J	152	ARG	CA-CB-CG	6.42	126.94	114.10
1	E	293	LYS	CA-C-O	-6.42	112.81	121.02
1	K	108	LEU	CA-C-O	6.42	125.83	118.97
1	N	75	GLY	CA-C-N	-6.42	113.45	122.75
1	N	75	GLY	C-N-CA	-6.42	113.45	122.75
1	O	120	LYS	N-CA-C	6.42	120.40	111.74
1	O	230	PRO	CB-CA-C	-6.42	100.97	111.56
1	A	72	SER	CA-C-N	-6.42	114.53	122.93
1	A	72	SER	C-N-CA	-6.42	114.53	122.93
1	N	148	ARG	CA-C-O	-6.42	113.26	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	THR	N-CA-CB	-6.41	99.39	111.00
1	C	319	ASN	CA-CB-CG	-6.41	106.19	112.60
1	D	307	ALA	CA-C-O	6.41	127.51	120.90
1	E	123	THR	N-CA-C	-6.41	97.14	110.80
1	H	2	HIS	CA-C-O	-6.41	111.34	120.51
1	J	239	CYS	O-C-N	6.41	130.71	122.89
1	K	75	GLY	O-C-N	-6.41	116.65	123.45
1	P	238	ALA	CA-C-N	-6.41	111.61	120.71
1	P	238	ALA	C-N-CA	-6.41	111.61	120.71
1	B	60	GLU	O-C-N	6.41	128.67	122.07
1	N	291	LEU	O-C-N	6.41	126.77	121.32
1	R	317	ALA	CA-C-O	6.41	127.55	120.63
1	C	288	LEU	O-C-N	-6.41	113.53	122.37
1	F	313	TRP	CA-C-O	6.41	127.73	121.00
1	K	150	VAL	O-C-N	-6.41	115.60	123.10
1	N	61	ILE	CA-C-O	-6.41	114.06	120.85
1	D	162	ALA	CA-C-O	-6.41	114.10	120.70
1	R	136	GLN	OE1-CD-NE2	6.41	129.01	122.60
1	K	45	ARG	NE-CZ-NH2	-6.41	113.43	119.20
1	L	191	ILE	N-CA-CB	-6.41	102.24	111.21
1	N	324	GLN	CA-C-O	6.40	127.34	120.55
1	C	66	ASP	O-C-N	-6.40	115.16	122.97
1	J	303	ARG	CD-NE-CZ	-6.40	115.44	124.40
1	B	114	PRO	CB-CA-C	-6.40	102.70	111.21
1	B	153	ILE	CA-C-O	-6.40	113.72	120.57
1	D	221	VAL	CA-CB-CG2	-6.40	99.52	110.40
1	H	330	ARG	CA-C-N	-6.40	111.20	120.29
1	H	330	ARG	C-N-CA	-6.40	111.20	120.29
1	L	115	LEU	CA-C-O	6.40	127.58	120.92
1	Q	235	ALA	O-C-N	6.40	130.41	122.86
1	F	24	ALA	N-CA-C	6.40	119.07	111.71
1	G	118	THR	CA-CB-OG1	-6.40	100.00	109.60
1	H	179	GLN	O-C-N	-6.40	114.01	122.33
1	O	277	GLU	CA-C-N	-6.40	112.12	120.44
1	O	277	GLU	C-N-CA	-6.40	112.12	120.44
1	P	261	PRO	CA-C-N	6.40	129.49	120.28
1	P	261	PRO	C-N-CA	6.40	129.49	120.28
1	B	278	ASP	CA-C-O	-6.40	114.11	120.70
1	D	319	ASN	CA-CB-CG	-6.40	106.20	112.60
1	A	159	SER	CA-C-O	6.39	129.28	121.99
1	E	273	GLY	CA-C-O	6.39	126.12	119.02
1	O	251	ALA	CA-C-O	6.39	127.33	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	217	ASN	CA-C-O	-6.39	114.11	120.82
1	D	280	THR	O-C-N	-6.39	115.48	122.07
1	J	340	GLY	CA-C-N	6.39	132.21	122.37
1	J	340	GLY	C-N-CA	6.39	132.21	122.37
1	R	336	GLN	O-C-N	6.39	128.65	122.07
1	E	224	GLU	CA-C-O	-6.39	111.37	120.51
1	A	245	PRO	O-C-N	6.39	129.59	122.24
1	F	132	GLU	CA-C-N	6.39	129.17	120.54
1	F	132	GLU	C-N-CA	6.39	129.17	120.54
1	L	26	GLY	CA-C-N	-6.39	107.78	121.45
1	L	26	GLY	C-N-CA	-6.39	107.78	121.45
1	M	212	VAL	N-CA-CB	-6.39	101.00	110.58
1	Q	178	GLN	O-C-N	-6.39	115.35	122.12
1	E	232	MET	CA-C-O	-6.39	114.71	121.99
1	B	16	SER	CA-C-O	6.39	127.32	120.55
1	C	184	PRO	CA-C-N	-6.39	114.38	122.43
1	C	184	PRO	C-N-CA	-6.39	114.38	122.43
1	I	89	GLN	CB-CG-CD	-6.39	101.74	112.60
1	J	53	GLU	N-CA-C	6.39	118.24	111.28
1	R	119	ASN	CA-C-O	6.39	129.72	122.37
1	R	226	THR	N-CA-CB	-6.39	100.99	111.66
1	A	167	ALA	CA-C-O	6.38	127.19	120.42
1	M	160	SER	O-C-N	6.38	130.12	122.27
1	M	182	LEU	O-C-N	-6.38	115.72	123.19
1	O	104	VAL	CB-CA-C	-6.38	101.98	110.98
1	G	137	TYR	N-CA-C	-6.38	104.42	111.82
1	E	258	ARG	CA-C-O	-6.38	112.26	119.79
1	I	14	GLU	O-C-N	6.38	128.64	122.07
1	J	299	PHE	CA-C-O	6.38	128.58	121.11
1	N	191	ILE	O-C-N	-6.38	113.83	121.10
1	O	133	ARG	CA-C-N	-6.38	111.23	120.29
1	O	133	ARG	C-N-CA	-6.38	111.23	120.29
1	R	109	ASP	O-C-N	6.38	130.50	122.65
1	F	29	ILE	CA-C-O	6.38	128.13	120.67
1	K	19	ALA	CA-C-N	-6.38	111.09	120.28
1	K	19	ALA	C-N-CA	-6.38	111.09	120.28
1	O	181	GLY	N-CA-C	6.38	124.11	114.61
1	F	70	ASN	CB-CG-ND2	6.38	125.97	116.40
1	K	330	ARG	CA-C-O	-6.38	111.54	119.38
1	O	131	SER	N-CA-CB	6.38	119.26	110.01
1	A	300	SER	N-CA-C	-6.38	96.80	107.32
1	M	230	PRO	CB-CA-C	-6.38	100.89	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	295	TRP	N-CA-CB	-6.38	101.20	110.70
1	R	290	PRO	N-CA-CB	-6.38	97.50	102.28
1	G	190	VAL	CA-C-N	6.37	132.53	119.72
1	G	190	VAL	C-N-CA	6.37	132.53	119.72
1	B	187	GLU	CB-CA-C	-6.37	104.02	110.65
1	F	10	GLU	CB-CG-CD	-6.37	101.77	112.60
1	N	178	GLN	N-CA-CB	6.37	119.62	110.06
1	Q	165	GLU	CG-CD-OE2	-6.37	103.75	118.40
1	K	80	HIS	CB-CA-C	-6.37	100.17	110.74
1	L	262	ALA	CA-C-O	6.37	127.26	119.11
1	G	271	SER	N-CA-C	-6.37	105.82	113.97
1	H	2	HIS	O-C-N	-6.37	114.12	122.59
1	F	284	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	L	160	SER	CA-C-N	-6.37	111.94	120.54
1	L	160	SER	C-N-CA	-6.37	111.94	120.54
1	F	326	ALA	N-CA-CB	-6.37	100.78	110.01
1	L	9	GLN	OE1-CD-NE2	6.37	128.97	122.60
1	A	342	TYR	CA-C-O	6.36	127.79	120.60
1	B	22	ILE	CA-C-O	-6.36	111.46	119.48
1	B	119	ASN	OD1-CG-ND2	6.36	128.96	122.60
1	F	56	ARG	N-CA-C	-6.36	103.86	111.69
1	L	115	LEU	N-CA-CB	-6.36	100.87	110.35
1	E	148	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	L	25	ASN	CA-C-N	-6.36	111.34	122.09
1	L	25	ASN	C-N-CA	-6.36	111.34	122.09
1	N	343	VAL	CA-C-O	-6.36	113.83	120.64
1	B	91	LYS	CA-CB-CG	-6.36	101.38	114.10
1	O	40	GLY	O-C-N	6.36	128.34	122.17
1	D	63	PHE	CA-CB-CG	6.36	120.16	113.80
1	D	136	GLN	OE1-CD-NE2	6.36	128.96	122.60
1	N	186	VAL	CA-CB-CG1	6.36	121.21	110.40
1	N	150	VAL	O-C-N	-6.36	116.39	123.26
1	N	231	ASN	CA-C-O	-6.36	114.31	121.81
1	Q	95	ASN	OD1-CG-ND2	6.36	128.96	122.60
1	D	209	LEU	CA-C-N	-6.35	111.27	120.29
1	D	209	LEU	C-N-CA	-6.35	111.27	120.29
1	K	187	GLU	CB-CG-CD	6.35	123.40	112.60
1	F	168	ASN	CA-CB-CG	-6.35	106.25	112.60
1	G	166	ASN	O-C-N	6.35	130.65	122.39
1	L	344	HIS	CA-C-O	-6.35	110.00	120.80
1	H	282	ASN	CA-CB-CG	-6.35	106.25	112.60
1	Q	214	LYS	O-C-N	6.35	129.39	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	THR	O-C-N	6.35	128.61	122.07
1	A	358	THR	CA-C-N	6.35	133.67	121.54
1	A	358	THR	C-N-CA	6.35	133.67	121.54
1	Q	231	ASN	O-C-N	6.35	130.17	123.06
1	B	279	ALA	N-CA-CB	6.35	120.17	110.14
1	B	342	TYR	N-CA-CB	6.35	121.22	110.49
1	E	114	PRO	CA-C-O	-6.35	114.44	121.23
1	E	135	ALA	CA-C-O	6.35	129.59	120.51
1	H	154	ALA	CA-C-N	-6.35	111.87	120.82
1	H	154	ALA	C-N-CA	-6.35	111.87	120.82
1	R	323	THR	CA-C-O	6.35	127.49	120.82
1	N	65	VAL	O-C-N	-6.35	114.64	122.57
1	B	78	LEU	O-C-N	6.34	131.44	123.19
1	D	63	PHE	O-C-N	-6.34	113.71	122.46
1	E	292	PRO	O-C-N	6.34	130.31	123.01
1	G	205	THR	O-C-N	6.34	128.84	122.12
1	K	29	ILE	CA-C-N	-6.34	113.74	122.30
1	K	29	ILE	C-N-CA	-6.34	113.74	122.30
1	N	178	GLN	O-C-N	6.34	128.85	122.12
1	G	224	GLU	CB-CG-CD	6.34	123.38	112.60
1	H	152	ARG	CD-NE-CZ	-6.34	115.52	124.40
1	O	105	GLY	CA-C-O	6.34	128.29	121.76
1	B	257	HIS	CA-CB-CG	6.34	120.14	113.80
1	I	266	GLY	N-CA-C	-6.34	101.10	110.87
1	G	295	TRP	O-C-N	-6.34	115.48	122.84
1	H	201	CYS	N-CA-C	-6.34	104.47	111.82
1	L	11	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	L	169	ALA	CA-C-N	6.34	129.10	120.54
1	L	169	ALA	C-N-CA	6.34	129.10	120.54
1	A	45	ARG	CG-CD-NE	-6.34	98.06	112.00
1	D	124	ILE	N-CA-CB	-6.34	101.05	111.44
1	H	340	GLY	CA-C-O	6.34	125.80	118.96
1	I	284	ASN	CA-C-N	-6.34	111.79	120.28
1	I	284	ASN	C-N-CA	-6.34	111.79	120.28
1	M	180	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	P	328	MET	O-C-N	6.34	128.84	122.12
1	M	70	ASN	CB-CG-ND2	-6.33	106.90	116.40
1	R	182	LEU	CA-C-O	-6.33	114.00	120.71
1	C	300	SER	CA-C-O	-6.33	111.82	122.20
1	F	194	GLY	CA-C-O	-6.33	115.99	122.26
1	J	116	ALA	O-C-N	6.33	130.12	122.96
1	F	266	GLY	O-C-N	6.33	130.93	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	168	ASN	N-CA-CB	6.33	119.53	110.16
1	N	90	GLY	O-C-N	6.33	130.77	122.35
1	P	27	LYS	CA-CB-CG	-6.33	101.44	114.10
1	P	72	SER	CB-CA-C	-6.33	98.78	109.03
1	Q	88	SER	CA-C-N	6.33	133.63	121.54
1	Q	88	SER	C-N-CA	6.33	133.63	121.54
1	D	148	ARG	NH1-CZ-NH2	6.33	127.52	119.30
1	F	299	PHE	CA-C-O	6.33	128.84	121.44
1	J	224	GLU	CA-CB-CG	6.33	126.75	114.10
1	A	1	ALA	CA-C-N	6.32	133.61	121.54
1	A	1	ALA	C-N-CA	6.32	133.61	121.54
1	B	18	ILE	CA-C-N	-6.32	112.22	120.44
1	B	18	ILE	C-N-CA	-6.32	112.22	120.44
1	D	158	PRO	N-CA-CB	-6.32	95.65	102.60
1	F	213	TYR	O-C-N	-6.32	115.42	122.12
1	M	90	GLY	CA-C-N	-6.32	112.73	122.09
1	M	90	GLY	C-N-CA	-6.32	112.73	122.09
1	O	94	ARG	CA-C-N	-6.32	110.16	120.71
1	O	94	ARG	C-N-CA	-6.32	110.16	120.71
1	R	50	ASN	N-CA-CB	6.32	119.43	110.46
1	A	306	GLN	CA-C-N	6.32	129.57	120.79
1	A	306	GLN	C-N-CA	6.32	129.57	120.79
1	C	42	ARG	N-CA-CB	6.32	119.41	110.12
1	E	292	PRO	CB-CA-C	-6.32	103.68	111.64
1	G	183	VAL	N-CA-CB	-6.32	103.19	111.21
1	Q	94	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	D	260	VAL	O-C-N	-6.32	117.07	121.55
1	G	3	ARG	NE-CZ-NH1	-6.32	115.19	121.50
1	J	45	ARG	NE-CZ-NH2	-6.32	113.52	119.20
1	J	232	MET	N-CA-C	-6.32	102.19	110.53
1	K	9	GLN	O-C-N	6.32	128.81	122.12
1	N	17	GLU	CA-C-N	-6.32	111.81	120.46
1	N	17	GLU	C-N-CA	-6.32	111.81	120.46
1	Q	93	PHE	O-C-N	-6.32	115.52	122.09
1	A	337	ALA	N-CA-C	-6.31	104.28	112.23
1	F	23	VAL	CG1-CB-CG2	-6.31	96.91	110.80
1	J	113	ALA	N-CA-C	-6.31	98.15	108.82
1	Q	234	THR	O-C-N	6.31	130.92	122.96
1	L	125	GLN	CG-CD-OE1	6.31	133.42	120.80
1	L	152	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	Q	225	GLY	O-C-N	6.31	130.91	122.70
1	F	4	PHE	CA-C-N	6.31	126.68	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	4	PHE	C-N-CA	6.31	126.68	119.93
1	F	151	LEU	CD1-CG-CD2	-6.31	96.92	110.80
1	J	263	ALA	CA-C-N	-6.31	112.52	121.23
1	J	263	ALA	C-N-CA	-6.31	112.52	121.23
1	K	237	HIS	CA-CB-CG	-6.31	107.49	113.80
1	P	105	GLY	O-C-N	-6.31	114.50	122.70
1	E	179	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	E	223	LEU	O-C-N	6.31	128.65	122.09
1	P	99	GLU	CA-C-O	-6.31	113.86	120.55
1	M	259	THR	CA-C-N	-6.31	115.66	122.85
1	M	259	THR	C-N-CA	-6.31	115.66	122.85
1	N	59	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	D	85	GLN	N-CA-CB	6.30	119.08	110.38
1	I	258	ARG	CG-CD-NE	-6.30	98.13	112.00
1	G	128	ASP	O-C-N	6.30	130.68	122.93
1	O	207	LYS	CB-CA-C	6.30	121.57	110.85
1	C	108	LEU	O-C-N	-6.30	114.86	122.48
1	D	181	GLY	CA-C-O	-6.30	111.81	119.06
1	E	132	GLU	N-CA-CB	6.30	119.49	110.16
1	H	93	PHE	CA-C-O	6.30	127.44	120.63
1	O	53	GLU	CA-C-O	-6.30	113.74	120.42
1	P	123	THR	OG1-CB-CG2	6.30	121.90	109.30
1	A	321	GLU	CA-C-O	-6.30	114.14	121.07
1	F	31	ALA	CA-C-O	-6.30	114.33	121.39
1	M	14	GLU	CB-CG-CD	6.30	123.31	112.60
1	A	94	ARG	CA-CB-CG	-6.30	101.50	114.10
1	B	118	THR	CA-CB-CG2	6.30	121.20	110.50
1	D	52	GLU	N-CA-C	-6.30	103.34	111.02
1	D	176	ILE	N-CA-C	6.30	116.47	110.42
1	J	16	SER	CA-CB-OG	6.30	123.69	111.10
1	R	119	ASN	O-C-N	-6.30	114.97	122.46
1	F	138	LYS	CA-CB-CG	6.29	126.69	114.10
1	C	179	GLN	CB-CG-CD	6.29	123.30	112.60
1	C	194	GLY	N-CA-C	6.29	119.94	112.33
1	D	160	SER	CA-C-O	-6.29	113.88	120.55
1	G	219	HIS	CA-CB-CG	-6.29	107.51	113.80
1	J	125	GLN	CG-CD-OE1	-6.29	108.21	120.80
1	L	99	GLU	CA-C-O	-6.29	111.64	119.38
1	D	247	GLN	N-CA-C	-6.29	103.95	111.69
1	J	164	GLN	CB-CG-CD	6.29	123.30	112.60
1	J	70	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	O	305	LEU	CA-C-N	-6.29	110.58	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	305	LEU	C-N-CA	-6.29	110.58	121.52
1	D	285	ALA	CB-CA-C	-6.29	100.35	110.79
1	O	55	ARG	CD-NE-CZ	-6.29	115.60	124.40
1	P	203	TYR	CB-CG-CD2	6.29	130.23	120.80
1	A	9	GLN	CA-C-N	-6.29	110.75	120.31
1	A	9	GLN	C-N-CA	-6.29	110.75	120.31
1	G	2	HIS	N-CA-CB	6.29	121.11	110.49
1	C	150	VAL	CA-C-N	6.29	132.99	122.87
1	C	150	VAL	C-N-CA	6.29	132.99	122.87
1	L	6	ALA	CB-CA-C	-6.29	100.36	110.79
1	N	293	LYS	CA-C-O	-6.29	113.90	121.00
1	P	93	PHE	CA-C-N	-6.29	111.86	120.28
1	P	93	PHE	C-N-CA	-6.29	111.86	120.28
1	Q	229	LYS	CA-C-N	6.29	127.70	119.84
1	Q	229	LYS	C-N-CA	6.29	127.70	119.84
1	D	89	GLN	CA-C-O	-6.28	111.53	120.51
1	G	101	GLY	CA-C-N	-6.28	115.01	122.93
1	G	101	GLY	C-N-CA	-6.28	115.01	122.93
1	K	195	ASP	CB-CA-C	-6.28	97.04	109.67
1	L	292	PRO	CB-CA-C	-6.28	103.58	111.56
1	M	118	THR	CA-CB-CG2	6.28	121.18	110.50
1	O	178	GLN	CA-CB-CG	-6.28	101.53	114.10
1	I	334	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	M	60	GLU	O-C-N	6.28	129.31	122.15
1	O	182	LEU	O-C-N	-6.28	115.91	122.94
1	D	341	GLN	CG-CD-NE2	-6.28	106.98	116.40
1	E	19	ALA	CB-CA-C	-6.28	100.77	110.81
1	M	242	LYS	CA-C-O	-6.28	114.02	121.11
1	O	156	GLN	CA-C-O	-6.28	113.04	120.57
1	E	201	CYS	N-CA-C	-6.28	104.44	111.28
1	E	333	ALA	CA-C-O	-6.28	114.23	120.82
1	I	91	LYS	CA-C-N	-6.28	112.53	121.50
1	I	91	LYS	C-N-CA	-6.28	112.53	121.50
1	L	226	THR	CA-C-O	-6.28	114.44	121.40
1	H	345	THR	CB-CA-C	6.27	122.91	110.42
1	D	70	ASN	N-CA-CB	-6.27	99.89	110.49
1	G	231	ASN	CB-CG-ND2	6.27	125.81	116.40
1	H	33	ASP	CA-CB-CG	-6.27	106.33	112.60
1	I	164	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	P	142	VAL	CA-CB-CG1	6.27	121.06	110.40
1	A	119	ASN	CA-CB-CG	-6.27	106.33	112.60
1	N	132	GLU	OE1-CD-OE2	-6.27	107.86	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	166	ASN	CB-CG-ND2	-6.27	107.00	116.40
1	C	119	ASN	CA-C-O	-6.27	114.33	121.66
1	C	165	GLU	CB-CA-C	6.27	120.80	110.90
1	L	218	ASP	CA-C-N	-6.27	111.78	122.56
1	L	218	ASP	C-N-CA	-6.27	111.78	122.56
1	A	73	ILE	N-CA-C	6.26	116.84	107.51
1	D	249	ALA	CA-C-N	6.26	128.96	120.44
1	D	249	ALA	C-N-CA	6.26	128.96	120.44
1	K	348	SER	CA-C-N	-6.26	109.13	121.41
1	K	348	SER	C-N-CA	-6.26	109.13	121.41
1	P	80	HIS	ND1-CE1-NE2	-6.26	102.14	108.40
1	E	65	VAL	CA-C-O	6.26	128.61	120.78
1	O	152	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	B	53	GLU	CB-CG-CD	6.26	123.25	112.60
1	E	165	GLU	CG-CD-OE2	-6.26	104.00	118.40
1	G	136	GLN	CB-CG-CD	-6.26	101.95	112.60
1	B	232	MET	CG-SD-CE	-6.26	87.13	100.90
1	I	21	SER	CA-CB-OG	-6.26	98.58	111.10
1	J	141	GLY	O-C-N	-6.26	114.22	122.42
1	J	51	THR	CA-CB-CG2	6.26	121.14	110.50
1	K	87	ASP	OD1-CG-OD2	-6.26	107.88	122.90
1	J	352	SER	N-CA-CB	6.26	121.06	110.49
1	K	9	GLN	CB-CA-C	-6.26	100.41	110.79
1	M	324	GLN	CA-C-N	6.26	128.66	120.28
1	M	324	GLN	C-N-CA	6.26	128.66	120.28
1	Q	100	LYS	CB-CA-C	-6.26	99.65	110.72
1	D	303	ARG	N-CA-CB	6.25	119.14	110.07
1	K	188	PRO	CA-C-N	-6.25	112.56	121.50
1	K	188	PRO	C-N-CA	-6.25	112.56	121.50
1	H	70	ASN	N-CA-C	6.25	120.47	112.34
1	I	22	ILE	CA-CB-CG2	6.25	121.13	110.50
1	J	219	HIS	O-C-N	-6.25	114.66	122.35
1	O	186	VAL	O-C-N	-6.25	115.86	122.68
1	B	269	PHE	CA-CB-CG	-6.25	107.55	113.80
1	K	235	ALA	O-C-N	6.25	129.91	122.79
1	D	151	LEU	O-C-N	-6.25	115.07	123.19
1	D	164	GLN	CG-CD-NE2	6.25	125.77	116.40
1	B	136	GLN	CB-CA-C	6.24	121.16	110.86
1	F	240	THR	CA-C-O	-6.24	111.97	119.27
1	I	164	GLN	CA-CB-CG	6.24	126.59	114.10
1	J	190	VAL	CA-C-N	6.24	133.68	122.13
1	J	190	VAL	C-N-CA	6.24	133.68	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	79	PHE	CA-CB-CG	6.24	120.04	113.80
1	R	91	LYS	O-C-N	6.24	130.40	123.16
1	G	215	ALA	CA-C-O	-6.24	114.27	120.82
1	J	74	GLY	O-C-N	-6.24	114.59	122.70
1	L	180	ASN	CB-CG-ND2	6.24	125.76	116.40
1	R	216	LEU	CA-C-N	-6.24	112.33	120.44
1	R	216	LEU	C-N-CA	-6.24	112.33	120.44
1	A	15	LEU	CA-C-O	6.24	127.15	119.79
1	D	33	ASP	CA-CB-CG	-6.24	106.36	112.60
1	K	164	GLN	CA-CB-CG	6.24	126.58	114.10
1	L	148	ARG	N-CA-C	6.24	119.41	109.24
1	Q	177	CYS	O-C-N	-6.24	115.51	122.12
1	C	3	ARG	N-CA-C	-6.24	97.52	110.80
1	A	119	ASN	OD1-CG-ND2	6.24	128.84	122.60
1	D	168	ASN	N-CA-CB	6.24	119.95	110.28
1	H	109	ASP	O-C-N	6.24	129.90	122.79
1	Q	181	GLY	CA-C-O	-6.24	111.33	119.44
1	R	165	GLU	N-CA-CB	-6.24	100.95	110.12
1	Q	117	GLY	CA-C-N	-6.23	112.80	122.59
1	Q	117	GLY	C-N-CA	-6.23	112.80	122.59
1	B	94	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	C	13	LYS	CA-C-N	-6.23	111.44	120.29
1	C	13	LYS	C-N-CA	-6.23	111.44	120.29
1	L	20	GLN	CA-C-O	6.23	127.04	119.31
1	Q	187	GLU	O-C-N	6.23	127.15	121.04
1	E	247	GLN	CB-CG-CD	-6.23	102.01	112.60
1	H	329	LYS	CB-CG-CD	6.23	125.63	111.30
1	Q	296	LYS	CB-CA-C	-6.23	99.38	109.72
1	N	110	GLN	CA-CB-CG	-6.23	101.64	114.10
1	B	148	ARG	CB-CA-C	-6.23	99.48	109.75
1	A	220	HIS	CA-C-O	-6.22	113.87	121.28
1	B	106	ILE	CA-C-N	-6.22	112.28	121.24
1	B	106	ILE	C-N-CA	-6.22	112.28	121.24
1	D	87	ASP	CA-C-O	-6.22	111.61	120.51
1	R	265	PRO	CA-C-N	-6.22	109.21	121.41
1	R	265	PRO	C-N-CA	-6.22	109.21	121.41
1	C	5	PRO	CA-C-O	-6.22	114.33	121.36
1	H	98	LYS	CA-C-O	6.22	127.13	120.10
1	J	92	LEU	CA-C-O	6.22	128.03	121.19
1	N	4	PHE	CA-C-N	6.22	126.25	119.90
1	N	4	PHE	C-N-CA	6.22	126.25	119.90
1	B	278	ASP	CA-CB-CG	-6.22	106.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	172	ARG	NE-CZ-NH2	6.22	124.80	119.20
1	N	180	ASN	N-CA-CB	-6.22	100.94	111.20
1	N	287	ASN	OD1-CG-ND2	6.22	128.82	122.60
1	D	165	GLU	CA-C-O	-6.22	113.83	120.42
1	G	296	LYS	CA-C-N	6.22	132.34	123.14
1	G	296	LYS	C-N-CA	6.22	132.34	123.14
1	J	230	PRO	CB-CA-C	-6.22	101.12	110.20
1	M	230	PRO	CA-C-N	-6.22	111.17	120.94
1	M	230	PRO	C-N-CA	-6.22	111.17	120.94
1	O	174	ALA	N-CA-C	-6.22	104.42	111.07
1	Q	211	ALA	CA-C-O	6.22	127.14	120.24
1	D	123	THR	N-CA-CB	6.22	121.00	110.49
1	E	103	VAL	CA-C-O	-6.22	113.71	121.11
1	M	209	LEU	CA-C-N	-6.22	111.46	120.29
1	M	209	LEU	C-N-CA	-6.22	111.46	120.29
1	N	235	ALA	O-C-N	6.22	130.03	122.75
1	K	98	LYS	CB-CG-CD	-6.22	97.00	111.30
1	L	124	ILE	N-CA-CB	-6.22	100.43	111.93
1	O	296	LYS	CD-CE-NZ	6.22	131.79	111.90
1	A	24	ALA	N-CA-C	6.21	117.72	111.07
1	A	172	ARG	NE-CZ-NH1	-6.21	115.28	121.50
1	I	194	GLY	CA-C-N	6.21	129.76	120.31
1	I	194	GLY	C-N-CA	6.21	129.76	120.31
1	E	195	ASP	CA-CB-CG	-6.21	106.39	112.60
1	N	37	GLY	CA-C-O	6.21	126.74	120.09
1	O	82	THR	CA-C-O	6.21	127.12	120.10
1	R	156	GLN	CA-C-O	-6.21	112.99	120.32
1	B	220	HIS	CE1-NE2-CD2	6.21	115.21	109.00
1	E	334	ASN	CA-CB-CG	-6.21	106.39	112.60
1	J	307	ALA	CA-C-O	-6.21	114.30	120.82
1	O	258	ARG	CD-NE-CZ	6.21	133.10	124.40
1	O	81	GLU	CA-CB-CG	6.21	126.52	114.10
1	R	238	ALA	CA-C-N	-6.21	112.62	121.50
1	R	238	ALA	C-N-CA	-6.21	112.62	121.50
1	B	269	PHE	CA-C-O	-6.21	114.97	121.55
1	D	147	TRP	CA-C-N	-6.21	114.43	123.00
1	D	147	TRP	C-N-CA	-6.21	114.43	123.00
1	F	133	ARG	CD-NE-CZ	-6.21	115.71	124.40
1	N	3	ARG	N-CA-C	6.21	124.02	110.80
1	Q	243	TYR	CB-CG-CD1	6.21	130.11	120.80
1	A	338	ALA	O-C-N	6.21	131.02	122.46
1	I	137	TYR	O-C-N	6.21	129.22	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	H	238	ALA	CA-C-O	-6.21	111.92	119.43
1	Q	59	ARG	NE-CZ-NH2	6.21	124.78	119.20
1	A	254	THR	O-C-N	6.20	128.48	122.03
1	B	33	ASP	O-C-N	6.20	130.31	122.37
1	B	341	GLN	CB-CA-C	6.20	121.25	111.39
1	D	353	THR	CA-C-N	6.20	133.39	121.54
1	D	353	THR	C-N-CA	6.20	133.39	121.54
1	E	172	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	Q	87	ASP	CB-CA-C	-6.20	98.07	110.42
1	J	99	GLU	CA-C-O	-6.20	113.09	120.10
1	J	193	ASP	O-C-N	6.20	130.50	122.87
1	J	334	ASN	N-CA-C	-6.20	104.60	111.36
1	L	343	VAL	CB-CA-C	6.20	121.46	111.29
1	P	61	ILE	O-C-N	6.20	127.99	121.91
1	C	168	ASN	CA-C-O	-6.20	113.85	120.42
1	J	188	PRO	CA-C-N	-6.20	112.92	122.09
1	J	188	PRO	C-N-CA	-6.20	112.92	122.09
1	P	82	THR	O-C-N	-6.20	115.13	122.20
1	R	4	PHE	CB-CA-C	-6.20	97.96	110.17
1	K	135	ALA	CA-C-O	6.20	127.10	120.10
1	J	3	ARG	CB-CG-CD	6.20	125.55	111.30
1	J	178	GLN	CA-C-O	6.19	127.10	119.79
1	E	125	GLN	CA-C-O	-6.19	114.03	121.89
1	E	160	SER	N-CA-CB	-6.19	100.99	110.16
1	F	66	ASP	CA-CB-CG	6.19	118.79	112.60
1	K	107	LYS	CA-C-O	-6.19	113.31	120.49
1	L	291	LEU	CA-C-O	-6.19	115.57	121.08
1	M	88	SER	CA-C-N	-6.19	111.43	123.13
1	M	88	SER	C-N-CA	-6.19	111.43	123.13
1	M	10	GLU	CA-C-O	-6.19	114.32	120.82
1	O	82	THR	CA-CB-CG2	-6.19	99.97	110.50
1	N	163	ILE	CA-C-N	-6.19	112.39	120.44
1	N	163	ILE	C-N-CA	-6.19	112.39	120.44
1	L	283	LEU	CA-C-O	6.19	127.09	120.10
1	N	130	LEU	O-C-N	-6.19	115.56	122.12
1	O	177	CYS	O-C-N	-6.19	115.66	122.09
1	D	149	ALA	N-CA-C	-6.18	100.83	110.42
1	I	4	PHE	CA-C-N	6.18	126.51	119.83
1	I	4	PHE	C-N-CA	6.18	126.51	119.83
1	O	70	ASN	N-CA-CB	6.18	119.54	110.57
1	O	76	VAL	CA-C-O	-6.18	113.96	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	THR	N-CA-C	6.18	122.29	114.31
1	L	9	GLN	CA-CB-CG	-6.18	101.74	114.10
1	L	229	LYS	CB-CA-C	-6.18	100.95	111.15
1	L	244	THR	N-CA-CB	-6.18	98.48	110.10
1	D	108	LEU	CA-C-O	6.18	125.58	118.97
1	E	303	ARG	CG-CD-NE	6.18	125.60	112.00
1	J	4	PHE	N-CA-CB	-6.18	99.37	110.37
1	A	140	ASP	CB-CG-OD1	-6.18	104.19	118.40
1	C	161	LEU	O-C-N	-6.18	115.66	122.09
1	L	177	CYS	O-C-N	-6.18	114.72	122.20
1	H	39	MET	CA-C-O	6.18	127.10	120.55
1	B	23	VAL	N-CA-C	-6.18	96.49	109.34
1	B	77	ILE	CB-CA-C	-6.18	103.25	110.91
1	L	152	ARG	CD-NE-CZ	-6.18	115.75	124.40
1	R	306	GLN	O-C-N	-6.18	114.75	122.35
1	D	35	SER	N-CA-CB	-6.17	101.85	110.25
1	I	88	SER	N-CA-CB	6.17	121.29	110.42
1	J	126	GLY	CA-C-N	-6.17	110.19	120.68
1	J	126	GLY	C-N-CA	-6.17	110.19	120.68
1	F	348	SER	N-CA-C	6.17	123.94	110.80
1	H	116	ALA	CA-C-O	-6.17	111.69	120.51
1	L	327	PHE	O-C-N	-6.17	115.67	122.09
1	N	171	ALA	N-CA-CB	6.17	119.19	110.12
1	K	188	PRO	CB-CA-C	-6.17	101.38	111.56
1	Q	258	ARG	CA-CB-CG	6.17	126.44	114.10
1	R	300	SER	N-CA-C	-6.17	98.31	108.49
1	A	149	ALA	CB-CA-C	-6.17	99.08	109.50
1	D	308	SER	CB-CA-C	6.17	122.04	110.63
1	E	308	SER	CB-CA-C	6.17	122.04	110.63
1	O	198	LEU	N-CA-CB	-6.17	101.07	110.01
1	Q	55	ARG	CD-NE-CZ	-6.17	115.77	124.40
1	A	106	ILE	O-C-N	-6.17	116.21	123.05
1	R	306	GLN	N-CA-CB	-6.17	101.59	110.65
1	D	111	GLY	N-CA-C	6.16	123.67	112.58
1	F	342	TYR	CA-C-O	6.16	127.64	120.80
1	K	171	ALA	CA-C-N	6.16	128.54	120.28
1	K	171	ALA	C-N-CA	6.16	128.54	120.28
1	L	267	ILE	CB-CA-C	6.16	118.74	110.42
1	M	123	THR	N-CA-C	-6.16	100.43	109.18
1	P	35	SER	N-CA-C	-6.16	100.17	109.79
1	A	257	HIS	CA-CB-CG	6.16	119.96	113.80
1	B	10	GLU	N-CA-C	6.16	118.79	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ASN	CA-CB-CG	-6.16	106.44	112.60
1	C	267	ILE	N-CA-C	-6.16	99.25	108.12
1	F	303	ARG	N-CA-C	6.16	117.99	111.28
1	G	237	HIS	CB-CA-C	-6.16	100.95	110.81
1	N	216	LEU	CA-CB-CG	6.16	137.85	116.30
1	O	214	LYS	CG-CD-CE	-6.16	97.14	111.30
1	R	3	ARG	O-C-N	6.16	130.78	122.59
1	R	50	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	A	11	GLN	CB-CG-CD	-6.16	102.14	112.60
1	B	172	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	O	280	THR	CA-C-N	-6.16	112.07	120.44
1	O	280	THR	C-N-CA	-6.16	112.07	120.44
1	D	193	ASP	CB-CA-C	-6.15	99.79	109.70
1	F	147	TRP	CA-C-O	-6.15	112.71	120.28
1	M	253	VAL	CA-C-O	6.15	126.90	120.25
1	B	226	THR	CA-CB-CG2	6.15	120.96	110.50
1	D	308	SER	CA-C-O	-6.15	113.15	120.10
1	E	195	ASP	CB-CA-C	-6.15	98.86	110.67
1	I	123	THR	CA-C-N	-6.15	115.08	123.14
1	I	123	THR	C-N-CA	-6.15	115.08	123.14
1	N	226	THR	N-CA-CB	-6.15	101.84	111.56
1	R	97	LEU	CA-C-O	6.15	127.03	120.70
1	A	106	ILE	CA-C-N	6.15	130.09	121.24
1	A	106	ILE	C-N-CA	6.15	130.09	121.24
1	F	164	GLN	CA-C-O	6.15	127.07	120.55
1	H	16	SER	O-C-N	6.15	128.40	122.07
1	I	323	THR	O-C-N	-6.15	115.50	122.08
1	P	109	ASP	CA-C-O	-6.15	114.74	121.87
1	C	123	THR	CA-C-N	-6.15	115.09	123.14
1	C	123	THR	C-N-CA	-6.15	115.09	123.14
1	F	191	ILE	N-CA-CB	-6.15	102.60	111.21
1	I	336	GLN	CG-CD-OE1	6.15	133.09	120.80
1	K	4	PHE	N-CA-CB	-6.15	100.05	110.50
1	O	76	VAL	O-C-N	6.15	129.87	123.05
1	L	204	VAL	CA-CB-CG2	-6.15	99.95	110.40
1	M	177	CYS	CA-CB-SG	6.15	128.54	114.40
1	E	343	VAL	CA-C-N	-6.14	109.80	121.54
1	E	343	VAL	C-N-CA	-6.14	109.80	121.54
1	N	221	VAL	CA-CB-CG1	-6.14	99.95	110.40
1	H	3	ARG	CB-CG-CD	6.14	125.43	111.30
1	N	336	GLN	N-CA-C	-6.14	104.21	111.03
1	P	358	THR	CA-CB-CG2	6.14	120.94	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	GLN	OE1-CD-NE2	6.14	128.74	122.60
1	D	281	LEU	O-C-N	6.14	128.63	122.12
1	I	194	GLY	CA-C-O	6.14	126.85	122.37
1	J	182	LEU	CA-C-O	6.14	127.62	120.80
1	O	184	PRO	CB-CA-C	-6.14	105.81	111.40
1	O	270	LEU	N-CA-CB	6.14	119.75	110.42
1	P	189	GLU	OE1-CD-OE2	-6.14	108.17	122.90
1	P	221	VAL	CA-CB-CG2	-6.14	99.96	110.40
1	P	9	GLN	CB-CG-CD	-6.14	102.17	112.60
1	Q	10	GLU	CA-C-N	-6.14	112.06	120.28
1	Q	10	GLU	C-N-CA	-6.14	112.06	120.28
1	A	228	LEU	O-C-N	6.14	130.85	123.36
1	B	344	HIS	CA-C-N	6.14	133.26	121.54
1	B	344	HIS	C-N-CA	6.14	133.26	121.54
1	J	154	ALA	CB-CA-C	-6.14	99.63	111.78
1	K	48	VAL	O-C-N	-6.14	116.88	123.14
1	M	292	PRO	CA-C-N	-6.14	116.88	122.28
1	M	292	PRO	C-N-CA	-6.14	116.88	122.28
1	H	306	GLN	CB-CG-CD	-6.13	102.17	112.60
1	Q	4	PHE	CA-C-N	6.13	126.16	119.90
1	Q	4	PHE	C-N-CA	6.13	126.16	119.90
1	R	29	ILE	O-C-N	-6.13	116.58	123.20
1	D	215	ALA	CA-C-N	-6.13	111.45	120.28
1	D	215	ALA	C-N-CA	-6.13	111.45	120.28
1	D	221	VAL	CA-C-O	-6.13	113.81	121.11
1	G	316	LYS	CG-CD-CE	6.13	125.40	111.30
1	J	226	THR	CA-C-O	-6.13	114.71	121.33
1	D	28	GLY	O-C-N	-6.13	114.73	122.70
1	D	240	THR	CA-C-O	-6.13	112.10	119.27
1	N	167	ALA	O-C-N	6.13	129.14	122.15
1	O	30	LEU	N-CA-C	-6.13	99.25	109.24
1	O	315	GLY	CA-C-O	-6.13	112.22	119.02
1	C	123	THR	CB-CA-C	-6.13	98.84	111.22
1	H	238	ALA	N-CA-C	-6.13	105.67	113.02
1	M	24	ALA	N-CA-CB	6.13	118.90	110.01
1	Q	175	SER	O-C-N	-6.13	115.76	122.07
1	E	293	LYS	CB-CG-CD	-6.13	97.21	111.30
1	I	157	CYS	CA-C-O	-6.13	113.12	120.41
1	R	3	ARG	N-CA-CB	6.13	120.84	110.49
1	H	195	ASP	CB-CA-C	-6.12	98.91	110.67
1	N	163	ILE	O-C-N	6.12	127.91	121.91
1	B	57	GLN	O-C-N	6.12	129.13	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	96	ILE	CB-CG1-CD1	6.12	126.66	113.80
1	Q	319	ASN	CA-CB-CG	-6.12	106.48	112.60
1	D	3	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	L	330	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	Q	85	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	B	262	ALA	O-C-N	-6.12	115.06	122.22
1	D	319	ASN	N-CA-CB	-6.12	101.60	110.47
1	M	69	ILE	CG1-CB-CG2	-6.12	92.34	110.70
1	I	190	VAL	O-C-N	-6.12	115.57	122.36
1	G	151	LEU	O-C-N	-6.12	115.28	123.23
1	B	179	GLN	CA-C-O	-6.12	112.09	119.49
1	C	36	VAL	CB-CA-C	-6.12	104.03	112.04
1	N	46	ILE	CA-C-O	-6.12	113.14	120.78
1	R	27	LYS	O-C-N	-6.11	115.82	122.79
1	B	226	THR	CA-C-O	-6.11	111.77	120.51
1	C	195	ASP	N-CA-C	6.11	120.34	113.01
1	F	160	SER	CA-C-O	-6.11	114.07	120.55
1	I	197	ASP	CA-C-O	-6.11	113.94	121.88
1	Q	4	PHE	N-CA-C	6.11	123.31	109.81
1	B	115	LEU	N-CA-CB	-6.11	100.29	110.37
1	D	325	GLU	CA-C-N	6.11	128.75	120.44
1	D	325	GLU	C-N-CA	6.11	128.75	120.44
1	H	333	ALA	CA-C-O	-6.11	114.41	120.70
1	I	118	THR	O-C-N	-6.11	115.47	123.16
1	I	339	LYS	CA-C-O	6.11	126.59	119.32
1	L	143	ASP	OD1-CG-OD2	6.11	137.56	122.90
1	N	72	SER	CA-CB-OG	-6.11	98.88	111.10
1	C	87	ASP	CA-C-O	-6.11	111.78	120.51
1	M	53	GLU	N-CA-C	6.11	117.94	111.28
1	M	205	THR	CA-C-O	-6.11	114.08	120.55
1	N	165	GLU	CA-C-O	-6.11	114.41	120.82
1	K	127	LEU	CA-C-N	-6.10	112.21	120.82
1	K	127	LEU	C-N-CA	-6.10	112.21	120.82
1	E	330	ARG	N-CA-C	-6.10	104.74	111.82
1	I	10	GLU	CB-CA-C	-6.10	99.34	110.63
1	K	121	GLU	N-CA-C	6.10	119.51	110.48
1	Q	133	ARG	CA-C-N	6.10	128.74	120.44
1	Q	133	ARG	C-N-CA	6.10	128.74	120.44
1	I	180	ASN	N-CA-CB	-6.10	101.28	110.73
1	I	29	ILE	O-C-N	6.10	129.62	123.10
1	J	184	PRO	CA-C-N	6.10	131.40	123.11
1	J	184	PRO	C-N-CA	6.10	131.40	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	34	GLU	O-C-N	-6.09	115.31	122.81
1	A	69	ILE	CA-CB-CG1	-6.09	100.04	110.40
1	C	226	THR	CA-CB-CG2	6.09	120.86	110.50
1	G	4	PHE	CA-C-N	6.09	126.11	119.89
1	G	4	PHE	C-N-CA	6.09	126.11	119.89
1	I	102	ILE	N-CA-C	6.09	116.64	107.80
1	R	212	VAL	O-C-N	-6.09	115.96	121.87
1	B	71	GLN	N-CA-CB	6.09	119.29	110.88
1	I	131	SER	O-C-N	6.09	128.60	122.08
1	K	126	GLY	CA-C-N	-6.09	110.48	121.14
1	K	126	GLY	C-N-CA	-6.09	110.48	121.14
1	M	264	VAL	CA-C-O	-6.09	111.79	119.95
1	R	148	ARG	CA-C-N	6.09	132.49	122.07
1	R	148	ARG	C-N-CA	6.09	132.49	122.07
1	K	217	ASN	CB-CG-OD1	6.09	132.98	120.80
1	O	181	GLY	CA-C-O	-6.09	111.96	119.69
1	A	287	ASN	CB-CG-OD1	6.09	132.98	120.80
1	D	97	LEU	O-C-N	-6.09	115.52	122.09
1	A	182	LEU	CA-C-N	-6.09	118.21	122.59
1	A	182	LEU	C-N-CA	-6.09	118.21	122.59
1	G	196	HIS	CA-CB-CG	-6.09	107.71	113.80
1	M	161	LEU	N-CA-C	-6.09	104.73	111.36
1	F	14	GLU	CB-CG-CD	6.08	122.94	112.60
1	K	188	PRO	O-C-N	6.08	130.85	122.64
1	K	297	LEU	CA-C-O	6.08	126.97	120.46
1	O	214	LYS	CA-C-O	6.08	126.97	119.79
1	Q	210	ALA	CB-CA-C	-6.08	99.37	110.63
1	B	271	SER	N-CA-C	-6.08	106.83	114.56
1	C	243	TYR	CA-C-O	-6.08	114.53	121.40
1	J	270	LEU	CA-C-O	-6.08	114.63	121.81
1	K	41	ASN	CA-C-O	-6.08	114.10	120.55
1	B	180	ASN	N-CA-CB	-6.08	102.43	111.43
1	H	61	ILE	CA-C-N	-6.08	112.53	120.44
1	H	61	ILE	C-N-CA	-6.08	112.53	120.44
1	I	255	ALA	CA-C-N	-6.08	111.65	120.29
1	I	255	ALA	C-N-CA	-6.08	111.65	120.29
1	N	43	LEU	CA-C-O	6.08	126.96	119.97
1	N	154	ALA	CA-C-O	-6.08	111.81	120.51
1	L	31	ALA	O-C-N	6.08	130.05	122.63
1	F	353	THR	N-CA-CB	-6.08	100.22	110.49
1	J	161	LEU	CB-CA-C	-6.08	100.52	110.85
1	N	248	VAL	CA-C-N	-6.08	111.07	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	248	VAL	C-N-CA	-6.08	111.07	120.31
1	N	341	GLN	CA-CB-CG	-6.08	101.94	114.10
1	O	272	GLY	CA-C-N	-6.08	113.77	123.31
1	O	272	GLY	C-N-CA	-6.08	113.77	123.31
1	L	260	VAL	CB-CA-C	-6.08	103.79	110.78
1	B	3	ARG	N-CA-C	-6.08	97.86	110.80
1	K	220	HIS	N-CA-CB	-6.08	102.91	112.08
1	M	334	ASN	CA-CB-CG	-6.08	106.53	112.60
1	O	132	GLU	CB-CG-CD	6.08	122.93	112.60
1	P	330	ARG	CG-CD-NE	6.08	125.37	112.00
1	D	346	GLY	CA-C-O	6.07	131.14	120.57
1	H	69	ILE	CA-CB-CG1	-6.07	100.08	110.40
1	L	159	SER	O-C-N	-6.07	116.26	123.06
1	C	268	CYS	CA-C-N	6.07	129.38	120.82
1	C	268	CYS	C-N-CA	6.07	129.38	120.82
1	B	228	LEU	CA-C-O	-6.07	114.01	121.11
1	M	343	VAL	CA-C-N	6.07	133.14	121.54
1	M	343	VAL	C-N-CA	6.07	133.14	121.54
1	P	348	SER	CB-CA-C	6.07	122.12	109.68
1	G	151	LEU	CA-C-O	6.07	127.25	120.70
1	H	3	ARG	CB-CA-C	-6.07	98.34	110.42
1	N	340	GLY	O-C-N	6.07	129.74	122.34
1	B	117	GLY	CA-C-O	6.07	126.62	119.46
1	G	241	LYS	CA-C-O	-6.07	114.95	121.56
1	H	267	ILE	CB-CG1-CD1	-6.07	101.06	113.80
1	M	217	ASN	CA-C-O	6.07	127.04	120.55
1	P	303	ARG	O-C-N	6.07	129.06	122.15
1	R	202	GLN	O-C-N	-6.07	115.23	122.15
1	J	165	GLU	CA-C-O	-6.06	113.99	120.42
1	C	132	GLU	CG-CD-OE1	6.06	132.34	118.40
1	F	125	GLN	CG-CD-NE2	6.06	125.49	116.40
1	Q	290	PRO	CB-CA-C	-6.06	104.85	113.09
1	R	205	THR	N-CA-C	-6.06	104.23	111.69
1	B	197	ASP	CA-C-O	6.06	127.61	120.89
1	C	170	LEU	CA-C-N	-6.06	112.36	120.54
1	C	170	LEU	C-N-CA	-6.06	112.36	120.54
1	P	4	PHE	CA-CB-CG	-6.06	107.74	113.80
1	C	103	VAL	CB-CA-C	-6.06	102.05	111.26
1	C	109	ASP	CA-C-O	-6.06	115.08	121.99
1	N	204	VAL	O-C-N	-6.06	115.59	121.83
1	O	134	CYS	CA-C-O	6.06	126.84	120.42
1	P	89	GLN	CB-CA-C	-6.06	100.92	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	199	GLU	CB-CG-CD	6.06	122.90	112.60
1	F	325	GLU	CA-C-O	6.06	127.18	120.82
1	L	4	PHE	CA-C-N	6.06	125.82	119.76
1	L	4	PHE	C-N-CA	6.06	125.82	119.76
1	M	26	GLY	CA-C-N	-6.06	109.95	120.97
1	M	26	GLY	C-N-CA	-6.06	109.95	120.97
1	G	337	ALA	CA-C-O	-6.05	114.46	120.82
1	J	223	LEU	CA-C-O	-6.05	114.13	120.55
1	K	191	ILE	CB-CG1-CD1	-6.05	101.08	113.80
1	R	150	VAL	CA-C-O	-6.05	114.03	120.39
1	A	51	THR	N-CA-C	6.05	119.76	110.20
1	I	315	GLY	N-CA-C	-6.05	107.54	115.47
1	B	146	LYS	CA-C-O	-6.05	113.34	120.60
1	G	73	ILE	CA-C-O	6.05	127.00	120.53
1	J	152	ARG	NE-CZ-NH1	-6.05	115.45	121.50
1	C	2	HIS	N-CA-C	6.05	119.39	108.69
1	C	118	THR	OG1-CB-CG2	6.05	121.39	109.30
1	H	165	GLU	CA-C-N	6.05	128.99	120.28
1	H	165	GLU	C-N-CA	6.05	128.99	120.28
1	H	208	VAL	CB-CA-C	-6.05	104.14	111.88
1	C	195	ASP	CB-CA-C	-6.04	97.84	110.17
1	A	303	ARG	N-CA-C	6.04	117.54	111.07
1	E	324	GLN	CA-C-O	6.04	126.92	119.97
1	I	68	SER	N-CA-CB	-6.04	100.28	110.49
1	J	196	HIS	CA-CB-CG	6.04	119.84	113.80
1	L	333	ALA	CA-C-N	-6.04	111.58	120.28
1	L	333	ALA	C-N-CA	-6.04	111.58	120.28
1	I	113	ALA	O-C-N	6.04	128.28	121.94
1	E	258	ARG	CG-CD-NE	-6.04	98.71	112.00
1	N	241	LYS	CB-CG-CD	6.04	125.19	111.30
1	B	3	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	F	22	ILE	N-CA-C	-6.04	104.96	110.82
1	Q	159	SER	CA-C-O	-6.04	115.00	121.94
1	D	119	ASN	CB-CG-ND2	6.04	125.45	116.40
1	H	132	GLU	CG-CD-OE1	6.04	132.29	118.40
1	O	255	ALA	N-CA-CB	-6.04	100.94	109.94
1	A	283	LEU	CA-C-O	6.04	126.82	120.42
1	B	109	ASP	CA-CB-CG	6.04	118.64	112.60
1	D	15	LEU	CA-C-N	-6.04	110.42	120.68
1	D	15	LEU	C-N-CA	-6.04	110.42	120.68
1	H	125	GLN	OE1-CD-NE2	-6.04	116.56	122.60
1	J	163	ILE	CA-C-O	6.04	127.75	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	135	ALA	CA-C-O	6.04	127.36	120.90
1	A	228	LEU	N-CA-C	-6.03	98.01	108.69
1	D	187	GLU	CG-CD-OE1	-6.03	104.53	118.40
1	F	279	ALA	CA-C-N	6.03	128.36	120.28
1	F	279	ALA	C-N-CA	6.03	128.36	120.28
1	I	61	ILE	CB-CG1-CD1	6.03	126.47	113.80
1	M	65	VAL	O-C-N	-6.03	115.03	122.57
1	O	271	SER	O-C-N	6.03	129.06	121.64
1	O	321	GLU	CA-C-N	-6.03	112.40	120.79
1	O	321	GLU	C-N-CA	-6.03	112.40	120.79
1	Q	34	GLU	CB-CG-CD	6.03	122.86	112.60
1	A	24	ALA	N-CA-CB	6.03	118.76	110.01
1	F	152	ARG	NH1-CZ-NH2	6.03	127.14	119.30
1	N	295	TRP	CA-C-N	-6.03	111.64	120.75
1	N	295	TRP	C-N-CA	-6.03	111.64	120.75
1	B	202	GLN	CA-CB-CG	-6.03	102.04	114.10
1	D	187	GLU	CA-CB-CG	-6.03	102.04	114.10
1	K	152	ARG	O-C-N	6.03	130.99	123.15
1	I	77	ILE	N-CA-CB	6.03	117.87	111.00
1	P	323	THR	CA-C-O	6.03	127.33	121.00
1	I	30	LEU	CA-C-N	-6.03	114.47	122.85
1	I	30	LEU	C-N-CA	-6.03	114.47	122.85
1	Q	12	LYS	CB-CG-CD	-6.03	97.44	111.30
1	Q	42	ARG	NH1-CZ-NH2	-6.02	111.47	119.30
1	A	224	GLU	O-C-N	6.02	129.07	122.20
1	G	62	LEU	N-CA-C	-6.02	104.80	111.36
1	B	123	THR	CB-CA-C	-6.02	99.98	112.44
1	J	19	ALA	N-CA-C	-6.02	104.79	111.71
1	N	65	VAL	N-CA-CB	-6.02	101.30	111.23
1	N	299	PHE	O-C-N	-6.02	115.33	123.10
1	M	44	GLN	CA-C-O	6.02	127.13	120.63
1	M	341	GLN	O-C-N	-6.02	114.96	122.24
1	H	54	ASN	CA-CB-CG	-6.02	106.58	112.60
1	D	211	ALA	O-C-N	-6.01	115.83	122.09
1	E	190	VAL	CA-CB-CG2	6.01	120.62	110.40
1	J	218	ASP	N-CA-CB	-6.01	100.33	110.49
1	K	247	GLN	CA-C-N	6.01	128.70	120.46
1	K	247	GLN	C-N-CA	6.01	128.70	120.46
1	N	164	GLN	OE1-CD-NE2	-6.01	116.58	122.60
1	N	203	TYR	CA-C-O	6.01	126.80	120.42
1	K	354	GLN	O-C-N	-6.01	115.34	123.10
1	O	198	LEU	O-C-N	-6.01	115.88	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	305	LEU	N-CA-CB	6.01	119.69	110.61
1	R	52	GLU	N-CA-CB	6.01	118.90	109.94
1	B	172	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	F	128	ASP	OD1-CG-OD2	6.01	137.33	122.90
1	K	301	TYR	CA-C-O	6.01	128.57	121.36
1	O	16	SER	CA-CB-OG	6.01	123.12	111.10
1	O	119	ASN	OD1-CG-ND2	6.01	128.61	122.60
1	B	201	CYS	CA-C-O	6.01	126.88	119.97
1	D	108	LEU	O-C-N	-6.01	115.21	122.48
1	E	153	ILE	CA-CB-CG1	-6.01	100.18	110.40
1	L	339	LYS	N-CA-C	-6.01	105.13	112.88
1	N	324	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	F	149	ALA	O-C-N	-6.01	116.19	123.10
1	F	152	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	H	66	ASP	CA-CB-CG	6.01	118.61	112.60
1	O	310	LEU	CA-C-O	6.00	127.12	120.82
1	A	41	ASN	OD1-CG-ND2	6.00	128.60	122.60
1	D	126	GLY	CA-C-N	-6.00	110.63	121.14
1	D	126	GLY	C-N-CA	-6.00	110.63	121.14
1	H	51	THR	CA-CB-OG1	-6.00	100.59	109.60
1	N	166	ASN	CB-CG-ND2	6.00	125.41	116.40
1	P	200	HIS	CG-CD2-NE2	6.00	113.20	107.20
1	Q	240	THR	O-C-N	6.00	130.75	122.46
1	B	179	GLN	OE1-CD-NE2	6.00	128.60	122.60
1	M	69	ILE	N-CA-C	-6.00	96.86	109.34
1	Q	168	ASN	N-CA-C	6.00	117.62	111.14
1	I	66	ASP	N-CA-CB	6.00	120.63	110.49
1	B	150	VAL	CB-CA-C	-6.00	102.25	110.77
1	G	335	CYS	CA-C-O	6.00	126.87	119.97
1	D	320	LYS	O-C-N	-6.00	114.61	122.59
1	E	2	HIS	O-C-N	-6.00	114.61	122.59
1	H	229	LYS	O-C-N	6.00	126.77	121.37
1	P	169	ALA	O-C-N	6.00	129.65	122.27
1	D	159	SER	O-C-N	-6.00	115.74	122.75
1	O	276	GLU	N-CA-C	-6.00	104.75	111.28
1	A	80	HIS	N-CA-C	5.99	118.58	111.33
1	C	226	THR	O-C-N	-5.99	116.21	123.10
1	G	267	ILE	CA-CB-CG1	-5.99	100.21	110.40
1	O	93	PHE	CA-C-O	5.99	126.90	120.55
1	P	55	ARG	CA-C-N	5.99	128.31	120.28
1	P	55	ARG	C-N-CA	5.99	128.31	120.28
1	B	248	VAL	CA-C-N	-5.99	112.65	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	VAL	C-N-CA	-5.99	112.65	120.44
1	G	231	ASN	CA-C-O	-5.99	114.17	121.36
1	I	36	VAL	CA-CB-CG1	-5.99	100.22	110.40
1	L	83	LEU	CA-C-O	5.99	126.74	119.49
1	N	79	PHE	CA-C-N	5.99	132.98	121.54
1	N	79	PHE	C-N-CA	5.99	132.98	121.54
1	N	87	ASP	N-CA-CB	-5.99	100.37	110.49
1	R	65	VAL	CA-C-O	5.99	128.27	120.78
1	B	79	PHE	CA-CB-CG	-5.99	107.81	113.80
1	L	266	GLY	O-C-N	5.99	128.08	123.23
1	Q	198	LEU	CD1-CG-CD2	-5.99	97.63	110.80
1	B	325	GLU	CA-C-O	5.99	127.28	121.00
1	D	233	VAL	CA-C-O	-5.99	113.80	120.74
1	I	286	ILE	CA-C-N	-5.99	109.91	121.58
1	I	286	ILE	C-N-CA	-5.99	109.91	121.58
1	L	184	PRO	O-C-N	-5.99	117.12	122.93
1	M	9	GLN	CA-C-O	5.99	127.11	120.82
1	M	258	ARG	NE-CZ-NH1	5.99	127.49	121.50
1	C	6	ALA	O-C-N	5.98	128.97	122.15
1	I	109	ASP	O-C-N	5.98	130.38	122.36
1	F	221	VAL	O-C-N	-5.98	116.17	122.57
1	M	126	GLY	CA-C-N	-5.98	110.51	120.68
1	M	126	GLY	C-N-CA	-5.98	110.51	120.68
1	M	195	ASP	CB-CA-C	-5.98	99.18	110.67
1	Q	319	ASN	CB-CG-ND2	5.98	125.37	116.40
1	F	131	SER	CB-CA-C	-5.98	101.41	110.92
1	N	168	ASN	O-C-N	5.98	128.46	122.12
1	N	249	ALA	CA-C-N	-5.98	111.80	120.29
1	N	249	ALA	C-N-CA	-5.98	111.80	120.29
1	L	237	HIS	CB-CA-C	-5.98	100.86	110.79
1	Q	244	THR	CA-CB-OG1	-5.98	100.63	109.60
1	I	277	GLU	CA-C-N	-5.98	112.67	120.44
1	I	277	GLU	C-N-CA	-5.98	112.67	120.44
1	Q	120	LYS	N-CA-C	5.98	120.15	112.86
1	G	217	ASN	O-C-N	-5.98	115.91	122.07
1	L	293	LYS	N-CA-CB	-5.98	103.96	110.71
1	B	309	ALA	CA-C-O	5.97	126.88	120.55
1	C	89	GLN	O-C-N	5.97	130.44	122.26
1	C	336	GLN	OE1-CD-NE2	-5.97	116.62	122.60
1	K	152	ARG	CB-CA-C	-5.97	97.54	109.79
1	R	219	HIS	N-CA-CB	-5.97	102.32	110.56
1	K	357	PHE	CB-CA-C	-5.97	98.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	90	GLY	CA-C-O	-5.97	111.61	119.25
1	F	49	GLU	O-C-N	5.97	130.28	122.93
1	F	165	GLU	N-CA-CB	-5.97	101.30	110.20
1	P	355	SER	O-C-N	5.97	130.53	122.59
1	Q	29	ILE	O-C-N	-5.97	117.05	123.14
1	G	20	GLN	N-CA-CB	-5.97	101.03	110.22
1	H	166	ASN	CB-CG-OD1	5.97	132.74	120.80
1	I	180	ASN	CA-CB-CG	-5.97	106.63	112.60
1	J	352	SER	CA-C-N	5.97	130.93	121.44
1	J	352	SER	C-N-CA	5.97	130.93	121.44
1	M	122	THR	N-CA-C	5.97	117.28	108.86
1	N	99	GLU	CA-C-O	-5.97	113.36	120.10
1	Q	66	ASP	CA-CB-CG	5.97	118.57	112.60
1	C	214	LYS	O-C-N	-5.97	115.79	122.12
1	N	323	THR	O-C-N	-5.97	115.69	122.08
1	O	170	LEU	CA-C-N	-5.97	110.75	120.72
1	O	170	LEU	C-N-CA	-5.97	110.75	120.72
1	Q	277	GLU	O-C-N	-5.97	114.47	122.23
1	A	210	ALA	CA-C-O	-5.97	114.52	120.90
1	G	341	GLN	OE1-CD-NE2	5.97	128.57	122.60
1	J	167	ALA	N-CA-CB	-5.97	101.03	110.28
1	J	317	ALA	CA-C-N	5.97	128.55	120.38
1	J	317	ALA	C-N-CA	5.97	128.55	120.38
1	K	201	CYS	N-CA-C	-5.97	104.86	111.36
1	O	190	VAL	N-CA-CB	5.97	118.46	111.66
1	Q	54	ASN	CA-CB-CG	-5.97	106.63	112.60
1	Q	191	ILE	N-CA-CB	-5.97	102.86	111.21
1	B	44	GLN	OE1-CD-NE2	5.96	128.56	122.60
1	R	295	TRP	CA-C-O	-5.96	114.66	121.58
1	D	213	TYR	O-C-N	5.96	129.60	122.27
1	G	226	THR	CA-C-O	-5.96	114.83	121.51
1	Q	199	GLU	CA-CB-CG	5.96	126.03	114.10
1	C	308	SER	CA-C-O	-5.96	114.10	120.42
1	D	324	GLN	O-C-N	-5.96	115.80	122.12
1	E	287	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	J	223	LEU	N-CA-C	5.96	117.78	111.28
1	O	233	VAL	O-C-N	5.96	129.18	122.68
1	C	235	ALA	CA-C-N	-5.96	113.13	120.64
1	C	235	ALA	C-N-CA	-5.96	113.13	120.64
1	G	92	LEU	CA-C-O	-5.96	113.85	120.70
1	P	356	LEU	CA-C-O	-5.96	109.29	121.03
1	D	100	LYS	CA-C-N	5.96	130.57	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	LYS	C-N-CA	5.96	130.57	121.51
1	N	257	HIS	CA-CB-CG	5.96	119.76	113.80
1	G	96	ILE	N-CA-C	-5.96	104.70	110.42
1	N	199	GLU	CB-CG-CD	5.96	122.72	112.60
1	B	123	THR	N-CA-CB	5.96	120.66	110.65
1	G	86	LYS	N-CA-C	5.96	118.46	109.41
1	H	330	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	I	229	LYS	N-CA-CB	-5.96	101.71	110.88
1	M	199	GLU	CA-C-O	5.96	126.69	119.31
1	A	292	PRO	CA-C-N	5.95	129.40	122.85
1	A	292	PRO	C-N-CA	5.95	129.40	122.85
1	F	32	ALA	N-CA-CB	-5.95	101.50	110.91
1	I	154	ALA	CA-C-O	-5.95	112.00	120.51
1	N	330	ARG	CA-C-N	-5.95	111.26	120.31
1	N	330	ARG	C-N-CA	-5.95	111.26	120.31
1	O	25	ASN	CA-C-N	-5.95	112.03	122.09
1	O	25	ASN	C-N-CA	-5.95	112.03	122.09
1	Q	3	ARG	CB-CA-C	5.95	122.27	110.42
1	E	123	THR	CB-CA-C	-5.95	98.58	110.42
1	G	271	SER	CA-C-O	5.95	125.34	118.97
1	O	123	THR	N-CA-C	-5.95	100.36	109.65
1	C	36	VAL	CA-CB-CG1	-5.95	100.28	110.40
1	I	140	ASP	CA-C-N	-5.95	112.74	122.20
1	I	140	ASP	C-N-CA	-5.95	112.74	122.20
1	L	59	ARG	CA-CB-CG	-5.95	102.20	114.10
1	O	262	ALA	CB-CA-C	5.95	122.75	110.31
1	P	267	ILE	CB-CA-C	-5.95	102.39	110.42
1	A	270	LEU	CA-C-N	-5.95	111.97	122.26
1	A	270	LEU	C-N-CA	-5.95	111.97	122.26
1	B	281	LEU	O-C-N	5.95	128.20	122.07
1	F	335	CYS	O-C-N	-5.95	115.81	122.12
1	J	123	THR	N-CA-C	-5.95	98.13	110.80
1	M	300	SER	N-CA-C	-5.95	98.68	108.49
1	N	271	SER	N-CA-CB	-5.95	102.67	110.88
1	B	218	ASP	O-C-N	5.95	129.18	122.22
1	F	65	VAL	N-CA-CB	-5.94	97.51	111.30
1	A	357	PHE	CB-CG-CD1	-5.94	110.60	120.70
1	B	166	ASN	CA-C-N	-5.94	111.85	120.29
1	B	166	ASN	C-N-CA	-5.94	111.85	120.29
1	B	183	VAL	CA-CB-CG1	5.94	120.50	110.40
1	K	122	THR	N-CA-C	5.94	118.44	109.41
1	D	264	VAL	N-CA-C	-5.94	103.13	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	291	LEU	CA-CB-CG	5.94	137.09	116.30
1	Q	189	GLU	N-CA-C	5.94	119.20	109.76
1	M	125	GLN	CA-C-O	-5.94	114.16	121.88
1	B	269	PHE	CG-CD1-CE1	5.94	130.79	120.70
1	D	226	THR	CA-CB-OG1	-5.94	100.69	109.60
1	F	330	ARG	CB-CG-CD	5.94	124.96	111.30
1	M	204	VAL	N-CA-CB	-5.94	101.67	110.58
1	K	257	HIS	N-CA-CB	5.94	120.78	110.39
1	D	259	THR	CA-C-N	-5.93	118.56	122.60
1	D	259	THR	C-N-CA	-5.93	118.56	122.60
1	O	89	GLN	N-CA-C	-5.93	98.18	107.73
1	Q	118	THR	OG1-CB-CG2	5.93	121.17	109.30
1	R	286	ILE	O-C-N	-5.93	115.15	122.57
1	F	22	ILE	O-C-N	5.93	129.61	121.90
1	G	182	LEU	CA-C-O	-5.93	114.46	121.16
1	D	93	PHE	CA-C-O	5.93	127.03	120.63
1	I	310	LEU	CA-C-O	5.93	126.80	120.10
1	P	136	GLN	CA-CB-CG	-5.93	102.24	114.10
1	D	191	ILE	N-CA-CB	-5.93	102.91	111.21
1	E	336	GLN	O-C-N	5.93	128.91	122.15
1	E	249	ALA	CB-CA-C	5.93	120.93	110.85
1	L	110	GLN	CA-C-N	-5.93	113.46	122.06
1	L	110	GLN	C-N-CA	-5.93	113.46	122.06
1	D	347	SER	CA-CB-OG	5.93	122.95	111.10
1	H	147	TRP	CA-CB-CG	5.93	124.86	113.60
1	L	96	ILE	N-CA-CB	-5.93	103.93	110.51
1	D	61	ILE	CA-C-N	5.92	128.14	120.44
1	D	61	ILE	C-N-CA	5.92	128.14	120.44
1	F	291	LEU	O-C-N	-5.92	117.70	121.85
1	K	188	PRO	N-CA-CB	5.92	109.47	103.25
1	M	156	GLN	CA-CB-CG	-5.92	102.25	114.10
1	P	187	GLU	CB-CG-CD	5.92	122.67	112.60
1	G	72	SER	N-CA-CB	-5.92	100.44	110.51
1	B	20	GLN	CA-C-O	5.92	126.65	119.31
1	F	8	THR	CA-CB-CG2	-5.92	100.43	110.50
1	L	205	THR	CA-C-O	-5.92	113.41	120.10
1	O	1	ALA	CA-C-N	5.92	132.85	121.54
1	O	1	ALA	C-N-CA	5.92	132.85	121.54
1	Q	123	THR	N-CA-C	-5.92	100.77	109.18
1	R	270	LEU	CA-C-N	-5.92	112.40	122.11
1	R	270	LEU	C-N-CA	-5.92	112.40	122.11
1	G	110	GLN	CB-CG-CD	5.92	122.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	GLN	N-CA-C	5.92	117.73	111.28
1	J	278	ASP	CA-CB-CG	-5.92	106.68	112.60
1	K	163	ILE	CA-C-O	5.92	127.62	121.05
1	M	207	LYS	CA-C-N	5.92	128.13	120.56
1	M	207	LYS	C-N-CA	5.92	128.13	120.56
1	B	34	GLU	O-C-N	-5.92	115.25	122.82
1	D	186	VAL	CA-C-O	-5.92	114.14	120.59
1	O	116	ALA	CB-CA-C	-5.92	100.27	109.61
1	L	16	SER	CA-C-O	5.91	126.82	120.55
1	J	189	GLU	O-C-N	5.91	130.02	123.16
1	O	76	VAL	CA-C-N	-5.91	115.48	122.93
1	O	76	VAL	C-N-CA	-5.91	115.48	122.93
1	E	348	SER	CA-C-N	5.91	132.99	121.41
1	E	348	SER	C-N-CA	5.91	132.99	121.41
1	L	199	GLU	N-CA-CB	-5.91	101.19	110.06
1	A	344	HIS	N-CA-CB	-5.91	100.50	110.49
1	B	211	ALA	N-CA-C	5.91	117.52	111.14
1	H	232	MET	CA-C-O	-5.91	115.14	121.94
1	H	250	MET	N-CA-C	-5.91	104.78	112.23
1	F	139	LYS	CA-C-O	-5.91	113.43	120.10
1	D	80	HIS	ND1-CE1-NE2	5.90	114.30	108.40
1	I	291	LEU	CD1-CG-CD2	-5.90	97.81	110.80
1	J	327	PHE	N-CA-C	-5.90	104.84	111.28
1	B	216	LEU	N-CA-C	-5.90	104.85	111.28
1	E	1	ALA	O-C-N	-5.90	113.56	123.00
1	E	255	ALA	CA-C-O	-5.90	114.29	120.55
1	F	255	ALA	CA-C-O	5.90	126.68	120.42
1	P	169	ALA	N-CA-C	-5.90	104.97	111.82
1	A	4	PHE	N-CA-C	-5.90	100.35	109.79
1	H	343	VAL	N-CA-CB	5.90	119.84	111.82
1	J	157	CYS	O-C-N	-5.90	116.11	121.66
1	K	33	ASP	CB-CG-OD1	-5.90	104.83	118.40
1	L	102	ILE	CB-CG1-CD1	-5.90	101.41	113.80
1	O	240	THR	CA-C-O	-5.90	112.37	119.27
1	Q	300	SER	CA-C-N	-5.90	111.60	121.39
1	Q	300	SER	C-N-CA	-5.90	111.60	121.39
1	G	325	GLU	CA-C-N	5.90	128.11	120.44
1	G	325	GLU	C-N-CA	5.90	128.11	120.44
1	M	176	ILE	CB-CA-C	-5.90	104.42	111.97
1	R	86	LYS	CA-C-N	-5.90	110.87	122.02
1	R	86	LYS	C-N-CA	-5.90	110.87	122.02
1	F	224	GLU	CB-CG-CD	5.90	122.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	16	SER	CA-C-N	-5.90	112.42	120.44
1	I	16	SER	C-N-CA	-5.90	112.42	120.44
1	L	298	SER	N-CA-CB	-5.90	100.53	110.49
1	R	13	LYS	O-C-N	-5.90	115.87	122.12
1	B	141	GLY	CA-C-N	5.89	129.97	122.37
1	B	141	GLY	C-N-CA	5.89	129.97	122.37
1	F	118	THR	CA-C-N	-5.89	111.94	122.32
1	F	118	THR	C-N-CA	-5.89	111.94	122.32
1	F	250	MET	CG-SD-CE	-5.89	87.93	100.90
1	J	146	LYS	CB-CG-CD	-5.89	97.74	111.30
1	O	330	ARG	CA-C-O	5.89	126.80	120.55
1	R	19	ALA	O-C-N	5.89	128.14	122.07
1	B	200	HIS	CA-C-N	-5.89	111.35	120.31
1	B	200	HIS	C-N-CA	-5.89	111.35	120.31
1	C	154	ALA	CA-C-O	-5.89	114.81	120.94
1	D	323	THR	CA-CB-OG1	-5.89	100.76	109.60
1	K	213	TYR	N-CA-C	5.89	117.78	111.36
1	K	324	GLN	N-CA-C	5.89	118.49	111.71
1	M	114	PRO	CA-C-N	5.89	131.67	123.07
1	M	114	PRO	C-N-CA	5.89	131.67	123.07
1	P	98	LYS	CA-C-O	5.89	127.01	120.82
1	D	221	VAL	O-C-N	5.89	129.67	122.72
1	F	77	ILE	N-CA-CB	5.89	117.72	111.00
1	I	221	VAL	O-C-N	-5.89	116.19	122.61
1	J	65	VAL	CB-CA-C	-5.89	104.85	111.45
1	A	195	ASP	O-C-N	5.89	129.26	122.25
1	M	152	ARG	CA-CB-CG	5.89	125.88	114.10
1	Q	160	SER	CA-C-O	5.89	126.79	120.55
1	R	207	LYS	CA-CB-CG	5.89	125.88	114.10
1	J	219	HIS	CB-CG-CD2	5.89	138.85	131.20
1	A	13	LYS	CA-C-N	-5.89	111.36	120.31
1	A	13	LYS	C-N-CA	-5.89	111.36	120.31
1	A	192	PRO	CA-C-O	5.89	126.46	118.81
1	M	231	ASN	CA-CB-CG	5.89	118.49	112.60
1	O	213	TYR	CA-CB-CG	-5.89	103.30	113.90
1	A	29	ILE	CA-C-O	5.88	127.56	120.67
1	C	185	ILE	N-CA-CB	-5.88	104.07	111.31
1	K	169	ALA	N-CA-C	-5.88	104.95	111.36
1	E	67	SER	N-CA-C	-5.88	98.27	110.80
1	G	172	ARG	N-CA-C	-5.88	104.79	111.14
1	J	274	MET	O-C-N	-5.88	115.79	122.97
1	H	90	GLY	O-C-N	5.88	130.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	10	GLU	N-CA-CB	5.88	118.77	110.12
1	P	12	LYS	CA-C-O	5.88	126.73	119.97
1	B	2	HIS	O-C-N	-5.88	114.77	122.59
1	R	274	MET	CA-C-O	-5.88	114.71	121.47
1	A	256	LEU	CA-C-O	-5.88	114.19	120.42
1	B	155	ASP	CA-CB-CG	5.88	118.48	112.60
1	L	58	PHE	O-C-N	-5.88	115.74	122.09
1	M	244	THR	OG1-CB-CG2	-5.88	97.54	109.30
1	E	151	LEU	CA-C-O	-5.88	114.48	120.71
1	I	291	LEU	O-C-N	5.88	128.08	121.32
1	K	175	SER	CA-C-N	5.88	127.89	120.72
1	K	175	SER	C-N-CA	5.88	127.89	120.72
1	L	60	GLU	CA-C-O	-5.88	114.65	120.82
1	N	3	ARG	CG-CD-NE	5.88	124.93	112.00
1	Q	91	LYS	CA-CB-CG	-5.88	102.35	114.10
1	A	138	LYS	O-C-N	5.88	128.12	122.07
1	N	258	ARG	N-CA-CB	5.88	119.61	110.44
1	D	232	MET	CA-C-O	-5.87	115.29	121.99
1	I	214	LYS	N-CA-C	-5.87	104.47	111.69
1	N	148	ARG	NE-CZ-NH2	-5.87	113.91	119.20
1	C	70	ASN	CA-CB-CG	5.87	118.47	112.60
1	D	270	LEU	CB-CA-C	5.87	119.55	109.51
1	L	267	ILE	CA-C-O	-5.87	114.34	120.27
1	N	228	LEU	CA-C-N	-5.87	115.94	123.16
1	N	228	LEU	C-N-CA	-5.87	115.94	123.16
1	O	257	HIS	CA-C-N	-5.87	111.14	122.06
1	O	257	HIS	C-N-CA	-5.87	111.14	122.06
1	C	25	ASN	CA-C-O	-5.87	110.84	122.23
1	E	9	GLN	N-CA-C	-5.87	104.96	111.71
1	E	258	ARG	N-CA-CB	5.87	119.34	110.30
1	F	24	ALA	CA-C-O	-5.87	113.47	120.10
1	F	258	ARG	CA-CB-CG	5.87	125.84	114.10
1	I	32	ALA	N-CA-CB	-5.87	101.55	111.17
1	O	132	GLU	CG-CD-OE1	5.87	131.90	118.40
1	B	3	ARG	N-CA-CB	5.87	120.41	110.49
1	A	162	ALA	CA-C-N	-5.87	113.05	120.56
1	A	162	ALA	C-N-CA	-5.87	113.05	120.56
1	A	352	SER	CA-CB-OG	-5.87	99.37	111.10
1	B	322	ALA	CA-C-N	5.87	128.94	120.79
1	B	322	ALA	C-N-CA	5.87	128.94	120.79
1	C	9	GLN	CA-C-N	-5.87	112.42	120.28
1	C	9	GLN	C-N-CA	-5.87	112.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	319	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	K	38	THR	CA-C-N	-5.86	111.82	120.38
1	K	38	THR	C-N-CA	-5.86	111.82	120.38
1	O	178	GLN	CA-C-N	-5.86	111.40	120.31
1	O	178	GLN	C-N-CA	-5.86	111.40	120.31
1	M	353	THR	N-CA-C	-5.86	98.31	110.80
1	B	4	PHE	CA-C-N	5.86	125.80	119.76
1	B	4	PHE	C-N-CA	5.86	125.80	119.76
1	K	140	ASP	N-CA-C	-5.86	105.71	112.92
1	D	188	PRO	N-CA-C	-5.86	100.40	112.47
1	H	150	VAL	N-CA-CB	-5.86	104.52	111.90
1	O	101	GLY	CA-C-O	-5.86	111.96	119.58
1	J	259	THR	CA-C-N	-5.86	116.93	123.02
1	J	259	THR	C-N-CA	-5.86	116.93	123.02
1	L	265	PRO	CA-C-N	-5.86	114.23	121.38
1	L	265	PRO	C-N-CA	-5.86	114.23	121.38
1	E	20	GLN	CA-CB-CG	-5.86	102.39	114.10
1	H	95	ASN	OD1-CG-ND2	5.86	128.46	122.60
1	A	76	VAL	O-C-N	5.85	129.76	123.03
1	E	214	LYS	N-CA-C	-5.85	104.90	111.28
1	E	109	ASP	CA-C-O	-5.85	115.08	121.87
1	Q	256	LEU	N-CA-CB	5.85	119.23	110.22
1	H	20	GLN	CA-C-O	-5.85	113.24	119.97
1	M	220	HIS	N-CA-C	5.85	119.50	111.54
1	P	269	PHE	CA-C-O	-5.85	115.18	121.56
1	B	343	VAL	N-CA-CB	5.85	120.88	111.23
1	C	156	GLN	OE1-CD-NE2	5.85	128.45	122.60
1	D	9	GLN	N-CA-C	-5.85	104.98	111.36
1	E	147	TRP	O-C-N	5.85	130.96	123.24
1	Q	99	GLU	O-C-N	5.85	129.06	122.22
1	R	165	GLU	OE1-CD-OE2	5.85	136.94	122.90
1	A	125	GLN	CA-C-O	-5.85	114.82	121.72
1	B	18	ILE	CB-CG1-CD1	5.85	126.08	113.80
1	C	173	TYR	N-CA-CB	-5.85	101.53	110.01
1	K	184	PRO	O-C-N	5.85	128.60	122.93
1	P	201	CYS	O-C-N	5.85	128.82	122.15
1	R	105	GLY	CA-C-O	-5.85	115.05	121.77
1	G	258	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	I	37	GLY	CA-C-N	-5.85	112.84	120.44
1	I	37	GLY	C-N-CA	-5.85	112.84	120.44
1	C	303	ARG	CD-NE-CZ	5.84	132.58	124.40
1	D	69	ILE	O-C-N	5.84	127.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	295	TRP	O-C-N	-5.84	115.56	123.10
1	N	299	PHE	CA-CB-CG	-5.84	107.96	113.80
1	R	331	ALA	CA-C-O	-5.84	114.68	120.82
1	H	356	LEU	O-C-N	5.84	129.35	122.34
1	R	232	MET	O-C-N	-5.84	114.53	122.36
1	F	18	ILE	CA-C-O	-5.84	115.19	121.27
1	J	277	GLU	CA-C-N	-5.84	112.85	120.44
1	J	277	GLU	C-N-CA	-5.84	112.85	120.44
1	K	293	LYS	O-C-N	-5.84	116.14	121.34
1	L	305	LEU	N-CA-C	-5.84	105.47	113.30
1	M	14	GLU	N-CA-C	-5.84	104.83	111.14
1	D	88	SER	O-C-N	-5.84	115.51	122.63
1	G	31	ALA	CA-C-O	-5.84	114.85	120.92
1	I	137	TYR	N-CA-CB	-5.84	101.52	110.16
1	L	261	PRO	N-CA-CB	5.84	108.22	103.32
1	O	141	GLY	O-C-N	-5.84	115.62	122.45
1	A	156	GLN	CB-CG-CD	-5.84	102.68	112.60
1	A	219	HIS	O-C-N	-5.84	114.90	122.37
1	C	249	ALA	CA-C-O	5.84	126.68	119.97
1	J	92	LEU	N-CA-CB	-5.84	101.02	109.83
1	B	42	ARG	CA-C-O	-5.83	114.69	120.82
1	D	16	SER	CB-CA-C	5.83	122.28	110.38
1	M	134	CYS	CA-C-O	5.83	126.73	120.55
1	Q	186	VAL	CA-CB-CG2	-5.83	100.48	110.40
1	E	2	HIS	CA-C-N	5.83	132.68	121.54
1	E	2	HIS	C-N-CA	5.83	132.68	121.54
1	I	98	LYS	CD-CE-NZ	5.83	130.56	111.90
1	L	233	VAL	CA-C-O	-5.83	113.86	120.74
1	O	182	LEU	CA-C-N	-5.83	117.01	123.43
1	O	182	LEU	C-N-CA	-5.83	117.01	123.43
1	G	247	GLN	N-CA-C	-5.83	104.52	111.69
1	H	188	PRO	CA-C-N	-5.83	113.16	121.50
1	H	188	PRO	C-N-CA	-5.83	113.16	121.50
1	H	243	TYR	CA-C-O	-5.83	114.80	121.68
1	K	191	ILE	CA-C-N	5.83	126.34	120.04
1	K	191	ILE	C-N-CA	5.83	126.34	120.04
1	R	170	LEU	O-C-N	5.83	128.30	122.12
1	H	206	GLU	CA-C-O	-5.83	114.70	120.82
1	I	38	THR	CA-C-N	-5.83	112.39	120.38
1	I	38	THR	C-N-CA	-5.83	112.39	120.38
1	N	133	ARG	CA-C-O	5.83	126.94	120.82
1	R	177	CYS	CA-CB-SG	5.83	127.80	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	257	HIS	CA-CB-CG	5.83	119.63	113.80
1	N	260	VAL	CA-CB-CG1	-5.83	100.50	110.40
1	B	61	ILE	O-C-N	5.83	127.94	121.94
1	D	199	GLU	O-C-N	-5.83	115.10	122.27
1	J	211	ALA	CA-C-O	5.83	127.13	120.90
1	R	164	GLN	CB-CG-CD	5.83	122.50	112.60
1	B	280	THR	CA-CB-CG2	5.82	120.40	110.50
1	F	134	CYS	CA-C-O	-5.82	114.38	120.55
1	L	338	ALA	CA-C-O	-5.82	112.74	119.61
1	A	200	HIS	O-C-N	5.82	128.79	122.15
1	C	130	LEU	CA-C-O	5.82	126.68	120.10
1	D	163	ILE	CA-C-N	-5.82	112.02	120.29
1	D	163	ILE	C-N-CA	-5.82	112.02	120.29
1	M	165	GLU	CG-CD-OE1	5.82	131.79	118.40
1	C	164	GLN	CA-C-N	-5.82	112.53	120.44
1	C	164	GLN	C-N-CA	-5.82	112.53	120.44
1	I	190	VAL	N-CA-CB	-5.82	106.41	112.06
1	K	10	GLU	CA-C-N	-5.82	112.41	120.38
1	K	10	GLU	C-N-CA	-5.82	112.41	120.38
1	N	260	VAL	CB-CA-C	-5.82	104.20	110.95
1	F	231	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	G	250	MET	CB-CG-SD	5.82	130.16	112.70
1	H	216	LEU	CA-C-O	5.82	126.66	119.97
1	H	277	GLU	O-C-N	5.82	128.28	122.12
1	D	159	SER	N-CA-CB	5.81	118.57	110.26
1	Q	125	GLN	CA-CB-CG	5.81	125.73	114.10
1	D	3	ARG	N-CA-C	-5.81	98.42	110.80
1	E	277	GLU	N-CA-CB	5.81	118.76	110.16
1	E	352	SER	N-CA-CB	5.81	120.31	110.49
1	M	260	VAL	O-C-N	5.81	125.03	121.37
1	N	86	LYS	CA-C-O	5.81	128.32	121.58
1	P	324	GLN	CA-C-N	5.81	128.00	120.44
1	P	324	GLN	C-N-CA	5.81	128.00	120.44
1	N	93	PHE	O-C-N	-5.81	114.86	122.59
1	F	325	GLU	CB-CG-CD	-5.81	102.72	112.60
1	J	70	ASN	CB-CG-OD1	5.81	132.42	120.80
1	L	145	GLY	CA-C-N	-5.81	111.56	121.85
1	L	145	GLY	C-N-CA	-5.81	111.56	121.85
1	R	174	ALA	N-CA-C	-5.81	104.31	111.40
1	C	100	LYS	N-CA-CB	5.81	118.90	110.65
1	F	202	GLN	OE1-CD-NE2	-5.81	116.79	122.60
1	F	291	LEU	CA-C-O	5.81	125.83	119.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	211	ALA	CA-C-N	-5.81	113.11	120.60
1	I	211	ALA	C-N-CA	-5.81	113.11	120.60
1	N	42	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	R	103	VAL	O-C-N	5.81	129.57	122.72
1	R	123	THR	CB-CA-C	-5.81	98.86	110.42
1	R	248	VAL	CB-CA-C	-5.81	104.30	112.14
1	B	160	SER	N-CA-C	-5.81	105.03	111.36
1	B	14	GLU	CB-CG-CD	5.80	122.47	112.60
1	B	340	GLY	CA-C-N	-5.80	112.19	120.89
1	B	340	GLY	C-N-CA	-5.80	112.19	120.89
1	G	339	LYS	N-CA-C	-5.80	105.52	113.30
1	L	4	PHE	CA-CB-CG	-5.80	108.00	113.80
1	N	325	GLU	CB-CG-CD	-5.80	102.73	112.60
1	P	191	ILE	CA-C-N	5.80	126.31	120.04
1	P	191	ILE	C-N-CA	5.80	126.31	120.04
1	P	265	PRO	CA-C-N	-5.80	113.02	121.26
1	P	265	PRO	C-N-CA	-5.80	113.02	121.26
1	Q	212	VAL	N-CA-CB	-5.80	103.76	110.55
1	Q	279	ALA	CA-C-O	-5.80	114.40	120.55
1	H	24	ALA	N-CA-CB	5.80	119.16	110.22
1	H	334	ASN	OD1-CG-ND2	5.80	128.40	122.60
1	L	71	GLN	CA-C-N	5.80	131.26	122.56
1	L	71	GLN	C-N-CA	5.80	131.26	122.56
1	O	116	ALA	CA-C-O	-5.80	114.80	121.07
1	A	183	VAL	CA-CB-CG2	-5.80	100.54	110.40
1	B	203	TYR	CA-C-N	5.80	128.66	120.42
1	B	203	TYR	C-N-CA	5.80	128.66	120.42
1	E	40	GLY	N-CA-C	-5.80	105.77	112.73
1	E	184	PRO	O-C-N	5.80	130.47	122.64
1	F	5	PRO	CA-C-O	-5.80	115.00	121.32
1	N	272	GLY	CA-C-N	-5.80	110.04	121.41
1	N	272	GLY	C-N-CA	-5.80	110.04	121.41
1	O	248	VAL	CA-CB-CG2	-5.80	100.54	110.40
1	O	316	LYS	N-CA-C	5.80	118.69	109.24
1	R	27	LYS	CD-CE-NZ	5.80	130.47	111.90
1	O	148	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	B	40	GLY	CA-C-N	-5.80	112.51	120.28
1	B	40	GLY	C-N-CA	-5.80	112.51	120.28
1	E	156	GLN	O-C-N	-5.80	112.90	122.23
1	N	254	THR	O-C-N	5.80	128.35	122.09
1	G	45	ARG	CA-C-O	-5.80	114.70	120.90
1	R	241	LYS	CA-C-O	5.79	127.69	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	GLN	N-CA-CB	-5.79	101.37	110.06
1	D	249	ALA	CB-CA-C	5.79	120.05	110.90
1	K	187	GLU	CA-CB-CG	5.79	125.69	114.10
1	L	114	PRO	N-CD-CG	-5.79	94.51	103.20
1	F	336	GLN	CA-C-O	5.79	126.56	120.42
1	H	123	THR	CB-CA-C	-5.79	101.09	114.41
1	J	133	ARG	CA-CB-CG	-5.79	102.52	114.10
1	O	326	ALA	N-CA-CB	-5.79	101.02	109.82
1	D	320	LYS	CA-C-O	5.79	128.79	120.51
1	I	23	VAL	CA-C-O	5.79	125.24	119.97
1	M	60	GLU	N-CA-C	-5.79	105.05	111.36
1	Q	175	SER	CA-CB-OG	-5.79	99.52	111.10
1	A	280	THR	CA-CB-OG1	-5.79	100.92	109.60
1	I	115	LEU	N-CA-CB	-5.79	99.80	110.56
1	P	45	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	Q	173	TYR	CA-C-O	5.79	126.64	120.10
1	R	201	CYS	CA-C-O	5.79	126.62	119.79
1	H	267	ILE	N-CA-C	-5.78	99.31	107.75
1	H	299	PHE	O-C-N	-5.78	116.13	123.24
1	N	205	THR	N-CA-CB	5.78	118.72	110.16
1	O	201	CYS	CA-C-N	-5.78	112.46	120.38
1	O	201	CYS	C-N-CA	-5.78	112.46	120.38
1	P	357	PHE	O-C-N	-5.78	114.93	122.97
1	R	117	GLY	CA-C-N	-5.78	113.11	122.36
1	R	117	GLY	C-N-CA	-5.78	113.11	122.36
1	B	10	GLU	CB-CA-C	-5.78	99.93	110.63
1	D	148	ARG	CG-CD-NE	5.78	124.72	112.00
1	I	130	LEU	O-C-N	-5.78	116.11	122.07
1	P	278	ASP	CA-CB-CG	-5.78	106.82	112.60
1	D	304	ALA	O-C-N	-5.78	114.74	122.43
1	F	257	HIS	CA-CB-CG	5.78	119.58	113.80
1	G	341	GLN	CG-CD-NE2	-5.78	107.73	116.40
1	I	6	ALA	CA-C-O	-5.78	114.42	120.55
1	K	26	GLY	O-C-N	5.78	129.32	122.50
1	N	215	ALA	N-CA-C	-5.78	105.06	111.36
1	R	3	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	P	4	PHE	O-C-N	-5.78	114.67	121.32
1	D	14	GLU	O-C-N	5.78	128.33	122.09
1	H	329	LYS	CB-CA-C	5.78	120.67	110.85
1	K	329	LYS	CA-C-O	-5.78	114.42	120.55
1	N	304	ALA	O-C-N	5.78	130.11	122.43
1	Q	212	VAL	N-CA-C	5.78	115.97	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ASN	O-C-N	-5.78	114.15	121.95
1	D	17	GLU	N-CA-CB	5.78	118.61	110.12
1	E	94	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	H	6	ALA	O-C-N	5.78	128.02	122.07
1	J	295	TRP	N-CA-C	5.78	118.98	109.85
1	L	164	GLN	CA-C-O	-5.78	114.30	120.42
1	A	224	GLU	CA-CB-CG	-5.77	102.55	114.10
1	B	335	CYS	CA-C-N	5.77	127.95	120.44
1	B	335	CYS	C-N-CA	5.77	127.95	120.44
1	G	76	VAL	CA-C-N	-5.77	115.15	122.37
1	G	76	VAL	C-N-CA	-5.77	115.15	122.37
1	H	108	LEU	O-C-N	-5.77	115.25	122.35
1	D	232	MET	N-CA-C	-5.77	103.31	110.41
1	L	284	ASN	CA-CB-CG	-5.77	106.83	112.60
1	J	57	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	K	175	SER	O-C-N	-5.77	116.00	122.12
1	L	210	ALA	N-CA-CB	-5.77	101.34	110.28
1	O	8	THR	CA-C-N	-5.77	112.75	120.54
1	O	8	THR	C-N-CA	-5.77	112.75	120.54
1	R	59	ARG	NH1-CZ-NH2	5.77	126.80	119.30
1	B	282	ASN	CB-CG-OD1	-5.77	109.26	120.80
1	B	327	PHE	CA-C-O	5.77	126.61	119.97
1	D	89	GLN	CA-CB-CG	-5.77	102.56	114.10
1	H	89	GLN	O-C-N	-5.77	114.92	122.59
1	R	321	GLU	N-CA-C	5.77	118.31	111.33
1	C	3	ARG	CG-CD-NE	5.77	124.69	112.00
1	J	190	VAL	CA-C-O	5.77	127.43	120.74
1	Q	139	LYS	O-C-N	5.77	128.97	122.22
1	B	167	ALA	CA-C-N	-5.77	111.98	120.28
1	B	167	ALA	C-N-CA	-5.77	111.98	120.28
1	F	156	GLN	CA-CB-CG	-5.77	102.57	114.10
1	I	38	THR	CB-CA-C	-5.77	101.83	110.88
1	B	50	ASN	CA-C-O	5.76	127.27	120.58
1	O	41	ASN	CA-C-O	5.76	126.53	120.42
1	B	305	LEU	CA-C-N	-5.76	110.62	121.63
1	B	305	LEU	C-N-CA	-5.76	110.62	121.63
1	E	141	GLY	CA-C-O	-5.76	112.61	119.01
1	D	188	PRO	CA-C-N	-5.76	113.26	121.50
1	D	188	PRO	C-N-CA	-5.76	113.26	121.50
1	L	104	VAL	CA-C-N	-5.76	116.63	121.58
1	L	104	VAL	C-N-CA	-5.76	116.63	121.58
1	Q	289	CYS	O-C-N	-5.76	116.17	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	HIS	CA-C-N	5.76	132.22	122.26
1	A	237	HIS	C-N-CA	5.76	132.22	122.26
1	G	258	ARG	CD-NE-CZ	-5.76	116.34	124.40
1	H	195	ASP	CA-C-N	5.76	132.54	121.54
1	H	195	ASP	C-N-CA	5.76	132.54	121.54
1	L	314	GLY	N-CA-C	-5.76	107.01	115.30
1	D	95	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	O	140	ASP	CA-CB-CG	-5.76	106.84	112.60
1	Q	63	PHE	N-CA-C	5.76	119.56	112.54
1	R	70	ASN	CA-CB-CG	-5.76	106.84	112.60
1	A	53	GLU	N-CA-C	5.76	117.64	111.36
1	H	84	TYR	CA-C-O	-5.76	112.69	119.48
1	H	98	LYS	CA-CB-CG	5.76	125.61	114.10
1	R	215	ALA	O-C-N	5.76	128.71	122.15
1	P	175	SER	N-CA-C	5.75	117.23	111.07
1	D	156	GLN	CA-CB-CG	-5.75	102.59	114.10
1	E	226	THR	CA-C-O	-5.75	115.07	121.51
1	F	214	LYS	CD-CE-NZ	-5.75	93.49	111.90
1	N	244	THR	OG1-CB-CG2	-5.75	97.79	109.30
1	A	336	GLN	CA-CB-CG	5.75	125.60	114.10
1	B	6	ALA	N-CA-CB	5.75	118.56	109.82
1	N	119	ASN	CA-CB-CG	-5.75	106.85	112.60
1	N	242	LYS	O-C-N	-5.75	116.46	123.19
1	R	17	GLU	CB-CG-CD	5.75	122.38	112.60
1	F	249	ALA	O-C-N	-5.75	116.03	122.12
1	L	296	LYS	CA-C-O	-5.75	115.55	121.87
1	N	156	GLN	N-CA-C	5.75	119.88	112.86
1	E	254	THR	CA-CB-OG1	-5.75	100.98	109.60
1	F	102	ILE	N-CA-C	5.75	116.86	108.58
1	F	196	HIS	CA-C-N	-5.75	110.63	122.82
1	F	196	HIS	C-N-CA	-5.75	110.63	122.82
1	H	5	PRO	CA-C-N	5.75	127.91	120.44
1	H	5	PRO	C-N-CA	5.75	127.91	120.44
1	J	75	GLY	CA-C-N	5.75	130.98	122.99
1	J	75	GLY	C-N-CA	5.75	130.98	122.99
1	O	236	GLY	CA-C-O	5.75	130.01	122.31
1	K	15	LEU	CA-C-O	5.75	126.85	120.82
1	K	325	GLU	CA-C-O	-5.75	114.78	120.70
1	O	6	ALA	CA-C-N	-5.75	113.57	122.59
1	O	6	ALA	C-N-CA	-5.75	113.57	122.59
1	H	264	VAL	CB-CA-C	5.75	117.61	110.95
1	B	252	THR	CA-CB-CG2	-5.74	100.74	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	ALA	O-C-N	5.74	128.06	122.09
1	G	233	VAL	O-C-N	-5.74	116.42	122.68
1	M	120	LYS	CA-C-O	-5.74	114.88	121.54
1	N	139	LYS	N-CA-CB	5.74	119.76	110.40
1	K	353	THR	CB-CA-C	5.74	119.98	109.99
1	I	93	PHE	N-CA-CB	-5.74	100.42	109.78
1	O	236	GLY	CA-C-N	5.74	128.25	120.38
1	O	236	GLY	C-N-CA	5.74	128.25	120.38
1	A	195	ASP	CA-C-O	-5.74	112.82	119.59
1	E	109	ASP	CA-CB-CG	5.74	118.34	112.60
1	E	176	ILE	CA-C-N	-5.74	112.52	120.38
1	E	176	ILE	C-N-CA	-5.74	112.52	120.38
1	E	242	LYS	CA-C-N	-5.74	112.53	123.32
1	E	242	LYS	C-N-CA	-5.74	112.53	123.32
1	O	203	TYR	CB-CG-CD1	-5.74	112.19	120.80
1	Q	165	GLU	N-CA-CB	-5.74	101.65	110.20
1	G	42	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	M	126	GLY	CA-C-O	-5.74	110.59	120.57
1	C	26	GLY	CA-C-N	-5.74	109.17	121.45
1	C	26	GLY	C-N-CA	-5.74	109.17	121.45
1	D	131	SER	CB-CA-C	-5.74	101.88	110.88
1	F	81	GLU	O-C-N	5.74	128.20	122.12
1	F	86	LYS	CA-C-N	-5.74	112.68	121.74
1	F	86	LYS	C-N-CA	-5.74	112.68	121.74
1	I	267	ILE	O-C-N	-5.73	117.22	123.18
1	P	3	ARG	CA-C-O	-5.73	112.31	120.51
1	I	102	ILE	N-CA-CB	-5.73	104.24	111.46
1	J	294	PRO	CA-C-O	-5.73	110.95	118.86
1	L	18	ILE	O-C-N	5.73	127.73	121.83
1	L	282	ASN	OD1-CG-ND2	5.73	128.33	122.60
1	N	62	LEU	CA-C-O	-5.73	113.38	119.97
1	I	269	PHE	CA-C-O	5.73	127.49	121.19
1	N	292	PRO	O-C-N	-5.73	116.09	123.03
1	R	13	LYS	CA-C-O	5.73	126.62	120.55
1	R	147	TRP	CE3-CZ3-CH2	5.73	128.55	121.10
1	D	265	PRO	CA-C-N	-5.73	110.18	121.41
1	D	265	PRO	C-N-CA	-5.73	110.18	121.41
1	E	43	LEU	CA-C-O	5.73	126.43	119.38
1	O	50	ASN	N-CA-C	-5.73	100.90	109.15
1	H	165	GLU	N-CA-CB	-5.73	101.70	110.01
1	P	355	SER	CA-CB-OG	5.73	122.55	111.10
1	R	271	SER	CA-CB-OG	-5.73	99.64	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	56	ARG	CA-C-O	5.73	126.62	120.55
1	Q	137	TYR	CA-C-O	5.73	126.62	120.55
1	Q	340	GLY	CA-C-O	-5.73	112.59	119.00
1	B	75	GLY	O-C-N	-5.72	118.24	123.56
1	D	11	GLN	CA-C-O	5.72	126.62	120.55
1	F	267	ILE	O-C-N	-5.72	117.13	123.20
1	J	300	SER	N-CA-C	-5.72	95.59	107.67
1	M	142	VAL	O-C-N	5.72	129.47	122.72
1	I	270	LEU	CA-C-O	-5.72	115.41	121.88
1	N	125	GLN	CA-CB-CG	-5.72	102.66	114.10
1	Q	203	TYR	CA-C-O	-5.72	113.89	120.24
1	H	286	ILE	CA-C-N	5.72	129.00	120.31
1	H	286	ILE	C-N-CA	5.72	129.00	120.31
1	O	60	GLU	O-C-N	5.72	127.96	122.07
1	D	110	GLN	CA-CB-CG	-5.72	102.66	114.10
1	J	26	GLY	N-CA-C	-5.72	107.78	115.21
1	O	296	LYS	N-CA-C	-5.72	102.98	110.53
1	G	252	THR	N-CA-CB	-5.71	101.78	110.07
1	I	133	ARG	CG-CD-NE	5.71	124.57	112.00
1	L	204	VAL	O-C-N	5.71	127.72	121.83
1	D	65	VAL	N-CA-CB	-5.71	98.59	110.64
1	H	55	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	P	243	TYR	CA-C-O	-5.71	114.78	121.46
1	R	335	CYS	CA-C-O	5.71	126.47	120.42
1	B	243	TYR	O-C-N	-5.71	116.53	123.10
1	C	197	ASP	CA-CB-CG	-5.71	106.89	112.60
1	F	140	ASP	CB-CG-OD1	-5.71	105.27	118.40
1	H	180	ASN	CA-CB-CG	-5.71	106.89	112.60
1	I	124	ILE	N-CA-C	5.71	116.10	108.11
1	C	297	LEU	CA-C-N	-5.71	114.62	122.16
1	C	297	LEU	C-N-CA	-5.71	114.62	122.16
1	I	76	VAL	O-C-N	5.71	129.43	123.26
1	K	287	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	L	207	LYS	CB-CA-C	5.71	120.56	110.85
1	P	199	GLU	CA-C-O	5.71	126.79	120.63
1	B	271	SER	O-C-N	5.71	128.15	122.10
1	D	321	GLU	CA-C-N	-5.71	112.63	120.28
1	D	321	GLU	C-N-CA	-5.71	112.63	120.28
1	E	276	GLU	CA-C-N	-5.71	112.19	120.29
1	E	276	GLU	C-N-CA	-5.71	112.19	120.29
1	L	267	ILE	N-CA-CB	5.71	119.58	111.82
1	J	172	ARG	NE-CZ-NH2	-5.71	114.07	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	42	ARG	NE-CZ-NH2	5.71	124.33	119.20
1	M	218	ASP	CA-C-N	-5.70	114.05	122.83
1	M	218	ASP	C-N-CA	-5.70	114.05	122.83
1	J	297	LEU	CA-C-N	5.70	130.67	122.23
1	J	297	LEU	C-N-CA	5.70	130.67	122.23
1	L	200	HIS	O-C-N	-5.70	115.93	122.09
1	P	51	THR	CA-CB-OG1	-5.70	101.05	109.60
1	B	203	TYR	CA-C-O	5.70	126.81	120.82
1	N	113	ALA	CA-C-N	5.70	125.46	119.76
1	N	113	ALA	C-N-CA	5.70	125.46	119.76
1	A	29	ILE	CB-CG1-CD1	-5.70	101.83	113.80
1	F	41	ASN	O-C-N	5.70	128.89	122.22
1	H	153	ILE	CA-C-O	-5.70	114.43	120.53
1	I	258	ARG	N-CA-CB	5.70	118.92	110.49
1	L	341	GLN	CA-C-N	-5.70	112.97	120.95
1	L	341	GLN	C-N-CA	-5.70	112.97	120.95
1	P	205	THR	CA-C-N	-5.70	111.65	120.31
1	P	205	THR	C-N-CA	-5.70	111.65	120.31
1	M	344	HIS	CA-C-O	-5.70	112.36	120.51
1	P	90	GLY	CA-C-O	-5.70	112.03	119.44
1	E	292	PRO	CA-C-O	-5.70	115.14	121.23
1	M	143	ASP	N-CA-CB	5.70	119.15	110.95
1	N	316	LYS	CG-CD-CE	5.70	124.40	111.30
1	N	339	LYS	CA-C-O	5.70	126.31	119.59
1	O	100	LYS	CA-C-O	5.70	126.56	119.78
1	O	155	ASP	O-C-N	-5.70	115.01	122.59
1	G	82	THR	CA-C-O	-5.69	113.42	119.97
1	H	137	TYR	CA-CB-CG	5.69	124.15	113.90
1	J	290	PRO	CB-CA-C	-5.69	105.35	113.09
1	B	60	GLU	N-CA-CB	5.69	118.26	110.01
1	R	316	LYS	CA-C-O	-5.69	114.27	120.36
1	C	143	ASP	CA-C-O	-5.69	112.45	118.77
1	C	221	VAL	CA-CB-CG2	-5.69	100.73	110.40
1	C	327	PHE	CA-CB-CG	-5.69	108.11	113.80
1	E	237	HIS	O-C-N	5.69	128.15	122.12
1	F	56	ARG	CA-CB-CG	5.69	125.48	114.10
1	H	149	ALA	O-C-N	5.69	130.59	123.19
1	I	62	LEU	N-CA-CB	5.69	118.48	110.12
1	M	277	GLU	CG-CD-OE1	5.69	131.49	118.40
1	M	25	ASN	N-CA-C	-5.69	96.75	108.53
1	A	156	GLN	N-CA-CB	-5.69	103.66	112.30
1	A	287	ASN	CB-CG-ND2	-5.69	107.87	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	GLU	N-CA-C	-5.69	105.08	111.28
1	C	31	ALA	CA-C-N	-5.69	114.70	123.17
1	C	31	ALA	C-N-CA	-5.69	114.70	123.17
1	E	11	GLN	CG-CD-NE2	-5.69	107.87	116.40
1	K	186	VAL	CA-C-N	-5.69	115.11	123.30
1	K	186	VAL	C-N-CA	-5.69	115.11	123.30
1	Q	168	ASN	CB-CG-OD1	5.69	132.18	120.80
1	D	160	SER	CB-CA-C	-5.69	101.35	110.79
1	Q	71	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	G	190	VAL	CA-C-O	-5.68	113.81	120.75
1	H	221	VAL	CA-C-N	5.68	132.40	121.54
1	H	221	VAL	C-N-CA	5.68	132.40	121.54
1	R	303	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	B	23	VAL	CG1-CB-CG2	-5.68	98.31	110.80
1	C	135	ALA	O-C-N	5.68	128.14	122.12
1	C	295	TRP	CB-CA-C	-5.68	98.97	109.37
1	E	89	GLN	N-CA-C	5.68	122.90	110.80
1	E	202	GLN	CB-CG-CD	-5.68	102.94	112.60
1	I	124	ILE	CA-C-O	-5.68	114.43	120.39
1	J	215	ALA	CA-C-O	5.68	126.44	120.42
1	M	306	GLN	OE1-CD-NE2	5.68	128.28	122.60
1	B	283	LEU	CA-C-O	5.68	126.76	120.63
1	D	341	GLN	CG-CD-OE1	5.68	132.15	120.80
1	Q	276	GLU	O-C-N	5.68	128.62	122.15
1	B	345	THR	CB-CA-C	5.67	121.71	110.42
1	C	286	ILE	O-C-N	5.67	127.61	121.94
1	G	11	GLN	CG-CD-NE2	-5.67	107.89	116.40
1	K	306	GLN	CA-C-N	5.67	127.81	120.44
1	K	306	GLN	C-N-CA	5.67	127.81	120.44
1	M	260	VAL	N-CA-C	5.67	113.17	107.55
1	O	217	ASN	CB-CG-ND2	5.67	124.91	116.40
1	D	63	PHE	N-CA-C	5.67	119.82	113.01
1	F	122	THR	CB-CA-C	-5.67	98.04	111.65
1	J	287	ASN	OD1-CG-ND2	5.67	128.27	122.60
1	L	223	LEU	CA-C-O	-5.67	114.50	120.63
1	P	309	ALA	N-CA-CB	5.67	118.46	110.12
1	J	268	CYS	O-C-N	-5.67	115.99	123.13
1	J	308	SER	CB-CA-C	5.67	121.08	110.70
1	A	267	ILE	CB-CA-C	5.67	118.07	110.42
1	B	93	PHE	CB-CA-C	-5.67	101.05	110.68
1	F	343	VAL	CA-C-N	-5.67	112.91	120.90
1	F	343	VAL	C-N-CA	-5.67	112.91	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	32	ALA	N-CA-C	-5.67	106.26	112.72
1	O	258	ARG	CA-CB-CG	5.67	125.44	114.10
1	Q	138	LYS	O-C-N	5.67	127.91	122.07
1	D	2	HIS	N-CA-C	5.67	118.69	110.42
1	E	172	ARG	NH1-CZ-NH2	5.67	126.67	119.30
1	F	319	ASN	CA-CB-CG	-5.67	106.93	112.60
1	J	62	LEU	CA-C-O	-5.67	114.87	120.82
1	N	39	MET	CB-CA-C	-5.67	101.05	110.68
1	N	106	ILE	N-CA-CB	-5.67	101.33	111.92
1	E	341	GLN	O-C-N	-5.67	115.51	122.25
1	E	350	ALA	N-CA-CB	-5.67	100.92	110.49
1	I	218	ASP	O-C-N	-5.67	116.20	122.09
1	I	295	TRP	CA-C-O	-5.67	114.81	121.44
1	J	214	LYS	CG-CD-CE	-5.67	98.27	111.30
1	A	94	ARG	NE-CZ-NH2	-5.66	114.10	119.20
1	J	136	GLN	N-CA-CB	-5.66	101.76	110.20
1	O	147	TRP	CZ3-CH2-CZ2	-5.66	114.14	121.50
1	O	339	LYS	CB-CG-CD	-5.66	98.28	111.30
1	P	328	MET	N-CA-C	-5.66	105.11	111.28
1	Q	267	ILE	CA-C-O	5.66	125.86	120.31
1	R	44	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	93	PHE	CA-C-N	-5.66	112.13	120.28
1	A	93	PHE	C-N-CA	-5.66	112.13	120.28
1	E	212	VAL	CB-CA-C	5.66	119.22	111.97
1	E	238	ALA	CA-C-N	-5.66	113.32	121.42
1	E	238	ALA	C-N-CA	-5.66	113.32	121.42
1	A	357	PHE	O-C-N	-5.66	115.06	122.59
1	M	3	ARG	CB-CG-CD	5.66	124.32	111.30
1	J	185	ILE	N-CA-C	-5.66	98.99	107.37
1	L	123	THR	N-CA-C	-5.66	100.82	109.65
1	N	8	THR	CA-C-N	-5.66	112.63	120.38
1	N	8	THR	C-N-CA	-5.66	112.63	120.38
1	R	210	ALA	O-C-N	-5.66	116.24	122.07
1	R	231	ASN	O-C-N	5.66	129.35	122.96
1	K	200	HIS	CB-CA-C	5.66	121.53	110.67
1	N	92	LEU	CA-C-O	5.66	127.14	120.69
1	O	95	ASN	CA-C-N	-5.66	113.30	120.60
1	O	95	ASN	C-N-CA	-5.66	113.30	120.60
1	Q	123	THR	CA-C-O	-5.66	114.93	121.49
1	F	205	THR	CA-C-O	-5.66	114.42	120.42
1	G	165	GLU	OE1-CD-OE2	5.66	136.47	122.90
1	K	301	TYR	CA-CB-CG	5.66	124.08	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	HIS	CA-C-O	5.65	126.74	120.63
1	D	244	THR	N-CA-CB	-5.65	97.73	110.56
1	G	330	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	K	212	VAL	O-C-N	5.65	127.45	121.91
1	M	336	GLN	N-CA-C	-5.65	105.04	111.14
1	B	331	ALA	O-C-N	-5.65	115.61	122.22
1	F	23	VAL	CA-C-O	5.65	125.79	120.14
1	G	59	ARG	CA-CB-CG	-5.65	102.80	114.10
1	G	191	ILE	N-CA-CB	-5.65	103.38	110.33
1	L	19	ALA	CA-C-N	-5.65	111.25	121.14
1	L	19	ALA	C-N-CA	-5.65	111.25	121.14
1	N	154	ALA	CA-C-N	-5.65	112.66	121.02
1	N	154	ALA	C-N-CA	-5.65	112.66	121.02
1	Q	45	ARG	CA-C-O	-5.65	114.59	120.92
1	B	132	GLU	CB-CG-CD	5.65	122.20	112.60
1	E	230	PRO	O-C-N	5.65	129.50	123.23
1	G	231	ASN	N-CA-C	-5.65	101.34	110.32
1	Q	246	GLU	O-C-N	-5.65	115.61	122.22
1	F	55	ARG	CA-C-N	-5.65	110.93	120.58
1	F	55	ARG	C-N-CA	-5.65	110.93	120.58
1	H	183	VAL	CA-C-O	5.65	127.52	119.95
1	M	18	ILE	CA-CB-CG2	5.65	120.10	110.50
1	Q	341	GLN	N-CA-C	5.65	119.48	112.59
1	A	131	SER	CA-CB-OG	-5.64	99.81	111.10
1	K	331	ALA	CA-C-N	5.64	128.30	120.29
1	K	331	ALA	C-N-CA	5.64	128.30	120.29
1	M	41	ASN	CA-CB-CG	-5.64	106.96	112.60
1	Q	161	LEU	CB-CA-C	5.64	120.44	110.85
1	B	231	ASN	CA-C-O	5.64	128.38	121.72
1	C	244	THR	CA-CB-OG1	5.64	118.06	109.60
1	H	142	VAL	N-CA-C	5.64	116.88	109.21
1	H	227	LEU	N-CA-CB	5.64	121.64	111.37
1	J	334	ASN	CB-CA-C	5.64	120.44	110.85
1	P	175	SER	CA-C-O	5.64	126.75	120.82
1	E	222	TYR	CA-CB-CG	5.64	124.05	113.90
1	K	356	LEU	CA-C-O	-5.64	113.64	119.51
1	Q	243	TYR	CB-CG-CD2	-5.64	112.34	120.80
1	B	205	THR	N-CA-C	-5.64	105.21	111.36
1	E	76	VAL	O-C-N	-5.64	117.17	123.26
1	H	355	SER	N-CA-CB	5.64	120.02	110.49
1	I	97	LEU	N-CA-C	5.64	117.51	111.36
1	Q	201	CYS	N-CA-C	-5.64	105.22	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	GLU	O-C-N	5.64	128.11	122.08
1	D	122	THR	CB-CA-C	-5.64	99.27	111.11
1	H	158	PRO	N-CA-CB	-5.64	96.40	102.60
1	J	110	GLN	O-C-N	5.64	128.98	121.99
1	L	100	LYS	N-CA-C	-5.64	106.61	112.93
1	Q	179	GLN	CG-CD-NE2	-5.64	107.94	116.40
1	G	339	LYS	CA-CB-CG	5.64	125.38	114.10
1	R	55	ARG	NH1-CZ-NH2	5.64	126.63	119.30
1	B	138	LYS	N-CA-C	-5.63	105.14	111.28
1	D	154	ALA	CB-CA-C	-5.63	99.21	110.42
1	E	64	SER	CA-C-N	-5.63	111.83	121.97
1	E	64	SER	C-N-CA	-5.63	111.83	121.97
1	H	347	SER	N-CA-CB	5.63	120.01	110.49
1	F	28	GLY	O-C-N	-5.63	115.38	122.70
1	F	226	THR	N-CA-C	5.63	117.97	109.41
1	H	11	GLN	OE1-CD-NE2	5.63	128.23	122.60
1	J	283	LEU	CA-C-O	5.63	126.45	119.97
1	K	42	ARG	NH1-CZ-NH2	-5.63	111.98	119.30
1	O	90	GLY	CA-C-O	-5.63	110.77	120.57
1	O	239	CYS	CB-CA-C	-5.63	100.37	109.72
1	P	25	ASN	CB-CA-C	-5.63	100.76	111.97
1	B	310	LEU	CA-C-N	-5.63	113.12	120.44
1	B	310	LEU	C-N-CA	-5.63	113.12	120.44
1	C	39	MET	CA-C-O	5.63	126.46	120.10
1	E	352	SER	CA-CB-OG	-5.63	99.84	111.10
1	G	103	VAL	CA-CB-CG1	-5.63	100.83	110.40
1	J	262	ALA	N-CA-C	-5.63	106.12	112.87
1	L	209	LEU	O-C-N	-5.63	115.64	122.22
1	N	260	VAL	CG1-CB-CG2	5.63	123.18	110.80
1	Q	164	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	A	263	ALA	O-C-N	-5.63	114.89	122.43
1	C	133	ARG	O-C-N	-5.63	116.16	122.12
1	D	88	SER	CB-CA-C	5.63	121.08	111.68
1	D	119	ASN	CA-C-O	5.63	128.56	120.51
1	E	54	ASN	CA-CB-CG	-5.63	106.97	112.60
1	K	233	VAL	N-CA-CB	5.63	117.92	111.39
1	N	195	ASP	N-CA-C	5.63	119.40	112.54
1	P	262	ALA	CA-C-O	5.63	126.46	120.10
1	A	19	ALA	CA-C-N	-5.62	111.76	120.31
1	A	19	ALA	C-N-CA	-5.62	111.76	120.31
1	Q	100	LYS	N-CA-CB	5.62	118.73	110.57
1	B	181	GLY	CA-C-O	-5.62	110.79	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	LYS	CA-C-N	-5.62	112.65	121.87
1	B	242	LYS	C-N-CA	-5.62	112.65	121.87
1	C	161	LEU	N-CA-CB	-5.62	101.56	109.94
1	G	72	SER	O-C-N	-5.62	114.56	122.10
1	I	153	ILE	N-CA-CB	-5.62	104.63	111.21
1	I	179	GLN	CA-C-N	5.62	131.37	122.60
1	I	179	GLN	C-N-CA	5.62	131.37	122.60
1	I	269	PHE	O-C-N	-5.62	115.95	122.87
1	K	21	SER	O-C-N	5.62	128.80	122.22
1	M	269	PHE	N-CA-C	5.62	118.00	110.35
1	P	337	ALA	N-CA-C	-5.62	105.23	111.36
1	P	165	GLU	N-CA-CB	-5.62	101.92	110.07
1	C	185	ILE	O-C-N	-5.62	115.80	122.77
1	E	6	ALA	CA-C-N	-5.62	113.77	122.59
1	E	6	ALA	C-N-CA	-5.62	113.77	122.59
1	G	148	ARG	CB-CA-C	-5.62	101.09	110.19
1	K	13	LYS	CA-C-N	-5.62	113.14	120.44
1	K	13	LYS	C-N-CA	-5.62	113.14	120.44
1	O	38	THR	CA-C-N	-5.62	112.75	120.28
1	O	38	THR	C-N-CA	-5.62	112.75	120.28
1	O	322	ALA	O-C-N	5.62	128.09	122.08
1	P	80	HIS	CE1-NE2-CD2	5.62	114.62	109.00
1	Q	214	LYS	N-CA-CB	5.62	118.48	110.16
1	E	163	ILE	CA-C-O	5.62	127.80	120.78
1	E	310	LEU	CA-C-O	5.62	126.37	120.42
1	H	26	GLY	CA-C-N	-5.62	111.38	120.87
1	H	26	GLY	C-N-CA	-5.62	111.38	120.87
1	A	334	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	B	291	LEU	CA-C-N	5.62	125.80	119.90
1	B	291	LEU	C-N-CA	5.62	125.80	119.90
1	K	203	TYR	O-C-N	5.62	127.85	122.07
1	M	144	PHE	CA-C-O	-5.62	115.22	121.23
1	R	181	GLY	CA-C-O	-5.62	112.28	119.58
1	C	230	PRO	CB-CA-C	-5.61	102.30	111.56
1	E	128	ASP	CA-CB-CG	5.61	118.21	112.60
1	N	274	MET	CA-CB-CG	-5.61	102.88	114.10
1	C	173	TYR	CB-CG-CD1	5.61	129.21	120.80
1	E	342	TYR	CA-C-O	-5.61	114.36	120.81
1	D	206	GLU	N-CA-C	5.61	117.39	111.28
1	E	81	GLU	CA-CB-CG	5.61	125.32	114.10
1	B	156	GLN	CB-CG-CD	-5.61	103.07	112.60
1	D	92	LEU	CA-C-O	5.61	127.36	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	234	THR	CA-C-O	-5.61	114.99	121.49
1	F	340	GLY	O-C-N	5.61	128.47	122.41
1	G	209	LEU	CA-C-N	-5.61	112.77	120.28
1	G	209	LEU	C-N-CA	-5.61	112.77	120.28
1	G	218	ASP	CA-C-O	-5.61	114.61	120.55
1	O	71	GLN	O-C-N	-5.61	115.45	122.35
1	A	152	ARG	CB-CA-C	-5.61	98.30	109.79
1	I	135	ALA	CA-C-O	5.61	126.28	119.38
1	K	258	ARG	N-CA-C	-5.61	106.28	113.23
1	M	204	VAL	CA-C-O	-5.61	114.91	120.85
1	P	266	GLY	O-C-N	5.61	128.70	123.54
1	D	119	ASN	N-CA-CB	-5.60	101.02	110.49
1	H	338	ALA	CA-C-O	-5.60	112.71	119.49
1	L	227	LEU	CA-C-O	-5.60	115.45	121.45
1	B	212	VAL	CA-CB-CG2	-5.60	100.88	110.40
1	B	213	TYR	CB-CG-CD2	-5.60	112.40	120.80
1	C	307	ALA	N-CA-C	5.60	117.06	111.07
1	D	45	ARG	NH1-CZ-NH2	5.60	126.58	119.30
1	E	181	GLY	CA-C-N	-5.60	113.85	122.87
1	E	181	GLY	C-N-CA	-5.60	113.85	122.87
1	J	330	ARG	NH1-CZ-NH2	5.60	126.58	119.30
1	K	231	ASN	CA-C-O	5.60	128.08	121.36
1	L	249	ALA	O-C-N	5.60	128.06	122.12
1	M	208	VAL	N-CA-C	-5.60	105.26	110.53
1	M	352	SER	CB-CA-C	5.60	121.57	110.42
1	Q	50	ASN	N-CA-CB	5.60	118.73	109.88
1	G	191	ILE	CA-C-N	5.60	127.67	120.89
1	G	191	ILE	C-N-CA	5.60	127.67	120.89
1	B	202	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	P	21	SER	CA-C-N	-5.60	111.12	120.30
1	P	21	SER	C-N-CA	-5.60	111.12	120.30
1	R	258	ARG	CA-CB-CG	5.60	125.30	114.10
1	G	93	PHE	CB-CA-C	-5.60	99.28	110.42
1	G	295	TRP	CB-CA-C	-5.60	100.77	110.45
1	M	236	GLY	N-CA-C	-5.60	105.10	112.82
1	B	276	GLU	CA-C-N	-5.60	112.34	120.29
1	B	276	GLU	C-N-CA	-5.60	112.34	120.29
1	H	219	HIS	ND1-CE1-NE2	5.60	114.00	108.40
1	D	157	CYS	N-CA-C	-5.59	101.54	110.10
1	E	17	GLU	CB-CG-CD	5.59	122.11	112.60
1	F	109	ASP	CA-C-O	-5.59	115.21	121.81
1	I	286	ILE	O-C-N	5.59	127.52	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	72	SER	CA-C-O	5.59	125.56	119.24
1	Q	309	ALA	N-CA-CB	5.59	118.18	110.07
1	R	14	GLU	N-CA-C	-5.59	105.10	111.14
1	F	214	LYS	CB-CG-CD	5.59	124.16	111.30
1	L	44	GLN	CA-C-O	-5.59	114.92	120.90
1	D	24	ALA	CB-CA-C	-5.59	102.07	110.90
1	N	81	GLU	CA-CB-CG	5.59	125.28	114.10
1	O	102	ILE	N-CA-C	5.59	116.63	108.53
1	P	56	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	Q	149	ALA	N-CA-C	-5.59	101.06	109.95
1	B	301	TYR	N-CA-CB	-5.59	102.25	110.85
1	D	211	ALA	N-CA-CB	-5.59	101.61	109.94
1	J	202	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	L	113	ALA	N-CA-CB	5.59	120.31	110.37
1	P	103	VAL	CB-CA-C	-5.59	102.77	111.26
1	A	147	TRP	CA-C-N	-5.58	115.29	123.00
1	A	147	TRP	C-N-CA	-5.58	115.29	123.00
1	B	191	ILE	CA-C-N	5.58	126.07	120.04
1	B	191	ILE	C-N-CA	5.58	126.07	120.04
1	F	100	LYS	CA-C-O	-5.58	112.32	119.80
1	K	252	THR	O-C-N	5.58	128.52	122.15
1	Q	204	VAL	CA-C-N	5.58	128.03	120.38
1	Q	204	VAL	C-N-CA	5.58	128.03	120.38
1	F	228	LEU	CA-C-O	5.58	126.39	120.36
1	R	104	VAL	CB-CA-C	-5.58	102.32	110.81
1	E	183	VAL	CA-CB-CG2	5.58	119.89	110.40
1	E	282	ASN	CB-CG-ND2	-5.58	108.03	116.40
1	F	109	ASP	N-CA-CB	5.58	118.93	110.45
1	F	255	ALA	CA-C-N	-5.58	112.80	120.28
1	F	255	ALA	C-N-CA	-5.58	112.80	120.28
1	J	319	ASN	CA-CB-CG	-5.58	107.02	112.60
1	L	131	SER	N-CA-CB	5.58	118.06	109.91
1	L	140	ASP	CA-CB-CG	-5.58	107.02	112.60
1	N	60	GLU	O-C-N	-5.58	115.69	122.22
1	O	69	ILE	N-CA-C	-5.58	105.67	112.76
1	R	149	ALA	O-C-N	5.58	129.31	123.06
1	E	202	GLN	CA-CB-CG	-5.58	102.94	114.10
1	E	295	TRP	CB-CG-CD1	-5.58	118.53	126.90
1	A	2	HIS	CA-C-N	5.58	132.20	121.54
1	A	2	HIS	C-N-CA	5.58	132.20	121.54
1	A	191	ILE	CB-CG1-CD1	-5.58	102.09	113.80
1	A	279	ALA	O-C-N	5.58	129.13	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	10	GLU	O-C-N	5.58	128.03	122.12
1	E	201	CYS	O-C-N	-5.58	116.21	122.12
1	F	124	ILE	CG1-CB-CG2	-5.58	93.96	110.70
1	I	205	THR	CA-C-N	-5.58	111.40	120.72
1	I	205	THR	C-N-CA	-5.58	111.40	120.72
1	P	149	ALA	CB-CA-C	-5.58	100.11	109.48
1	C	267	ILE	CA-CB-CG1	5.58	119.88	110.40
1	O	123	THR	N-CA-CB	5.58	120.02	110.65
1	O	205	THR	N-CA-C	-5.58	105.28	111.36
1	H	99	GLU	CA-C-O	-5.58	114.64	120.55
1	J	300	SER	O-C-N	5.58	132.59	122.44
1	K	118	THR	O-C-N	-5.57	116.42	123.17
1	M	66	ASP	CA-CB-CG	5.57	118.17	112.60
1	P	86	LYS	O-C-N	-5.57	115.64	123.11
1	D	325	GLU	O-C-N	-5.57	115.80	122.15
1	K	339	LYS	CB-CG-CD	-5.57	98.48	111.30
1	J	161	LEU	N-CA-CB	-5.57	101.91	110.16
1	O	61	ILE	N-CA-CB	5.57	117.70	110.57
1	Q	167	ALA	CA-C-O	-5.57	114.64	120.55
1	B	16	SER	CA-C-N	-5.57	113.20	120.44
1	B	16	SER	C-N-CA	-5.57	113.20	120.44
1	B	306	GLN	O-C-N	5.57	128.91	121.67
1	C	302	GLY	CA-C-N	-5.57	112.87	120.44
1	C	302	GLY	C-N-CA	-5.57	112.87	120.44
1	K	100	LYS	N-CA-CB	5.57	118.64	110.57
1	O	177	CYS	CA-C-O	5.57	126.86	120.90
1	E	125	GLN	N-CA-CB	-5.57	101.83	110.46
1	E	321	GLU	CA-C-N	5.57	128.19	120.29
1	E	321	GLU	C-N-CA	5.57	128.19	120.29
1	F	144	PHE	N-CA-CB	5.57	121.09	111.13
1	F	334	ASN	CB-CG-ND2	5.57	124.75	116.40
1	H	273	GLY	N-CA-C	5.57	121.70	115.08
1	H	276	GLU	CB-CA-C	-5.57	101.91	110.81
1	J	186	VAL	O-C-N	-5.57	115.87	122.77
1	O	166	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	R	258	ARG	NH1-CZ-NH2	-5.57	112.06	119.30
1	B	158	PRO	O-C-N	5.56	131.67	121.10
1	N	64	SER	CA-C-O	5.56	126.23	119.11
1	B	147	TRP	CA-C-N	-5.56	115.04	122.72
1	B	147	TRP	C-N-CA	-5.56	115.04	122.72
1	D	3	ARG	CG-CD-NE	5.56	124.24	112.00
1	H	259	THR	CA-CB-OG1	-5.56	101.25	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	143	ASP	CA-CB-CG	-5.56	107.04	112.60
1	Q	31	ALA	CA-C-O	-5.56	115.16	121.39
1	P	187	GLU	O-C-N	5.56	126.38	121.32
1	P	329	LYS	CG-CD-CE	5.56	124.09	111.30
1	G	11	GLN	CG-CD-OE1	5.56	131.92	120.80
1	G	253	VAL	CA-C-N	-5.56	113.21	120.44
1	G	253	VAL	C-N-CA	-5.56	113.21	120.44
1	H	76	VAL	O-C-N	-5.56	117.40	123.18
1	J	14	GLU	CB-CG-CD	5.56	122.05	112.60
1	K	182	LEU	CA-C-O	-5.56	114.63	120.80
1	K	292	PRO	CB-CA-C	-5.56	104.58	111.64
1	K	349	GLY	O-C-N	5.56	129.93	122.70
1	B	265	PRO	O-C-N	-5.56	115.56	122.23
1	C	127	LEU	N-CA-C	-5.56	106.34	113.23
1	D	80	HIS	O-C-N	-5.56	116.13	122.08
1	G	322	ALA	O-C-N	5.56	127.81	122.03
1	J	198	LEU	O-C-N	5.56	128.09	122.09
1	B	70	ASN	CB-CG-ND2	-5.56	108.07	116.40
1	D	292	PRO	CB-CA-C	-5.56	104.74	111.46
1	G	67	SER	CA-CB-OG	-5.56	99.99	111.10
1	H	207	LYS	CG-CD-CE	5.56	124.08	111.30
1	N	230	PRO	CB-CA-C	-5.56	102.39	111.56
1	D	262	ALA	N-CA-C	-5.55	105.38	111.82
1	D	303	ARG	CD-NE-CZ	-5.55	116.62	124.40
1	I	70	ASN	CA-CB-CG	5.55	118.16	112.60
1	K	278	ASP	CA-CB-CG	-5.55	107.05	112.60
1	N	141	GLY	N-CA-C	5.55	122.43	115.21
1	O	179	GLN	CA-C-O	-5.55	113.58	119.97
1	Q	174	ALA	CA-C-O	5.55	126.31	120.42
1	A	133	ARG	CB-CG-CD	5.55	124.06	111.30
1	B	195	ASP	CB-CG-OD2	5.55	131.16	118.40
1	B	235	ALA	CA-C-O	-5.55	115.43	121.87
1	C	172	ARG	CD-NE-CZ	-5.55	116.63	124.40
1	C	215	ALA	CA-C-N	-5.55	112.29	120.28
1	C	215	ALA	C-N-CA	-5.55	112.29	120.28
1	E	200	HIS	CA-C-O	5.55	126.40	120.24
1	F	231	ASN	O-C-N	5.55	129.16	122.94
1	L	209	LEU	CA-C-O	5.55	126.37	120.10
1	C	78	LEU	O-C-N	5.55	130.15	123.16
1	D	204	VAL	N-CA-CB	-5.55	103.00	110.54
1	D	217	ASN	N-CA-C	-5.55	104.87	111.69
1	G	51	THR	N-CA-CB	-5.55	101.22	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	231	ASN	CA-CB-CG	-5.55	107.05	112.60
1	Q	33	ASP	CB-CA-C	5.55	120.09	110.94
1	Q	232	MET	CA-C-N	5.55	129.42	122.43
1	Q	232	MET	C-N-CA	5.55	129.42	122.43
1	G	34	GLU	N-CA-CB	5.54	118.17	109.69
1	N	106	ILE	CB-CG1-CD1	-5.54	102.16	113.80
1	D	52	GLU	CA-C-O	-5.54	114.97	121.07
1	H	146	LYS	CA-C-O	-5.54	113.46	120.28
1	K	52	GLU	O-C-N	-5.54	115.88	122.20
1	R	97	LEU	CA-C-N	-5.54	112.30	120.28
1	R	97	LEU	C-N-CA	-5.54	112.30	120.28
1	G	202	GLN	O-C-N	-5.54	116.25	122.12
1	H	202	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	J	267	ILE	CB-CA-C	5.54	118.64	110.77
1	L	133	ARG	CA-C-N	-5.54	112.30	120.28
1	L	133	ARG	C-N-CA	-5.54	112.30	120.28
1	O	270	LEU	N-CA-C	-5.54	102.55	110.59
1	Q	324	GLN	CG-CD-NE2	5.54	124.71	116.40
1	L	118	THR	OG1-CB-CG2	5.54	120.38	109.30
1	M	296	LYS	CB-CA-C	-5.54	100.52	109.72
1	A	292	PRO	CA-C-O	5.54	127.62	121.36
1	F	138	LYS	O-C-N	5.54	128.46	122.15
1	K	132	GLU	N-CA-CB	5.54	118.36	110.16
1	K	195	ASP	OD1-CG-OD2	5.54	136.19	122.90
1	C	72	SER	CA-C-N	-5.54	115.58	123.11
1	C	72	SER	C-N-CA	-5.54	115.58	123.11
1	C	188	PRO	CA-C-O	-5.54	115.43	123.07
1	D	195	ASP	N-CA-C	5.54	119.34	112.59
1	F	221	VAL	CA-C-N	-5.54	114.27	122.41
1	F	221	VAL	C-N-CA	-5.54	114.27	122.41
1	F	270	LEU	CA-C-O	-5.54	115.19	121.72
1	L	131	SER	CA-C-N	5.54	127.70	120.28
1	L	131	SER	C-N-CA	5.54	127.70	120.28
1	M	136	GLN	CA-C-O	5.54	126.40	120.70
1	P	295	TRP	CB-CA-C	-5.54	100.50	110.36
1	Q	290	PRO	N-CA-CB	5.54	106.28	102.35
1	F	254	THR	O-C-N	5.53	128.46	122.15
1	J	287	ASN	CB-CG-ND2	-5.53	108.10	116.40
1	M	160	SER	CA-C-O	-5.53	113.61	119.97
1	P	287	ASN	CB-CG-ND2	-5.53	108.10	116.40
1	Q	168	ASN	CA-CB-CG	-5.53	107.07	112.60
1	L	71	GLN	N-CA-C	-5.53	106.58	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	100	LYS	CA-CB-CG	5.53	125.16	114.10
1	D	128	ASP	O-C-N	-5.53	116.13	122.93
1	E	347	SER	O-C-N	5.53	129.94	122.59
1	C	94	ARG	CG-CD-NE	5.53	124.17	112.00
1	M	351	ALA	CA-C-O	5.53	127.49	121.02
1	N	59	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	O	14	GLU	CA-C-N	-5.53	112.87	120.28
1	O	14	GLU	C-N-CA	-5.53	112.87	120.28
1	A	343	VAL	CA-C-O	5.53	127.69	120.78
1	D	113	ALA	O-C-N	5.53	128.68	122.16
1	D	336	GLN	CG-CD-OE1	5.53	131.86	120.80
1	R	178	GLN	CB-CG-CD	5.53	122.00	112.60
1	B	95	ASN	CA-C-N	-5.53	112.74	120.53
1	B	95	ASN	C-N-CA	-5.53	112.74	120.53
1	B	307	ALA	CB-CA-C	-5.53	101.57	110.74
1	J	94	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	K	176	ILE	CA-C-O	-5.53	114.77	121.18
1	K	214	LYS	CA-C-N	-5.53	113.26	120.44
1	K	214	LYS	C-N-CA	-5.53	113.26	120.44
1	L	34	GLU	O-C-N	-5.53	116.23	122.97
1	A	223	LEU	CA-C-O	-5.52	114.69	120.55
1	F	110	GLN	CA-CB-CG	5.52	125.15	114.10
1	L	126	GLY	CA-C-N	-5.52	110.24	121.18
1	L	126	GLY	C-N-CA	-5.52	110.24	121.18
1	P	228	LEU	N-CA-C	-5.52	100.01	109.24
1	C	42	ARG	O-C-N	5.52	127.97	122.12
1	C	248	VAL	N-CA-CB	-5.52	103.03	110.54
1	H	142	VAL	N-CA-CB	-5.52	102.69	110.26
1	I	149	ALA	O-C-N	-5.52	116.88	123.06
1	I	180	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	I	322	ALA	CA-C-N	5.52	128.47	120.79
1	I	322	ALA	C-N-CA	5.52	128.47	120.79
1	J	327	PHE	CA-C-N	-5.52	112.88	120.28
1	J	327	PHE	C-N-CA	-5.52	112.88	120.28
1	R	184	PRO	CB-CA-C	-5.52	104.65	111.11
1	I	281	LEU	CA-C-O	-5.52	115.02	120.82
1	I	325	GLU	N-CA-CB	-5.52	101.85	109.91
1	Q	335	CYS	CA-C-N	-5.52	112.88	120.28
1	Q	335	CYS	C-N-CA	-5.52	112.88	120.28
1	E	93	PHE	O-C-N	-5.52	116.27	122.12
1	I	283	LEU	O-C-N	5.52	127.97	122.12
1	K	13	LYS	CB-CA-C	5.52	119.95	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	VAL	CA-C-O	5.52	126.71	120.42
1	H	118	THR	OG1-CB-CG2	5.52	120.33	109.30
1	H	158	PRO	O-C-N	5.52	131.58	121.10
1	N	135	ALA	O-C-N	5.52	127.97	122.12
1	N	217	ASN	O-C-N	5.52	129.40	122.23
1	P	118	THR	N-CA-CB	-5.52	101.27	111.53
1	P	154	ALA	O-C-N	-5.52	117.30	123.04
1	Q	190	VAL	CB-CA-C	-5.52	104.25	111.81
1	D	29	ILE	N-CA-CB	-5.52	101.79	111.39
1	D	220	HIS	N-CA-C	5.52	119.30	112.24
1	H	10	GLU	O-C-N	5.52	128.44	122.15
1	N	89	GLN	OE1-CD-NE2	5.52	128.12	122.60
1	Q	335	CYS	N-CA-C	-5.52	105.27	111.28
1	C	214	LYS	CG-CD-CE	-5.51	98.62	111.30
1	D	69	ILE	CB-CG1-CD1	5.51	125.38	113.80
1	E	284	ASN	CA-C-O	5.51	126.27	120.42
1	G	55	ARG	CG-CD-NE	5.51	124.13	112.00
1	M	203	TYR	CA-C-N	-5.51	112.59	120.42
1	M	203	TYR	C-N-CA	-5.51	112.59	120.42
1	C	173	TYR	CA-C-N	-5.51	112.89	120.28
1	C	173	TYR	C-N-CA	-5.51	112.89	120.28
1	O	291	LEU	CA-C-O	-5.51	112.61	120.16
1	F	169	ALA	CA-C-O	-5.51	114.58	120.42
1	G	188	PRO	CA-C-O	-5.51	110.57	120.60
1	H	231	ASN	OD1-CG-ND2	5.51	128.11	122.60
1	I	54	ASN	N-CA-CB	-5.51	102.02	110.12
1	K	10	GLU	N-CA-CB	5.51	118.00	110.01
1	P	70	ASN	OD1-CG-ND2	5.51	128.11	122.60
1	R	306	GLN	CA-C-O	5.51	125.11	119.05
1	K	95	ASN	CA-C-N	-5.51	112.60	120.42
1	K	95	ASN	C-N-CA	-5.51	112.60	120.42
1	K	343	VAL	O-C-N	-5.51	117.20	123.10
1	R	145	GLY	CA-C-O	5.51	127.47	121.57
1	A	198	LEU	CA-C-N	-5.51	111.94	120.31
1	A	198	LEU	C-N-CA	-5.51	111.94	120.31
1	Q	227	LEU	CA-C-O	-5.51	114.89	121.11
1	B	256	LEU	CA-C-N	-5.51	111.50	121.14
1	B	256	LEU	C-N-CA	-5.51	111.50	121.14
1	E	39	MET	N-CA-CB	-5.51	102.01	110.16
1	G	222	TYR	CA-C-N	-5.51	112.90	120.28
1	G	222	TYR	C-N-CA	-5.51	112.90	120.28
1	I	125	GLN	OE1-CD-NE2	-5.51	117.09	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	33	ASP	CA-C-O	-5.51	112.64	120.51
1	K	35	SER	O-C-N	5.51	129.37	122.65
1	P	140	ASP	CB-CG-OD2	5.51	131.07	118.40
1	R	6	ALA	CA-C-N	-5.50	113.21	122.29
1	R	6	ALA	C-N-CA	-5.50	113.21	122.29
1	J	200	HIS	CB-CA-C	5.50	120.77	110.70
1	L	70	ASN	O-C-N	-5.50	115.27	122.59
1	L	132	GLU	CA-C-N	-5.50	112.47	120.29
1	L	132	GLU	C-N-CA	-5.50	112.47	120.29
1	O	153	ILE	N-CA-CB	-5.50	104.77	111.21
1	Q	200	HIS	CA-CB-CG	5.50	119.30	113.80
1	R	24	ALA	CA-C-O	-5.50	115.01	120.90
1	B	69	ILE	CA-C-O	-5.50	113.90	120.78
1	C	65	VAL	CA-C-O	5.50	127.66	120.78
1	D	356	LEU	N-CA-CB	-5.50	101.15	110.50
1	I	69	ILE	CB-CA-C	5.50	120.31	111.29
1	J	132	GLU	CG-CD-OE1	5.50	131.06	118.40
1	N	293	LYS	O-C-N	5.50	125.67	121.27
1	O	217	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	O	253	VAL	CA-C-N	-5.50	113.29	120.44
1	O	253	VAL	C-N-CA	-5.50	113.29	120.44
1	D	300	SER	CA-C-N	-5.50	113.29	122.64
1	D	300	SER	C-N-CA	-5.50	113.29	122.64
1	J	257	HIS	CA-C-O	-5.50	112.49	119.31
1	N	163	ILE	CB-CA-C	-5.50	104.93	111.97
1	N	189	GLU	N-CA-C	5.50	118.89	110.20
1	H	38	THR	CA-CB-OG1	-5.50	101.35	109.60
1	H	300	SER	N-CA-C	-5.50	97.15	108.53
1	M	114	PRO	O-C-N	-5.50	116.19	123.01
1	E	33	ASP	CA-CB-CG	-5.50	107.10	112.60
1	E	116	ALA	N-CA-CB	5.50	118.12	110.04
1	F	344	HIS	N-CA-C	-5.50	102.49	110.24
1	I	229	LYS	CA-C-N	5.50	126.71	119.84
1	I	229	LYS	C-N-CA	5.50	126.71	119.84
1	M	20	GLN	CG-CD-NE2	-5.50	108.16	116.40
1	O	89	GLN	CA-C-O	-5.50	115.10	121.26
1	G	166	ASN	CA-C-O	-5.50	112.84	119.49
1	H	253	VAL	CA-C-N	-5.50	113.30	120.44
1	H	253	VAL	C-N-CA	-5.50	113.30	120.44
1	L	10	GLU	O-C-N	5.50	127.94	122.12
1	M	96	ILE	CA-C-O	-5.50	115.03	120.85
1	M	182	LEU	CA-C-O	5.50	126.90	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	GLY	CA-C-N	-5.49	113.96	122.86
1	C	272	GLY	C-N-CA	-5.49	113.96	122.86
1	F	136	GLN	CB-CG-CD	-5.49	103.26	112.60
1	I	78	LEU	CA-C-N	5.49	129.94	122.19
1	I	78	LEU	C-N-CA	5.49	129.94	122.19
1	O	330	ARG	CA-C-N	-5.49	112.37	120.28
1	O	330	ARG	C-N-CA	-5.49	112.37	120.28
1	R	193	ASP	O-C-N	5.49	129.67	122.97
1	A	168	ASN	OD1-CG-ND2	5.49	128.09	122.60
1	B	249	ALA	N-CA-C	5.49	116.95	111.07
1	F	109	ASP	CA-C-N	-5.49	113.45	123.34
1	F	109	ASP	C-N-CA	-5.49	113.45	123.34
1	L	165	GLU	N-CA-CB	-5.49	102.11	110.07
1	N	160	SER	CA-C-N	-5.49	113.16	120.79
1	N	160	SER	C-N-CA	-5.49	113.16	120.79
1	C	316	LYS	CA-CB-CG	-5.49	103.12	114.10
1	H	33	ASP	CA-C-O	-5.49	113.91	120.55
1	I	86	LYS	CA-C-N	-5.49	111.12	121.66
1	I	86	LYS	C-N-CA	-5.49	111.12	121.66
1	M	24	ALA	CB-CA-C	-5.49	102.26	110.88
1	R	308	SER	CB-CA-C	5.49	120.01	110.68
1	A	157	CYS	N-CA-CB	-5.49	98.20	110.27
1	B	96	ILE	N-CA-CB	-5.49	103.61	110.47
1	O	111	GLY	CA-C-O	5.49	127.62	122.57
1	R	258	ARG	CB-CA-C	-5.49	99.18	110.38
1	G	152	ARG	NH1-CZ-NH2	5.49	126.43	119.30
1	J	264	VAL	CA-C-N	5.49	124.83	118.85
1	J	264	VAL	C-N-CA	5.49	124.83	118.85
1	B	232	MET	N-CA-C	-5.49	101.60	110.32
1	E	315	GLY	N-CA-C	-5.49	107.75	115.32
1	K	230	PRO	CB-CA-C	-5.49	102.51	111.56
1	O	30	LEU	CA-C-O	-5.49	114.45	120.43
1	O	250	MET	CB-CA-C	-5.49	102.03	110.81
1	M	223	LEU	O-C-N	5.48	127.93	122.12
1	E	52	GLU	CA-C-O	-5.48	115.03	120.90
1	E	195	ASP	N-CA-CB	-5.48	101.78	110.28
1	J	285	ALA	CA-C-N	5.48	127.97	120.46
1	J	285	ALA	C-N-CA	5.48	127.97	120.46
1	K	194	GLY	CA-C-N	5.48	131.61	121.52
1	K	194	GLY	C-N-CA	5.48	131.61	121.52
1	R	73	ILE	N-CA-CB	-5.48	104.56	111.41
1	B	238	ALA	CA-C-O	-5.48	112.94	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	89	GLN	OE1-CD-NE2	5.48	128.08	122.60
1	H	282	ASN	CB-CG-ND2	-5.48	108.18	116.40
1	P	86	LYS	CA-C-N	5.48	132.01	121.54
1	P	86	LYS	C-N-CA	5.48	132.01	121.54
1	A	134	CYS	O-C-N	-5.48	115.90	122.15
1	Q	236	GLY	CA-C-N	5.48	128.41	120.79
1	Q	236	GLY	C-N-CA	5.48	128.41	120.79
1	A	236	GLY	N-CA-C	-5.48	105.53	112.54
1	D	89	GLN	CA-C-N	5.48	132.15	121.41
1	D	89	GLN	C-N-CA	5.48	132.15	121.41
1	I	132	GLU	CG-CD-OE1	5.48	131.00	118.40
1	K	99	GLU	OE1-CD-OE2	5.48	136.05	122.90
1	M	201	CYS	N-CA-C	-5.48	105.47	111.82
1	N	194	GLY	O-C-N	-5.48	116.63	123.37
1	P	89	GLN	O-C-N	5.48	129.76	122.26
1	Q	294	PRO	N-CA-CB	-5.48	98.26	103.41
1	E	162	ALA	CA-C-N	-5.48	112.11	121.97
1	E	162	ALA	C-N-CA	-5.48	112.11	121.97
1	F	124	ILE	CA-C-O	-5.48	114.54	120.67
1	F	145	GLY	CA-C-O	5.48	128.07	121.77
1	M	284	ASN	CA-CB-CG	-5.48	107.12	112.60
1	J	169	ALA	N-CA-C	-5.47	105.39	111.36
1	H	335	CYS	CB-CA-C	-5.47	101.71	110.79
1	M	154	ALA	O-C-N	-5.47	117.35	123.04
1	N	284	ASN	CA-C-O	5.47	126.34	120.70
1	R	310	LEU	CA-C-N	5.47	127.56	120.44
1	R	310	LEU	C-N-CA	5.47	127.56	120.44
1	B	274	MET	CA-C-O	5.47	127.17	121.15
1	B	275	SER	N-CA-C	-5.47	103.27	110.43
1	D	307	ALA	CB-CA-C	-5.47	102.47	110.95
1	D	341	GLN	O-C-N	-5.47	115.74	122.25
1	F	349	GLY	N-CA-C	-5.47	100.22	113.18
1	H	148	ARG	CA-C-O	5.47	126.51	120.71
1	I	56	ARG	NH1-CZ-NH2	5.47	126.41	119.30
1	L	15	LEU	O-C-N	5.47	127.92	122.12
1	L	232	MET	O-C-N	5.47	129.19	123.06
1	Q	138	LYS	N-CA-CB	5.47	117.94	110.01
1	Q	226	THR	O-C-N	-5.47	116.04	123.15
1	R	214	LYS	CG-CD-CE	-5.47	98.72	111.30
1	D	219	HIS	CA-CB-CG	5.47	119.27	113.80
1	H	220	HIS	CA-CB-CG	-5.47	108.33	113.80
1	I	172	ARG	O-C-N	5.47	128.00	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	179	GLN	CA-C-O	-5.47	111.94	119.05
1	F	29	ILE	CB-CG1-CD1	-5.47	102.32	113.80
1	H	326	ALA	CA-C-O	5.47	126.74	121.00
1	M	13	LYS	CA-C-O	5.47	126.34	120.55
1	O	120	LYS	CA-C-N	5.47	131.42	122.07
1	O	120	LYS	C-N-CA	5.47	131.42	122.07
1	O	187	GLU	CG-CD-OE2	5.47	130.97	118.40
1	O	328	MET	O-C-N	-5.47	114.92	122.46
1	A	11	GLN	CA-C-N	-5.46	112.53	120.29
1	A	11	GLN	C-N-CA	-5.46	112.53	120.29
1	C	299	PHE	CA-CB-CG	-5.46	108.33	113.80
1	E	87	ASP	CA-C-O	-5.46	115.21	121.82
1	J	344	HIS	N-CA-C	-5.46	101.00	109.14
1	O	210	ALA	CB-CA-C	5.46	121.53	110.38
1	P	212	VAL	N-CA-CB	5.46	116.36	110.62
1	A	132	GLU	N-CA-C	-5.46	105.41	111.36
1	B	34	GLU	CG-CD-OE1	5.46	130.96	118.40
1	E	53	GLU	N-CA-C	5.46	117.23	111.28
1	N	319	ASN	CA-CB-CG	-5.46	107.14	112.60
1	H	107	LYS	CA-C-O	-5.46	114.70	120.92
1	J	156	GLN	CA-CB-CG	-5.46	103.18	114.10
1	J	219	HIS	ND1-CG-CD2	-5.46	100.64	106.10
1	R	3	ARG	NH1-CZ-NH2	5.46	126.40	119.30
1	C	341	GLN	N-CA-CB	5.46	119.45	111.54
1	M	55	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	N	313	TRP	CB-CA-C	-5.46	102.24	110.92
1	P	227	LEU	CA-C-O	-5.46	115.23	121.40
1	B	335	CYS	O-C-N	-5.46	115.93	122.15
1	G	128	ASP	N-CA-C	-5.46	101.78	109.96
1	I	321	GLU	CB-CA-C	-5.46	102.28	110.90
1	D	17	GLU	CB-CG-CD	5.46	121.87	112.60
1	D	282	ASN	N-CA-CB	5.46	117.98	110.07
1	H	295	TRP	N-CA-C	5.46	118.47	109.85
1	A	127	LEU	CA-C-O	-5.45	113.36	119.79
1	B	62	LEU	N-CA-CB	5.45	118.14	110.12
1	N	168	ASN	N-CA-CB	5.45	118.14	110.12
1	N	259	THR	N-CA-CB	-5.45	102.74	110.81
1	R	153	ILE	N-CA-CB	-5.45	104.83	111.21
1	D	296	LYS	CB-CG-CD	-5.45	98.76	111.30
1	N	285	ALA	CA-C-N	-5.45	112.84	120.53
1	N	285	ALA	C-N-CA	-5.45	112.84	120.53
1	E	44	GLN	OE1-CD-NE2	-5.45	117.15	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	299	PHE	CA-C-O	5.45	127.82	121.44
1	H	288	LEU	CA-C-O	-5.45	112.69	119.28
1	I	15	LEU	O-C-N	5.45	128.97	122.27
1	J	3	ARG	NH1-CZ-NH2	-5.45	112.22	119.30
1	A	277	GLU	O-C-N	5.45	128.36	122.15
1	B	81	GLU	CB-CG-CD	5.45	121.86	112.60
1	E	197	ASP	CA-C-N	5.45	127.84	120.65
1	E	197	ASP	C-N-CA	5.45	127.84	120.65
1	G	199	GLU	CB-CG-CD	5.45	121.86	112.60
1	H	34	GLU	CA-C-O	5.45	127.18	121.19
1	I	108	LEU	N-CA-C	-5.45	107.18	113.88
1	E	64	SER	CA-C-O	-5.45	112.89	119.59
1	G	284	ASN	CA-CB-CG	-5.45	107.16	112.60
1	H	271	SER	CA-C-O	5.45	124.89	118.90
1	L	27	LYS	CB-CG-CD	5.45	123.83	111.30
1	M	37	GLY	N-CA-C	5.45	119.26	112.73
1	N	165	GLU	CG-CD-OE2	-5.45	105.88	118.40
1	N	217	ASN	OD1-CG-ND2	-5.45	117.16	122.60
1	O	169	ALA	CA-C-N	5.45	127.58	120.28
1	O	169	ALA	C-N-CA	5.45	127.58	120.28
1	E	6	ALA	O-C-N	5.44	129.31	122.23
1	K	234	THR	O-C-N	5.44	129.82	122.96
1	C	331	ALA	N-CA-C	-5.44	105.51	111.82
1	D	203	TYR	CB-CG-CD2	5.44	128.97	120.80
1	F	321	GLU	N-CA-C	5.44	116.89	111.07
1	K	220	HIS	CE1-NE2-CD2	5.44	114.44	109.00
1	O	307	ALA	CA-C-N	-5.44	111.43	120.68
1	O	307	ALA	C-N-CA	-5.44	111.43	120.68
1	Q	180	ASN	OD1-CG-ND2	5.44	128.04	122.60
1	R	46	ILE	CA-C-O	5.44	125.58	120.14
1	A	177	CYS	CA-C-N	-5.44	112.04	120.31
1	A	177	CYS	C-N-CA	-5.44	112.04	120.31
1	B	53	GLU	CA-C-O	-5.44	114.65	120.42
1	B	68	SER	CA-C-O	-5.44	112.73	120.51
1	D	38	THR	N-CA-C	-5.44	105.43	111.36
1	D	193	ASP	CA-CB-CG	5.44	118.04	112.60
1	F	56	ARG	CG-CD-NE	5.44	123.97	112.00
1	P	119	ASN	CA-C-O	-5.44	116.11	122.37
1	R	332	MET	CA-C-O	5.44	126.32	120.55
1	A	98	LYS	O-C-N	-5.44	116.36	122.12
1	E	136	GLN	CB-CG-CD	-5.44	103.36	112.60
1	F	5	PRO	O-C-N	5.44	129.48	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	44	GLN	N-CA-C	-5.44	104.58	111.11
1	L	160	SER	CB-CA-C	-5.44	101.44	110.68
1	O	227	LEU	CA-C-N	-5.44	114.28	122.81
1	O	227	LEU	C-N-CA	-5.44	114.28	122.81
1	A	118	THR	CA-C-O	-5.43	114.76	121.06
1	B	328	MET	CA-C-O	5.43	126.22	119.97
1	C	64	SER	O-C-N	-5.43	114.87	122.37
1	D	121	GLU	CB-CA-C	5.43	118.77	109.80
1	F	42	ARG	CG-CD-NE	5.43	123.95	112.00
1	J	94	ARG	CB-CA-C	-5.43	99.61	110.42
1	K	99	GLU	CB-CA-C	-5.43	100.57	110.63
1	K	176	ILE	CB-CG1-CD1	5.43	125.21	113.80
1	L	172	ARG	CA-C-O	5.43	126.53	120.82
1	B	213	TYR	CG-CD2-CE2	-5.43	113.05	121.20
1	G	213	TYR	N-CA-CB	5.43	118.70	110.28
1	H	95	ASN	CA-C-N	5.43	127.40	120.56
1	H	95	ASN	C-N-CA	5.43	127.40	120.56
1	M	190	VAL	CB-CA-C	-5.43	104.37	111.81
1	E	166	ASN	CA-CB-CG	-5.43	107.17	112.60
1	N	44	GLN	O-C-N	5.43	127.74	122.09
1	P	56	ARG	CD-NE-CZ	5.43	132.00	124.40
1	F	117	GLY	CA-C-O	5.43	126.55	120.03
1	I	94	ARG	O-C-N	-5.43	116.37	122.12
1	I	166	ASN	CA-CB-CG	5.43	118.03	112.60
1	K	241	LYS	N-CA-C	-5.43	102.85	110.50
1	P	248	VAL	O-C-N	5.43	127.14	121.87
1	A	184	PRO	CB-CA-C	-5.43	104.89	111.46
1	A	308	SER	CA-C-O	-5.43	115.12	120.82
1	H	81	GLU	CB-CG-CD	5.43	121.83	112.60
1	J	218	ASP	CA-C-N	-5.43	113.99	122.73
1	J	218	ASP	C-N-CA	-5.43	113.99	122.73
1	G	75	GLY	CA-C-N	-5.43	116.03	123.14
1	G	75	GLY	C-N-CA	-5.43	116.03	123.14
1	H	214	LYS	CG-CD-CE	-5.43	98.82	111.30
1	J	89	GLN	CG-CD-OE1	-5.42	109.95	120.80
1	D	331	ALA	CA-C-O	5.42	126.51	120.82
1	E	83	LEU	CA-C-N	-5.42	114.02	122.37
1	E	83	LEU	C-N-CA	-5.42	114.02	122.37
1	O	246	GLU	CA-C-O	-5.42	114.80	120.55
1	B	125	GLN	O-C-N	5.42	129.16	123.03
1	G	73	ILE	N-CA-C	5.42	115.66	107.80
1	N	194	GLY	N-CA-C	5.42	118.64	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	THR	O-C-N	5.42	129.79	122.96
1	J	335	CYS	CA-C-O	5.42	126.16	120.42
1	Q	88	SER	O-C-N	-5.42	115.20	122.19
1	C	36	VAL	N-CA-C	5.42	116.80	110.62
1	D	103	VAL	CA-C-N	-5.42	115.16	122.91
1	D	103	VAL	C-N-CA	-5.42	115.16	122.91
1	D	146	LYS	CA-C-O	-5.42	113.62	120.28
1	H	159	SER	CA-C-N	-5.42	112.60	120.29
1	H	159	SER	C-N-CA	-5.42	112.60	120.29
1	L	133	ARG	CB-CG-CD	5.42	123.76	111.30
1	L	299	PHE	CA-CB-CG	-5.42	108.38	113.80
1	M	271	SER	CA-C-N	5.42	132.03	121.41
1	M	271	SER	C-N-CA	5.42	132.03	121.41
1	P	119	ASN	OD1-CG-ND2	5.42	128.02	122.60
1	P	348	SER	N-CA-C	-5.42	103.38	110.53
1	C	56	ARG	O-C-N	5.42	127.65	122.07
1	P	358	THR	CA-C-N	5.42	128.53	120.95
1	P	358	THR	C-N-CA	5.42	128.53	120.95
1	C	142	VAL	N-CA-C	5.41	116.78	108.71
1	I	118	THR	N-CA-C	5.41	118.56	109.95
1	N	267	ILE	CB-CG1-CD1	-5.41	102.43	113.80
1	O	239	CYS	CA-C-O	-5.41	115.23	121.19
1	P	59	ARG	CA-CB-CG	-5.41	103.27	114.10
1	P	159	SER	CA-C-O	5.41	128.15	121.87
1	B	137	TYR	CB-CA-C	-5.41	102.15	110.81
1	J	301	TYR	N-CA-CB	-5.41	102.12	110.56
1	M	4	PHE	CA-C-N	5.41	125.33	119.76
1	M	4	PHE	C-N-CA	5.41	125.33	119.76
1	Q	209	LEU	O-C-N	-5.41	116.50	122.07
1	E	161	LEU	CA-C-N	-5.41	112.61	120.29
1	E	161	LEU	C-N-CA	-5.41	112.61	120.29
1	H	204	VAL	CA-CB-CG2	-5.41	101.20	110.40
1	K	50	ASN	CB-CG-ND2	5.41	124.52	116.40
1	M	248	VAL	CA-CB-CG2	-5.41	101.20	110.40
1	O	248	VAL	CB-CA-C	-5.41	104.83	112.14
1	C	97	LEU	CA-C-O	5.41	126.50	120.82
1	Q	33	ASP	CA-CB-CG	-5.41	107.19	112.60
1	D	3	ARG	NH1-CZ-NH2	-5.41	112.27	119.30
1	Q	207	LYS	CA-CB-CG	5.41	124.91	114.10
1	D	90	GLY	CA-C-O	-5.41	111.17	120.57
1	K	109	ASP	CB-CG-OD1	5.41	130.83	118.40
1	C	25	ASN	OD1-CG-ND2	5.40	128.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	GLN	CB-CG-CD	-5.40	103.42	112.60
1	E	50	ASN	CA-C-O	-5.40	115.87	122.41
1	E	136	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	E	209	LEU	CA-C-O	5.40	126.15	120.42
1	N	20	GLN	CA-C-O	5.40	126.15	120.42
1	O	125	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	P	10	GLU	CA-C-N	-5.40	113.04	120.28
1	P	10	GLU	C-N-CA	-5.40	113.04	120.28
1	G	130	LEU	N-CA-CB	5.40	117.84	110.01
1	G	138	LYS	CB-CG-CD	5.40	123.72	111.30
1	I	98	LYS	CG-CD-CE	5.40	123.72	111.30
1	K	215	ALA	N-CA-CB	-5.40	102.18	110.01
1	M	284	ASN	CA-C-O	-5.40	114.69	120.42
1	O	65	VAL	CB-CA-C	-5.40	102.43	111.29
1	R	20	GLN	N-CA-CB	5.40	118.06	110.12
1	D	87	ASP	CB-CG-OD1	-5.40	105.98	118.40
1	F	155	ASP	CA-CB-CG	5.40	118.00	112.60
1	I	115	LEU	CA-C-O	5.40	127.75	121.11
1	J	53	GLU	CG-CD-OE1	5.40	130.81	118.40
1	L	156	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	E	335	CYS	CA-C-N	-5.40	112.63	120.29
1	E	335	CYS	C-N-CA	-5.40	112.63	120.29
1	J	66	ASP	CA-C-O	5.40	127.08	121.15
1	O	341	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	D	110	GLN	CA-C-O	-5.39	114.98	121.34
1	D	275	SER	N-CA-CB	-5.39	102.95	110.29
1	G	17	GLU	N-CA-CB	5.39	118.14	110.16
1	K	90	GLY	O-C-N	5.39	128.24	122.41
1	B	204	VAL	CA-CB-CG2	-5.39	101.23	110.40
1	D	346	GLY	O-C-N	-5.39	115.69	122.70
1	F	287	ASN	CA-C-O	-5.39	112.04	119.05
1	L	98	LYS	CA-C-N	-5.39	111.72	120.72
1	L	98	LYS	C-N-CA	-5.39	111.72	120.72
1	P	49	GLU	CB-CG-CD	5.39	121.77	112.60
1	Q	245	PRO	N-CA-C	-5.39	105.72	113.75
1	A	173	TYR	CA-C-N	-5.39	113.06	120.28
1	A	173	TYR	C-N-CA	-5.39	113.06	120.28
1	B	172	ARG	CA-C-O	5.39	126.22	120.24
1	E	148	ARG	N-CA-CB	-5.39	101.64	110.43
1	F	5	PRO	N-CD-CG	-5.39	95.12	103.20
1	H	342	TYR	O-C-N	5.39	129.35	123.04
1	I	251	ALA	N-CA-CB	5.39	118.04	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	286	ILE	CA-C-O	-5.39	114.80	120.57
1	K	41	ASN	OD1-CG-ND2	5.39	127.99	122.60
1	O	208	VAL	CA-CB-CG1	-5.39	101.24	110.40
1	Q	50	ASN	CB-CG-ND2	5.39	124.48	116.40
1	B	80	HIS	N-CA-C	5.39	122.28	110.80
1	D	282	ASN	CB-CG-OD1	-5.39	110.02	120.80
1	B	91	LYS	CA-C-O	-5.39	114.61	120.81
1	C	206	GLU	CG-CD-OE1	5.39	130.79	118.40
1	F	178	GLN	CA-C-O	5.39	126.45	120.63
1	H	258	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	H	327	PHE	CA-C-O	5.39	126.26	120.55
1	J	64	SER	CA-C-O	-5.39	112.97	119.59
1	L	231	ASN	N-CA-C	-5.39	103.28	110.55
1	O	172	ARG	CA-C-O	5.39	126.13	120.42
1	I	92	LEU	O-C-N	-5.38	116.74	123.04
1	J	115	LEU	O-C-N	-5.38	116.92	123.27
1	O	191	ILE	CB-CG1-CD1	-5.38	102.49	113.80
1	P	149	ALA	CA-C-N	5.38	130.43	123.11
1	P	149	ALA	C-N-CA	5.38	130.43	123.11
1	Q	210	ALA	O-C-N	5.38	128.52	122.22
1	Q	250	MET	CA-CB-CG	-5.38	103.33	114.10
1	E	10	GLU	O-C-N	-5.38	116.01	122.15
1	I	87	ASP	CB-CG-OD1	-5.38	106.02	118.40
1	H	140	ASP	CA-CB-CG	-5.38	107.22	112.60
1	H	347	SER	O-C-N	5.38	129.75	122.59
1	I	40	GLY	CA-C-N	-5.38	113.44	120.44
1	I	40	GLY	C-N-CA	-5.38	113.44	120.44
1	J	341	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	O	255	ALA	N-CA-C	5.38	117.57	111.11
1	R	9	GLN	CB-CA-C	-5.38	101.53	110.68
1	R	27	LYS	CA-C-N	5.38	131.96	121.41
1	R	27	LYS	C-N-CA	5.38	131.96	121.41
1	L	15	LEU	CA-C-N	-5.38	113.07	120.28
1	L	15	LEU	C-N-CA	-5.38	113.07	120.28
1	B	133	ARG	CA-C-N	-5.38	113.07	120.28
1	B	133	ARG	C-N-CA	-5.38	113.07	120.28
1	C	106	ILE	CB-CG1-CD1	-5.38	102.51	113.80
1	D	29	ILE	O-C-N	-5.38	117.37	123.18
1	D	93	PHE	CA-CB-CG	5.38	119.18	113.80
1	G	217	ASN	CB-CG-ND2	5.38	124.47	116.40
1	M	3	ARG	CA-CB-CG	5.38	124.86	114.10
1	M	10	GLU	CA-C-N	-5.38	113.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	10	GLU	C-N-CA	-5.38	113.07	120.28
1	N	62	LEU	N-CA-C	-5.38	105.58	111.82
1	P	125	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	R	42	ARG	CA-C-O	-5.38	114.72	120.42
1	B	118	THR	O-C-N	-5.38	115.57	122.94
1	E	4	PHE	O-C-N	5.38	125.74	121.17
1	G	172	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	I	206	GLU	CA-CB-CG	5.38	124.85	114.10
1	J	354	GLN	N-CA-C	5.38	118.06	111.82
1	Q	5	PRO	CB-CA-C	-5.38	104.73	111.56
1	G	226	THR	CA-CB-CG2	5.38	119.64	110.50
1	M	258	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	A	200	HIS	CE1-NE2-CD2	5.37	114.37	109.00
1	B	334	ASN	CA-C-N	-5.37	112.66	120.29
1	B	334	ASN	C-N-CA	-5.37	112.66	120.29
1	G	1	ALA	CA-C-N	5.37	131.80	121.54
1	G	1	ALA	C-N-CA	5.37	131.80	121.54
1	J	108	LEU	N-CA-CB	-5.37	103.46	110.88
1	L	288	LEU	CA-C-O	5.37	125.64	119.35
1	C	172	ARG	CA-C-O	5.37	126.65	120.90
1	D	194	GLY	N-CA-C	5.37	118.58	111.70
1	E	185	ILE	N-CA-CB	5.37	117.12	111.00
1	F	162	ALA	CA-C-N	-5.37	112.79	120.42
1	F	162	ALA	C-N-CA	-5.37	112.79	120.42
1	G	5	PRO	O-C-N	5.37	129.81	122.99
1	I	152	ARG	CD-NE-CZ	-5.37	116.88	124.40
1	J	347	SER	CA-C-N	5.37	131.80	121.54
1	J	347	SER	C-N-CA	5.37	131.80	121.54
1	M	214	LYS	CG-CD-CE	-5.37	98.94	111.30
1	N	316	LYS	CA-CB-CG	-5.37	103.36	114.10
1	O	87	ASP	CA-CB-CG	5.37	117.97	112.60
1	Q	32	ALA	N-CA-CB	-5.37	102.42	110.91
1	F	253	VAL	O-C-N	-5.37	116.66	121.87
1	L	41	ASN	O-C-N	5.37	128.27	122.15
1	B	328	MET	N-CA-CB	-5.37	101.96	110.28
1	E	255	ALA	O-C-N	5.37	127.81	122.12
1	H	2	HIS	ND1-CG-CD2	-5.37	100.73	106.10
1	H	73	ILE	N-CA-CB	-5.37	104.70	111.41
1	I	182	LEU	N-CA-CB	-5.37	101.88	110.63
1	J	247	GLN	CB-CG-CD	-5.37	103.47	112.60
1	K	342	TYR	N-CA-CB	-5.37	101.95	110.06
1	O	246	GLU	N-CA-C	-5.37	105.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	PRO	O-C-N	-5.37	116.97	123.03
1	O	54	ASN	CA-CB-CG	-5.37	107.23	112.60
1	B	230	PRO	CB-CA-C	-5.37	102.39	110.17
1	E	207	LYS	CD-CE-NZ	5.37	129.07	111.90
1	I	305	LEU	N-CA-C	-5.37	106.41	113.17
1	J	325	GLU	CB-CG-CD	-5.37	103.48	112.60
1	K	169	ALA	O-C-N	5.37	128.27	122.15
1	K	179	GLN	OE1-CD-NE2	5.37	127.97	122.60
1	N	247	GLN	CG-CD-NE2	-5.37	108.35	116.40
1	P	326	ALA	CA-C-N	-5.37	113.47	120.44
1	P	326	ALA	C-N-CA	-5.37	113.47	120.44
1	B	179	GLN	CA-CB-CG	-5.36	103.38	114.10
1	E	195	ASP	N-CA-C	5.36	118.04	111.82
1	G	48	VAL	CA-C-O	5.36	126.28	120.43
1	G	76	VAL	CA-CB-CG2	-5.36	101.28	110.40
1	H	255	ALA	CA-C-N	-5.36	112.67	120.29
1	H	255	ALA	C-N-CA	-5.36	112.67	120.29
1	J	73	ILE	N-CA-C	5.36	116.44	108.23
1	C	89	GLN	CB-CG-CD	-5.36	103.48	112.60
1	H	169	ALA	O-C-N	5.36	128.26	122.15
1	I	264	VAL	N-CA-CB	-5.36	103.70	111.21
1	N	296	LYS	CB-CA-C	-5.36	100.02	109.62
1	Q	218	ASP	N-CA-C	5.36	118.04	111.82
1	B	255	ALA	CA-C-O	5.36	126.45	120.82
1	C	249	ALA	CA-C-N	-5.36	112.68	120.29
1	C	249	ALA	C-N-CA	-5.36	112.68	120.29
1	D	248	VAL	CA-CB-CG2	-5.36	101.29	110.40
1	E	10	GLU	CA-CB-CG	5.36	124.82	114.10
1	F	56	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	G	59	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	I	175	SER	N-CA-CB	-5.36	101.97	110.28
1	J	52	GLU	CB-CG-CD	5.36	121.71	112.60
1	N	193	ASP	CA-C-N	5.36	131.33	122.65
1	N	193	ASP	C-N-CA	5.36	131.33	122.65
1	R	165	GLU	N-CA-C	5.36	117.12	111.28
1	A	132	GLU	CA-C-O	-5.36	114.74	120.42
1	N	165	GLU	CB-CA-C	5.36	119.29	110.88
1	B	148	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	G	89	GLN	CG-CD-NE2	-5.36	108.36	116.40
1	G	261	PRO	O-C-N	5.36	129.65	123.01
1	H	17	GLU	CA-C-N	-5.36	114.18	120.72
1	H	17	GLU	C-N-CA	-5.36	114.18	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	192	PRO	CB-CA-C	-5.36	102.95	111.04
1	N	178	GLN	CA-CB-CG	-5.36	103.39	114.10
1	Q	132	GLU	CA-CB-CG	5.36	124.81	114.10
1	R	61	ILE	N-CA-C	-5.36	105.16	111.00
1	C	250	MET	O-C-N	5.36	128.25	122.15
1	D	336	GLN	OE1-CD-NE2	-5.36	117.25	122.60
1	G	10	GLU	CA-C-N	-5.36	112.17	120.31
1	G	10	GLU	C-N-CA	-5.36	112.17	120.31
1	I	133	ARG	CA-C-O	5.36	126.44	120.82
1	L	104	VAL	CA-CB-CG2	-5.36	101.29	110.40
1	N	231	ASN	CA-CB-CG	-5.36	107.24	112.60
1	P	283	LEU	N-CA-C	-5.36	105.61	111.82
1	F	284	ASN	CA-CB-CG	-5.35	107.25	112.60
1	G	168	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	H	195	ASP	CA-CB-CG	-5.35	107.25	112.60
1	B	42	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	G	292	PRO	CB-CA-C	-5.35	104.84	111.64
1	M	190	VAL	CA-C-O	5.35	127.34	120.97
1	R	341	GLN	O-C-N	-5.35	115.88	122.25
1	L	142	VAL	CA-C-N	-5.35	113.94	122.29
1	L	142	VAL	C-N-CA	-5.35	113.94	122.29
1	B	34	GLU	CB-CG-CD	5.35	121.69	112.60
1	B	213	TYR	CB-CA-C	5.35	119.67	110.79
1	E	171	ALA	N-CA-C	-5.35	105.53	111.36
1	F	254	THR	N-CA-C	-5.35	105.53	111.36
1	G	169	ALA	N-CA-C	-5.35	105.36	111.14
1	G	185	ILE	CB-CA-C	-5.35	104.98	111.88
1	N	233	VAL	O-C-N	-5.35	116.85	122.68
1	N	306	GLN	CG-CD-NE2	-5.35	108.38	116.40
1	A	254	THR	CA-C-N	-5.35	113.49	120.44
1	A	254	THR	C-N-CA	-5.35	113.49	120.44
1	K	277	GLU	CG-CD-OE1	5.35	130.70	118.40
1	M	156	GLN	CB-CG-CD	-5.35	103.51	112.60
1	O	85	GLN	CA-C-O	5.35	128.15	121.89
1	R	134	CYS	CA-C-O	5.35	126.09	120.42
1	I	122	THR	CA-C-O	5.35	127.69	121.44
1	J	128	ASP	CA-CB-CG	5.35	117.95	112.60
1	N	287	ASN	CA-CB-CG	-5.35	107.25	112.60
1	B	3	ARG	NH1-CZ-NH2	-5.34	112.35	119.30
1	F	52	GLU	O-C-N	5.34	127.80	122.08
1	N	109	ASP	CA-C-O	-5.34	112.87	120.51
1	N	217	ASN	CB-CG-ND2	5.34	124.42	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	ILE	O-C-N	-5.34	117.27	122.99
1	A	123	THR	CA-C-O	-5.34	114.13	121.98
1	C	124	ILE	N-CA-CB	-5.34	104.04	111.41
1	D	1	ALA	N-CA-C	5.34	125.95	111.00
1	H	199	GLU	CA-CB-CG	5.34	124.78	114.10
1	I	12	LYS	CB-CG-CD	-5.34	99.01	111.30
1	R	172	ARG	CD-NE-CZ	-5.34	116.92	124.40
1	D	126	GLY	O-C-N	5.34	129.64	122.70
1	E	156	GLN	N-CA-C	5.34	118.95	111.90
1	G	133	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	G	343	VAL	N-CA-CB	5.34	121.81	111.93
1	J	343	VAL	N-CA-CB	5.34	120.04	111.23
1	L	287	ASN	CA-C-N	-5.34	113.73	122.54
1	L	287	ASN	C-N-CA	-5.34	113.73	122.54
1	N	160	SER	N-CA-C	-5.34	105.36	111.07
1	O	78	LEU	CA-C-O	-5.34	115.08	121.11
1	C	172	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	G	150	VAL	CA-C-N	5.34	130.94	122.94
1	G	150	VAL	C-N-CA	5.34	130.94	122.94
1	H	86	LYS	CA-C-N	-5.34	111.94	122.02
1	H	86	LYS	C-N-CA	-5.34	111.94	122.02
1	L	329	LYS	CA-C-O	-5.34	115.40	120.90
1	N	42	ARG	N-CA-CB	5.34	117.96	110.12
1	N	330	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
1	R	224	GLU	CG-CD-OE2	5.34	130.67	118.40
1	J	343	VAL	CA-C-N	-5.33	113.82	122.36
1	J	343	VAL	C-N-CA	-5.33	113.82	122.36
1	K	291	LEU	O-C-N	-5.33	117.76	121.65
1	Q	267	ILE	CB-CG1-CD1	-5.33	102.60	113.80
1	D	65	VAL	O-C-N	-5.33	117.13	122.62
1	F	176	ILE	CA-C-O	-5.33	115.20	120.85
1	I	223	LEU	N-CA-CB	5.33	117.74	110.01
1	K	10	GLU	CB-CG-CD	-5.33	103.53	112.60
1	K	62	LEU	O-C-N	-5.33	115.50	122.59
1	K	212	VAL	CA-CB-CG2	-5.33	101.33	110.40
1	O	16	SER	CA-C-N	-5.33	113.51	120.44
1	O	16	SER	C-N-CA	-5.33	113.51	120.44
1	Q	264	VAL	O-C-N	-5.33	115.02	121.10
1	I	290	PRO	N-CA-CB	-5.33	98.56	102.35
1	J	184	PRO	O-C-N	-5.33	116.70	123.10
1	M	201	CYS	CA-C-N	-5.33	113.14	120.28
1	M	201	CYS	C-N-CA	-5.33	113.14	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	218	ASP	CA-CB-CG	-5.33	107.27	112.60
1	D	10	GLU	CA-C-O	-5.33	114.90	120.55
1	G	296	LYS	N-CA-CB	5.33	117.79	109.85
1	B	132	GLU	CG-CD-OE1	5.33	130.66	118.40
1	C	108	LEU	CA-C-N	-5.33	111.04	121.06
1	C	108	LEU	C-N-CA	-5.33	111.04	121.06
1	E	327	PHE	CA-CB-CG	-5.33	108.47	113.80
1	F	103	VAL	N-CA-C	5.33	116.56	109.37
1	F	244	THR	CA-CB-OG1	-5.33	101.61	109.60
1	I	49	GLU	N-CA-C	5.33	117.90	109.96
1	Q	226	THR	N-CA-C	5.33	117.78	109.52
1	D	332	MET	CA-C-N	5.33	127.42	120.28
1	D	332	MET	C-N-CA	5.33	127.42	120.28
1	K	104	VAL	CB-CA-C	-5.33	102.89	110.83
1	C	173	TYR	CB-CG-CD2	-5.33	112.81	120.80
1	D	355	SER	N-CA-CB	5.33	119.49	110.49
1	E	154	ALA	CA-C-N	-5.33	113.14	121.02
1	E	154	ALA	C-N-CA	-5.33	113.14	121.02
1	E	282	ASN	CA-C-O	5.33	126.15	120.24
1	G	92	LEU	CB-CA-C	-5.33	102.49	110.16
1	H	306	GLN	O-C-N	-5.33	115.80	122.35
1	K	160	SER	CA-CB-OG	-5.33	100.45	111.10
1	M	81	GLU	CA-C-O	5.33	126.59	121.00
1	Q	228	LEU	O-C-N	-5.33	117.01	123.29
1	D	128	ASP	CA-C-O	5.32	126.93	120.81
1	E	125	GLN	CG-CD-NE2	5.32	124.39	116.40
1	E	139	LYS	CA-C-N	-5.32	113.98	122.66
1	E	139	LYS	C-N-CA	-5.32	113.98	122.66
1	F	152	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	I	103	VAL	CA-C-N	-5.32	116.59	123.19
1	I	103	VAL	C-N-CA	-5.32	116.59	123.19
1	M	11	GLN	CB-CG-CD	5.32	121.65	112.60
1	Q	157	CYS	CA-C-O	-5.32	114.44	120.46
1	R	214	LYS	N-CA-CB	5.32	118.46	109.78
1	B	184	PRO	CB-CA-C	-5.32	103.35	110.85
1	D	221	VAL	CA-C-N	5.32	130.85	122.34
1	D	221	VAL	C-N-CA	5.32	130.85	122.34
1	G	272	GLY	CA-C-N	-5.32	110.98	121.41
1	G	272	GLY	C-N-CA	-5.32	110.98	121.41
1	M	176	ILE	CA-C-N	-5.32	113.09	120.38
1	M	176	ILE	C-N-CA	-5.32	113.09	120.38
1	N	96	ILE	CA-CB-CG2	-5.32	101.45	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	167	ALA	CA-C-O	5.32	126.19	120.55
1	P	54	ASN	CA-CB-CG	-5.32	107.28	112.60
1	P	258	ARG	NH1-CZ-NH2	-5.32	112.38	119.30
1	P	341	GLN	CB-CG-CD	5.32	121.64	112.60
1	H	134	CYS	O-C-N	-5.32	116.09	122.15
1	I	194	GLY	N-CA-C	5.32	117.45	112.08
1	O	189	GLU	CA-CB-CG	-5.32	103.46	114.10
1	O	248	VAL	O-C-N	5.32	127.03	121.87
1	Q	109	ASP	N-CA-C	-5.32	103.87	110.41
1	Q	140	ASP	CA-CB-CG	-5.32	107.28	112.60
1	E	168	ASN	CA-C-N	-5.32	113.15	120.28
1	E	168	ASN	C-N-CA	-5.32	113.15	120.28
1	M	63	PHE	N-CA-C	5.32	119.61	113.18
1	B	54	ASN	CA-C-N	5.32	127.35	120.44
1	B	54	ASN	C-N-CA	5.32	127.35	120.44
1	E	118	THR	O-C-N	-5.32	116.74	123.17
1	E	121	GLU	CA-C-O	5.32	127.58	121.47
1	H	277	GLU	CA-C-N	-5.32	112.63	120.28
1	H	277	GLU	C-N-CA	-5.32	112.63	120.28
1	J	86	LYS	N-CA-C	5.32	118.25	109.85
1	Q	4	PHE	O-C-N	-5.32	115.21	121.32
1	A	125	GLN	CB-CA-C	-5.31	100.53	109.83
1	F	75	GLY	O-C-N	-5.31	118.62	123.56
1	O	36	VAL	CA-C-O	-5.31	115.88	121.41
1	A	29	ILE	N-CA-C	5.31	116.13	108.48
1	A	134	CYS	CA-C-O	5.31	126.05	120.42
1	B	39	MET	CA-C-O	-5.31	114.25	120.20
1	C	58	PHE	CA-C-N	-5.31	112.23	120.31
1	C	58	PHE	C-N-CA	-5.31	112.23	120.31
1	E	20	GLN	CA-C-N	-5.31	112.23	120.31
1	E	20	GLN	C-N-CA	-5.31	112.23	120.31
1	L	198	LEU	N-CA-C	5.31	116.76	110.97
1	M	18	ILE	CA-C-N	-5.31	113.16	120.28
1	M	18	ILE	C-N-CA	-5.31	113.16	120.28
1	M	95	ASN	CA-C-N	-5.31	112.88	120.42
1	M	95	ASN	C-N-CA	-5.31	112.88	120.42
1	P	338	ALA	CA-C-N	-5.31	114.31	122.60
1	P	338	ALA	C-N-CA	-5.31	114.31	122.60
1	K	283	LEU	CD1-CG-CD2	-5.31	99.12	110.80
1	C	250	MET	N-CA-C	-5.31	105.57	111.36
1	O	287	ASN	CA-C-N	-5.31	113.78	122.54
1	O	287	ASN	C-N-CA	-5.31	113.78	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	54	ASN	CA-C-N	-5.31	113.54	120.44
1	P	54	ASN	C-N-CA	-5.31	113.54	120.44
1	R	303	ARG	N-CA-C	5.31	116.87	111.14
1	C	8	THR	CA-CB-OG1	5.31	117.56	109.60
1	C	20	GLN	CA-C-N	-5.31	111.86	120.72
1	C	20	GLN	C-N-CA	-5.31	111.86	120.72
1	G	323	THR	CA-CB-CG2	-5.31	101.48	110.50
1	K	79	PHE	CA-C-O	-5.31	115.02	121.28
1	L	307	ALA	CB-CA-C	-5.31	99.86	110.42
1	O	149	ALA	O-C-N	5.31	129.20	123.10
1	P	98	LYS	N-CA-C	5.31	116.75	111.07
1	P	258	ARG	CA-CB-CG	5.31	124.72	114.10
1	K	327	PHE	CB-CA-C	-5.31	102.32	110.81
1	P	231	ASN	CB-CG-ND2	5.31	124.36	116.40
1	A	267	ILE	N-CA-CB	5.30	119.03	111.82
1	D	10	GLU	CB-CG-CD	-5.30	103.58	112.60
1	D	137	TYR	O-C-N	-5.30	116.50	122.12
1	E	96	ILE	O-C-N	5.30	127.11	121.91
1	F	231	ASN	N-CA-C	-5.30	102.67	110.52
1	O	81	GLU	CB-CG-CD	5.30	121.62	112.60
1	E	169	ALA	CA-C-O	-5.30	114.93	120.55
1	B	4	PHE	CA-CB-CG	-5.30	108.50	113.80
1	H	99	GLU	CG-CD-OE2	-5.30	106.21	118.40
1	H	207	LYS	CD-CE-NZ	5.30	128.87	111.90
1	M	110	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	R	94	ARG	NH1-CZ-NH2	5.30	126.19	119.30
1	A	306	GLN	N-CA-C	5.30	122.08	114.39
1	C	41	ASN	O-C-N	5.30	127.53	122.07
1	E	326	ALA	CA-C-N	-5.30	113.55	120.44
1	E	326	ALA	C-N-CA	-5.30	113.55	120.44
1	F	146	LYS	CG-CD-CE	5.30	123.49	111.30
1	G	85	GLN	CG-CD-OE1	5.30	131.40	120.80
1	G	107	LYS	O-C-N	5.30	129.71	122.82
1	G	160	SER	CA-C-O	5.30	126.06	119.97
1	L	59	ARG	CA-C-O	-5.30	114.93	120.55
1	R	109	ASP	N-CA-CB	5.30	118.02	110.44
1	E	220	HIS	CA-C-O	-5.30	114.24	120.81
1	G	203	TYR	CA-C-O	-5.30	114.80	120.42
1	H	142	VAL	CA-C-N	-5.30	113.91	122.23
1	H	142	VAL	C-N-CA	-5.30	113.91	122.23
1	J	282	ASN	N-CA-C	-5.30	105.59	111.36
1	I	118	THR	OG1-CB-CG2	5.30	119.89	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	259	THR	O-C-N	-5.30	116.48	122.10
1	D	96	ILE	CA-C-N	5.29	127.64	120.44
1	D	96	ILE	C-N-CA	5.29	127.64	120.44
1	K	195	ASP	CB-CG-OD1	-5.29	106.22	118.40
1	M	52	GLU	N-CA-CB	5.29	117.83	109.94
1	N	122	THR	O-C-N	5.29	130.03	123.15
1	R	215	ALA	CB-CA-C	-5.29	101.85	110.85
1	A	205	THR	CA-CB-OG1	5.29	117.54	109.60
1	H	138	LYS	O-C-N	-5.29	116.51	122.12
1	H	187	GLU	N-CA-C	5.29	120.09	108.66
1	H	345	THR	O-C-N	-5.29	115.55	122.59
1	N	110	GLN	CA-C-N	-5.29	110.50	122.04
1	N	110	GLN	C-N-CA	-5.29	110.50	122.04
1	Q	142	VAL	O-C-N	-5.29	115.99	122.61
1	A	285	ALA	O-C-N	-5.29	116.51	122.12
1	C	11	GLN	OE1-CD-NE2	5.29	127.89	122.60
1	E	257	HIS	N-CA-C	-5.29	106.33	112.89
1	J	100	LYS	CA-C-N	5.29	129.48	120.91
1	J	100	LYS	C-N-CA	5.29	129.48	120.91
1	J	137	TYR	CA-C-O	5.29	126.03	120.42
1	L	61	ILE	N-CA-CB	5.29	116.38	110.51
1	O	187	GLU	OE1-CD-OE2	-5.29	110.20	122.90
1	P	180	ASN	OD1-CG-ND2	5.29	127.89	122.60
1	B	287	ASN	CA-C-N	-5.29	112.22	122.06
1	B	287	ASN	C-N-CA	-5.29	112.22	122.06
1	C	258	ARG	O-C-N	5.29	129.42	122.33
1	G	159	SER	N-CA-CB	-5.29	102.40	110.49
1	K	301	TYR	O-C-N	-5.29	117.14	123.06
1	P	87	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	303	ARG	CA-C-N	5.29	128.10	120.38
1	C	303	ARG	C-N-CA	5.29	128.10	120.38
1	E	295	TRP	CD2-CE2-CZ2	5.29	127.69	122.40
1	G	20	GLN	CA-C-O	5.29	126.07	120.10
1	J	109	ASP	CB-CG-OD2	-5.29	106.24	118.40
1	J	57	GLN	CG-CD-OE1	5.29	131.37	120.80
1	J	193	ASP	CA-C-O	-5.29	115.38	121.19
1	L	118	THR	O-C-N	-5.29	115.62	122.97
1	N	4	PHE	N-CA-C	-5.29	98.13	109.81
1	B	131	SER	CA-C-N	5.28	127.31	120.44
1	B	131	SER	C-N-CA	5.28	127.31	120.44
1	B	197	ASP	O-C-N	-5.28	116.39	122.20
1	R	292	PRO	CA-C-N	-5.28	117.14	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	292	PRO	C-N-CA	-5.28	117.14	122.74
1	B	82	THR	CB-CA-C	5.28	120.40	110.63
1	F	219	HIS	N-CA-C	5.28	119.44	113.15
1	D	205	THR	N-CA-CB	5.28	117.67	110.01
1	E	26	GLY	CA-C-N	-5.28	111.36	120.97
1	E	26	GLY	C-N-CA	-5.28	111.36	120.97
1	E	87	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	277	GLU	CA-C-N	-5.28	112.80	120.29
1	A	277	GLU	C-N-CA	-5.28	112.80	120.29
1	D	18	ILE	N-CA-C	-5.28	105.57	110.53
1	E	9	GLN	CB-CG-CD	-5.28	103.63	112.60
1	K	164	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	C	8	THR	OG1-CB-CG2	-5.28	98.75	109.30
1	C	127	LEU	CA-C-N	-5.28	113.21	121.02
1	C	127	LEU	C-N-CA	-5.28	113.21	121.02
1	C	156	GLN	N-CA-C	5.28	119.30	112.86
1	F	256	LEU	N-CA-C	-5.28	105.53	111.28
1	H	354	GLN	OE1-CD-NE2	5.28	127.88	122.60
1	I	80	HIS	CA-CB-CG	5.28	119.08	113.80
1	N	195	ASP	CB-CA-C	-5.28	99.28	110.31
1	P	351	ALA	CA-C-N	-5.28	110.40	122.95
1	P	351	ALA	C-N-CA	-5.28	110.40	122.95
1	E	103	VAL	CB-CA-C	-5.27	103.85	111.34
1	I	176	ILE	N-CA-CB	-5.27	101.75	110.56
1	B	132	GLU	CA-C-N	-5.27	113.42	120.54
1	B	132	GLU	C-N-CA	-5.27	113.42	120.54
1	D	196	HIS	CA-C-O	-5.27	115.75	121.87
1	E	178	GLN	N-CA-CB	5.27	117.96	110.16
1	F	179	GLN	OE1-CD-NE2	5.27	127.87	122.60
1	I	110	GLN	CA-C-N	-5.27	114.42	122.06
1	I	110	GLN	C-N-CA	-5.27	114.42	122.06
1	Q	306	GLN	N-CA-CB	-5.27	103.89	110.90
1	A	261	PRO	O-C-N	-5.27	116.47	123.01
1	B	198	LEU	N-CA-CB	-5.27	102.35	110.20
1	B	226	THR	N-CA-CB	-5.27	101.58	110.49
1	N	102	ILE	CA-C-N	5.27	128.15	120.98
1	N	102	ILE	C-N-CA	5.27	128.15	120.98
1	P	27	LYS	N-CA-CB	-5.27	102.82	110.36
1	Q	18	ILE	N-CA-C	-5.27	105.58	110.53
1	Q	156	GLN	OE1-CD-NE2	5.27	127.87	122.60
1	N	178	GLN	OE1-CD-NE2	5.27	127.87	122.60
1	O	18	ILE	CB-CA-C	-5.27	105.23	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	HIS	CA-C-N	-5.27	111.72	120.68
1	C	257	HIS	C-N-CA	-5.27	111.72	120.68
1	E	232	MET	N-CA-C	-5.27	103.93	110.41
1	G	134	CYS	CA-C-O	-5.27	115.29	120.82
1	E	42	ARG	O-C-N	5.27	127.49	122.07
1	K	188	PRO	CA-C-O	-5.27	111.02	120.60
1	D	161	LEU	N-CA-CB	-5.26	102.12	110.28
1	G	85	GLN	CA-C-N	5.26	131.66	122.82
1	G	85	GLN	C-N-CA	5.26	131.66	122.82
1	J	356	LEU	N-CA-CB	-5.26	101.55	110.50
1	M	51	THR	CA-CB-CG2	5.26	119.45	110.50
1	D	34	GLU	CA-C-O	5.26	126.92	120.92
1	D	35	SER	CA-C-O	-5.26	116.48	122.01
1	D	94	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	K	116	ALA	CA-C-O	-5.26	115.82	121.56
1	M	335	CYS	CA-C-O	5.26	126.02	119.97
1	N	26	GLY	CA-C-N	-5.26	111.17	121.06
1	N	26	GLY	C-N-CA	-5.26	111.17	121.06
1	O	300	SER	N-CA-C	-5.26	96.57	107.67
1	B	55	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	C	186	VAL	CA-C-N	5.26	130.88	123.30
1	C	186	VAL	C-N-CA	5.26	130.88	123.30
1	D	55	ARG	O-C-N	-5.26	116.54	122.12
1	E	130	LEU	CA-C-N	-5.26	113.60	120.44
1	E	130	LEU	C-N-CA	-5.26	113.60	120.44
1	M	118	THR	CA-CB-OG1	-5.26	101.71	109.60
1	M	254	THR	CA-C-N	5.26	127.59	120.38
1	M	254	THR	C-N-CA	5.26	127.59	120.38
1	O	192	PRO	CA-C-N	-5.26	113.08	120.82
1	O	192	PRO	C-N-CA	-5.26	113.08	120.82
1	P	354	GLN	CB-CG-CD	-5.26	103.66	112.60
1	B	39	MET	O-C-N	5.26	128.20	122.20
1	F	208	VAL	CA-CB-CG2	5.26	119.34	110.40
1	G	12	LYS	CB-CG-CD	-5.26	99.20	111.30
1	I	108	LEU	CA-C-O	5.26	125.18	119.24
1	N	95	ASN	N-CA-C	-5.26	105.61	112.23
1	A	42	ARG	CB-CG-CD	5.26	123.39	111.30
1	B	321	GLU	N-CA-CB	5.26	117.77	109.94
1	G	54	ASN	O-C-N	-5.26	116.16	122.15
1	J	114	PRO	CA-C-O	-5.26	115.45	121.86
1	K	28	GLY	CA-C-O	5.26	129.72	120.57
1	M	20	GLN	CA-C-O	-5.26	113.92	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	2	HIS	O-C-N	-5.26	115.60	122.59
1	Q	166	ASN	O-C-N	5.26	128.74	122.27
1	R	315	GLY	N-CA-C	-5.26	108.37	115.36
1	C	44	GLN	N-CA-C	-5.25	104.80	111.11
1	G	255	ALA	CB-CA-C	-5.25	102.63	110.88
1	I	300	SER	N-CA-C	-5.25	96.49	107.37
1	K	223	LEU	O-C-N	5.25	127.69	122.12
1	C	303	ARG	CG-CD-NE	5.25	123.56	112.00
1	D	152	ARG	NH1-CZ-NH2	-5.25	112.47	119.30
1	H	160	SER	CA-C-N	-5.25	112.83	120.29
1	H	160	SER	C-N-CA	-5.25	112.83	120.29
1	J	270	LEU	N-CA-C	-5.25	103.46	110.55
1	M	230	PRO	CA-C-O	-5.25	115.50	121.96
1	F	279	ALA	N-CA-CB	5.25	117.58	109.91
1	F	328	MET	N-CA-C	5.25	117.00	111.28
1	I	124	ILE	N-CA-CB	-5.25	104.16	111.41
1	L	212	VAL	CA-CB-CG1	-5.25	101.47	110.40
1	N	253	VAL	CA-C-O	5.25	126.36	119.85
1	R	141	GLY	CA-C-N	-5.25	112.93	122.43
1	R	141	GLY	C-N-CA	-5.25	112.93	122.43
1	R	254	THR	CA-C-N	-5.25	113.24	120.28
1	R	254	THR	C-N-CA	-5.25	113.24	120.28
1	C	76	VAL	O-C-N	5.25	128.88	123.05
1	C	191	ILE	O-C-N	-5.25	115.11	121.10
1	I	291	LEU	N-CA-CB	-5.25	101.03	110.37
1	R	259	THR	CA-CB-OG1	-5.25	101.72	109.60
1	F	269	PHE	N-CA-C	5.25	117.49	110.35
1	G	78	LEU	N-CA-C	5.25	118.56	110.42
1	H	319	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	84	TYR	CA-C-O	-5.25	113.40	119.59
1	F	84	TYR	O-C-N	-5.25	116.01	122.20
1	F	199	GLU	CA-C-O	5.25	125.98	120.42
1	F	271	SER	O-C-N	5.25	129.52	122.49
1	J	76	VAL	CA-CB-CG2	-5.25	101.48	110.40
1	L	201	CYS	CA-C-N	-5.25	113.46	120.54
1	L	201	CYS	C-N-CA	-5.25	113.46	120.54
1	N	152	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	E	217	ASN	O-C-N	-5.25	116.56	122.12
1	R	145	GLY	O-C-N	-5.25	119.04	123.60
1	A	310	LEU	N-CA-C	-5.24	105.46	111.07
1	C	40	GLY	N-CA-C	-5.24	106.42	112.50
1	C	116	ALA	CA-C-O	-5.24	115.99	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	68	SER	CA-C-O	5.24	125.63	119.28
1	G	230	PRO	CB-CA-C	-5.24	102.91	111.56
1	I	207	LYS	N-CA-CB	5.24	118.01	110.20
1	B	143	ASP	CA-C-O	-5.24	113.08	119.32
1	C	168	ASN	N-CA-CB	5.24	117.92	110.16
1	D	149	ALA	N-CA-CB	5.24	118.73	110.56
1	D	151	LEU	CA-C-N	5.24	130.82	122.59
1	D	151	LEU	C-N-CA	5.24	130.82	122.59
1	E	203	TYR	CB-CG-CD1	-5.24	112.94	120.80
1	H	191	ILE	N-CA-CB	-5.24	103.89	110.33
1	I	101	GLY	CA-C-N	-5.24	116.31	123.12
1	I	101	GLY	C-N-CA	-5.24	116.31	123.12
1	Q	339	LYS	CA-CB-CG	5.24	124.58	114.10
1	D	279	ALA	N-CA-CB	5.24	118.62	109.72
1	D	337	ALA	N-CA-CB	5.24	117.82	110.12
1	G	102	ILE	N-CA-C	5.24	115.85	108.36
1	K	338	ALA	CA-C-O	5.24	125.70	119.10
1	N	136	GLN	CB-CA-C	5.24	119.76	110.85
1	R	74	GLY	CA-C-N	-5.24	111.14	121.41
1	R	74	GLY	C-N-CA	-5.24	111.14	121.41
1	R	139	LYS	O-C-N	5.24	128.12	122.15
1	R	297	LEU	O-C-N	-5.24	115.00	122.96
1	D	324	GLN	OE1-CD-NE2	5.24	127.84	122.60
1	E	183	VAL	O-C-N	-5.24	117.01	121.57
1	H	156	GLN	N-CA-CB	-5.24	104.29	112.41
1	L	148	ARG	NH1-CZ-NH2	-5.24	112.49	119.30
1	M	120	LYS	CA-C-N	-5.24	113.61	122.67
1	M	120	LYS	C-N-CA	-5.24	113.61	122.67
1	D	269	PHE	CA-C-O	-5.24	116.00	121.55
1	H	113	ALA	O-C-N	-5.24	116.95	121.71
1	H	197	ASP	CA-C-N	5.24	127.56	120.44
1	H	197	ASP	C-N-CA	5.24	127.56	120.44
1	H	349	GLY	CA-C-N	5.24	131.54	121.54
1	H	349	GLY	C-N-CA	5.24	131.54	121.54
1	J	300	SER	CA-C-O	-5.24	112.35	121.62
1	K	38	THR	O-C-N	5.24	127.46	122.07
1	K	354	GLN	CB-CG-CD	-5.24	103.70	112.60
1	R	20	GLN	CA-C-N	-5.24	113.26	120.28
1	R	20	GLN	C-N-CA	-5.24	113.26	120.28
1	E	162	ALA	CB-CA-C	-5.23	101.95	110.85
1	H	248	VAL	CA-C-N	-5.23	112.86	120.29
1	H	248	VAL	C-N-CA	-5.23	112.86	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	261	PRO	N-CA-CB	5.23	107.90	103.35
1	Q	261	PRO	N-CA-CB	5.23	108.31	103.39
1	R	4	PHE	O-C-N	-5.23	115.30	121.32
1	C	182	LEU	N-CA-CB	-5.23	102.09	110.46
1	E	11	GLN	CA-C-O	-5.23	115.00	120.55
1	E	308	SER	N-CA-C	-5.23	105.69	111.71
1	F	248	VAL	CA-CB-CG2	-5.23	101.51	110.40
1	J	194	GLY	CA-C-O	5.23	126.79	122.13
1	A	82	THR	CA-C-O	-5.23	114.34	120.20
1	H	237	HIS	CA-CB-CG	-5.23	108.57	113.80
1	Q	93	PHE	CA-C-N	-5.23	112.75	120.28
1	Q	93	PHE	C-N-CA	-5.23	112.75	120.28
1	H	214	LYS	N-CA-C	-5.23	105.58	111.28
1	K	313	TRP	CB-CA-C	-5.23	102.91	110.96
1	M	92	LEU	O-C-N	-5.23	116.69	122.86
1	J	164	GLN	N-CA-C	-5.23	105.48	111.07
1	J	248	VAL	CB-CA-C	-5.23	101.81	111.79
1	L	57	GLN	N-CA-CB	-5.23	102.41	110.20
1	M	223	LEU	CA-C-O	-5.23	114.98	120.63
1	P	154	ALA	CA-C-O	5.23	126.95	121.25
1	P	202	GLN	CA-C-O	5.23	126.31	120.82
1	A	151	LEU	CA-C-O	-5.23	115.06	120.70
1	A	348	SER	CB-CA-C	5.23	118.42	109.80
1	E	125	GLN	CB-CA-C	-5.23	101.41	110.45
1	E	132	GLU	N-CA-C	-5.23	105.66	111.36
1	M	205	THR	CA-C-N	-5.23	112.75	120.28
1	M	205	THR	C-N-CA	-5.23	112.75	120.28
1	D	119	ASN	CB-CG-OD1	-5.22	110.35	120.80
1	I	165	GLU	N-CA-CB	-5.22	102.43	110.16
1	K	108	LEU	N-CA-CB	-5.22	103.41	110.67
1	K	115	LEU	CB-CG-CD1	5.22	126.38	110.70
1	L	215	ALA	O-C-N	5.22	128.10	122.15
1	N	190	VAL	CA-C-N	5.22	131.79	122.13
1	N	190	VAL	C-N-CA	5.22	131.79	122.13
1	O	315	GLY	N-CA-C	-5.22	108.41	115.36
1	Q	200	HIS	N-CA-C	-5.22	105.66	111.36
1	C	174	ALA	N-CA-CB	5.22	117.80	110.12
1	F	171	ALA	CA-C-N	-5.22	113.53	120.79
1	F	171	ALA	C-N-CA	-5.22	113.53	120.79
1	F	308	SER	O-C-N	5.22	128.33	122.22
1	G	82	THR	CA-CB-OG1	-5.22	101.77	109.60
1	O	98	LYS	CD-CE-NZ	5.22	128.61	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	238	ALA	CA-C-O	-5.22	112.97	119.18
1	R	226	THR	CA-C-O	-5.22	115.69	121.33
1	B	225	GLY	N-CA-C	5.22	125.55	113.18
1	B	38	THR	N-CA-CB	5.22	117.53	109.91
1	B	175	SER	CA-C-N	-5.22	114.18	120.70
1	B	175	SER	C-N-CA	-5.22	114.18	120.70
1	C	110	GLN	OE1-CD-NE2	5.22	127.82	122.60
1	H	12	LYS	CA-CB-CG	-5.22	103.66	114.10
1	K	103	VAL	CA-C-O	-5.22	115.62	121.36
1	O	186	VAL	CA-C-N	-5.22	115.78	123.30
1	O	186	VAL	C-N-CA	-5.22	115.78	123.30
1	O	256	LEU	CD1-CG-CD2	-5.22	99.32	110.80
1	H	282	ASN	OD1-CG-ND2	5.22	127.82	122.60
1	J	331	ALA	O-C-N	-5.22	116.69	122.07
1	M	250	MET	O-C-N	5.22	128.10	122.15
1	N	87	ASP	CB-CG-OD2	-5.22	106.40	118.40
1	P	7	LEU	CA-C-O	-5.22	115.50	121.40
1	C	296	LYS	CB-CA-C	-5.22	100.04	110.42
1	G	40	GLY	O-C-N	-5.22	117.18	122.19
1	G	138	LYS	CA-C-O	5.22	125.99	120.10
1	G	194	GLY	CA-C-N	5.22	130.84	121.66
1	G	194	GLY	C-N-CA	5.22	130.84	121.66
1	L	237	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	R	6	ALA	CA-C-O	-5.22	114.45	120.24
1	A	183	VAL	O-C-N	5.21	126.11	121.57
1	E	335	CYS	CB-CA-C	-5.21	100.98	110.63
1	F	59	ARG	CD-NE-CZ	-5.21	117.10	124.40
1	I	68	SER	CB-CA-C	-5.21	100.05	110.42
1	J	14	GLU	N-CA-C	-5.21	105.68	111.36
1	L	234	THR	O-C-N	-5.21	117.10	123.10
1	L	282	ASN	CA-CB-CG	-5.21	107.39	112.60
1	M	178	GLN	CA-C-N	-5.21	110.85	121.18
1	M	178	GLN	C-N-CA	-5.21	110.85	121.18
1	P	148	ARG	NE-CZ-NH1	5.21	126.72	121.50
1	J	34	GLU	CA-C-N	-5.21	111.65	121.66
1	J	34	GLU	C-N-CA	-5.21	111.65	121.66
1	L	223	LEU	O-C-N	5.21	127.65	122.12
1	P	297	LEU	N-CA-CB	5.21	118.89	110.65
1	H	321	GLU	O-C-N	5.21	127.44	122.07
1	I	160	SER	O-C-N	5.21	128.09	122.15
1	K	238	ALA	N-CA-C	-5.21	106.60	113.17
1	L	262	ALA	O-C-N	-5.21	114.82	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	257	HIS	CE1-NE2-CD2	-5.21	103.79	109.00
1	N	21	SER	CA-C-N	-5.21	111.75	120.30
1	N	21	SER	C-N-CA	-5.21	111.75	120.30
1	O	150	VAL	CA-C-O	5.21	125.89	120.36
1	R	128	ASP	CA-C-O	-5.21	114.98	120.92
1	R	258	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	B	337	ALA	CA-C-N	-5.21	111.59	121.54
1	B	337	ALA	C-N-CA	-5.21	111.59	121.54
1	C	122	THR	OG1-CB-CG2	-5.21	98.88	109.30
1	F	267	ILE	CG1-CB-CG2	-5.21	95.07	110.70
1	M	146	LYS	CA-CB-CG	5.21	124.52	114.10
1	N	82	THR	CA-CB-OG1	5.21	117.42	109.60
1	R	214	LYS	CD-CE-NZ	-5.21	95.23	111.90
1	C	258	ARG	N-CA-CB	5.21	118.32	110.30
1	E	42	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	G	287	ASN	CA-C-O	-5.21	112.44	119.11
1	H	155	ASP	CA-C-N	-5.21	114.87	123.05
1	H	155	ASP	C-N-CA	-5.21	114.87	123.05
1	M	116	ALA	O-C-N	5.21	128.84	122.75
1	M	143	ASP	CB-CA-C	-5.21	100.79	109.75
1	O	53	GLU	O-C-N	5.21	128.09	122.15
1	C	121	GLU	O-C-N	-5.21	116.59	122.68
1	F	167	ALA	N-CA-CB	5.21	117.56	110.01
1	F	243	TYR	CB-CG-CD2	-5.21	112.99	120.80
1	G	274	MET	CB-CA-C	-5.21	101.38	109.61
1	I	8	THR	CA-CB-OG1	5.21	117.41	109.60
1	L	275	SER	N-CA-C	-5.21	103.66	110.53
1	O	312	ALA	O-C-N	-5.21	116.67	122.09
1	Q	280	THR	CA-CB-OG1	-5.21	101.79	109.60
1	A	277	GLU	CA-C-O	-5.20	114.90	120.42
1	D	124	ILE	N-CA-C	5.20	116.21	108.46
1	F	325	GLU	CA-CB-CG	-5.20	103.69	114.10
1	I	249	ALA	CB-CA-C	5.20	119.70	110.85
1	Q	81	GLU	N-CA-CB	5.20	117.56	110.01
1	A	353	THR	CA-C-O	-5.20	113.22	119.15
1	C	100	LYS	N-CA-C	-5.20	107.46	112.97
1	M	47	LYS	CA-C-N	5.20	130.22	122.99
1	M	47	LYS	C-N-CA	5.20	130.22	122.99
1	P	103	VAL	CA-C-N	5.20	129.64	123.19
1	P	103	VAL	C-N-CA	5.20	129.64	123.19
1	C	248	VAL	CA-CB-CG2	-5.20	101.56	110.40
1	C	313	TRP	O-C-N	5.20	127.43	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	164	GLN	CG-CD-OE1	5.20	131.20	120.80
1	F	169	ALA	N-CA-CB	5.20	117.86	110.16
1	F	258	ARG	CB-CG-CD	-5.20	99.34	111.30
1	F	84	TYR	CA-C-O	5.20	125.31	119.18
1	I	187	GLU	O-C-N	-5.20	115.95	121.04
1	L	10	GLU	CA-C-N	-5.20	113.52	120.54
1	L	10	GLU	C-N-CA	-5.20	113.52	120.54
1	L	207	LYS	O-C-N	5.20	128.08	122.15
1	N	153	ILE	CA-CB-CG2	-5.20	101.66	110.50
1	P	191	ILE	CB-CA-C	5.20	116.66	110.68
1	C	3	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	C	209	LEU	CA-C-O	-5.20	113.66	119.79
1	D	298	SER	N-CA-C	5.20	118.27	108.65
1	N	286	ILE	CA-C-N	-5.20	112.04	120.72
1	N	286	ILE	C-N-CA	-5.20	112.04	120.72
1	R	71	GLN	O-C-N	5.20	129.58	122.46
1	D	344	HIS	CA-C-O	5.20	127.94	120.51
1	E	84	TYR	CA-C-O	-5.20	113.35	119.48
1	F	156	GLN	CG-CD-OE1	-5.20	110.41	120.80
1	G	90	GLY	N-CA-C	-5.20	107.82	115.30
1	G	295	TRP	CA-C-O	-5.20	115.29	121.89
1	K	135	ALA	O-C-N	-5.20	116.14	122.22
1	M	190	VAL	CA-C-N	5.20	131.74	122.13
1	M	190	VAL	C-N-CA	5.20	131.74	122.13
1	N	56	ARG	CB-CA-C	-5.20	102.12	110.74
1	E	342	TYR	CB-CA-C	-5.19	101.58	109.89
1	K	313	TRP	CA-C-O	-5.19	115.55	121.00
1	A	110	GLN	CA-C-O	-5.19	113.08	120.51
1	C	223	LEU	N-CA-C	5.19	117.68	111.71
1	J	125	GLN	CG-CD-NE2	5.19	124.19	116.40
1	M	277	GLU	OE1-CD-OE2	-5.19	110.44	122.90
1	O	65	VAL	CA-CB-CG2	5.19	119.23	110.40
1	Q	55	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	12	LYS	CA-C-O	5.19	125.92	120.42
1	D	342	TYR	O-C-N	-5.19	117.14	123.16
1	F	104	VAL	O-C-N	-5.19	117.73	123.18
1	F	348	SER	CA-C-N	5.19	131.58	121.41
1	F	348	SER	C-N-CA	5.19	131.58	121.41
1	G	16	SER	CA-C-N	-5.19	112.92	120.29
1	G	16	SER	C-N-CA	-5.19	112.92	120.29
1	H	303	ARG	O-C-N	5.19	127.49	122.09
1	K	79	PHE	CA-C-N	-5.19	113.03	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	79	PHE	C-N-CA	-5.19	113.03	120.82
1	P	42	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
1	Q	61	ILE	O-C-N	5.19	126.91	121.87
1	R	38	THR	CA-CB-OG1	-5.19	101.81	109.60
1	R	213	TYR	CA-CB-CG	-5.19	104.56	113.90
1	D	37	GLY	O-C-N	5.19	127.22	122.19
1	E	189	GLU	N-CA-C	5.19	117.19	109.25
1	G	60	GLU	CA-C-O	-5.19	114.00	119.97
1	J	49	GLU	O-C-N	-5.19	116.52	122.95
1	K	318	ALA	O-C-N	5.19	129.13	122.39
1	L	60	GLU	N-CA-CB	5.19	117.53	110.01
1	M	277	GLU	CA-C-O	5.19	126.00	120.24
1	N	161	LEU	CA-C-O	5.19	126.78	121.07
1	N	341	GLN	OE1-CD-NE2	5.19	127.79	122.60
1	P	215	ALA	O-C-N	5.19	128.06	122.15
1	R	99	GLU	CA-C-O	-5.19	114.00	119.97
1	B	324	GLN	OE1-CD-NE2	5.19	127.79	122.60
1	G	118	THR	N-CA-CB	-5.19	103.19	111.43
1	N	202	GLN	CA-CB-CG	-5.19	103.73	114.10
1	O	113	ALA	CA-C-N	5.19	125.34	119.90
1	O	113	ALA	C-N-CA	5.19	125.34	119.90
1	R	8	THR	CA-CB-CG2	-5.19	101.68	110.50
1	F	111	GLY	O-C-N	5.18	128.65	122.64
1	F	195	ASP	CB-CG-OD2	5.18	130.32	118.40
1	K	194	GLY	O-C-N	5.18	127.98	123.06
1	K	336	GLN	N-CA-C	-5.18	105.71	111.36
1	N	16	SER	N-CA-CB	-5.18	102.49	110.01
1	N	330	ARG	CG-CD-NE	5.18	123.41	112.00
1	O	185	ILE	CB-CA-C	-5.18	105.63	111.23
1	C	136	GLN	CB-CA-C	5.18	119.02	110.88
1	E	154	ALA	CA-C-O	-5.18	115.60	121.25
1	E	165	GLU	N-CA-CB	-5.18	102.25	110.28
1	F	42	ARG	NH1-CZ-NH2	-5.18	112.56	119.30
1	B	209	LEU	CD1-CG-CD2	-5.18	99.40	110.80
1	C	74	GLY	CA-C-O	5.18	128.19	119.59
1	G	68	SER	CA-C-O	5.18	125.79	119.05
1	N	172	ARG	CD-NE-CZ	-5.18	117.15	124.40
1	O	307	ALA	N-CA-CB	-5.18	101.33	109.78
1	C	332	MET	CA-C-O	-5.18	114.93	120.42
1	D	80	HIS	CA-C-O	5.18	126.77	121.07
1	D	121	GLU	CG-CD-OE2	-5.18	106.49	118.40
1	J	109	ASP	OD1-CG-OD2	5.18	135.33	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	136	GLN	OE1-CD-NE2	5.18	127.78	122.60
1	Q	71	GLN	CA-C-O	5.18	124.84	119.14
1	F	123	THR	CA-C-N	-5.18	115.74	122.94
1	F	123	THR	C-N-CA	-5.18	115.74	122.94
1	A	154	ALA	CA-C-N	-5.18	113.36	121.02
1	A	154	ALA	C-N-CA	-5.18	113.36	121.02
1	B	80	HIS	CB-CA-C	-5.18	100.12	110.42
1	H	33	ASP	O-C-N	5.18	128.82	122.20
1	J	1	ALA	O-C-N	-5.18	114.72	123.00
1	J	9	GLN	N-CA-CB	5.18	117.82	110.16
1	P	210	ALA	CA-C-O	-5.18	115.36	120.90
1	R	108	LEU	O-C-N	-5.18	115.98	122.35
1	A	203	TYR	CB-CG-CD2	5.17	128.56	120.80
1	A	218	ASP	CA-CB-CG	-5.17	107.42	112.60
1	A	335	CYS	N-CA-CB	-5.17	102.33	110.30
1	G	119	ASN	CA-C-O	5.17	127.38	121.58
1	J	167	ALA	N-CA-C	-5.17	105.82	111.82
1	K	66	ASP	OD1-CG-OD2	-5.17	110.48	122.90
1	M	293	LYS	N-CA-CB	-5.17	104.66	111.23
1	N	49	GLU	CA-C-O	5.17	126.76	120.81
1	D	257	HIS	N-CA-C	-5.17	106.92	113.18
1	K	129	GLY	N-CA-C	5.17	122.32	114.61
1	N	331	ALA	N-CA-C	-5.17	105.82	111.82
1	O	101	GLY	CA-C-N	-5.17	116.43	123.10
1	O	101	GLY	C-N-CA	-5.17	116.43	123.10
1	B	71	GLN	CG-CD-OE1	5.17	131.14	120.80
1	E	337	ALA	CA-C-O	-5.17	115.07	120.55
1	G	193	ASP	CA-CB-CG	5.17	117.77	112.60
1	P	294	PRO	N-CA-C	5.17	120.56	113.84
1	Q	179	GLN	CA-C-N	-5.17	114.45	122.67
1	Q	179	GLN	C-N-CA	-5.17	114.45	122.67
1	R	200	HIS	CA-C-N	-5.17	111.89	120.68
1	R	200	HIS	C-N-CA	-5.17	111.89	120.68
1	Q	49	GLU	O-C-N	5.17	129.09	123.04
1	Q	300	SER	CA-C-O	-5.17	114.51	122.32
1	C	25	ASN	CA-C-N	-5.17	111.35	121.53
1	C	25	ASN	C-N-CA	-5.17	111.35	121.53
1	D	103	VAL	O-C-N	5.17	128.55	122.81
1	E	234	THR	CB-CA-C	-5.17	99.34	110.45
1	H	168	ASN	CA-C-N	-5.17	112.95	120.29
1	H	168	ASN	C-N-CA	-5.17	112.95	120.29
1	J	223	LEU	N-CA-CB	5.17	117.72	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	322	ALA	CB-CA-C	-5.17	102.70	110.92
1	Q	55	ARG	CA-CB-CG	-5.17	103.76	114.10
1	B	61	ILE	N-CA-CB	5.17	116.25	110.62
1	D	180	ASN	OD1-CG-ND2	5.17	127.77	122.60
1	K	235	ALA	N-CA-CB	5.17	117.75	110.36
1	L	264	VAL	CA-C-O	-5.17	114.91	119.71
1	P	208	VAL	CB-CA-C	5.17	118.58	111.97
1	Q	332	MET	O-C-N	-5.17	116.17	122.22
1	G	334	ASN	CA-C-O	-5.17	114.26	120.10
1	F	57	GLN	OE1-CD-NE2	5.16	127.76	122.60
1	M	103	VAL	O-C-N	5.16	128.54	122.81
1	O	277	GLU	CA-C-O	5.16	126.24	120.82
1	O	338	ALA	N-CA-CB	5.16	119.22	110.49
1	R	149	ALA	CB-CA-C	-5.16	100.68	109.51
1	B	204	VAL	CB-CA-C	-5.16	105.10	112.22
1	B	303	ARG	CG-CD-NE	5.16	123.36	112.00
1	C	297	LEU	N-CA-CB	5.16	118.61	110.71
1	J	319	ASN	N-CA-CB	-5.16	102.51	110.46
1	O	334	ASN	CB-CA-C	5.16	119.36	110.79
1	B	123	THR	N-CA-C	-5.16	101.60	109.65
1	I	82	THR	CA-CB-CG2	-5.16	101.73	110.50
1	J	216	LEU	CA-C-N	-5.16	112.09	120.71
1	J	216	LEU	C-N-CA	-5.16	112.09	120.71
1	K	156	GLN	CB-CG-CD	-5.16	103.83	112.60
1	P	162	ALA	CA-C-N	-5.16	113.96	120.56
1	P	162	ALA	C-N-CA	-5.16	113.96	120.56
1	Q	53	GLU	CB-CA-C	5.16	119.62	110.85
1	A	219	HIS	CA-CB-CG	5.16	118.96	113.80
1	F	14	GLU	CA-C-O	5.16	126.42	121.00
1	F	136	GLN	OE1-CD-NE2	5.16	127.76	122.60
1	J	2	HIS	O-C-N	-5.16	115.73	122.59
1	P	201	CYS	N-CA-C	-5.16	105.74	111.36
1	Q	77	ILE	CA-CB-CG2	5.16	119.27	110.50
1	Q	101	GLY	CA-C-N	-5.16	116.79	123.19
1	Q	101	GLY	C-N-CA	-5.16	116.79	123.19
1	B	284	ASN	CA-CB-CG	-5.16	107.44	112.60
1	I	278	ASP	CA-C-O	5.16	126.23	120.82
1	A	39	MET	CA-C-N	5.16	125.70	119.98
1	A	39	MET	C-N-CA	5.16	125.70	119.98
1	C	159	SER	CA-C-N	-5.16	113.74	120.44
1	C	159	SER	C-N-CA	-5.16	113.74	120.44
1	K	125	GLN	CB-CA-C	-5.16	100.81	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	331	ALA	CA-C-O	5.16	125.90	119.97
1	M	308	SER	CA-C-O	-5.16	113.04	119.38
1	O	194	GLY	O-C-N	-5.16	117.03	123.37
1	R	344	HIS	CA-C-O	-5.16	112.03	120.80
1	A	157	CYS	O-C-N	-5.15	116.43	121.38
1	B	339	LYS	CA-C-O	5.15	125.45	119.32
1	D	8	THR	N-CA-CB	5.15	117.81	110.44
1	F	304	ALA	CA-C-O	-5.15	112.35	119.05
1	G	207	LYS	CA-CB-CG	5.15	124.41	114.10
1	L	196	HIS	ND1-CE1-NE2	5.15	113.55	108.40
1	O	211	ALA	N-CA-C	5.15	116.71	111.14
1	Q	204	VAL	O-C-N	-5.15	116.42	121.94
1	C	191	ILE	CB-CG1-CD1	-5.15	102.98	113.80
1	E	306	GLN	N-CA-C	5.15	120.42	113.72
1	F	196	HIS	CA-C-O	5.15	127.88	120.51
1	P	86	LYS	N-CA-C	5.15	117.99	109.85
1	Q	300	SER	N-CA-C	-5.15	100.08	109.56
1	D	327	PHE	CG-CD1-CE1	5.15	129.46	120.70
1	G	3	ARG	CA-C-N	-5.15	117.98	124.21
1	G	3	ARG	C-N-CA	-5.15	117.98	124.21
1	L	81	GLU	CA-CB-CG	5.15	124.40	114.10
1	M	308	SER	N-CA-C	-5.15	106.26	112.54
1	P	116	ALA	N-CA-CB	-5.15	102.40	109.97
1	P	259	THR	CA-C-O	-5.15	113.14	120.51
1	Q	139	LYS	CB-CA-C	-5.15	101.10	110.63
1	Q	172	ARG	N-CA-C	-5.15	105.56	111.07
1	G	110	GLN	CG-CD-OE1	5.15	131.09	120.80
1	G	336	GLN	CA-C-N	-5.15	113.75	120.44
1	G	336	GLN	C-N-CA	-5.15	113.75	120.44
1	O	19	ALA	O-C-N	-5.15	116.77	122.07
1	C	172	ARG	NH1-CZ-NH2	5.15	125.99	119.30
1	D	163	ILE	CA-CB-CG1	-5.15	101.65	110.40
1	F	99	GLU	CA-C-O	-5.15	114.28	120.10
1	H	113	ALA	N-CA-CB	-5.15	105.70	111.10
1	J	336	GLN	N-CA-CB	5.15	117.69	110.12
1	M	163	ILE	CA-CB-CG1	-5.15	101.65	110.40
1	D	143	ASP	O-C-N	5.14	127.84	122.23
1	F	180	ASN	O-C-N	5.14	128.91	122.22
1	F	351	ALA	N-CA-C	5.14	121.76	110.80
1	J	167	ALA	CA-C-N	-5.14	112.99	120.29
1	J	167	ALA	C-N-CA	-5.14	112.99	120.29
1	O	328	MET	N-CA-C	-5.14	106.84	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	249	ALA	CA-C-O	5.14	126.00	120.55
1	R	286	ILE	CA-CB-CG2	5.14	119.25	110.50
1	C	248	VAL	CA-C-N	-5.14	112.49	120.31
1	C	248	VAL	C-N-CA	-5.14	112.49	120.31
1	I	209	LEU	CA-C-N	-5.14	112.49	120.31
1	I	209	LEU	C-N-CA	-5.14	112.49	120.31
1	J	170	LEU	CA-C-O	5.14	126.40	120.90
1	L	301	TYR	N-CA-CB	-5.14	102.23	110.46
1	M	346	GLY	N-CA-C	-5.14	101.00	113.18
1	Q	153	ILE	CA-CB-CG2	-5.14	101.76	110.50
1	Q	171	ALA	N-CA-CB	5.14	117.86	110.20
1	D	254	THR	CA-CB-OG1	-5.14	101.89	109.60
1	L	69	ILE	O-C-N	-5.14	116.20	122.06
1	J	188	PRO	CA-C-O	-5.14	111.25	120.60
1	L	80	HIS	ND1-CE1-NE2	5.14	113.54	108.40
1	O	183	VAL	CB-CA-C	-5.14	104.87	110.37
1	I	66	ASP	CB-CG-OD1	5.14	130.22	118.40
1	J	342	TYR	O-C-N	-5.14	116.70	123.02
1	M	300	SER	CA-CB-OG	5.14	121.38	111.10
1	R	245	PRO	CB-CA-C	-5.14	103.70	112.64
1	A	194	GLY	CA-C-N	-5.14	114.59	122.60
1	A	194	GLY	C-N-CA	-5.14	114.59	122.60
1	A	295	TRP	CA-C-N	-5.14	112.99	120.75
1	A	295	TRP	C-N-CA	-5.14	112.99	120.75
1	C	207	LYS	CA-C-O	5.14	125.94	120.24
1	F	186	VAL	CA-C-O	-5.14	114.99	120.59
1	F	334	ASN	O-C-N	-5.14	115.95	122.27
1	G	301	TYR	N-CA-C	5.14	117.88	110.28
1	I	248	VAL	CA-C-N	-5.14	113.00	120.29
1	I	248	VAL	C-N-CA	-5.14	113.00	120.29
1	I	285	ALA	N-CA-CB	5.14	117.67	110.12
1	P	253	VAL	CG1-CB-CG2	-5.14	99.50	110.80
1	Q	143	ASP	CA-CB-CG	-5.14	107.46	112.60
1	R	340	GLY	N-CA-C	-5.14	107.17	115.08
1	A	20	GLN	N-CA-CB	-5.13	102.32	110.28
1	G	207	LYS	CG-CD-CE	5.13	123.11	111.30
1	G	276	GLU	O-C-N	5.13	127.56	122.12
1	K	213	TYR	CA-CB-CG	-5.13	104.66	113.90
1	L	73	ILE	N-CA-CB	-5.13	104.93	110.53
1	L	336	GLN	O-C-N	5.13	127.36	122.07
1	B	5	PRO	CA-C-O	5.13	127.19	121.34
1	L	266	GLY	CA-C-O	-5.13	116.52	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	55	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	D	187	GLU	CB-CG-CD	-5.13	103.88	112.60
1	F	190	VAL	N-CA-CB	-5.13	106.55	111.89
1	J	156	GLN	CG-CD-NE2	5.13	124.10	116.40
1	N	126	GLY	CA-C-N	-5.13	111.57	121.58
1	N	126	GLY	C-N-CA	-5.13	111.57	121.58
1	O	168	ASN	CB-CG-ND2	-5.13	108.70	116.40
1	O	204	VAL	N-CA-CB	-5.13	101.48	110.77
1	R	95	ASN	CB-CG-ND2	5.13	124.10	116.40
1	L	133	ARG	CD-NE-CZ	-5.13	117.22	124.40
1	B	101	GLY	CA-C-N	-5.13	116.42	123.14
1	B	101	GLY	C-N-CA	-5.13	116.42	123.14
1	D	7	LEU	N-CA-C	5.13	117.60	109.50
1	D	277	GLU	CB-CG-CD	5.13	121.32	112.60
1	I	300	SER	N-CA-CB	5.13	120.75	111.11
1	Q	123	THR	CA-CB-OG1	5.13	117.29	109.60
1	R	250	MET	CA-C-O	5.13	125.86	120.42
1	A	353	THR	CB-CA-C	-5.13	100.73	109.65
1	B	218	ASP	OD1-CG-OD2	5.13	135.21	122.90
1	D	185	ILE	CA-CB-CG1	5.13	119.12	110.40
1	E	350	ALA	O-C-N	-5.13	115.77	122.59
1	F	223	LEU	N-CA-C	5.13	117.53	111.33
1	F	278	ASP	CA-C-N	-5.13	113.88	120.65
1	F	278	ASP	C-N-CA	-5.13	113.88	120.65
1	K	309	ALA	O-C-N	-5.13	115.96	122.27
1	O	39	MET	O-C-N	5.13	127.55	122.12
1	O	189	GLU	N-CA-C	5.13	117.09	109.25
1	R	280	THR	O-C-N	-5.13	116.31	122.15
1	R	329	LYS	N-CA-CB	-5.13	102.64	110.07
1	R	344	HIS	CB-CA-C	-5.13	100.36	110.10
1	O	174	ALA	O-C-N	-5.12	116.79	122.07
1	F	71	GLN	CG-CD-OE1	5.12	131.05	120.80
1	J	344	HIS	CB-CA-C	5.12	122.09	110.67
1	P	82	THR	CA-C-O	-5.12	114.46	120.20
1	J	164	GLN	CA-CB-CG	5.12	124.34	114.10
1	E	215	ALA	CA-C-O	-5.12	114.99	120.42
1	E	284	ASN	OD1-CG-ND2	5.12	127.72	122.60
1	G	317	ALA	O-C-N	5.12	128.21	122.22
1	J	12	LYS	N-CA-CB	-5.12	102.31	109.94
1	K	172	ARG	CB-CA-C	-5.12	102.29	110.79
1	P	193	ASP	CB-CG-OD1	5.12	130.18	118.40
1	P	338	ALA	N-CA-C	-5.12	106.87	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	225	GLY	CA-C-N	-5.12	114.55	122.59
1	Q	225	GLY	C-N-CA	-5.12	114.55	122.59
1	R	144	PHE	CA-C-O	-5.12	115.78	121.51
1	D	306	GLN	OE1-CD-NE2	5.12	127.72	122.60
1	N	153	ILE	CA-C-N	-5.12	111.76	121.54
1	N	153	ILE	C-N-CA	-5.12	111.76	121.54
1	O	191	ILE	CA-CB-CG1	-5.12	101.70	110.40
1	D	336	GLN	N-CA-C	-5.12	105.40	111.69
1	H	261	PRO	N-CA-CB	-5.12	97.88	103.25
1	J	354	GLN	CA-C-O	-5.12	114.09	119.97
1	P	154	ALA	N-CA-CB	-5.12	102.48	111.49
1	B	102	ILE	CA-C-O	-5.12	115.02	120.39
1	C	287	ASN	CA-C-N	-5.12	113.12	122.38
1	C	287	ASN	C-N-CA	-5.12	113.12	122.38
1	D	261	PRO	O-C-N	-5.12	115.73	122.64
1	I	292	PRO	CA-C-N	-5.12	116.48	122.00
1	I	292	PRO	C-N-CA	-5.12	116.48	122.00
1	L	89	GLN	N-CA-CB	-5.12	104.49	111.65
1	A	199	GLU	CA-C-O	5.11	125.85	119.97
1	D	53	GLU	N-CA-C	5.11	117.52	111.33
1	D	278	ASP	CA-CB-CG	-5.11	107.49	112.60
1	G	270	LEU	CA-C-N	-5.11	113.72	122.11
1	G	270	LEU	C-N-CA	-5.11	113.72	122.11
1	H	6	ALA	CB-CA-C	-5.11	102.85	110.88
1	I	109	ASP	N-CA-CB	5.11	117.21	110.25
1	I	233	VAL	O-C-N	-5.11	116.43	122.77
1	O	301	TYR	N-CA-CB	-5.11	102.67	110.85
1	P	216	LEU	N-CA-C	-5.11	105.14	111.33
1	K	219	HIS	CA-C-N	-5.11	114.56	122.08
1	K	219	HIS	C-N-CA	-5.11	114.56	122.08
1	C	115	LEU	O-C-N	-5.11	116.39	122.63
1	C	194	GLY	CA-C-O	5.11	126.56	122.52
1	E	94	ARG	CG-CD-NE	-5.11	100.76	112.00
1	E	106	ILE	N-CA-CB	-5.11	102.36	111.92
1	G	195	ASP	N-CA-C	5.11	119.57	113.23
1	M	14	GLU	N-CA-CB	5.11	117.48	110.07
1	O	221	VAL	CA-CB-CG2	-5.11	101.71	110.40
1	Q	24	ALA	CB-CA-C	-5.11	101.18	110.63
1	R	109	ASP	N-CA-C	-5.11	103.94	110.53
1	F	89	GLN	CG-CD-NE2	-5.11	108.74	116.40
1	Q	147	TRP	CA-C-N	-5.11	115.95	123.00
1	Q	147	TRP	C-N-CA	-5.11	115.95	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	ALA	N-CA-C	5.11	125.30	111.00
1	F	85	GLN	CA-C-O	5.11	127.75	121.72
1	I	156	GLN	CA-CB-CG	-5.11	103.88	114.10
1	I	180	ASN	O-C-N	-5.11	116.17	122.25
1	J	190	VAL	O-C-N	-5.11	115.25	122.76
1	L	59	ARG	CA-C-N	-5.11	113.80	120.44
1	L	59	ARG	C-N-CA	-5.11	113.80	120.44
1	O	137	TYR	CA-C-O	5.11	125.97	120.55
1	Q	20	GLN	CB-CG-CD	-5.11	103.92	112.60
1	C	298	SER	CA-CB-OG	-5.11	100.89	111.10
1	D	148	ARG	CA-C-O	-5.11	114.81	120.38
1	F	29	ILE	CA-CB-CG1	5.11	119.08	110.40
1	I	138	LYS	CB-CG-CD	5.11	123.05	111.30
1	M	156	GLN	CG-CD-OE1	-5.11	110.59	120.80
1	C	217	ASN	CA-C-N	-5.10	112.55	120.31
1	C	217	ASN	C-N-CA	-5.10	112.55	120.31
1	G	37	GLY	N-CA-C	5.10	118.42	112.50
1	B	329	LYS	CA-C-N	-5.10	113.39	120.38
1	B	329	LYS	C-N-CA	-5.10	113.39	120.38
1	E	261	PRO	O-C-N	-5.10	116.68	123.01
1	F	180	ASN	CB-CG-ND2	5.10	124.05	116.40
1	G	248	VAL	O-C-N	-5.10	116.91	121.91
1	H	166	ASN	CA-C-O	-5.10	114.33	120.10
1	I	57	GLN	CA-C-O	-5.10	115.46	120.82
1	K	193	ASP	CA-C-N	-5.10	114.45	122.92
1	K	193	ASP	C-N-CA	-5.10	114.45	122.92
1	L	211	ALA	CA-C-N	-5.10	114.02	120.60
1	L	211	ALA	C-N-CA	-5.10	114.02	120.60
1	O	276	GLU	CB-CG-CD	5.10	121.28	112.60
1	B	73	ILE	N-CA-C	5.10	115.62	108.89
1	H	44	GLN	O-C-N	5.10	127.53	122.12
1	L	172	ARG	CG-CD-NE	-5.10	100.78	112.00
1	M	264	VAL	CA-CB-CG1	-5.10	101.73	110.40
1	P	57	GLN	CA-C-O	-5.10	115.65	121.00
1	A	277	GLU	CG-CD-OE2	-5.10	106.67	118.40
1	L	314	GLY	CA-C-N	-5.10	111.49	121.53
1	L	314	GLY	C-N-CA	-5.10	111.49	121.53
1	L	325	GLU	CA-C-O	5.10	126.35	121.00
1	M	233	VAL	CA-C-O	-5.10	114.90	120.97
1	M	237	HIS	N-CA-CB	-5.10	102.09	110.14
1	O	291	LEU	CD1-CG-CD2	-5.10	99.59	110.80
1	Q	126	GLY	CA-C-N	-5.10	112.21	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	126	GLY	C-N-CA	-5.10	112.21	120.72
1	A	63	PHE	CA-C-N	-5.09	114.50	122.65
1	A	63	PHE	C-N-CA	-5.09	114.50	122.65
1	B	10	GLU	CB-CG-CD	-5.09	103.94	112.60
1	C	110	GLN	CA-C-O	-5.09	114.52	120.53
1	C	249	ALA	CB-CA-C	5.09	120.45	110.67
1	D	305	LEU	O-C-N	-5.09	116.08	122.24
1	H	208	VAL	O-C-N	5.09	127.03	121.94
1	I	95	ASN	CA-C-N	-5.09	114.03	120.60
1	I	95	ASN	C-N-CA	-5.09	114.03	120.60
1	I	232	MET	CA-C-N	-5.09	116.01	122.43
1	I	232	MET	C-N-CA	-5.09	116.01	122.43
1	J	171	ALA	CA-C-O	-5.09	115.02	120.42
1	L	152	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	O	103	VAL	CA-C-O	-5.09	115.05	121.11
1	P	170	LEU	CA-C-O	5.09	125.83	119.97
1	B	284	ASN	CB-CG-ND2	-5.09	108.76	116.40
1	F	197	ASP	CA-CB-CG	-5.09	107.51	112.60
1	K	337	ALA	CA-C-O	-5.09	115.15	120.55
1	M	20	GLN	O-C-N	5.09	128.53	122.27
1	N	191	ILE	N-CA-CB	-5.09	104.08	111.21
1	P	13	LYS	CG-CD-CE	5.09	123.01	111.30
1	Q	89	GLN	CB-CG-CD	-5.09	103.94	112.60
1	B	287	ASN	CA-CB-CG	-5.09	107.51	112.60
1	E	11	GLN	N-CA-CB	-5.09	102.64	110.12
1	E	147	TRP	CA-CB-CG	5.09	123.27	113.60
1	J	47	LYS	N-CA-CB	-5.09	103.61	111.65
1	M	103	VAL	CA-C-N	-5.09	115.63	122.91
1	M	103	VAL	C-N-CA	-5.09	115.63	122.91
1	M	133	ARG	CA-CB-CG	-5.09	103.92	114.10
1	Q	9	GLN	CG-CD-NE2	5.09	124.03	116.40
1	R	244	THR	CA-C-N	5.09	125.12	119.32
1	R	244	THR	C-N-CA	5.09	125.12	119.32
1	P	125	GLN	CG-CD-NE2	5.09	124.03	116.40
1	B	174	ALA	CA-C-N	-5.09	113.67	120.54
1	B	174	ALA	C-N-CA	-5.09	113.67	120.54
1	G	273	GLY	CA-C-O	-5.09	111.72	120.57
1	I	42	ARG	N-CA-CB	5.09	118.06	110.22
1	L	25	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	L	96	ILE	O-C-N	5.09	127.03	121.94
1	N	109	ASP	CA-CB-CG	5.09	117.69	112.60
1	N	204	VAL	N-CA-C	-5.09	105.58	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	299	PHE	CA-C-O	5.09	127.39	121.44
1	R	202	GLN	CA-C-O	5.09	125.81	120.42
1	B	30	LEU	O-C-N	5.08	129.02	123.22
1	I	49	GLU	O-C-N	-5.08	116.25	123.01
1	Q	195	ASP	N-CA-CB	5.08	118.61	110.73
1	B	54	ASN	O-C-N	-5.08	116.80	122.09
1	C	90	GLY	CA-C-N	-5.08	115.02	122.19
1	C	90	GLY	C-N-CA	-5.08	115.02	122.19
1	K	167	ALA	O-C-N	-5.08	116.74	122.03
1	M	172	ARG	O-C-N	5.08	127.95	122.15
1	M	214	LYS	CB-CG-CD	5.08	122.99	111.30
1	O	336	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	P	89	GLN	CA-C-O	-5.08	113.88	119.78
1	A	138	LYS	N-CA-C	-5.08	105.63	111.07
1	C	72	SER	CA-CB-OG	-5.08	100.94	111.10
1	H	162	ALA	O-C-N	5.08	128.84	122.23
1	K	188	PRO	N-CA-C	-5.08	102.00	112.47
1	M	172	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	Q	190	VAL	CA-CB-CG1	-5.08	101.76	110.40
1	R	342	TYR	CA-C-O	-5.08	115.26	121.05
1	A	115	LEU	CB-CA-C	-5.08	102.65	110.78
1	B	272	GLY	CA-C-N	-5.08	111.45	121.41
1	B	272	GLY	C-N-CA	-5.08	111.45	121.41
1	C	300	SER	N-CA-C	-5.08	98.30	107.60
1	G	138	LYS	N-CA-C	-5.08	105.87	111.71
1	R	63	PHE	CA-CB-CG	5.08	118.88	113.80
1	D	257	HIS	ND1-CE1-NE2	5.08	113.48	108.40
1	E	169	ALA	N-CA-C	-5.08	105.74	111.28
1	E	328	MET	N-CA-CB	-5.08	102.40	110.22
1	F	161	LEU	CA-C-N	-5.08	113.08	120.29
1	F	161	LEU	C-N-CA	-5.08	113.08	120.29
1	K	128	ASP	O-C-N	-5.08	116.65	122.95
1	O	329	LYS	N-CA-CB	-5.08	102.32	110.19
1	R	102	ILE	CA-C-O	-5.08	114.95	120.84
1	B	233	VAL	N-CA-CB	5.08	119.61	111.23
1	L	248	VAL	CA-C-O	5.08	126.33	121.05
1	L	322	ALA	N-CA-CB	5.08	117.50	109.94
1	C	125	GLN	N-CA-C	5.08	117.08	110.53
1	C	211	ALA	CA-C-N	-5.08	114.05	120.60
1	C	211	ALA	C-N-CA	-5.08	114.05	120.60
1	I	217	ASN	CA-C-N	-5.08	113.69	120.54
1	I	217	ASN	C-N-CA	-5.08	113.69	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	115	LEU	CD1-CG-CD2	-5.08	99.63	110.80
1	M	330	ARG	CD-NE-CZ	-5.08	117.30	124.40
1	N	87	ASP	CA-C-N	-5.08	113.19	122.38
1	N	87	ASP	C-N-CA	-5.08	113.19	122.38
1	N	248	VAL	N-CA-C	-5.08	105.55	110.42
1	O	336	GLN	N-CA-C	-5.08	105.83	111.36
1	F	147	TRP	O-C-N	5.07	129.55	123.36
1	G	4	PHE	N-CA-C	5.07	122.59	111.53
1	G	124	ILE	N-CA-CB	-5.07	102.54	111.93
1	I	336	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	J	156	GLN	CB-CG-CD	-5.07	103.97	112.60
1	K	94	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	P	55	ARG	O-C-N	-5.07	116.84	122.07
1	R	215	ALA	CA-C-O	-5.07	115.04	120.42
1	H	330	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	B	261	PRO	N-CA-CB	5.07	107.76	103.35
1	H	91	LYS	CA-C-O	-5.07	114.75	120.43
1	J	119	ASN	OD1-CG-ND2	5.07	127.67	122.60
1	L	125	GLN	CB-CG-CD	-5.07	103.98	112.60
1	Q	140	ASP	CB-CG-OD1	-5.07	106.74	118.40
1	K	42	ARG	CA-C-N	5.07	127.07	120.28
1	K	42	ARG	C-N-CA	5.07	127.07	120.28
1	R	328	MET	CA-CB-CG	-5.07	103.96	114.10
1	F	228	LEU	O-C-N	-5.07	117.27	123.30
1	G	310	LEU	CA-C-N	-5.07	113.55	120.44
1	G	310	LEU	C-N-CA	-5.07	113.55	120.44
1	J	137	TYR	O-C-N	-5.07	116.37	122.15
1	K	77	ILE	CB-CA-C	-5.07	103.95	110.84
1	K	119	ASN	O-C-N	-5.07	116.43	122.46
1	R	64	SER	CA-C-N	-5.07	112.85	121.97
1	R	64	SER	C-N-CA	-5.07	112.85	121.97
1	A	13	LYS	O-C-N	5.07	127.49	122.12
1	H	337	ALA	O-C-N	-5.07	116.29	122.22
1	L	182	LEU	CA-C-O	5.07	126.75	120.92
1	N	133	ARG	O-C-N	-5.07	116.85	122.07
1	A	122	THR	N-CA-C	5.06	116.98	109.69
1	I	127	LEU	CA-C-N	-5.06	113.53	121.02
1	I	127	LEU	C-N-CA	-5.06	113.53	121.02
1	L	24	ALA	N-CA-CB	5.06	118.03	109.78
1	N	304	ALA	CA-C-O	-5.06	112.72	119.10
1	Q	90	GLY	N-CA-C	-5.06	101.18	113.18
1	A	59	ARG	O-C-N	-5.06	116.05	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	178	GLN	CG-CD-OE1	5.06	130.92	120.80
1	G	248	VAL	CA-C-O	5.06	126.53	121.17
1	G	337	ALA	O-C-N	5.06	127.28	122.07
1	Q	47	LYS	CA-C-N	5.06	131.17	122.67
1	Q	47	LYS	C-N-CA	5.06	131.17	122.67
1	Q	165	GLU	CB-CG-CD	-5.06	104.00	112.60
1	C	268	CYS	CA-C-O	5.06	126.94	120.57
1	E	71	GLN	O-C-N	5.06	129.54	122.36
1	L	88	SER	CA-C-O	5.06	127.02	119.23
1	O	52	GLU	CB-CA-C	-5.06	102.08	110.68
1	O	339	LYS	N-CA-C	-5.06	106.36	112.88
1	B	252	THR	CA-CB-OG1	-5.06	102.02	109.60
1	C	209	LEU	CA-C-N	-5.06	112.62	120.31
1	C	209	LEU	C-N-CA	-5.06	112.62	120.31
1	O	6	ALA	CB-CA-C	-5.06	102.25	110.85
1	Q	193	ASP	CA-C-O	-5.06	115.59	121.15
1	E	97	LEU	CA-C-O	5.05	126.13	120.82
1	F	148	ARG	N-CA-CB	-5.05	102.77	110.65
1	K	99	GLU	CA-C-N	-5.05	112.29	122.55
1	K	99	GLU	C-N-CA	-5.05	112.29	122.55
1	O	93	PHE	N-CA-CB	-5.05	102.69	110.12
1	O	204	VAL	CA-CB-CG1	-5.05	101.81	110.40
1	C	62	LEU	CA-C-O	-5.05	115.06	120.42
1	J	89	GLN	N-CA-C	-5.05	105.82	112.94
1	K	272	GLY	CA-C-N	-5.05	116.26	123.08
1	K	272	GLY	C-N-CA	-5.05	116.26	123.08
1	Q	235	ALA	CA-C-N	5.05	125.95	120.44
1	Q	235	ALA	C-N-CA	5.05	125.95	120.44
1	E	16	SER	CA-C-O	-5.05	115.20	120.55
1	F	270	LEU	CA-C-N	-5.05	113.18	121.92
1	F	270	LEU	C-N-CA	-5.05	113.18	121.92
1	G	8	THR	CA-C-O	-5.05	115.85	121.81
1	J	246	GLU	N-CA-CB	5.05	117.64	110.16
1	O	124	ILE	O-C-N	-5.05	117.69	123.10
1	Q	212	VAL	CA-C-O	5.05	126.53	121.17
1	A	131	SER	N-CA-CB	-5.05	102.70	110.12
1	K	248	VAL	CA-C-N	-5.05	113.12	120.29
1	K	248	VAL	C-N-CA	-5.05	113.12	120.29
1	N	261	PRO	N-CA-C	5.05	119.14	111.11
1	H	26	GLY	N-CA-C	-5.05	108.65	115.36
1	K	234	THR	CB-CA-C	-5.05	99.41	110.67
1	M	170	LEU	CA-C-O	5.05	126.08	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	GLU	CA-C-O	-5.05	115.20	120.55
1	B	247	GLN	CG-CD-OE1	5.05	130.89	120.80
1	C	70	ASN	CA-C-O	5.05	127.00	119.23
1	I	163	ILE	CA-C-O	5.05	126.69	121.29
1	K	52	GLU	CA-C-O	-5.05	114.55	120.20
1	M	61	ILE	CA-C-N	5.05	127.45	120.29
1	M	61	ILE	C-N-CA	5.05	127.45	120.29
1	D	187	GLU	OE1-CD-OE2	5.04	135.01	122.90
1	D	345	THR	CA-C-O	-5.04	113.30	120.51
1	P	114	PRO	CB-CA-C	5.04	117.01	111.11
1	C	56	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	F	87	ASP	CB-CG-OD2	5.04	130.00	118.40
1	I	116	ALA	CA-C-O	-5.04	115.99	121.44
1	I	334	ASN	CA-CB-CG	-5.04	107.56	112.60
1	O	38	THR	O-C-N	5.04	127.26	122.07
1	B	233	VAL	CG1-CB-CG2	-5.04	99.71	110.80
1	G	310	LEU	CA-CB-CG	5.04	133.94	116.30
1	L	229	LYS	CA-C-O	-5.04	115.37	121.22
1	M	217	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	N	215	ALA	CA-C-N	-5.04	112.53	120.60
1	N	215	ALA	C-N-CA	-5.04	112.53	120.60
1	H	330	ARG	N-CA-C	-5.04	105.97	111.82
1	I	11	GLN	N-CA-C	-5.04	105.79	111.28
1	N	121	GLU	N-CA-C	5.04	117.35	110.55
1	A	33	ASP	O-C-N	-5.04	115.92	122.37
1	C	220	HIS	CA-CB-CG	-5.04	108.76	113.80
1	F	220	HIS	CE1-NE2-CD2	5.04	114.04	109.00
1	J	38	THR	O-C-N	5.04	127.89	122.15
1	J	87	ASP	N-CA-CB	5.04	119.01	110.49
1	Q	84	TYR	CA-C-O	5.04	125.12	119.18
1	A	343	VAL	N-CA-C	-5.04	98.86	109.34
1	I	333	ALA	CA-C-O	-5.04	115.19	120.63
1	P	114	PRO	N-CA-CB	-5.04	99.18	103.36
1	B	343	VAL	CA-C-O	5.04	127.08	120.78
1	D	181	GLY	CA-C-N	-5.04	115.15	122.65
1	D	181	GLY	C-N-CA	-5.04	115.15	122.65
1	H	204	VAL	CA-C-N	-5.04	113.53	120.28
1	H	204	VAL	C-N-CA	-5.04	113.53	120.28
1	I	25	ASN	N-CA-CB	5.04	121.68	111.36
1	L	23	VAL	CA-CB-CG1	5.04	118.96	110.40
1	L	191	ILE	CG1-CB-CG2	-5.04	95.59	110.70
1	R	154	ALA	CB-CA-C	-5.04	101.81	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	VAL	CA-C-O	-5.03	115.10	120.59
1	C	95	ASN	O-C-N	5.03	129.07	122.33
1	F	58	PHE	O-C-N	5.03	127.45	122.12
1	G	190	VAL	N-CA-CB	5.03	117.50	111.31
1	H	131	SER	O-C-N	5.03	127.47	122.03
1	L	42	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	N	72	SER	CA-C-N	-5.03	116.08	122.37
1	N	72	SER	C-N-CA	-5.03	116.08	122.37
1	R	91	LYS	CA-C-N	-5.03	114.30	121.50
1	R	91	LYS	C-N-CA	-5.03	114.30	121.50
1	E	267	ILE	CB-CG1-CD1	-5.03	103.23	113.80
1	B	21	SER	CA-C-N	-5.03	114.28	121.52
1	B	21	SER	C-N-CA	-5.03	114.28	121.52
1	C	9	GLN	CA-C-O	-5.03	114.42	120.10
1	C	222	TYR	N-CA-CB	-5.03	102.21	110.21
1	F	65	VAL	O-C-N	-5.03	118.22	122.65
1	F	261	PRO	O-C-N	5.03	129.25	123.01
1	I	244	THR	N-CA-CB	-5.03	101.86	110.72
1	J	173	TYR	N-CA-CB	-5.03	102.72	110.12
1	N	155	ASP	CA-C-O	5.03	126.48	120.70
1	O	94	ARG	CA-C-O	5.03	125.76	119.97
1	Q	287	ASN	CA-CB-CG	-5.03	107.57	112.60
1	R	102	ILE	N-CA-C	5.03	116.20	108.71
1	A	277	GLU	CG-CD-OE1	5.03	129.96	118.40
1	D	309	ALA	CA-C-O	5.03	125.75	120.42
1	H	304	ALA	CA-C-O	-5.03	112.51	119.05
1	K	328	MET	N-CA-CB	5.03	117.30	110.01
1	M	22	ILE	N-CA-C	5.03	117.33	111.05
1	L	18	ILE	CB-CA-C	-5.03	105.28	112.22
1	M	42	ARG	NH1-CZ-NH2	-5.03	112.77	119.30
1	O	217	ASN	CA-C-N	5.03	127.27	120.38
1	O	217	ASN	C-N-CA	5.03	127.27	120.38
1	P	125	GLN	CB-CA-C	-5.03	101.01	110.51
1	A	284	ASN	CB-CG-OD1	5.02	130.85	120.80
1	D	185	ILE	CA-C-O	-5.02	114.77	120.65
1	J	219	HIS	ND1-CE1-NE2	-5.02	103.38	108.40
1	M	194	GLY	CA-C-O	5.02	126.04	122.37
1	B	82	THR	N-CA-CB	-5.02	102.49	110.22
1	F	122	THR	OG1-CB-CG2	-5.02	99.26	109.30
1	O	145	GLY	CA-C-N	-5.02	113.10	121.94
1	O	145	GLY	C-N-CA	-5.02	113.10	121.94
1	R	108	LEU	CA-C-O	5.02	124.57	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	111	GLY	CA-C-O	-5.02	117.95	122.57
1	E	191	ILE	N-CA-CB	5.02	118.24	111.21
1	G	117	GLY	CA-C-N	-5.02	114.39	122.82
1	G	117	GLY	C-N-CA	-5.02	114.39	122.82
1	I	292	PRO	CA-C-O	5.02	127.33	121.31
1	I	341	GLN	OE1-CD-NE2	5.02	127.62	122.60
1	M	235	ALA	N-CA-CB	5.02	117.25	110.38
1	O	196	HIS	CA-CB-CG	-5.02	108.78	113.80
1	O	329	LYS	CA-C-N	-5.02	113.55	120.28
1	O	329	LYS	C-N-CA	-5.02	113.55	120.28
1	A	187	GLU	O-C-N	-5.02	116.12	121.04
1	A	270	LEU	N-CA-C	-5.02	103.78	110.55
1	A	339	LYS	CB-CG-CD	5.02	122.84	111.30
1	C	179	GLN	O-C-N	5.02	129.15	122.43
1	C	316	LYS	N-CA-CB	5.02	118.43	110.55
1	D	46	ILE	N-CA-CB	-5.02	106.52	112.39
1	F	91	LYS	O-C-N	5.02	128.93	123.01
1	H	50	ASN	CB-CA-C	-5.02	103.13	111.41
1	I	184	PRO	N-CA-CB	5.02	108.52	103.25
1	I	325	GLU	CB-CG-CD	-5.02	104.07	112.60
1	L	70	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	Q	131	SER	CA-CB-OG	-5.02	101.06	111.10
1	B	270	LEU	CA-C-N	-5.02	114.41	122.08
1	B	270	LEU	C-N-CA	-5.02	114.41	122.08
1	D	269	PHE	N-CA-C	5.02	117.17	110.35
1	K	244	THR	CA-C-N	5.02	124.62	119.05
1	K	244	THR	C-N-CA	5.02	124.62	119.05
1	R	22	ILE	O-C-N	5.02	126.94	121.87
1	C	271	SER	N-CA-C	-5.01	107.84	114.31
1	E	193	ASP	O-C-N	5.01	129.24	122.82
1	I	260	VAL	CG1-CB-CG2	5.01	121.83	110.80
1	L	260	VAL	N-CA-C	5.01	113.39	107.77
1	P	189	GLU	CG-CD-OE1	5.01	129.93	118.40
1	R	197	ASP	CA-C-N	5.01	127.41	120.29
1	R	197	ASP	C-N-CA	5.01	127.41	120.29
1	B	296	LYS	CB-CA-C	-5.01	101.40	109.72
1	E	19	ALA	CA-C-O	-5.01	115.54	120.90
1	F	120	LYS	CA-C-O	-5.01	114.40	120.32
1	J	108	LEU	CA-C-O	5.01	124.42	118.90
1	L	47	LYS	N-CA-C	5.01	118.36	111.54
1	M	117	GLY	O-C-N	5.01	128.46	122.34
1	A	31	ALA	CA-C-O	-5.01	115.78	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASN	CB-CA-C	-5.01	102.33	110.85
1	A	346	GLY	N-CA-C	-5.01	101.30	113.18
1	B	146	LYS	CG-CD-CE	5.01	122.82	111.30
1	G	132	GLU	CA-C-O	-5.01	115.54	120.90
1	J	26	GLY	CA-C-N	-5.01	111.85	120.97
1	J	26	GLY	C-N-CA	-5.01	111.85	120.97
1	M	321	GLU	CA-C-N	-5.01	113.17	120.29
1	M	321	GLU	C-N-CA	-5.01	113.17	120.29
1	P	3	ARG	CD-NE-CZ	5.01	131.41	124.40
1	P	114	PRO	CA-C-N	5.01	129.36	122.84
1	P	114	PRO	C-N-CA	5.01	129.36	122.84
1	Q	47	LYS	N-CA-C	5.01	118.12	111.30
1	R	258	ARG	CA-C-N	-5.01	114.37	122.24
1	R	258	ARG	C-N-CA	-5.01	114.37	122.24
1	E	325	GLU	CB-CG-CD	-5.01	104.08	112.60
1	I	191	ILE	CA-C-O	5.01	126.66	119.95
1	M	106	ILE	CA-C-O	-5.01	115.97	121.28
1	R	20	GLN	CA-C-O	-5.01	115.24	120.55
1	R	260	VAL	N-CA-C	5.01	112.12	107.56
1	D	279	ALA	CA-C-O	-5.01	115.16	121.02
1	F	71	GLN	N-CA-CB	-5.01	102.63	110.44
1	N	25	ASN	CA-CB-CG	5.01	117.61	112.60
1	Q	221	VAL	O-C-N	-5.01	117.32	122.63
1	R	165	GLU	CB-CG-CD	-5.01	104.09	112.60
1	C	198	LEU	N-CA-C	5.01	116.43	111.07
1	H	10	GLU	CB-CG-CD	-5.01	104.09	112.60
1	J	87	ASP	CB-CA-C	-5.01	100.45	110.42
1	K	89	GLN	CG-CD-NE2	-5.01	108.89	116.40
1	M	287	ASN	CA-C-O	5.01	125.68	119.12
1	D	195	ASP	CB-CG-OD1	-5.00	106.89	118.40
1	G	8	THR	CA-CB-CG2	-5.00	101.99	110.50
1	M	83	LEU	CA-C-N	-5.00	114.64	122.65
1	M	83	LEU	C-N-CA	-5.00	114.64	122.65
1	R	122	THR	N-CA-C	5.00	116.90	109.69
1	C	18	ILE	CB-CA-C	-5.00	105.39	112.14
1	C	22	ILE	CA-C-O	-5.00	114.85	120.25
1	E	276	GLU	O-C-N	5.00	127.42	122.12
1	H	170	LEU	CA-C-N	-5.00	113.94	120.44
1	H	170	LEU	C-N-CA	-5.00	113.94	120.44
1	I	13	LYS	CA-C-N	-5.00	113.94	120.44
1	I	13	LYS	C-N-CA	-5.00	113.94	120.44
1	K	20	GLN	OE1-CD-NE2	5.00	127.60	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	303	ARG	N-CA-CB	5.00	117.26	110.01
1	Q	212	VAL	O-C-N	-5.00	117.01	121.91
1	R	67	SER	N-CA-CB	-5.00	101.21	110.32
1	C	45	ARG	CA-C-O	-5.00	115.55	120.90
1	I	328	MET	CA-C-O	5.00	125.72	119.97
1	J	171	ALA	CA-C-N	-5.00	113.64	120.44
1	J	171	ALA	C-N-CA	-5.00	113.64	120.44
1	M	175	SER	N-CA-C	5.00	116.42	110.97
1	O	306	GLN	N-CA-CB	5.00	118.45	111.15
1	P	81	GLU	N-CA-C	-5.00	105.52	110.97
1	P	339	LYS	CG-CD-CE	5.00	122.80	111.30

There are no chirality outliers.

All (133) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	THR	Mainchain
1	A	153	ILE	Mainchain
1	A	159	SER	Mainchain
1	A	220	HIS	Mainchain
1	A	300	SER	Mainchain
1	A	356	LEU	Peptide
1	A	4	PHE	Mainchain
1	B	214	LYS	Mainchain
1	B	226	THR	Mainchain
1	B	248	VAL	Mainchain
1	B	267	ILE	Mainchain
1	B	292	PRO	Mainchain
1	B	300	SER	Mainchain
1	B	323	THR	Mainchain
1	B	334	ASN	Mainchain
1	B	341	GLN	Mainchain
1	B	345	THR	Mainchain
1	B	6	ALA	Mainchain
1	B	68	SER	Mainchain
1	B	69	ILE	Mainchain
1	C	115	LEU	Mainchain
1	C	263	ALA	Mainchain
1	C	296	LYS	Mainchain
1	C	300	SER	Mainchain
1	C	35	SER	Mainchain
1	C	87	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	D	1	ALA	Peptide
1	D	100	LYS	Mainchain
1	D	159	SER	Mainchain
1	D	18	ILE	Mainchain
1	D	195	ASP	Mainchain
1	D	226	THR	Mainchain
1	D	24	ALA	Mainchain
1	D	285	ALA	Mainchain
1	D	306	GLN	Mainchain
1	D	33	ASP	Mainchain
1	D	70	ASN	Mainchain
1	D	87	ASP	Mainchain
1	D	89	GLN	Mainchain
1	E	100	LYS	Mainchain
1	E	123	THR	Mainchain
1	E	196	HIS	Mainchain
1	E	247	GLN	Mainchain
1	E	258	ARG	Mainchain
1	E	88	SER	Peptide,Mainchain
1	F	190	VAL	Mainchain
1	F	26	GLY	Mainchain
1	F	319	ASN	Mainchain
1	F	70	ASN	Mainchain
1	G	113	ALA	Mainchain
1	G	229	LYS	Mainchain
1	G	3	ARG	Mainchain
1	G	300	SER	Mainchain
1	G	65	VAL	Mainchain
1	G	83	LEU	Mainchain
1	G	87	ASP	Mainchain
1	G	98	LYS	Mainchain
1	H	1	ALA	Peptide
1	H	166	ASN	Mainchain
1	H	3	ARG	Mainchain
1	H	300	SER	Mainchain
1	H	345	THR	Mainchain
1	H	70	ASN	Mainchain
1	H	89	GLN	Mainchain
1	I	109	ASP	Mainchain
1	I	115	LEU	Mainchain
1	I	148	ARG	Mainchain
1	I	154	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	I	176	ILE	Mainchain
1	I	204	VAL	Mainchain
1	I	331	ALA	Mainchain
1	I	338	ALA	Mainchain
1	I	66	ASP	Peptide
1	I	67	SER	Mainchain
1	I	69	ILE	Mainchain
1	J	108	LEU	Mainchain
1	J	24	ALA	Mainchain
1	J	33	ASP	Mainchain
1	J	70	ASN	Mainchain
1	K	189	GLU	Mainchain
1	K	300	SER	Mainchain
1	K	347	SER	Peptide,Mainchain
1	K	4	PHE	Mainchain
1	K	88	SER	Mainchain
1	L	12	LYS	Mainchain
1	L	180	ASN	Mainchain
1	L	296	LYS	Mainchain
1	L	333	ALA	Mainchain
1	L	338	ALA	Mainchain
1	L	87	ASP	Mainchain
1	M	282	ASN	Mainchain
1	M	344	HIS	Mainchain
1	M	352	SER	Peptide
1	M	356	LEU	Mainchain
1	M	358	THR	Mainchain
1	M	68	SER	Mainchain
1	M	69	ILE	Peptide
1	M	71	GLN	Mainchain
1	N	109	ASP	Mainchain
1	N	116	ALA	Mainchain
1	N	298	SER	Mainchain
1	N	3	ARG	Peptide
1	N	35	SER	Mainchain
1	N	87	ASP	Mainchain
1	O	116	ALA	Mainchain
1	O	180	ASN	Mainchain
1	O	267	ILE	Mainchain
1	O	297	LEU	Mainchain
1	O	300	SER	Mainchain
1	P	114	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	P	123	THR	Mainchain
1	P	285	ALA	Mainchain
1	P	295	TRP	Mainchain
1	P	352	SER	Mainchain
1	P	87	ASP	Mainchain
1	Q	134	CYS	Mainchain
1	Q	21	SER	Mainchain
1	Q	217	ASN	Mainchain
1	Q	300	SER	Mainchain
1	Q	87	ASP	Mainchain
1	Q	88	SER	Mainchain
1	R	113	ALA	Mainchain
1	R	134	CYS	Mainchain
1	R	161	LEU	Mainchain
1	R	171	ALA	Mainchain
1	R	220	HIS	Mainchain
1	R	237	HIS	Mainchain
1	R	266	GLY	Mainchain
1	R	300	SER	Mainchain
1	R	70	ASN	Mainchain
1	R	88	SER	Mainchain

5.2 Too-close contacts

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	2730	0	2739	252	0
1	B	2651	0	2665	279	0
1	C	2635	0	2651	227	0
1	D	2701	0	2713	235	0
1	E	2687	0	2696	205	0
1	F	2675	0	2685	174	0
1	G	2628	0	2645	163	0
1	H	2712	0	2721	224	0
1	I	2628	0	2644	260	0
1	J	2701	0	2714	199	0
1	K	2686	0	2694	154	0
1	L	2628	0	2645	202	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	2730	0	2739	255	0
1	N	2628	0	2644	243	0
1	O	2628	0	2645	218	0
1	P	2730	0	2740	186	0
1	Q	2628	0	2645	153	0
1	R	2628	0	2645	164	0
2	A	10	0	0	4	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	G	15	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	M	5	0	0	0	0
2	O	5	0	0	0	0
2	P	10	0	0	0	0
2	R	10	0	0	1	0
3	A	86	0	0	17	0
3	B	34	0	0	4	0
3	C	44	0	0	2	0
3	D	82	0	0	8	0
3	E	75	0	0	7	0
3	F	80	0	0	14	0
3	G	75	0	0	5	0
3	H	70	0	0	9	0
3	I	45	0	0	7	0
3	J	78	0	0	17	0
3	K	71	0	0	6	0
3	L	28	0	0	2	0
3	M	81	0	0	9	0
3	N	53	0	0	5	0
3	O	37	0	0	8	0
3	P	78	0	0	11	0
3	Q	80	0	0	10	0
3	R	72	0	0	10	0
All	All	49278	0	48270	3485	0

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 36.

All (3485) 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:D:70:ASN:CA	1:D:70:ASN:CB	1.74	1.64
1:D:70:ASN:CA	1:D:70:ASN:HD22	1.30	1.41
1:E:89:GLN:OE1	1:E:89:GLN:CB	1.72	1.36
1:D:70:ASN:CA	1:D:70:ASN:ND2	1.87	1.35
1:A:356:LEU:HD13	1:A:357:PHE:CE1	1.65	1.32
1:M:68:SER:CA	1:M:69:ILE:HG13	1.61	1.29
1:E:329:LYS:NZ	1:E:347:SER:HB3	1.48	1.28
1:F:69:ILE:HG22	3:F:457:HOH:O	1.24	1.28
1:D:70:ASN:CB	1:D:70:ASN:C	2.07	1.25
1:M:66:ASP:O	1:M:68:SER:HA	1.34	1.23
1:M:343:VAL:HG23	1:M:344:HIS:O	1.34	1.22
1:M:69:ILE:HD13	1:M:328:MET:CE	1.69	1.22
1:A:67:SER:CB	3:A:502:HOH:O	1.87	1.21
1:A:342:TYR:CE2	1:A:344:HIS:HB3	1.75	1.20
1:M:68:SER:O	1:M:69:ILE:C	1.78	1.18
1:D:70:ASN:HD22	1:D:70:ASN:HA	1.02	1.16
1:J:244:THR:HG22	1:J:247:GLN:H	1.09	1.16
1:R:51:THR:HG22	1:R:54:ASN:H	1.05	1.16
1:M:69:ILE:HD13	1:M:328:MET:HE1	1.27	1.16
1:M:68:SER:OG	1:M:69:ILE:HD12	1.42	1.15
1:I:3:ARG:HD3	1:J:156:GLN:HE22	1.05	1.14
1:N:2:HIS:HA	1:N:3:ARG:CZ	1.78	1.13
1:G:87:ASP:HB3	1:G:89:GLN:H	1.06	1.13
1:D:70:ASN:HB3	1:D:70:ASN:O	1.49	1.12
1:K:244:THR:HG22	1:K:247:GLN:N	1.64	1.13
1:M:69:ILE:CD1	1:M:328:MET:SD	2.37	1.12
1:B:342:TYR:CE2	1:B:344:HIS:HA	1.83	1.12
1:K:244:THR:CG2	1:K:247:GLN:H	1.63	1.11
1:R:244:THR:HG22	1:R:247:GLN:H	1.14	1.11
1:A:51:THR:HG22	1:A:54:ASN:H	0.99	1.11
1:P:51:THR:HG22	1:P:54:ASN:H	1.03	1.11
1:P:303:ARG:HH21	1:P:357:PHE:HA	1.08	1.11
1:A:2:HIS:HB2	1:A:3:ARG:HD2	1.31	1.11
1:L:51:THR:HG22	1:L:54:ASN:H	1.06	1.11
1:Q:119:ASN:N	1:R:1:ALA:HB1	1.65	1.10
1:D:88:SER:O	1:D:89:GLN:HB2	1.30	1.10
1:H:329:LYS:HD2	1:H:347:SER:HA	1.33	1.10
1:A:45:ARG:CZ	1:A:357:PHE:HA	1.80	1.10
1:A:307:ALA:CB	1:A:357:PHE:HZ	1.62	1.10
1:E:256:LEU:HD13	1:E:267:ILE:HD11	1.32	1.10
1:J:51:THR:HG22	1:J:54:ASN:H	1.05	1.10
1:M:329:LYS:HE3	1:M:347:SER:HB2	1.21	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:68:SER:HA	1:I:70:ASN:ND2	1.66	1.10
1:N:123:THR:HG22	1:N:124:ILE:H	1.07	1.09
1:C:51:THR:HG22	1:C:54:ASN:N	1.67	1.09
1:H:256:LEU:HD13	1:H:267:ILE:HD11	1.31	1.09
1:H:51:THR:HG22	1:H:54:ASN:H	0.98	1.09
1:N:256:LEU:HD13	1:N:267:ILE:HD11	1.29	1.09
1:B:51:THR:HG22	1:B:54:ASN:HB2	1.33	1.09
1:K:353:THR:HG22	3:O:509:HOH:O	1.51	1.09
1:K:51:THR:HG22	1:K:54:ASN:H	1.18	1.08
1:K:303:ARG:NH2	1:K:357:PHE:HB2	1.69	1.08
1:F:329:LYS:HE2	1:F:347:SER:HA	1.09	1.08
1:Q:51:THR:HG22	1:Q:54:ASN:H	1.07	1.08
1:A:244:THR:CG2	1:A:247:GLN:H	1.66	1.08
1:M:69:ILE:HD13	1:M:328:MET:SD	1.93	1.08
1:E:329:LYS:HZ2	1:E:347:SER:HB3	0.98	1.07
1:I:119:ASN:H	1:J:1:ALA:HB3	1.11	1.07
1:Q:50:ASN:ND2	1:Q:55:ARG:HH11	1.52	1.07
1:D:244:THR:HG22	1:D:247:GLN:H	1.18	1.07
1:H:330:ARG:HH11	1:H:347:SER:CB	1.68	1.07
1:D:70:ASN:CA	1:D:70:ASN:CG	2.27	1.07
1:Q:119:ASN:H	1:R:1:ALA:HB1	0.91	1.07
1:H:330:ARG:HH11	1:H:347:SER:HB2	1.18	1.06
1:P:3:ARG:HD3	1:P:4:PHE:H	1.19	1.06
1:A:307:ALA:HB2	1:A:357:PHE:CZ	1.90	1.05
1:I:68:SER:HB3	3:I:406:HOH:O	1.53	1.05
1:I:223:LEU:O	1:I:226:THR:HB	1.56	1.05
1:A:244:THR:HG22	1:A:247:GLN:N	1.69	1.05
1:F:50:ASN:ND2	1:F:55:ARG:HH11	1.52	1.05
1:F:329:LYS:CE	1:F:347:SER:HA	1.86	1.05
1:M:69:ILE:HA	1:M:71:GLN:H	1.14	1.05
1:A:307:ALA:CA	1:A:357:PHE:HZ	1.70	1.05
1:B:58:PHE:CE1	1:B:310:LEU:HD13	1.91	1.05
1:M:68:SER:CA	1:M:69:ILE:CG1	2.35	1.04
1:N:244:THR:HG22	1:N:247:GLN:HG3	1.38	1.04
1:C:51:THR:CG2	1:C:54:ASN:H	1.70	1.04
1:H:352:SER:HA	1:H:354:GLN:HB2	1.39	1.04
1:I:65:VAL:HG11	1:I:69:ILE:HD13	1.39	1.04
1:B:68:SER:O	1:B:70:ASN:N	1.92	1.03
1:L:118:THR:CG2	1:L:121:GLU:H	1.71	1.03
1:N:3:ARG:CZ	1:O:203:TYR:OH	2.07	1.03
1:A:41:ASN:HB3	1:A:358:THR:HB	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ASN:CB	1:D:70:ASN:O	2.06	1.02
1:E:253:VAL:HG12	1:E:291:LEU:HD23	1.40	1.02
1:M:51:THR:HG22	1:M:54:ASN:H	1.25	1.02
1:O:244:THR:HG22	1:O:247:GLN:H	1.24	1.02
1:Q:119:ASN:H	1:R:1:ALA:CB	1.72	1.02
1:D:51:THR:HG22	1:D:54:ASN:H	1.21	1.01
1:P:244:THR:HG22	1:P:247:GLN:H	1.25	1.01
1:A:244:THR:HG22	1:A:247:GLN:H	0.85	1.01
1:P:250:MET:HE3	1:P:291:LEU:HD11	1.37	1.01
1:F:71:GLN:NE2	3:F:401:HOH:O	1.68	1.01
1:E:89:GLN:OE1	1:E:90:GLY:N	1.92	1.01
1:E:66:ASP:O	1:E:67:SER:HB3	1.58	1.01
1:I:3:ARG:HD3	1:J:156:GLN:NE2	1.75	1.00
1:B:51:THR:CG2	1:B:54:ASN:H	1.75	1.00
1:E:329:LYS:NZ	1:E:347:SER:CB	2.24	1.00
1:I:123:THR:HG22	1:I:124:ILE:H	1.24	1.00
1:E:244:THR:HG22	1:E:247:GLN:H	1.26	1.00
1:H:3:ARG:O	1:H:3:ARG:HD3	1.60	1.00
1:D:191:ILE:N	1:D:191:ILE:HD12	1.76	0.99
1:D:88:SER:O	1:D:89:GLN:CB	2.08	0.99
1:C:51:THR:HG22	1:C:54:ASN:H	0.85	0.99
1:B:51:THR:HG22	1:B:54:ASN:H	1.28	0.99
1:L:51:THR:CG2	1:L:54:ASN:H	1.75	0.99
1:Q:2:HIS:O	1:Q:3:ARG:HB2	1.63	0.99
1:E:329:LYS:HZ2	1:E:347:SER:CB	1.75	0.99
1:P:51:THR:CG2	1:P:54:ASN:H	1.76	0.99
1:A:356:LEU:HD13	1:A:357:PHE:HE1	1.20	0.99
1:L:87:ASP:HB2	1:L:91:LYS:H	1.27	0.99
1:A:50:ASN:ND2	1:A:55:ARG:HH11	1.58	0.99
1:O:51:THR:HG22	1:O:54:ASN:HB2	1.42	0.98
1:B:50:ASN:HD21	1:B:55:ARG:HD3	1.27	0.98
1:K:244:THR:HG22	1:K:247:GLN:H	0.84	0.98
1:L:87:ASP:HB3	1:L:89:GLN:H	1.25	0.98
1:I:118:THR:HA	1:J:1:ALA:N	1.77	0.98
1:A:307:ALA:HB2	1:A:357:PHE:HZ	1.25	0.98
1:L:89:GLN:O	1:L:89:GLN:HG2	1.60	0.98
1:O:3:ARG:HG2	1:O:4:PHE:H	1.28	0.98
1:P:303:ARG:HH22	1:P:357:PHE:HD1	1.09	0.97
1:J:244:THR:HB	1:J:247:GLN:HE21	1.26	0.97
1:E:12:LYS:HB3	1:E:222:TYR:CE2	2.00	0.96
1:O:343:VAL:HG23	1:O:344:HIS:H	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ALA:HA	1:A:357:PHE:CZ	2.00	0.96
1:A:307:ALA:CB	1:A:357:PHE:CZ	2.46	0.96
1:B:330:ARG:HA	1:B:330:ARG:HE	1.31	0.96
1:D:1:ALA:N	1:D:220:HIS:HE1	1.62	0.96
1:E:329:LYS:CE	1:E:347:SER:HB3	1.94	0.96
1:N:87:ASP:HB3	1:N:89:GLN:H	1.30	0.96
1:N:223:LEU:O	1:N:226:THR:HB	1.65	0.95
1:M:66:ASP:O	1:M:68:SER:N	1.99	0.95
1:A:51:THR:CG2	1:A:54:ASN:H	1.78	0.95
1:C:123:THR:HG22	1:C:124:ILE:H	1.30	0.95
1:O:156:GLN:OE1	1:P:2:HIS:HB3	1.67	0.95
1:A:51:THR:HG22	1:A:54:ASN:N	1.80	0.95
1:B:281:LEU:HD21	1:B:344:HIS:ND1	1.82	0.95
1:A:42:ARG:CD	1:A:357:PHE:HB3	1.95	0.94
1:K:303:ARG:HH21	1:K:357:PHE:HB2	1.29	0.94
1:L:244:THR:CG2	1:L:247:GLN:H	1.79	0.94
1:Q:223:LEU:O	1:Q:226:THR:HB	1.68	0.94
1:B:203:TYR:OH	1:C:2:HIS:HA	1.67	0.94
1:M:118:THR:CG2	1:M:121:GLU:H	1.80	0.94
1:A:124:ILE:HD13	1:A:149:ALA:HA	1.50	0.94
1:E:329:LYS:HD3	1:E:347:SER:CB	1.97	0.94
1:F:67:SER:O	1:F:70:ASN:ND2	1.98	0.94
1:F:351:ALA:O	1:F:352:SER:HB2	1.66	0.94
1:M:1:ALA:HB3	1:N:119:ASN:H	1.32	0.94
1:A:67:SER:HB3	3:A:502:HOH:O	1.57	0.93
1:A:207:LYS:HE2	1:D:2:HIS:NE2	1.83	0.93
1:A:125:GLN:HE22	1:B:129:GLY:H	1.13	0.93
1:C:87:ASP:HB3	1:C:89:GLN:H	1.33	0.93
1:C:118:THR:CG2	1:C:121:GLU:H	1.82	0.93
1:H:256:LEU:HD13	1:H:267:ILE:CD1	1.99	0.93
1:A:342:TYR:HE2	1:A:344:HIS:HB3	1.31	0.93
1:B:342:TYR:C	1:B:344:HIS:H	1.75	0.93
1:D:189:GLU:HG2	1:D:191:ILE:HD12	1.51	0.93
1:P:51:THR:HG22	1:P:54:ASN:N	1.84	0.93
1:I:51:THR:HG22	1:I:53:GLU:N	1.84	0.93
1:A:115:LEU:O	1:A:118:THR:HB	1.69	0.92
1:D:189:GLU:HG2	1:D:191:ILE:CD1	1.97	0.92
1:G:119:ASN:H	1:H:1:ALA:N	1.66	0.92
1:C:159:SER:CB	1:D:1:ALA:HB3	1.98	0.92
1:E:12:LYS:HB3	1:E:222:TYR:CZ	2.04	0.92
1:N:123:THR:HG22	1:N:124:ILE:N	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:118:THR:HG23	1:M:121:GLU:H	1.34	0.92
1:Q:3:ARG:HD2	1:R:156:GLN:HE22	1.33	0.92
1:R:124:ILE:HG22	1:R:147:TRP:CZ2	2.04	0.92
1:G:223:LEU:O	1:G:226:THR:HB	1.70	0.92
1:R:190:VAL:H	1:R:231:ASN:ND2	1.67	0.92
1:E:329:LYS:HE2	1:E:346:GLY:O	1.70	0.92
1:H:51:THR:HG22	1:H:54:ASN:N	1.83	0.92
1:P:3:ARG:HD3	1:P:4:PHE:N	1.85	0.92
1:I:118:THR:CA	1:J:1:ALA:H3	1.83	0.91
1:A:307:ALA:CA	1:A:357:PHE:CZ	2.52	0.91
1:F:71:GLN:HG3	3:F:401:HOH:O	1.69	0.91
1:A:303:ARG:HG2	1:A:357:PHE:CD1	2.05	0.91
1:K:51:THR:HG22	1:K:54:ASN:N	1.86	0.91
1:N:3:ARG:HG2	1:O:203:TYR:HE1	1.36	0.91
1:L:51:THR:HG22	1:L:54:ASN:N	1.86	0.91
1:P:303:ARG:NH2	1:P:357:PHE:HD1	1.67	0.91
1:E:250:MET:CE	1:E:291:LEU:HD22	2.00	0.91
1:Q:129:GLY:H	1:R:125:GLN:NE2	1.67	0.91
1:R:58:PHE:CZ	1:R:310:LEU:HD13	2.04	0.91
1:A:207:LYS:HE2	1:D:2:HIS:CD2	2.06	0.91
1:B:8:THR:OG1	1:B:11:GLN:HG3	1.70	0.91
1:D:87:ASP:HB2	1:D:91:LYS:H	1.32	0.91
1:D:58:PHE:CZ	1:D:310:LEU:HD13	2.06	0.91
1:D:119:ASN:O	1:D:152:ARG:NH1	2.04	0.91
1:E:2:HIS:HB3	1:F:156:GLN:OE1	1.69	0.91
1:H:330:ARG:NH1	1:H:347:SER:HB2	1.86	0.91
1:M:67:SER:O	1:M:69:ILE:HG23	1.70	0.91
1:L:50:ASN:HD21	1:L:55:ARG:HD3	1.33	0.90
1:N:313:TRP:CE2	1:N:315:GLY:HA2	2.06	0.90
1:D:1:ALA:H2	1:D:220:HIS:HE1	1.14	0.90
1:A:223:LEU:O	1:A:226:THR:HB	1.71	0.90
1:N:3:ARG:NH1	1:O:203:TYR:CZ	2.39	0.90
1:P:291:LEU:O	1:P:293:LYS:HG3	1.72	0.90
1:R:343:VAL:O	1:R:344:HIS:ND1	2.04	0.90
1:Q:129:GLY:H	1:R:125:GLN:HE22	1.12	0.90
1:H:24:ALA:HA	3:H:434:HOH:O	1.70	0.90
1:I:213:TYR:OH	1:I:228:LEU:HD13	1.70	0.90
1:A:356:LEU:CD1	1:A:357:PHE:CE1	2.54	0.89
1:B:244:THR:CG2	1:B:247:GLN:H	1.85	0.89
1:B:244:THR:HG22	1:B:247:GLN:H	1.35	0.89
1:G:202:GLN:HB2	1:G:233:VAL:HG11	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:LYS:HZ3	1:E:347:SER:HA	1.36	0.89
1:H:329:LYS:CD	1:H:347:SER:HA	2.02	0.89
1:M:1:ALA:N	1:N:118:THR:HA	1.85	0.89
1:N:244:THR:CG2	1:N:247:GLN:HG3	2.01	0.89
1:B:51:THR:HG22	1:B:54:ASN:CB	2.01	0.89
1:B:61:ILE:HG21	1:B:323:THR:CG2	2.02	0.89
1:A:118:THR:HA	1:B:1:ALA:CB	2.02	0.89
1:N:3:ARG:HG2	1:O:203:TYR:CE1	2.08	0.89
1:N:51:THR:HG22	1:N:54:ASN:H	1.38	0.89
1:A:50:ASN:HD21	1:A:55:ARG:NH1	1.71	0.89
1:A:50:ASN:HD21	1:A:55:ARG:HH11	0.89	0.88
1:F:50:ASN:HD21	1:F:55:ARG:HH11	0.91	0.88
1:M:71:GLN:HG2	3:M:501:HOH:O	1.70	0.88
1:P:1:ALA:O	1:P:2:HIS:HB2	1.71	0.88
1:I:343:VAL:HG12	1:I:344:HIS:N	1.85	0.88
1:J:51:THR:HG22	1:J:54:ASN:N	1.89	0.88
1:J:230:PRO:HG3	1:J:267:ILE:HD12	1.55	0.88
1:F:69:ILE:CG2	3:F:457:HOH:O	1.95	0.88
1:A:45:ARG:HH21	1:A:358:THR:H	1.17	0.88
1:A:87:ASP:HB3	1:A:89:GLN:H	1.38	0.88
1:E:190:VAL:H	1:E:231:ASN:ND2	1.70	0.88
1:H:8:THR:HG22	1:H:10:GLU:H	1.37	0.88
1:M:69:ILE:HA	1:M:71:GLN:N	1.88	0.88
1:C:313:TRP:CE2	1:C:315:GLY:HA2	2.08	0.87
1:I:226:THR:HG23	3:I:423:HOH:O	1.74	0.87
1:M:69:ILE:HD11	1:M:328:MET:SD	2.13	0.87
2:A:401:SO4:O1	3:A:501:HOH:O	1.93	0.87
1:K:357:PHE:O	1:O:139:LYS:HE3	1.75	0.87
1:A:303:ARG:HG2	1:A:357:PHE:HD1	1.35	0.87
1:N:244:THR:HG22	1:N:247:GLN:H	1.38	0.87
1:B:344:HIS:CG	1:B:345:THR:H	1.88	0.87
1:E:125:GLN:NE2	1:F:129:GLY:H	1.72	0.87
1:P:87:ASP:HB3	1:P:89:GLN:H	1.40	0.87
1:I:68:SER:HA	1:I:70:ASN:HD22	1.33	0.87
1:I:118:THR:CA	1:J:1:ALA:N	2.36	0.87
1:Q:51:THR:HG22	1:Q:54:ASN:N	1.90	0.87
1:B:123:THR:HG23	1:B:165:GLU:HG3	1.55	0.86
1:M:69:ILE:CA	1:M:71:GLN:H	1.88	0.86
1:O:51:THR:CG2	1:O:54:ASN:H	1.88	0.86
1:B:67:SER:O	1:B:68:SER:C	2.15	0.86
1:E:129:GLY:H	1:F:125:GLN:NE2	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:THR:CG2	1:E:246:GLU:HB2	2.05	0.86
1:M:66:ASP:O	1:M:68:SER:CA	2.23	0.86
1:M:308:SER:HB3	1:M:351:ALA:HB1	1.55	0.86
1:N:256:LEU:HD13	1:N:267:ILE:CD1	2.05	0.86
1:H:352:SER:OG	1:H:354:GLN:HB3	1.75	0.86
1:J:8:THR:OG1	1:J:11:GLN:HG3	1.75	0.86
1:E:66:ASP:O	1:E:67:SER:CB	2.20	0.86
1:Q:1:ALA:N	3:Q:2001:HOH:O	2.08	0.86
1:O:51:THR:HG22	1:O:54:ASN:CB	2.04	0.86
1:D:1:ALA:N	1:D:220:HIS:CE1	2.42	0.86
1:B:123:THR:O	1:B:124:ILE:HD13	1.74	0.86
1:L:65:VAL:HG21	1:L:69:ILE:HG13	1.57	0.86
1:M:95:ASN:O	1:M:99:GLU:HG3	1.75	0.86
1:N:190:VAL:H	1:N:231:ASN:ND2	1.72	0.86
1:F:58:PHE:CZ	1:F:310:LEU:HD13	2.10	0.86
1:J:244:THR:HG22	1:J:247:GLN:N	1.89	0.86
1:L:244:THR:HG23	1:L:247:GLN:H	1.40	0.86
1:A:156:GLN:OE1	1:B:2:HIS:HB3	1.75	0.86
1:A:356:LEU:O	1:A:359:ALA:HB2	1.75	0.85
1:I:129:GLY:H	1:J:125:GLN:NE2	1.73	0.85
1:I:200:HIS:HE1	1:L:2:HIS:ND1	1.74	0.85
1:M:329:LYS:CE	1:M:347:SER:HB2	2.04	0.85
1:M:345:THR:HG21	1:M:347:SER:HB3	1.57	0.85
1:Q:2:HIS:HB3	1:R:156:GLN:OE1	1.75	0.85
1:R:51:THR:HG22	1:R:54:ASN:N	1.90	0.85
1:G:156:GLN:OE1	1:H:1:ALA:HB1	1.75	0.85
1:M:1:ALA:N	1:N:118:THR:CA	2.39	0.85
1:M:1:ALA:H3	1:N:118:THR:CA	1.88	0.85
1:E:51:THR:HG22	1:E:54:ASN:H	1.40	0.85
1:H:58:PHE:CZ	1:H:310:LEU:HD13	2.12	0.85
1:J:115:LEU:O	1:J:118:THR:HB	1.76	0.85
1:A:42:ARG:HD2	1:A:357:PHE:HB3	1.59	0.85
1:D:329:LYS:NZ	1:D:347:SER:HA	1.91	0.85
1:Q:271:SER:HA	1:Q:274:MET:HE3	1.59	0.85
1:P:303:ARG:NH2	1:P:357:PHE:HA	1.92	0.85
1:B:250:MET:HE3	1:B:291:LEU:HD21	1.58	0.85
1:Q:156:GLN:O	1:R:1:ALA:N	2.10	0.85
1:H:352:SER:HA	1:H:354:GLN:CB	2.07	0.85
1:M:68:SER:N	1:M:69:ILE:HG13	1.91	0.85
1:Q:156:GLN:NE2	1:R:3:ARG:HE	1.73	0.85
1:G:129:GLY:H	1:H:125:GLN:NE2	1.74	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:TYR:OH	1:C:228:LEU:HD13	1.76	0.84
1:L:277:GLU:OE2	1:L:342:TYR:OH	1.95	0.84
1:B:202:GLN:O	1:B:206:GLU:HG3	1.76	0.84
1:C:244:THR:HG22	1:C:247:GLN:CG	2.06	0.84
1:L:78:LEU:O	1:L:106:ILE:HD12	1.76	0.84
1:Q:159:SER:HB3	1:R:1:ALA:H3	1.43	0.84
1:A:42:ARG:HD3	1:A:357:PHE:HB3	1.59	0.84
1:N:244:THR:HG22	1:N:247:GLN:N	1.92	0.84
1:F:68:SER:O	1:F:71:GLN:HB2	1.78	0.84
1:G:18:ILE:HD13	1:G:143:ASP:HB3	1.57	0.84
1:J:71:GLN:CD	3:J:504:HOH:O	2.20	0.84
1:L:190:VAL:H	1:L:231:ASN:HD22	1.22	0.84
1:P:223:LEU:O	1:P:226:THR:HB	1.78	0.84
1:A:45:ARG:NH2	1:A:358:THR:H	1.75	0.83
1:E:87:ASP:OD1	1:E:89:GLN:CB	2.26	0.83
1:I:68:SER:CA	1:I:70:ASN:ND2	2.41	0.83
1:K:199:GLU:HB2	3:K:546:HOH:O	1.78	0.83
1:E:351:ALA:O	1:E:352:SER:HB2	1.76	0.83
1:M:123:THR:HG22	1:M:124:ILE:H	1.41	0.83
1:N:244:THR:CG2	1:N:247:GLN:H	1.90	0.83
1:M:68:SER:CA	1:M:69:ILE:CD1	2.56	0.83
1:C:224:GLU:N	1:C:224:GLU:OE1	2.11	0.83
1:E:271:SER:O	1:E:274:MET:HE2	1.78	0.83
1:G:51:THR:CG2	1:G:54:ASN:H	1.92	0.83
1:H:253:VAL:HG12	1:H:291:LEU:HD23	1.58	0.83
1:N:244:THR:HG22	1:N:247:GLN:CG	2.08	0.83
1:I:66:ASP:CG	1:I:67:SER:HB2	2.04	0.83
1:M:214:LYS:HE3	1:M:218:ASP:OD1	1.78	0.83
1:O:51:THR:HG22	1:O:54:ASN:H	1.41	0.83
1:Q:50:ASN:HD21	1:Q:55:ARG:HH11	1.23	0.83
1:P:303:ARG:HH21	1:P:357:PHE:CA	1.90	0.83
1:Q:50:ASN:HD21	1:Q:55:ARG:HD3	1.42	0.83
1:A:50:ASN:ND2	1:A:55:ARG:NH1	2.26	0.82
1:D:244:THR:HG22	1:D:247:GLN:N	1.93	0.82
1:G:87:ASP:HB3	1:G:89:GLN:N	1.92	0.82
1:L:281:LEU:HD23	1:L:342:TYR:HE2	1.45	0.82
1:N:313:TRP:CZ2	1:N:315:GLY:HA2	2.14	0.82
1:F:352:SER:OG	1:F:356:LEU:HD21	1.79	0.82
1:J:70:ASN:ND2	1:J:100:LYS:O	2.11	0.82
1:M:68:SER:CB	1:M:69:ILE:HD12	2.07	0.82
1:R:155:ASP:OD1	1:R:156:GLN:HG2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:330:ARG:NH1	1:J:346:GLY:HA3	1.95	0.82
1:A:118:THR:HA	1:B:1:ALA:HB3	1.60	0.82
1:E:51:THR:CG2	1:E:54:ASN:H	1.93	0.82
1:I:58:PHE:CZ	1:I:310:LEU:HD13	2.15	0.82
1:J:58:PHE:CZ	1:J:310:LEU:HD13	2.14	0.82
1:J:355:SER:N	3:J:501:HOH:O	2.13	0.82
1:B:277:GLU:OE2	1:B:342:TYR:OH	1.97	0.82
1:E:329:LYS:CD	1:E:347:SER:HB3	2.09	0.82
1:F:51:THR:CG2	1:F:54:ASN:H	1.92	0.82
1:B:118:THR:HG23	1:B:121:GLU:H	1.43	0.82
1:E:95:ASN:O	1:E:99:GLU:HG3	1.80	0.82
1:A:42:ARG:HD2	1:A:357:PHE:CB	2.10	0.82
1:H:330:ARG:NH1	1:H:347:SER:CB	2.43	0.82
1:I:118:THR:CG2	1:I:121:GLU:H	1.92	0.82
1:J:329:LYS:HD3	1:J:347:SER:HA	1.60	0.81
1:F:50:ASN:HD21	1:F:55:ARG:NH1	1.76	0.81
1:G:87:ASP:HB2	1:G:91:LYS:H	1.44	0.81
1:D:70:ASN:CB	1:D:70:ASN:N	2.43	0.81
1:E:344:HIS:NE2	3:E:501:HOH:O	2.13	0.81
1:K:156:GLN:HB3	1:L:1:ALA:CB	2.10	0.81
1:K:355:SER:CB	1:O:139:LYS:HE2	2.09	0.81
1:M:344:HIS:HB3	3:M:551:HOH:O	1.80	0.81
1:I:313:TRP:CZ2	1:I:315:GLY:HA2	2.14	0.81
1:I:313:TRP:CE2	1:I:315:GLY:HA2	2.15	0.81
1:K:355:SER:HB2	1:O:139:LYS:HE2	1.62	0.81
1:D:1:ALA:H2	1:D:220:HIS:CE1	1.98	0.81
1:Q:51:THR:CG2	1:Q:54:ASN:H	1.92	0.81
1:F:118:THR:HG23	1:F:121:GLU:HB2	1.61	0.81
1:I:2:HIS:O	1:I:3:ARG:O	1.98	0.81
1:L:115:LEU:O	1:L:118:THR:HB	1.81	0.81
1:A:226:THR:CG2	3:A:536:HOH:O	2.28	0.81
1:B:118:THR:CG2	1:B:121:GLU:H	1.93	0.81
1:M:68:SER:HA	1:M:69:ILE:HG13	1.61	0.81
1:N:199:GLU:HB2	3:N:442:HOH:O	1.79	0.81
1:C:189:GLU:HG2	1:C:191:ILE:HD13	1.63	0.81
1:D:274:MET:O	1:D:356:LEU:HD12	1.81	0.80
1:G:123:THR:C	1:G:124:ILE:HD12	2.06	0.80
1:I:271:SER:O	1:I:272:GLY:C	2.20	0.80
1:G:58:PHE:CZ	1:G:310:LEU:HD13	2.15	0.80
1:K:66:ASP:OD2	1:K:68:SER:OG	1.97	0.80
1:M:50:ASN:ND2	1:M:55:ARG:HH11	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:SER:HB3	1:D:1:ALA:HB3	1.62	0.80
1:L:58:PHE:CE1	1:L:310:LEU:HD13	2.16	0.80
1:D:191:ILE:N	1:D:191:ILE:CD1	2.44	0.80
1:M:345:THR:HG21	3:M:502:HOH:O	1.82	0.80
1:Q:2:HIS:O	1:Q:3:ARG:CB	2.27	0.80
1:O:70:ASN:HD22	1:O:70:ASN:N	1.77	0.80
1:I:190:VAL:H	1:I:231:ASN:ND2	1.79	0.80
1:O:2:HIS:HB3	1:P:156:GLN:OE1	1.82	0.80
1:B:67:SER:O	1:B:69:ILE:HG22	1.81	0.80
1:C:313:TRP:CZ2	1:C:315:GLY:HA2	2.15	0.80
1:G:244:THR:HG22	1:G:247:GLN:H	1.47	0.80
1:I:1:ALA:HB3	1:J:118:THR:HA	1.62	0.80
1:N:9:GLN:NE2	3:N:401:HOH:O	2.13	0.80
1:P:123:THR:HG22	1:P:124:ILE:H	1.47	0.80
1:N:87:ASP:HB3	1:N:89:GLN:N	1.96	0.80
1:R:87:ASP:OD1	1:R:89:GLN:HB3	1.80	0.80
1:A:307:ALA:HA	1:A:357:PHE:CE2	2.16	0.79
1:B:342:TYR:C	1:B:344:HIS:N	2.37	0.79
1:E:125:GLN:HE22	1:F:129:GLY:H	1.31	0.79
1:I:2:HIS:HB3	1:J:156:GLN:OE1	1.81	0.79
1:D:226:THR:HG23	3:D:541:HOH:O	1.81	0.79
1:E:250:MET:HE1	1:E:291:LEU:HD22	1.62	0.79
1:F:51:THR:HG22	1:F:54:ASN:H	1.47	0.79
1:F:118:THR:CG2	1:F:121:GLU:HB2	2.13	0.79
1:I:129:GLY:H	1:J:125:GLN:HE22	1.27	0.79
1:L:232:MET:SD	1:L:274:MET:HE1	2.23	0.79
1:H:123:THR:C	1:H:124:ILE:HD12	2.07	0.79
1:I:119:ASN:N	1:J:1:ALA:HB3	1.95	0.79
1:K:80:HIS:HD2	1:K:137:TYR:OH	1.65	0.79
1:L:8:THR:OG1	1:L:11:GLN:HG3	1.82	0.79
1:M:3:ARG:NH1	1:N:156:GLN:NE2	2.30	0.79
1:M:68:SER:O	1:M:69:ILE:O	1.99	0.79
1:O:123:THR:HG23	1:O:165:GLU:HG3	1.64	0.79
1:D:118:THR:CG2	1:D:121:GLU:H	1.95	0.79
1:H:277:GLU:HG2	1:H:345:THR:HG23	1.63	0.79
1:N:44:GLN:OE1	1:N:44:GLN:HA	1.82	0.79
1:N:256:LEU:CD1	1:N:267:ILE:HD11	2.11	0.79
1:A:2:HIS:HA	1:D:203:TYR:CZ	2.16	0.79
1:K:88:SER:O	1:K:89:GLN:CB	2.26	0.79
1:M:345:THR:CG2	3:M:502:HOH:O	2.31	0.79
1:E:329:LYS:HD3	1:E:347:SER:OG	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:244:THR:HG23	1:N:246:GLU:H	1.47	0.79
1:D:70:ASN:ND2	1:D:70:ASN:HA	1.67	0.78
1:E:58:PHE:CZ	1:E:310:LEU:HD13	2.18	0.78
1:D:191:ILE:CD1	1:D:191:ILE:H	1.96	0.78
1:B:89:GLN:O	1:B:91:LYS:N	2.15	0.78
1:B:330:ARG:HA	1:B:330:ARG:NE	1.98	0.78
1:C:123:THR:HG21	1:C:165:GLU:OE2	1.83	0.78
1:D:1:ALA:HB2	3:D:531:HOH:O	1.83	0.78
1:J:118:THR:CG2	1:J:121:GLU:H	1.96	0.78
1:B:190:VAL:H	1:B:231:ASN:HD22	1.28	0.78
1:B:250:MET:CE	1:B:291:LEU:HD21	2.13	0.78
1:O:50:ASN:HD21	1:O:55:ARG:HD3	1.49	0.78
1:C:244:THR:HG22	1:C:247:GLN:CB	2.14	0.78
1:M:276:GLU:HG3	1:M:352:SER:HB3	1.64	0.78
1:O:70:ASN:HD22	1:O:70:ASN:H	1.29	0.78
1:R:289:CYS:O	1:R:293:LYS:HE3	1.84	0.78
1:A:2:HIS:O	1:A:4:PHE:N	2.14	0.77
1:B:342:TYR:CD2	1:B:344:HIS:HA	2.18	0.77
1:P:313:TRP:CE2	1:P:315:GLY:HA2	2.18	0.77
1:Q:3:ARG:HD2	1:R:156:GLN:NE2	2.00	0.77
1:A:342:TYR:CE2	1:A:344:HIS:CB	2.65	0.77
1:E:1:ALA:HB3	1:F:159:SER:HB2	1.66	0.77
1:G:129:GLY:H	1:H:125:GLN:HE22	1.30	0.77
1:M:2:HIS:O	1:M:3:ARG:C	2.27	0.77
1:L:87:ASP:HB2	1:L:91:LYS:N	2.00	0.77
1:E:329:LYS:HZ3	1:E:347:SER:CA	1.96	0.77
1:B:27:LYS:HB3	1:B:72:SER:O	1.83	0.77
1:C:159:SER:HB2	1:D:1:ALA:CB	2.15	0.77
1:G:123:THR:HG23	1:G:165:GLU:HG3	1.65	0.77
1:I:118:THR:HA	1:J:1:ALA:H3	1.42	0.77
1:M:329:LYS:HZ1	1:M:348:SER:N	1.82	0.77
1:A:203:TYR:HE2	1:D:2:HIS:HD2	1.30	0.77
1:C:65:VAL:O	1:C:100:LYS:NZ	2.17	0.77
1:C:303:ARG:HH11	1:C:303:ARG:HG3	1.48	0.77
1:R:76:VAL:HG23	1:R:102:ILE:HG21	1.66	0.77
1:P:244:THR:CG2	1:P:247:GLN:H	1.97	0.77
1:A:125:GLN:HE21	1:B:128:ASP:HA	1.48	0.77
1:E:276:GLU:HG3	1:E:352:SER:HB3	1.66	0.77
1:N:244:THR:HG23	1:N:246:GLU:N	2.00	0.77
1:H:118:THR:CG2	1:H:121:GLU:H	1.96	0.77
1:O:244:THR:HG22	1:O:247:GLN:N	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:SO4:S	3:A:503:HOH:O	2.42	0.76
1:B:61:ILE:HG21	1:B:323:THR:HG22	1.66	0.76
1:C:159:SER:HB2	1:D:1:ALA:HB3	1.68	0.76
1:H:51:THR:CG2	1:H:54:ASN:H	1.90	0.76
1:J:276:GLU:HG3	1:J:352:SER:HB3	1.67	0.76
1:L:190:VAL:H	1:L:231:ASN:ND2	1.83	0.76
1:O:244:THR:CG2	1:O:247:GLN:H	1.98	0.76
1:Q:156:GLN:HE22	1:R:3:ARG:NE	1.83	0.76
1:A:2:HIS:HB2	1:A:3:ARG:CD	2.14	0.76
1:F:226:THR:HG23	3:F:449:HOH:O	1.83	0.76
1:G:244:THR:HG23	1:G:246:GLU:N	2.00	0.76
1:R:309:ALA:HB1	1:R:323:THR:HG23	1.67	0.76
1:E:329:LYS:CD	1:E:347:SER:CB	2.62	0.76
1:E:2:HIS:HB3	1:F:156:GLN:CD	2.09	0.76
1:G:119:ASN:H	1:H:1:ALA:H1	1.31	0.76
1:P:80:HIS:HD2	1:P:137:TYR:OH	1.68	0.76
1:Q:200:HIS:HB2	3:Q:2059:HOH:O	1.86	0.76
1:R:330:ARG:HA	1:R:330:ARG:HE	1.50	0.76
1:B:29:ILE:HB	1:B:300:SER:HB2	1.67	0.76
1:E:191:ILE:HB	1:E:192:PRO:HD2	1.68	0.76
1:G:125:GLN:NE2	1:H:129:GLY:H	1.83	0.76
1:K:50:ASN:ND2	1:K:55:ARG:HH11	1.83	0.76
1:M:68:SER:O	1:M:68:SER:OG	1.89	0.76
1:M:343:VAL:CG2	1:M:344:HIS:O	2.27	0.76
1:H:329:LYS:HD2	1:H:347:SER:CA	2.13	0.76
1:M:2:HIS:O	1:M:4:PHE:HB2	1.85	0.76
1:N:115:LEU:O	1:N:118:THR:HB	1.85	0.76
1:B:203:TYR:HH	1:C:2:HIS:HA	1.48	0.75
1:D:273:GLY:HA2	1:D:356:LEU:HB2	1.68	0.75
1:N:2:HIS:HA	1:N:3:ARG:NH1	2.00	0.75
1:N:123:THR:CG2	1:N:124:ILE:H	1.92	0.75
1:P:45:ARG:HH12	1:P:356:LEU:HA	1.51	0.75
1:I:44:GLN:HA	1:I:44:GLN:OE1	1.84	0.75
1:N:58:PHE:CZ	1:N:310:LEU:HD13	2.21	0.75
1:B:67:SER:O	1:B:68:SER:O	2.05	0.75
1:E:89:GLN:N	1:E:89:GLN:NE2	2.30	0.75
1:I:343:VAL:O	1:I:344:HIS:ND1	2.19	0.75
1:L:155:ASP:O	1:L:156:GLN:HB2	1.85	0.75
1:Q:267:ILE:HG12	1:Q:297:LEU:HD23	1.68	0.75
1:A:42:ARG:CD	1:A:357:PHE:CB	2.64	0.75
1:D:51:THR:HG22	1:D:54:ASN:N	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:PHE:CE2	1:D:310:LEU:HD13	2.21	0.75
1:N:1:ALA:O	1:N:3:ARG:NE	2.19	0.75
1:F:267:ILE:HG12	1:F:297:LEU:HD23	1.67	0.75
1:N:65:VAL:HG11	1:N:69:ILE:HG12	1.67	0.75
1:A:154:ALA:HB3	1:A:157:CYS:HB2	1.67	0.75
1:K:156:GLN:HB3	1:L:1:ALA:HB3	1.68	0.75
1:E:88:SER:O	1:E:89:GLN:NE2	2.19	0.75
1:H:124:ILE:HG22	1:H:147:TRP:CZ2	2.21	0.75
1:J:329:LYS:HD3	1:J:347:SER:CA	2.16	0.75
1:O:58:PHE:CE1	1:O:310:LEU:HD13	2.22	0.75
1:Q:4:PHE:HE1	1:R:156:GLN:HG3	1.51	0.75
1:K:51:THR:CG2	1:K:54:ASN:H	1.95	0.74
1:M:69:ILE:CD1	1:M:328:MET:HE1	2.14	0.74
1:A:118:THR:CG2	1:A:121:GLU:H	2.00	0.74
1:A:226:THR:HG23	3:A:536:HOH:O	1.86	0.74
1:B:58:PHE:CZ	1:B:62:LEU:HD21	2.21	0.74
1:H:80:HIS:HD2	1:H:137:TYR:OH	1.69	0.74
1:O:319:ASN:O	1:O:320:LYS:C	2.26	0.74
1:M:67:SER:O	1:M:69:ILE:N	2.14	0.74
1:M:244:THR:HG23	1:M:247:GLN:HG3	1.68	0.74
1:Q:1:ALA:O	1:Q:2:HIS:HB2	1.88	0.74
1:B:51:THR:HG22	1:B:54:ASN:N	2.00	0.74
1:P:199:GLU:HB2	3:P:540:HOH:O	1.88	0.74
1:A:125:GLN:NE2	1:B:128:ASP:HA	2.02	0.74
1:G:313:TRP:CE2	1:G:315:GLY:HA2	2.21	0.74
1:H:36:VAL:HG13	1:H:55:ARG:NH1	2.03	0.74
1:K:226:THR:CG2	3:K:512:HOH:O	2.34	0.74
1:L:50:ASN:HD21	1:L:55:ARG:HH11	1.35	0.74
1:M:67:SER:C	1:M:69:ILE:H	1.82	0.74
1:P:226:THR:CG2	3:P:520:HOH:O	2.36	0.74
1:C:244:THR:HG23	1:C:247:GLN:H	1.52	0.74
1:E:250:MET:HE3	1:E:291:LEU:HD22	1.70	0.74
1:H:2:HIS:O	1:H:3:ARG:HB2	1.85	0.74
1:O:118:THR:HA	1:P:1:ALA:N	2.03	0.74
1:G:190:VAL:H	1:G:231:ASN:ND2	1.85	0.74
1:I:67:SER:OG	1:I:68:SER:HB2	1.88	0.74
1:A:168:ASN:O	1:A:171:ALA:HB3	1.88	0.73
1:B:342:TYR:CZ	1:B:344:HIS:HA	2.23	0.73
1:E:276:GLU:OE1	1:E:330:ARG:HD3	1.88	0.73
1:G:68:SER:O	1:G:71:GLN:HB2	1.87	0.73
1:G:87:ASP:HB2	1:G:91:LYS:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:VAL:O	1:K:100:LYS:NZ	2.17	0.73
1:O:343:VAL:HG23	1:O:344:HIS:N	1.95	0.73
1:Q:50:ASN:ND2	1:Q:55:ARG:NH1	2.35	0.73
1:N:344:HIS:H	1:N:344:HIS:CD2	2.01	0.73
1:P:244:THR:HG22	1:P:247:GLN:N	2.02	0.73
1:A:277:GLU:CD	1:A:347:SER:HB2	2.13	0.73
1:F:50:ASN:HD21	1:F:55:ARG:HD3	1.53	0.73
1:I:51:THR:HG22	1:I:53:GLU:H	1.54	0.73
1:C:50:ASN:ND2	1:C:55:ARG:HH11	1.85	0.73
1:C:244:THR:HG22	1:C:247:GLN:HB2	1.71	0.73
1:L:12:LYS:HE2	1:L:222:TYR:CD1	2.23	0.73
1:O:3:ARG:HG2	1:O:4:PHE:N	2.03	0.73
1:D:2:HIS:O	1:D:3:ARG:HB3	1.87	0.73
1:P:42:ARG:HH12	1:P:358:THR:CB	2.01	0.73
1:H:89:GLN:O	1:H:91:LYS:N	2.20	0.73
1:O:67:SER:O	1:O:70:ASN:ND2	2.22	0.73
1:A:355:SER:O	1:A:356:LEU:HD23	1.89	0.73
3:J:564:HOH:O	1:K:200:HIS:HB2	1.89	0.73
1:O:156:GLN:O	1:P:1:ALA:HB1	1.89	0.73
1:Q:58:PHE:CZ	1:Q:310:LEU:HD13	2.24	0.73
1:E:244:THR:HG22	1:E:247:GLN:N	2.04	0.72
1:Q:55:ARG:O	1:Q:59:ARG:HG2	1.89	0.72
1:E:250:MET:CE	1:E:291:LEU:CD2	2.66	0.72
1:F:244:THR:CG2	1:F:247:GLN:H	2.02	0.72
1:L:89:GLN:O	1:L:89:GLN:CG	2.38	0.72
1:J:330:ARG:NH1	1:J:347:SER:H	1.86	0.72
1:C:129:GLY:H	1:D:125:GLN:HE22	1.36	0.72
1:G:3:ARG:HG2	1:G:3:ARG:HH11	1.53	0.72
1:D:244:THR:HG23	1:D:246:GLU:H	1.54	0.72
1:E:58:PHE:CE1	1:E:310:LEU:HD13	2.25	0.72
1:E:256:LEU:HD13	1:E:267:ILE:CD1	2.15	0.72
1:D:86:LYS:HD3	1:D:90:GLY:HA3	1.71	0.72
1:O:220:HIS:HE1	3:O:528:HOH:O	1.72	0.72
1:P:352:SER:N	3:P:501:HOH:O	2.22	0.72
1:H:50:ASN:HD21	1:H:55:ARG:HD3	1.53	0.72
1:I:115:LEU:O	1:I:118:THR:HB	1.90	0.72
1:H:62:LEU:O	1:H:65:VAL:HG13	1.89	0.72
1:K:88:SER:O	1:K:89:GLN:HB2	1.88	0.72
1:L:2:HIS:O	1:L:3:ARG:C	2.33	0.72
1:N:50:ASN:ND2	1:N:55:ARG:HH11	1.87	0.72
1:B:244:THR:HG22	1:B:247:GLN:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:GLY:H	1:D:125:GLN:NE2	1.88	0.72
1:C:156:GLN:NE2	1:D:3:ARG:HD2	2.04	0.72
1:I:322:ALA:O	1:I:325:GLU:HB2	1.90	0.71
1:J:330:ARG:CZ	1:J:346:GLY:HA3	2.20	0.71
1:N:78:LEU:O	1:N:106:ILE:HD12	1.90	0.71
1:C:244:THR:CG2	1:C:247:GLN:HG3	2.20	0.71
1:E:256:LEU:CD1	1:E:267:ILE:HD11	2.15	0.71
1:F:190:VAL:H	1:F:231:ASN:ND2	1.87	0.71
1:G:244:THR:HB	1:G:247:GLN:HE21	1.54	0.71
1:H:256:LEU:CD1	1:H:267:ILE:HD11	2.15	0.71
1:I:34:GLU:HB2	1:I:38:THR:HB	1.72	0.71
1:J:230:PRO:HG3	1:J:267:ILE:CD1	2.20	0.71
1:P:42:ARG:HH12	1:P:358:THR:HB	1.53	0.71
1:E:303:ARG:CG	1:E:303:ARG:HH11	2.03	0.71
1:G:70:ASN:ND2	1:G:100:LYS:O	2.22	0.71
1:G:313:TRP:CZ2	1:G:315:GLY:HA2	2.24	0.71
1:O:59:ARG:HB3	1:O:63:PHE:CE1	2.24	0.71
1:B:244:THR:HG22	1:B:247:GLN:HG3	1.73	0.71
1:H:172:ARG:NH2	1:H:176:ILE:HD11	2.04	0.71
1:I:119:ASN:H	1:J:1:ALA:CB	1.97	0.71
1:A:9:GLN:NE2	3:A:504:HOH:O	2.22	0.71
1:A:303:ARG:CG	1:A:357:PHE:HD1	2.04	0.71
1:A:203:TYR:HE2	1:D:2:HIS:CD2	2.07	0.71
1:C:1:ALA:HB3	1:D:118:THR:HA	1.72	0.71
1:F:274:MET:O	1:F:356:LEU:HD12	1.90	0.71
1:N:224:GLU:OE1	1:N:224:GLU:N	2.20	0.71
1:R:226:THR:CG2	3:R:520:HOH:O	2.39	0.71
1:A:118:THR:HA	1:B:1:ALA:HB2	1.72	0.71
1:A:191:ILE:HB	1:A:192:PRO:HD2	1.73	0.71
1:E:129:GLY:H	1:F:125:GLN:HE22	1.37	0.71
1:G:51:THR:HG22	1:G:54:ASN:H	1.54	0.71
1:I:123:THR:HG22	1:I:124:ILE:N	2.04	0.71
1:L:50:ASN:ND2	1:L:55:ARG:HH11	1.87	0.71
1:M:68:SER:C	1:M:69:ILE:CG1	2.42	0.71
1:M:329:LYS:HZ1	1:M:347:SER:C	1.98	0.71
1:N:2:HIS:HA	1:N:3:ARG:NH2	2.05	0.71
1:O:58:PHE:CZ	1:O:310:LEU:HD13	2.25	0.71
1:P:276:GLU:HB2	1:P:352:SER:HB3	1.73	0.71
1:J:330:ARG:HH11	1:J:347:SER:H	1.38	0.71
1:L:220:HIS:HE1	3:L:407:HOH:O	1.72	0.71
1:M:345:THR:OG1	3:M:502:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:115:LEU:O	1:O:118:THR:HB	1.91	0.70
1:Q:156:GLN:NE2	1:R:3:ARG:NE	2.39	0.70
1:B:244:THR:HG21	3:B:414:HOH:O	1.90	0.70
1:B:254:THR:O	1:B:258:ARG:HG2	1.91	0.70
1:C:271:SER:HB3	1:C:301:TYR:CE2	2.26	0.70
1:D:89:GLN:O	1:D:91:LYS:N	2.23	0.70
1:D:223:LEU:O	1:D:226:THR:HB	1.90	0.70
1:A:42:ARG:HD3	1:A:357:PHE:O	1.90	0.70
1:E:89:GLN:OE1	1:E:89:GLN:HB2	1.89	0.70
1:E:253:VAL:CG1	1:E:291:LEU:HD23	2.20	0.70
1:L:2:HIS:O	1:L:3:ARG:O	2.08	0.70
1:M:345:THR:CG2	1:M:347:SER:HB3	2.21	0.70
1:F:223:LEU:O	1:F:226:THR:HB	1.90	0.70
1:M:50:ASN:HD21	1:M:55:ARG:HH11	1.39	0.70
1:N:284:ASN:HD22	1:N:340:GLY:HA2	1.56	0.70
1:I:118:THR:HA	1:J:1:ALA:H2	1.57	0.70
1:J:329:LYS:NZ	1:J:347:SER:HA	2.06	0.70
1:K:345:THR:O	1:K:346:GLY:O	2.08	0.70
1:B:51:THR:O	1:B:55:ARG:HG3	1.92	0.70
1:E:50:ASN:HD21	1:E:55:ARG:HD3	1.56	0.70
1:L:58:PHE:CZ	1:L:62:LEU:HD21	2.27	0.70
1:L:87:ASP:CB	1:L:91:LYS:H	2.01	0.70
1:O:254:THR:O	1:O:258:ARG:HG2	1.92	0.70
1:P:12:LYS:HB3	1:P:222:TYR:CZ	2.26	0.70
1:B:61:ILE:HG21	1:B:323:THR:HG21	1.72	0.70
1:E:4:PHE:O	1:F:117:GLY:HA2	1.92	0.70
1:N:202:GLN:HB2	1:N:233:VAL:HG11	1.73	0.70
1:E:329:LYS:NZ	1:E:347:SER:CA	2.54	0.70
1:I:50:ASN:ND2	1:I:55:ARG:HH11	1.90	0.70
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.74	0.70
1:N:244:THR:CG2	1:N:247:GLN:N	2.53	0.70
1:B:190:VAL:H	1:B:231:ASN:ND2	1.89	0.70
1:C:244:THR:HG22	1:C:247:GLN:HG3	1.73	0.70
1:C:254:THR:O	1:C:258:ARG:HG2	1.92	0.70
1:H:226:THR:CG2	3:H:421:HOH:O	2.40	0.70
1:Q:190:VAL:H	1:Q:231:ASN:ND2	1.90	0.70
1:Q:250:MET:O	1:Q:250:MET:HG3	1.90	0.70
1:C:237:HIS:CG	3:C:403:HOH:O	2.45	0.69
1:E:78:LEU:O	1:E:106:ILE:HD12	1.92	0.69
1:H:329:LYS:CE	1:H:347:SER:HA	2.21	0.69
1:I:50:ASN:HD21	1:I:55:ARG:HD3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:357:PHE:H	1:O:139:LYS:HZ1	1.38	0.69
1:E:240:THR:O	1:E:242:LYS:HE3	1.92	0.69
1:F:351:ALA:O	1:F:352:SER:CB	2.40	0.69
1:H:354:GLN:HG2	1:H:356:LEU:CD2	2.22	0.69
1:J:95:ASN:O	1:J:99:GLU:HG3	1.91	0.69
1:Q:4:PHE:CE1	1:R:156:GLN:HG3	2.27	0.69
1:Q:256:LEU:HD13	1:Q:267:ILE:HD11	1.73	0.69
1:B:80:HIS:HD2	1:B:137:TYR:OH	1.75	0.69
1:C:2:HIS:HB2	1:D:156:GLN:OE1	1.92	0.69
1:I:320:LYS:O	1:I:324:GLN:HG3	1.93	0.69
1:O:129:GLY:H	1:P:125:GLN:HE22	1.39	0.69
1:P:50:ASN:ND2	1:P:55:ARG:HH11	1.90	0.69
1:B:61:ILE:HG23	1:B:324:GLN:HG2	1.74	0.69
1:B:69:ILE:HB	1:B:328:MET:HE1	1.72	0.69
1:N:202:GLN:O	1:N:206:GLU:HG3	1.93	0.69
1:R:214:LYS:HD2	1:R:214:LYS:O	1.91	0.69
1:A:207:LYS:HE2	1:D:2:HIS:HE2	1.55	0.69
1:D:87:ASP:HB2	1:D:91:LYS:N	2.07	0.69
1:E:344:HIS:CD2	3:E:501:HOH:O	2.43	0.69
1:M:159:SER:HB3	1:N:1:ALA:HA	1.74	0.69
1:D:351:ALA:O	1:D:354:GLN:HB2	1.91	0.69
1:E:87:ASP:OD1	1:E:89:GLN:HB2	1.93	0.69
1:M:67:SER:C	1:M:69:ILE:N	2.51	0.69
1:D:3:ARG:HD3	3:D:575:HOH:O	1.91	0.69
1:E:51:THR:HG22	1:E:54:ASN:HB2	1.72	0.69
1:E:344:HIS:CE1	3:E:501:HOH:O	2.45	0.69
1:F:51:THR:HG22	1:F:54:ASN:HB2	1.74	0.69
1:H:172:ARG:O	1:H:176:ILE:HG13	1.93	0.69
1:R:115:LEU:O	1:R:118:THR:HB	1.93	0.69
1:C:51:THR:HG23	1:C:53:GLU:H	1.57	0.69
1:C:87:ASP:HB3	1:C:89:GLN:N	2.08	0.69
1:G:118:THR:CG2	1:G:121:GLU:H	2.06	0.69
1:L:244:THR:HG22	1:L:247:GLN:CB	2.22	0.69
1:M:58:PHE:CZ	1:M:310:LEU:HD13	2.27	0.69
1:N:1:ALA:O	1:N:3:ARG:CZ	2.40	0.69
1:O:50:ASN:ND2	1:O:55:ARG:HH11	1.91	0.69
1:E:28:GLY:HA3	1:E:299:PHE:CZ	2.28	0.69
1:G:244:THR:HG23	1:G:246:GLU:H	1.56	0.69
1:H:223:LEU:O	1:H:226:THR:HB	1.93	0.69
1:I:65:VAL:O	1:I:66:ASP:C	2.32	0.69
1:I:67:SER:CB	3:I:406:HOH:O	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:197:ASP:C	1:I:197:ASP:OD1	2.34	0.69
1:K:244:THR:CG2	1:K:247:GLN:N	2.40	0.69
1:M:115:LEU:O	1:M:118:THR:HB	1.93	0.69
1:O:1:ALA:HA	3:O:528:HOH:O	1.92	0.69
1:R:244:THR:HG22	1:R:247:GLN:N	1.98	0.69
1:G:118:THR:HG23	1:G:121:GLU:H	1.58	0.69
1:K:355:SER:HB2	1:O:139:LYS:CE	2.23	0.69
1:I:65:VAL:CG1	1:I:69:ILE:HD13	2.21	0.68
1:N:200:HIS:CE1	1:O:2:HIS:NE2	2.61	0.68
1:A:271:SER:OG	3:A:503:HOH:O	2.03	0.68
1:I:12:LYS:HG2	1:I:222:TYR:CZ	2.27	0.68
1:L:271:SER:HA	1:L:274:MET:HE3	1.74	0.68
1:P:290:PRO:O	1:P:291:LEU:HG	1.92	0.68
1:J:276:GLU:CG	1:J:352:SER:HB3	2.23	0.68
1:L:87:ASP:HB3	1:L:89:GLN:N	2.05	0.68
1:M:119:ASN:H	1:N:1:ALA:HB3	1.57	0.68
1:M:350:ALA:H	1:M:353:THR:CG2	2.06	0.68
1:D:50:ASN:ND2	1:D:55:ARG:HH11	1.90	0.68
1:I:244:THR:HG23	1:I:246:GLU:H	1.59	0.68
1:L:118:THR:HG23	1:L:121:GLU:H	1.58	0.68
1:M:228:LEU:HG	1:M:230:PRO:HD3	1.74	0.68
1:O:128:ASP:HA	1:P:125:GLN:HE21	1.58	0.68
1:B:187:GLU:HG3	1:B:229:LYS:O	1.92	0.68
1:D:1:ALA:H1	1:D:220:HIS:CE1	2.11	0.68
1:N:274:MET:HE3	1:N:279:ALA:HA	1.75	0.68
1:O:276:GLU:OE2	1:O:307:ALA:HB3	1.93	0.68
1:B:2:HIS:NE2	1:C:200:HIS:CE1	2.61	0.68
1:D:2:HIS:O	1:D:4:PHE:HD1	1.77	0.68
1:F:354:GLN:O	1:F:355:SER:HB2	1.92	0.68
1:I:198:LEU:HD22	1:I:243:TYR:CD2	2.29	0.68
1:A:124:ILE:CD1	1:A:149:ALA:HA	2.22	0.68
1:B:244:THR:CG2	1:B:247:GLN:HG3	2.23	0.68
1:B:313:TRP:CZ2	1:B:315:GLY:HA2	2.28	0.68
1:C:36:VAL:O	1:C:36:VAL:HG12	1.93	0.68
1:L:51:THR:HG22	1:L:54:ASN:HB2	1.76	0.68
1:L:319:ASN:O	1:L:320:LYS:C	2.37	0.68
1:N:189:GLU:HG2	1:N:191:ILE:HD12	1.75	0.68
1:I:36:VAL:O	1:I:36:VAL:HG12	1.91	0.68
1:I:51:THR:HG22	1:I:54:ASN:H	1.57	0.68
1:I:67:SER:OG	1:I:68:SER:CB	2.42	0.68
1:N:190:VAL:H	1:N:231:ASN:HD22	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:124:ILE:HG21	1:R:147:TRP:NE1	2.09	0.68
1:R:257:HIS:CD2	1:R:292:PRO:HD2	2.28	0.68
1:A:303:ARG:HG2	1:A:357:PHE:HB2	1.74	0.68
1:C:191:ILE:HD13	1:C:191:ILE:N	2.07	0.68
1:K:357:PHE:N	1:O:139:LYS:HZ1	1.91	0.68
1:M:189:GLU:CG	1:M:191:ILE:HD13	2.23	0.68
1:R:223:LEU:O	1:R:226:THR:HB	1.94	0.68
1:A:343:VAL:C	1:A:344:HIS:O	2.34	0.68
1:B:313:TRP:CE2	1:B:315:GLY:HA2	2.29	0.68
1:D:329:LYS:HZ3	1:D:347:SER:HA	1.56	0.68
1:K:128:ASP:HB2	1:L:128:ASP:OD2	1.93	0.68
1:N:118:THR:CG2	1:N:121:GLU:H	2.07	0.68
1:O:18:ILE:HD13	1:O:143:ASP:HB3	1.76	0.68
1:O:330:ARG:HA	1:O:330:ARG:HE	1.59	0.68
1:O:343:VAL:O	1:O:344:HIS:ND1	2.27	0.68
1:B:2:HIS:NE2	1:C:200:HIS:HE1	1.91	0.67
1:B:344:HIS:CG	1:B:345:THR:N	2.61	0.67
1:D:191:ILE:HD12	1:D:191:ILE:H	1.52	0.67
1:F:214:LYS:HE3	1:F:218:ASP:OD1	1.94	0.67
1:F:354:GLN:O	1:F:355:SER:CB	2.42	0.67
1:I:53:GLU:OE1	1:I:53:GLU:HA	1.94	0.67
1:I:150:VAL:HG13	1:I:191:ILE:HG13	1.76	0.67
1:M:353:THR:HG23	1:M:353:THR:O	1.94	0.67
1:D:87:ASP:CB	1:D:91:LYS:H	2.04	0.67
1:J:170:LEU:HD22	1:J:186:VAL:HG13	1.76	0.67
1:K:44:GLN:OE1	1:K:44:GLN:HA	1.93	0.67
1:E:88:SER:C	1:E:89:GLN:CD	2.62	0.67
1:I:51:THR:CG2	1:I:53:GLU:H	2.07	0.67
1:L:244:THR:HG22	1:L:247:GLN:HB2	1.76	0.67
1:D:87:ASP:HB3	1:D:89:GLN:O	1.93	0.67
1:E:271:SER:HA	1:E:274:MET:CE	2.23	0.67
1:R:244:THR:CG2	1:R:247:GLN:H	2.00	0.67
1:I:68:SER:CA	1:I:70:ASN:HD22	2.04	0.67
1:I:274:MET:HE3	1:I:279:ALA:HA	1.77	0.67
1:N:118:THR:CG2	1:N:121:GLU:HB2	2.24	0.67
1:C:190:VAL:H	1:C:231:ASN:ND2	1.92	0.67
1:D:67:SER:O	1:D:68:SER:C	2.33	0.67
1:E:190:VAL:H	1:E:231:ASN:HD22	1.39	0.67
1:O:190:VAL:H	1:O:231:ASN:ND2	1.91	0.67
1:E:51:THR:HG22	1:E:54:ASN:CB	2.23	0.67
1:G:58:PHE:CE1	1:G:310:LEU:HD13	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:ASP:OD2	1:H:89:GLN:O	2.13	0.67
1:H:257:HIS:HD2	1:H:292:PRO:HD2	1.59	0.67
1:I:202:GLN:O	1:I:206:GLU:HG3	1.95	0.67
1:K:58:PHE:CZ	1:K:310:LEU:HD13	2.29	0.67
1:M:329:LYS:HE3	1:M:347:SER:CB	2.12	0.67
1:N:80:HIS:HD2	1:N:137:TYR:OH	1.76	0.67
1:F:50:ASN:ND2	1:F:55:ARG:NH1	2.35	0.67
1:J:3:ARG:O	1:J:4:PHE:C	2.36	0.67
1:N:68:SER:O	1:N:70:ASN:N	2.27	0.67
1:A:123:THR:HG23	1:A:165:GLU:HG3	1.77	0.67
1:D:244:THR:HB	1:D:247:GLN:OE1	1.95	0.67
1:M:128:ASP:HB2	1:N:128:ASP:OD2	1.93	0.67
1:G:33:ASP:HB3	1:G:77:ILE:HG22	1.77	0.67
1:P:303:ARG:NH2	1:P:357:PHE:CD1	2.53	0.67
1:A:3:ARG:HD3	1:B:156:GLN:CD	2.21	0.66
1:E:303:ARG:HH11	1:E:303:ARG:HG3	1.60	0.66
1:M:118:THR:HA	1:N:1:ALA:HB3	1.76	0.66
1:N:94:ARG:O	1:N:98:LYS:HG3	1.94	0.66
1:A:67:SER:CA	3:A:502:HOH:O	2.33	0.66
1:B:60:GLU:OE1	1:B:87:ASP:HB2	1.95	0.66
1:B:274:MET:HE3	1:B:279:ALA:HB2	1.77	0.66
1:M:189:GLU:HG2	1:M:191:ILE:HD13	1.77	0.66
1:P:28:GLY:HA3	1:P:299:PHE:CZ	2.30	0.66
1:P:250:MET:CE	1:P:291:LEU:HD11	2.21	0.66
1:Q:256:LEU:HD13	1:Q:267:ILE:CD1	2.26	0.66
1:I:277:GLU:O	1:I:281:LEU:HG	1.95	0.66
1:A:118:THR:HG23	1:A:121:GLU:H	1.60	0.66
1:B:207:LYS:CE	1:C:2:HIS:HE2	2.07	0.66
1:C:50:ASN:HD21	1:C:55:ARG:HD3	1.59	0.66
1:I:170:LEU:HD22	1:I:186:VAL:HG13	1.75	0.66
1:L:118:THR:CG2	1:L:121:GLU:N	2.53	0.66
1:L:281:LEU:HD23	1:L:342:TYR:CE2	2.29	0.66
1:M:16:SER:O	1:M:20:GLN:HG3	1.93	0.66
1:N:189:GLU:HG2	1:N:191:ILE:CD1	2.25	0.66
1:Q:226:THR:CG2	3:Q:2024:HOH:O	2.43	0.66
1:D:148:ARG:HA	1:D:187:GLU:HB3	1.78	0.66
1:D:250:MET:HE1	1:D:291:LEU:HD21	1.77	0.66
1:E:202:GLN:HB2	1:E:233:VAL:HG11	1.78	0.66
1:N:250:MET:HE3	1:N:291:LEU:HD21	1.77	0.66
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.77	0.66
1:C:159:SER:CB	1:D:1:ALA:CB	2.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:ASN:H	1:H:1:ALA:H3	1.41	0.66
1:H:195:ASP:O	1:H:239:CYS:HB2	1.96	0.66
1:G:125:GLN:HE22	1:H:129:GLY:H	1.42	0.66
1:H:257:HIS:CD2	1:H:292:PRO:HD2	2.30	0.66
1:R:124:ILE:CG2	1:R:147:TRP:CZ2	2.77	0.66
1:B:272:GLY:HA2	1:B:303:ARG:NH1	2.10	0.66
1:C:87:ASP:CB	1:C:89:GLN:H	2.05	0.66
1:K:88:SER:O	1:K:89:GLN:CG	2.44	0.66
1:M:1:ALA:N	1:N:118:THR:CB	2.59	0.66
1:M:1:ALA:H3	1:N:119:ASN:N	1.94	0.66
1:N:200:HIS:HE1	1:O:2:HIS:NE2	1.94	0.66
1:Q:118:THR:HG21	1:Q:121:GLU:HB2	1.77	0.66
1:R:80:HIS:HD2	1:R:137:TYR:OH	1.78	0.66
1:R:240:THR:O	1:R:242:LYS:HE3	1.95	0.66
1:B:244:THR:CG2	1:B:247:GLN:N	2.59	0.66
1:E:89:GLN:OE1	1:E:89:GLN:HB3	1.89	0.66
1:K:8:THR:N	1:K:11:GLN:OE1	2.24	0.66
1:M:119:ASN:HB2	1:N:4:PHE:CE1	2.31	0.66
1:P:3:ARG:O	1:P:4:PHE:C	2.39	0.66
1:Q:121:GLU:OE1	1:R:1:ALA:HB3	1.95	0.66
1:Q:218:ASP:O	1:R:161:LEU:HD22	1.96	0.66
1:A:128:ASP:OD2	1:B:128:ASP:HB2	1.96	0.66
1:B:50:ASN:ND2	1:B:55:ARG:HD3	2.07	0.66
1:D:123:THR:HG23	1:D:165:GLU:HG3	1.78	0.66
1:G:118:THR:HG21	1:G:121:GLU:HB2	1.78	0.66
1:I:330:ARG:HA	1:I:330:ARG:HE	1.60	0.66
1:B:207:LYS:CE	1:C:2:HIS:NE2	2.60	0.65
1:D:329:LYS:HD3	1:D:347:SER:CB	2.27	0.65
1:I:159:SER:O	1:I:163:ILE:HG13	1.96	0.65
1:L:48:VAL:CG1	1:L:54:ASN:ND2	2.59	0.65
1:N:8:THR:OG1	1:N:11:GLN:HG3	1.95	0.65
1:P:237:HIS:HE1	3:P:541:HOH:O	1.79	0.65
1:D:250:MET:HE1	1:D:291:LEU:CD2	2.26	0.65
1:E:38:THR:O	1:E:42:ARG:HG2	1.96	0.65
1:K:125:GLN:HE22	1:L:129:GLY:H	1.43	0.65
1:L:202:GLN:O	1:L:206:GLU:HG3	1.96	0.65
1:O:271:SER:HA	1:O:274:MET:CE	2.26	0.65
1:R:67:SER:O	1:R:70:ASN:HB2	1.96	0.65
1:A:187:GLU:HB2	1:A:229:LYS:HB3	1.78	0.65
1:B:50:ASN:ND2	1:B:55:ARG:HH11	1.93	0.65
1:B:342:TYR:CD2	1:B:344:HIS:CA	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:THR:O	1:G:242:LYS:HE3	1.95	0.65
1:I:12:LYS:HG2	1:I:222:TYR:CE1	2.31	0.65
1:E:343:VAL:O	1:E:344:HIS:HB2	1.96	0.65
1:H:244:THR:N	1:H:247:GLN:OE1	2.29	0.65
1:F:256:LEU:HD11	1:F:267:ILE:HD11	1.78	0.65
1:F:277:GLU:OE2	1:F:344:HIS:ND1	2.27	0.65
1:G:244:THR:CG2	1:G:247:GLN:H	2.09	0.65
1:J:223:LEU:O	1:J:226:THR:HB	1.95	0.65
1:L:123:THR:HG23	1:L:165:GLU:HG3	1.78	0.65
1:N:203:TYR:CZ	1:O:2:HIS:HA	2.32	0.65
1:B:123:THR:C	1:B:124:ILE:HD13	2.20	0.65
1:C:36:VAL:HG13	1:C:55:ARG:NH1	2.12	0.65
1:H:112:GLY:HA2	1:H:123:THR:O	1.97	0.65
1:I:133:ARG:O	1:I:134:CYS:C	2.35	0.65
1:I:156:GLN:HB3	1:J:1:ALA:HB1	1.77	0.65
1:O:202:GLN:O	1:O:206:GLU:HG3	1.96	0.65
1:A:3:ARG:HD3	1:B:156:GLN:OE1	1.96	0.65
1:A:220:HIS:HE1	3:A:559:HOH:O	1.80	0.65
1:C:244:THR:CG2	1:C:247:GLN:H	2.08	0.65
1:G:3:ARG:NE	1:H:156:GLN:NE2	2.44	0.65
1:K:223:LEU:O	1:K:226:THR:HB	1.96	0.65
1:K:353:THR:HG21	1:O:92:LEU:HD11	1.79	0.65
1:L:184:PRO:HD2	1:L:225:GLY:O	1.97	0.65
1:R:124:ILE:HG21	1:R:147:TRP:CE2	2.31	0.65
1:A:313:TRP:CE2	1:A:315:GLY:HA2	2.32	0.65
1:C:125:GLN:NE2	1:D:129:GLY:H	1.95	0.65
1:F:244:THR:HG22	1:F:247:GLN:HB2	1.77	0.65
1:A:58:PHE:CZ	1:A:310:LEU:HD13	2.32	0.65
1:E:89:GLN:N	1:E:89:GLN:HE22	1.95	0.65
1:G:188:PRO:O	1:G:188:PRO:HG2	1.97	0.65
1:I:244:THR:HG23	1:I:246:GLU:N	2.11	0.65
1:N:192:PRO:HD3	3:N:428:HOH:O	1.97	0.65
1:Q:87:ASP:OD2	1:Q:88:SER:N	2.30	0.65
1:R:244:THR:HG22	1:R:247:GLN:HG3	1.79	0.65
1:A:244:THR:HB	1:A:247:GLN:OE1	1.97	0.65
1:C:231:ASN:ND2	1:C:231:ASN:H	1.95	0.65
1:N:313:TRP:CD2	1:N:315:GLY:HA2	2.32	0.65
1:A:156:GLN:HE22	1:B:3:ARG:NE	1.93	0.64
1:E:89:GLN:NE2	1:E:89:GLN:H	1.93	0.64
1:F:256:LEU:CD1	1:F:267:ILE:HD11	2.28	0.64
1:L:254:THR:O	1:L:258:ARG:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:118:THR:HG23	1:N:121:GLU:H	1.62	0.64
1:R:36:VAL:HG13	1:R:55:ARG:NH1	2.11	0.64
1:C:118:THR:CG2	1:C:121:GLU:N	2.59	0.64
1:E:191:ILE:HB	1:E:192:PRO:CD	2.26	0.64
1:M:146:LYS:HE2	1:M:187:GLU:OE1	1.97	0.64
1:N:3:ARG:CZ	1:O:203:TYR:CZ	2.80	0.64
1:N:3:ARG:NE	1:O:203:TYR:OH	2.28	0.64
1:N:284:ASN:ND2	1:N:340:GLY:HA2	2.11	0.64
1:O:51:THR:HG22	1:O:54:ASN:N	2.12	0.64
1:O:118:THR:CG2	1:O:121:GLU:HB2	2.26	0.64
1:R:244:THR:CG2	1:R:246:GLU:HB2	2.27	0.64
1:A:191:ILE:HB	1:A:192:PRO:CD	2.28	0.64
1:B:244:THR:HG22	1:B:247:GLN:CG	2.27	0.64
1:H:330:ARG:HH11	1:H:347:SER:HB3	1.62	0.64
1:D:115:LEU:O	1:D:118:THR:HB	1.97	0.64
1:E:115:LEU:O	1:E:118:THR:HB	1.98	0.64
1:H:8:THR:HB	1:H:11:GLN:H	1.62	0.64
1:I:82:THR:O	1:I:82:THR:HG22	1.97	0.64
1:I:224:GLU:OE1	1:I:224:GLU:N	2.26	0.64
1:N:3:ARG:NH1	1:N:3:ARG:N	2.46	0.64
1:Q:320:LYS:O	1:Q:324:GLN:HG3	1.98	0.64
1:A:3:ARG:HD2	1:A:3:ARG:H	1.62	0.64
1:D:198:LEU:CD1	1:D:234:THR:HA	2.28	0.64
1:H:119:ASN:O	1:H:152:ARG:NH1	2.30	0.64
1:O:190:VAL:H	1:O:231:ASN:HD22	1.45	0.64
1:E:2:HIS:CB	1:F:156:GLN:OE1	2.45	0.64
1:E:124:ILE:HG22	1:E:147:TRP:CZ2	2.33	0.64
1:N:51:THR:O	1:N:54:ASN:N	2.31	0.64
1:N:118:THR:HG21	1:N:121:GLU:HB2	1.78	0.64
1:A:45:ARG:HH21	1:A:358:THR:N	1.91	0.64
1:E:50:ASN:ND2	1:E:55:ARG:HH11	1.96	0.64
1:F:80:HIS:HD2	1:F:137:TYR:OH	1.79	0.64
1:Q:313:TRP:CE2	1:Q:315:GLY:HA2	2.32	0.64
1:D:52:GLU:O	1:D:55:ARG:HB2	1.98	0.64
1:M:2:HIS:ND1	1:P:203:TYR:OH	2.23	0.64
1:M:123:THR:O	1:M:124:ILE:HD13	1.97	0.64
1:B:65:VAL:HG23	1:B:324:GLN:HB3	1.80	0.64
1:B:232:MET:HE2	1:B:286:ILE:HD12	1.80	0.64
1:J:12:LYS:O	1:J:13:LYS:C	2.41	0.64
1:O:25:ASN:H	1:O:27:LYS:HD2	1.63	0.64
1:Q:156:GLN:HE22	1:R:3:ARG:CD	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:244:THR:CG2	1:Q:247:GLN:H	2.10	0.64
1:D:75:GLY:HA2	1:D:103:VAL:O	1.97	0.64
1:N:34:GLU:HB3	1:N:38:THR:HB	1.80	0.64
1:N:171:ALA:HA	1:N:216:LEU:HD12	1.79	0.64
1:N:343:VAL:O	1:N:344:HIS:C	2.38	0.64
1:Q:313:TRP:CZ2	1:Q:315:GLY:HA2	2.32	0.64
1:A:303:ARG:HB3	1:A:357:PHE:CD1	2.33	0.63
1:H:250:MET:HE1	1:H:291:LEU:HD13	1.80	0.63
1:H:349:GLY:O	1:H:351:ALA:N	2.31	0.63
1:N:53:GLU:OE1	1:N:53:GLU:HA	1.98	0.63
1:A:202:GLN:O	1:A:206:GLU:HG3	1.98	0.63
1:A:203:TYR:CE2	1:D:2:HIS:CD2	2.86	0.63
1:B:66:ASP:O	1:B:67:SER:C	2.41	0.63
1:C:344:HIS:O	1:C:345:THR:C	2.41	0.63
1:H:308:SER:HB3	1:H:351:ALA:HB1	1.80	0.63
1:J:276:GLU:HG3	1:J:352:SER:CB	2.27	0.63
1:M:1:ALA:H3	1:N:118:THR:HA	1.51	0.63
1:O:70:ASN:H	1:O:70:ASN:ND2	1.96	0.63
1:F:115:LEU:O	1:F:118:THR:HB	1.98	0.63
1:L:123:THR:HG22	1:L:124:ILE:H	1.63	0.63
1:A:274:MET:HE3	1:A:279:ALA:HB2	1.80	0.63
1:C:44:GLN:OE1	1:C:44:GLN:HA	1.98	0.63
1:E:329:LYS:CE	1:E:347:SER:CB	2.74	0.63
1:L:244:THR:HG22	1:L:247:GLN:H	1.63	0.63
1:P:313:TRP:CZ2	1:P:315:GLY:HA2	2.33	0.63
1:Q:156:GLN:HB3	1:R:1:ALA:N	2.13	0.63
1:A:156:GLN:HE22	1:B:3:ARG:HE	1.47	0.63
1:C:118:THR:HG23	1:C:121:GLU:H	1.59	0.63
1:G:86:LYS:HD3	1:G:90:GLY:HA2	1.81	0.63
1:H:86:LYS:HB3	1:H:90:GLY:HA2	1.79	0.63
1:K:129:GLY:H	1:L:125:GLN:HE22	1.45	0.63
1:L:58:PHE:CZ	1:L:310:LEU:HD13	2.32	0.63
1:O:244:THR:HG23	1:O:246:GLU:H	1.64	0.63
1:O:342:TYR:O	1:O:342:TYR:CD2	2.51	0.63
1:D:50:ASN:HD21	1:D:55:ARG:HH11	1.46	0.63
1:D:71:GLN:OE1	3:D:501:HOH:O	2.15	0.63
1:G:189:GLU:HG2	1:G:191:ILE:HD12	1.80	0.63
1:I:65:VAL:HG23	1:I:324:GLN:HB3	1.80	0.63
1:Q:109:ASP:HB2	1:Q:124:ILE:HG21	1.80	0.63
1:A:80:HIS:HD2	1:A:137:TYR:OH	1.82	0.63
1:A:349:GLY:O	1:A:352:SER:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:308:SER:CB	1:H:351:ALA:HB1	2.29	0.63
1:J:146:LYS:HE2	1:J:187:GLU:OE1	1.98	0.63
1:M:68:SER:HA	1:M:69:ILE:CD1	2.29	0.63
1:D:123:THR:HG21	1:D:165:GLU:OE2	1.97	0.63
1:P:30:LEU:HB3	1:P:76:VAL:HG22	1.81	0.63
1:A:213:TYR:OH	1:A:228:LEU:HD13	1.99	0.63
1:C:223:LEU:O	1:C:226:THR:HB	1.98	0.63
1:E:87:ASP:O	1:E:89:GLN:CB	2.47	0.63
1:K:123:THR:HG22	1:K:124:ILE:H	1.64	0.63
1:M:121:GLU:OE1	1:N:1:ALA:HB2	1.99	0.63
1:Q:156:GLN:HB3	1:R:1:ALA:CA	2.28	0.63
1:A:303:ARG:CG	1:A:357:PHE:CD1	2.78	0.62
1:B:344:HIS:C	1:B:345:THR:O	2.40	0.62
1:D:278:ASP:O	1:D:279:ALA:C	2.42	0.62
1:I:51:THR:CG2	1:I:54:ASN:H	2.12	0.62
1:I:67:SER:HB3	3:I:406:HOH:O	1.99	0.62
1:J:25:ASN:H	1:J:27:LYS:HG3	1.64	0.62
1:M:69:ILE:C	1:M:71:GLN:N	2.55	0.62
1:P:352:SER:CA	3:P:501:HOH:O	2.47	0.62
1:Q:244:THR:HG23	1:Q:246:GLU:N	2.14	0.62
1:A:2:HIS:C	1:A:4:PHE:H	2.03	0.62
1:A:3:ARG:HD3	1:B:156:GLN:NE2	2.14	0.62
1:N:68:SER:O	1:N:69:ILE:C	2.42	0.62
1:O:50:ASN:HD21	1:O:55:ARG:HH11	1.48	0.62
1:A:344:HIS:HB2	1:A:345:THR:O	2.00	0.62
1:E:244:THR:HG23	1:E:246:GLU:H	1.65	0.62
1:G:33:ASP:O	1:G:107:LYS:HE3	1.98	0.62
1:H:66:ASP:O	1:H:67:SER:HB3	1.99	0.62
1:H:313:TRP:CZ2	1:H:315:GLY:HA2	2.34	0.62
1:P:229:LYS:HG3	1:P:268:CYS:O	1.98	0.62
1:A:356:LEU:CD1	1:A:357:PHE:HE1	2.04	0.62
1:B:58:PHE:CE1	1:B:310:LEU:CD1	2.78	0.62
1:B:207:LYS:CD	1:C:2:HIS:HE2	2.12	0.62
1:I:118:THR:C	1:J:1:ALA:H3	2.08	0.62
1:J:244:THR:HG23	1:J:246:GLU:H	1.62	0.62
1:O:125:GLN:HE22	1:P:129:GLY:H	1.47	0.62
1:A:356:LEU:HD13	1:A:357:PHE:CD1	2.31	0.62
1:B:106:ILE:HG22	1:B:142:VAL:HG11	1.81	0.62
1:B:244:THR:O	1:B:247:GLN:N	2.32	0.62
1:I:130:LEU:O	1:I:134:CYS:N	2.25	0.62
1:M:51:THR:HG22	1:M:54:ASN:N	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:276:GLU:H	1:P:352:SER:HB3	1.64	0.62
1:D:81:GLU:HG2	1:D:82:THR:N	2.15	0.62
1:H:250:MET:HE1	1:H:291:LEU:CD1	2.30	0.62
1:I:244:THR:CG2	1:I:247:GLN:H	2.13	0.62
1:N:51:THR:HG22	1:N:54:ASN:N	2.13	0.62
1:O:29:ILE:HB	1:O:300:SER:HA	1.81	0.62
1:P:123:THR:HG23	1:P:165:GLU:HG3	1.80	0.62
1:F:123:THR:CG2	1:F:165:GLU:HG3	2.30	0.62
1:H:88:SER:O	1:H:89:GLN:HB2	2.00	0.62
1:I:125:GLN:NE2	1:J:129:GLY:H	1.98	0.62
1:B:343:VAL:O	1:B:344:HIS:C	2.42	0.62
1:H:58:PHE:CE1	1:H:310:LEU:HD13	2.35	0.62
1:H:220:HIS:HE1	3:H:407:HOH:O	1.81	0.62
1:G:187:GLU:HG3	1:G:229:LYS:HG2	1.82	0.62
1:G:319:ASN:O	1:G:320:LYS:C	2.42	0.62
1:L:69:ILE:HD13	1:L:73:ILE:HG12	1.82	0.62
1:O:148:ARG:HB2	1:O:187:GLU:OE1	2.00	0.62
1:B:248:VAL:O	1:B:249:ALA:C	2.42	0.61
1:C:202:GLN:HB2	1:C:233:VAL:HG11	1.81	0.61
1:D:336:GLN:HB2	1:D:342:TYR:HB2	1.82	0.61
1:L:17:GLU:O	1:L:21:SER:HB3	2.00	0.61
1:L:244:THR:HG22	1:L:247:GLN:CG	2.30	0.61
1:L:312:ALA:HB1	1:L:322:ALA:HB3	1.82	0.61
1:O:244:THR:N	1:O:247:GLN:OE1	2.32	0.61
1:E:87:ASP:O	1:E:89:GLN:HB3	1.99	0.61
1:F:276:GLU:CG	1:F:352:SER:HB3	2.30	0.61
1:G:119:ASN:O	1:G:152:ARG:NH1	2.31	0.61
1:J:244:THR:H	1:J:247:GLN:NE2	1.98	0.61
1:G:50:ASN:ND2	1:G:55:ARG:HH11	1.97	0.61
1:N:271:SER:O	1:N:272:GLY:C	2.40	0.61
1:B:58:PHE:CZ	1:B:310:LEU:HD13	2.33	0.61
1:D:329:LYS:HD3	1:D:347:SER:H	1.65	0.61
1:I:2:HIS:O	1:I:3:ARG:C	2.43	0.61
1:I:319:ASN:O	1:I:320:LYS:C	2.43	0.61
1:O:118:THR:HA	1:P:1:ALA:H1	1.65	0.61
1:E:89:GLN:N	3:E:504:HOH:O	2.34	0.61
1:G:51:THR:HG23	1:G:54:ASN:H	1.65	0.61
1:M:3:ARG:NH1	1:N:156:GLN:HE22	1.97	0.61
1:N:3:ARG:HB2	1:N:3:ARG:HH11	1.66	0.61
1:O:144:PHE:HA	1:O:183:VAL:H	1.64	0.61
1:P:58:PHE:CZ	1:P:310:LEU:HD13	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:HIS:CD2	1:B:137:TYR:OH	2.54	0.61
1:C:118:THR:HG21	1:C:121:GLU:HB2	1.81	0.61
1:E:244:THR:HG23	1:E:246:GLU:HB2	1.79	0.61
1:L:67:SER:HA	1:L:100:LYS:HD3	1.82	0.61
1:L:313:TRP:CZ2	1:L:315:GLY:HA2	2.35	0.61
1:N:221:VAL:HG12	1:N:222:TYR:N	2.15	0.61
1:O:88:SER:O	1:O:89:GLN:HB2	1.98	0.61
1:Q:87:ASP:HB2	1:Q:91:LYS:O	2.01	0.61
1:R:244:THR:HG23	1:R:246:GLU:H	1.63	0.61
1:E:2:HIS:O	1:E:4:PHE:HD1	1.84	0.61
1:I:231:ASN:ND2	1:I:231:ASN:H	1.97	0.61
1:K:353:THR:CG2	1:O:92:LEU:HD11	2.31	0.61
1:M:58:PHE:CE2	1:M:310:LEU:HD13	2.36	0.61
1:P:276:GLU:HG3	1:P:352:SER:HB2	1.82	0.61
1:A:156:GLN:NE2	1:B:3:ARG:HE	1.99	0.61
1:C:189:GLU:HG2	1:C:191:ILE:CD1	2.28	0.61
1:D:119:ASN:HB3	1:D:157:CYS:SG	2.41	0.61
1:F:195:ASP:HB3	1:F:238:ALA:HB3	1.83	0.61
1:O:182:LEU:N	1:O:182:LEU:HD23	2.15	0.61
1:R:58:PHE:CE1	1:R:310:LEU:HD13	2.36	0.61
1:R:124:ILE:HD13	3:R:514:HOH:O	2.01	0.61
1:B:88:SER:O	1:B:89:GLN:HB2	2.00	0.61
1:E:1:ALA:N	1:E:220:HIS:HE1	1.98	0.61
1:K:12:LYS:HB3	1:K:222:TYR:CZ	2.36	0.61
1:A:202:GLN:HB2	1:A:233:VAL:HG11	1.83	0.61
1:M:272:GLY:HA2	1:M:303:ARG:NH1	2.16	0.61
1:R:95:ASN:O	1:R:99:GLU:HG3	2.00	0.61
1:R:276:GLU:HB3	1:R:330:ARG:HD3	1.82	0.61
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.36	0.60
1:B:78:LEU:O	1:B:106:ILE:HD12	2.01	0.60
1:F:80:HIS:CD2	1:F:137:TYR:OH	2.54	0.60
1:J:58:PHE:CE2	1:J:310:LEU:HD13	2.36	0.60
1:J:214:LYS:HG2	1:K:214:LYS:HG2	1.83	0.60
1:O:65:VAL:HG12	1:O:324:GLN:HB3	1.82	0.60
1:B:89:GLN:O	1:B:90:GLY:C	2.39	0.60
1:B:244:THR:HG22	1:B:247:GLN:CB	2.31	0.60
1:E:244:THR:HG21	1:E:246:GLU:HB2	1.82	0.60
1:I:28:GLY:HA3	1:I:299:PHE:CZ	2.35	0.60
1:I:123:THR:CG2	1:I:124:ILE:H	1.99	0.60
1:I:343:VAL:HG12	1:I:344:HIS:H	1.65	0.60
1:L:118:THR:HG22	1:L:121:GLU:H	1.61	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:345:THR:CB	3:M:502:HOH:O	2.49	0.60
1:R:271:SER:HA	1:R:274:MET:CE	2.31	0.60
1:R:313:TRP:CZ2	1:R:315:GLY:HA2	2.36	0.60
1:D:189:GLU:HG2	1:D:191:ILE:HD11	1.79	0.60
1:E:118:THR:HG23	1:E:121:GLU:HG3	1.82	0.60
1:E:123:THR:HG23	1:E:165:GLU:HG3	1.83	0.60
1:E:233:VAL:HG23	1:E:252:THR:HA	1.83	0.60
1:F:276:GLU:HG3	1:F:352:SER:HB3	1.82	0.60
1:J:329:LYS:HZ2	1:J:347:SER:HA	1.65	0.60
1:K:156:GLN:HE22	1:L:3:ARG:NE	1.99	0.60
1:M:349:GLY:O	1:M:350:ALA:HB3	2.01	0.60
1:O:324:GLN:O	1:O:328:MET:HB3	2.01	0.60
1:H:250:MET:CE	1:H:291:LEU:HD22	2.31	0.60
1:M:1:ALA:H2	1:N:118:THR:HA	1.64	0.60
1:Q:344:HIS:ND1	1:Q:344:HIS:N	2.48	0.60
1:M:1:ALA:CB	1:N:119:ASN:H	2.12	0.60
1:N:3:ARG:HH11	1:N:3:ARG:CB	2.14	0.60
1:N:61:ILE:CG2	1:N:324:GLN:HG2	2.32	0.60
1:P:68:SER:O	1:P:71:GLN:HG3	2.01	0.60
1:R:8:THR:OG1	1:R:11:GLN:HG3	2.01	0.60
1:E:89:GLN:HE22	1:E:89:GLN:H	1.48	0.60
1:H:189:GLU:HG2	1:H:191:ILE:HD12	1.82	0.60
1:J:113:ALA:O	1:J:122:THR:HB	2.02	0.60
1:L:51:THR:HG22	1:L:54:ASN:CB	2.32	0.60
1:A:344:HIS:O	1:A:344:HIS:CG	2.54	0.60
1:B:207:LYS:HD3	1:C:2:HIS:HE2	1.66	0.60
1:C:232:MET:HG3	1:C:269:PHE:CD2	2.36	0.60
1:I:124:ILE:HG22	1:I:147:TRP:CZ2	2.37	0.60
1:K:91:LYS:HD3	1:K:96:ILE:HG12	1.84	0.60
1:Q:125:GLN:NE2	1:R:129:GLY:H	2.00	0.60
1:R:343:VAL:O	1:R:344:HIS:CG	2.54	0.60
1:A:91:LYS:HD3	1:A:96:ILE:HG12	1.83	0.60
1:J:352:SER:HA	3:J:503:HOH:O	2.01	0.60
1:L:12:LYS:HE2	1:L:222:TYR:CE1	2.37	0.60
1:O:277:GLU:OE2	1:O:342:TYR:OH	2.20	0.60
1:A:45:ARG:NE	1:A:357:PHE:HA	2.17	0.60
1:A:244:THR:HG23	1:A:246:GLU:N	2.17	0.60
1:B:61:ILE:CG2	1:B:323:THR:HG22	2.31	0.60
1:F:329:LYS:HD2	1:F:346:GLY:O	2.02	0.60
1:G:128:ASP:OD1	1:H:125:GLN:HB3	2.02	0.60
1:I:244:THR:HG22	1:I:247:GLN:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:343:VAL:O	1:L:344:HIS:ND1	2.35	0.60
1:M:65:VAL:HG12	1:M:68:SER:HB2	1.83	0.60
1:O:61:ILE:CG2	1:O:324:GLN:HG2	2.31	0.60
1:O:278:ASP:O	1:O:281:LEU:N	2.35	0.60
1:Q:109:ASP:HB2	1:Q:124:ILE:CG2	2.32	0.60
1:H:50:ASN:ND2	1:H:55:ARG:HD3	2.17	0.60
1:L:72:SER:HB3	1:L:331:ALA:O	2.02	0.60
1:N:313:TRP:CE2	1:N:315:GLY:CA	2.83	0.60
1:O:70:ASN:N	1:O:70:ASN:ND2	2.50	0.60
1:O:203:TYR:C	1:O:203:TYR:CD2	2.79	0.60
1:O:278:ASP:O	1:O:279:ALA:C	2.45	0.60
1:R:18:ILE:HD13	1:R:143:ASP:HB3	1.83	0.60
1:B:207:LYS:HZ3	1:C:2:HIS:HE2	1.50	0.59
1:D:86:LYS:HD3	1:D:90:GLY:CA	2.31	0.59
1:L:91:LYS:HD3	1:L:96:ILE:CG1	2.32	0.59
1:L:272:GLY:HA2	1:L:303:ARG:NH1	2.17	0.59
1:M:80:HIS:HD2	1:M:137:TYR:OH	1.84	0.59
1:A:244:THR:CG2	1:A:247:GLN:N	2.46	0.59
1:C:50:ASN:HD21	1:C:55:ARG:HH11	1.48	0.59
1:F:33:ASP:HB3	1:F:77:ILE:HG22	1.84	0.59
1:I:61:ILE:CG2	1:I:324:GLN:HG2	2.31	0.59
1:I:271:SER:HB3	1:I:301:TYR:CE2	2.38	0.59
1:L:337:ALA:O	1:L:338:ALA:C	2.42	0.59
1:M:244:THR:HG23	1:M:247:GLN:OE1	2.01	0.59
1:Q:240:THR:O	1:Q:242:LYS:HE3	2.02	0.59
1:Q:330:ARG:HA	1:Q:330:ARG:HE	1.67	0.59
1:R:229:LYS:HA	1:R:268:CYS:O	2.02	0.59
1:C:118:THR:CG2	1:C:121:GLU:HB2	2.32	0.59
1:F:316:LYS:HB2	1:F:319:ASN:ND2	2.17	0.59
1:G:320:LYS:O	1:G:324:GLN:HG3	2.01	0.59
1:H:191:ILE:HD12	1:H:191:ILE:N	2.14	0.59
1:J:313:TRP:CE2	1:J:315:GLY:HA2	2.38	0.59
1:M:1:ALA:H3	1:N:119:ASN:H	1.50	0.59
1:M:3:ARG:O	1:M:4:PHE:C	2.45	0.59
1:B:66:ASP:O	1:B:67:SER:O	2.21	0.59
1:E:51:THR:HG22	1:E:54:ASN:N	2.14	0.59
1:E:276:GLU:HG3	1:E:352:SER:CB	2.32	0.59
1:F:60:GLU:OE1	1:F:87:ASP:HB2	2.02	0.59
1:I:46:ILE:HG21	1:I:310:LEU:O	2.03	0.59
1:C:123:THR:HG22	1:C:124:ILE:N	2.11	0.59
1:D:63:PHE:O	1:D:100:LYS:HE3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:SER:OG	1:F:356:LEU:HD11	2.02	0.59
1:M:2:HIS:NE2	1:P:207:LYS:HE2	2.17	0.59
1:C:58:PHE:CZ	1:C:310:LEU:HD13	2.37	0.59
1:F:51:THR:HG22	1:F:54:ASN:CB	2.33	0.59
1:G:244:THR:HG22	1:G:247:GLN:N	2.18	0.59
1:H:313:TRP:CH2	1:H:315:GLY:HA2	2.37	0.59
1:I:29:ILE:HB	1:I:300:SER:HB2	1.85	0.59
1:K:303:ARG:NH2	1:K:357:PHE:CB	2.57	0.59
1:L:313:TRP:CE2	1:L:315:GLY:HA2	2.38	0.59
1:M:303:ARG:HD2	1:M:356:LEU:HB2	1.85	0.59
1:Q:170:LEU:HD22	1:Q:186:VAL:HG13	1.84	0.59
1:D:190:VAL:H	1:D:231:ASN:ND2	2.00	0.59
1:H:115:LEU:O	1:H:118:THR:HB	2.03	0.59
1:I:58:PHE:CE2	1:I:62:LEU:HD11	2.36	0.59
1:J:224:GLU:OE1	1:J:224:GLU:N	2.31	0.59
1:L:123:THR:HG21	1:L:165:GLU:OE2	2.02	0.59
1:O:129:GLY:H	1:P:125:GLN:NE2	2.00	0.59
1:O:187:GLU:HG3	1:O:229:LYS:O	2.03	0.59
1:O:313:TRP:CZ2	1:O:315:GLY:HA2	2.38	0.59
1:P:313:TRP:CD2	1:P:315:GLY:HA2	2.38	0.59
1:C:12:LYS:HG2	1:C:222:TYR:CE1	2.37	0.59
1:C:271:SER:O	1:C:272:GLY:C	2.46	0.59
1:E:250:MET:HE1	1:E:291:LEU:CD2	2.32	0.59
1:H:281:LEU:HD22	1:H:344:HIS:CE1	2.37	0.59
1:B:2:HIS:CD2	1:B:2:HIS:O	2.55	0.59
1:B:29:ILE:HB	1:B:300:SER:HA	1.84	0.59
1:H:299:PHE:CD1	1:H:334:ASN:HB3	2.37	0.59
1:J:28:GLY:HA3	1:J:299:PHE:CZ	2.38	0.59
1:J:42:ARG:HH11	1:J:42:ARG:CG	2.14	0.59
1:R:124:ILE:CG2	1:R:147:TRP:CE2	2.86	0.59
1:D:1:ALA:HB1	1:D:2:HIS:ND1	2.17	0.59
1:G:188:PRO:O	1:G:188:PRO:CG	2.45	0.59
1:G:330:ARG:HA	1:G:330:ARG:HE	1.66	0.59
1:B:58:PHE:CE2	1:B:62:LEU:HD21	2.37	0.58
1:B:343:VAL:O	1:B:343:VAL:HG22	2.02	0.58
1:C:156:GLN:HE22	1:D:3:ARG:HD2	1.65	0.58
1:F:271:SER:O	1:F:274:MET:HB2	2.03	0.58
1:H:118:THR:HG23	1:H:121:GLU:H	1.66	0.58
1:I:258:ARG:NH1	1:L:224:GLU:OE2	2.32	0.58
1:N:63:PHE:HB3	1:N:97:LEU:HD21	1.85	0.58
1:Q:244:THR:HG22	1:Q:247:GLN:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ALA:O	1:B:218:ASP:HB2	2.03	0.58
1:E:223:LEU:O	1:E:226:THR:HB	2.03	0.58
1:F:123:THR:C	1:F:124:ILE:HD12	2.28	0.58
1:L:18:ILE:HD13	1:L:143:ASP:HB3	1.85	0.58
1:N:108:LEU:HD12	1:N:173:TYR:HE1	1.68	0.58
1:M:1:ALA:HB1	1:N:156:GLN:HB3	1.85	0.58
1:M:329:LYS:NZ	1:M:347:SER:C	2.61	0.58
1:A:125:GLN:NE2	1:B:129:GLY:H	1.94	0.58
1:B:87:ASP:CG	1:B:87:ASP:O	2.47	0.58
1:G:3:ARG:HH11	1:G:3:ARG:CG	2.16	0.58
1:G:12:LYS:HB3	1:G:222:TYR:CZ	2.38	0.58
1:J:123:THR:HG21	1:J:165:GLU:OE2	2.03	0.58
1:M:3:ARG:HG3	1:M:4:PHE:H	1.68	0.58
1:M:66:ASP:C	1:M:68:SER:N	2.58	0.58
1:N:58:PHE:CE1	1:N:310:LEU:CD1	2.86	0.58
1:O:118:THR:HG21	1:O:121:GLU:HB2	1.84	0.58
1:P:146:LYS:HE2	1:P:187:GLU:OE1	2.04	0.58
1:D:329:LYS:HZ2	1:D:347:SER:HA	1.67	0.58
1:D:343:VAL:HG12	1:D:344:HIS:N	2.19	0.58
1:I:2:HIS:CB	1:J:156:GLN:OE1	2.52	0.58
1:I:198:LEU:CD1	1:I:234:THR:HA	2.34	0.58
1:C:197:ASP:C	1:C:197:ASP:OD1	2.46	0.58
1:G:29:ILE:HB	1:G:300:SER:HA	1.84	0.58
1:L:244:THR:N	1:L:247:GLN:OE1	2.36	0.58
1:N:2:HIS:C	1:N:3:ARG:NH1	2.61	0.58
1:N:51:THR:O	1:N:52:GLU:C	2.45	0.58
1:Q:161:LEU:HB3	3:Q:2023:HOH:O	2.01	0.58
1:C:2:HIS:CB	1:D:156:GLN:OE1	2.51	0.58
1:M:1:ALA:H3	1:N:118:THR:C	2.11	0.58
1:M:3:ARG:HG2	1:M:4:PHE:CD1	2.39	0.58
1:M:69:ILE:HG22	1:M:71:GLN:HG2	1.84	0.58
1:O:123:THR:HG21	1:O:165:GLU:OE2	2.04	0.58
1:R:118:THR:HG23	1:R:121:GLU:HG3	1.84	0.58
1:A:307:ALA:HB2	1:A:357:PHE:CE1	2.38	0.58
1:F:50:ASN:ND2	1:F:55:ARG:HD3	2.19	0.58
1:L:281:LEU:CD2	1:L:342:TYR:HE2	2.14	0.58
1:N:253:VAL:O	1:N:257:HIS:HB3	2.03	0.58
1:O:51:THR:CG2	1:O:54:ASN:N	2.65	0.58
1:Q:91:LYS:NZ	1:Q:99:GLU:OE1	2.36	0.58
1:Q:202:GLN:HB2	1:Q:233:VAL:HG11	1.85	0.58
1:B:223:LEU:O	1:B:226:THR:HB	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:THR:HG23	1:C:53:GLU:N	2.19	0.58
1:E:89:GLN:CA	3:E:504:HOH:O	2.51	0.58
1:G:322:ALA:O	1:G:325:GLU:N	2.36	0.58
1:H:330:ARG:NH1	1:H:347:SER:HB3	2.19	0.58
1:I:138:LYS:HD2	3:I:412:HOH:O	2.02	0.58
1:K:87:ASP:OD2	1:K:89:GLN:HB2	2.04	0.58
1:O:128:ASP:HB2	1:P:128:ASP:OD2	2.03	0.58
1:P:50:ASN:HD21	1:P:55:ARG:HH11	1.49	0.58
1:B:51:THR:CG2	1:B:54:ASN:HB2	2.22	0.58
1:B:319:ASN:O	1:B:320:LYS:C	2.45	0.58
1:B:341:GLN:O	1:B:342:TYR:C	2.47	0.58
1:H:118:THR:HG23	1:H:121:GLU:HG3	1.85	0.58
1:I:51:THR:HB	1:I:54:ASN:HB2	1.86	0.58
1:K:51:THR:CG2	1:K:54:ASN:N	2.63	0.58
1:K:177:CYS:HB3	1:K:182:LEU:HB2	1.86	0.58
1:B:17:GLU:O	1:B:18:ILE:C	2.45	0.57
1:D:61:ILE:HG21	1:D:323:THR:CG2	2.33	0.57
1:K:118:THR:CG2	1:K:121:GLU:H	2.16	0.57
1:K:237:HIS:NE2	1:K:357:PHE:O	2.37	0.57
1:K:357:PHE:C	1:O:139:LYS:HE3	2.29	0.57
1:R:214:LYS:HD2	1:R:214:LYS:C	2.29	0.57
1:A:65:VAL:O	1:A:100:LYS:NZ	2.28	0.57
1:A:291:LEU:O	1:A:293:LYS:HG3	2.05	0.57
1:F:233:VAL:HG23	1:F:252:THR:HA	1.86	0.57
1:G:58:PHE:CE2	1:G:62:LEU:HD11	2.38	0.57
1:O:123:THR:CG2	1:O:165:GLU:HG3	2.34	0.57
1:A:277:GLU:HG2	1:A:347:SER:HB3	1.86	0.57
1:A:303:ARG:CB	1:A:357:PHE:CD1	2.87	0.57
1:C:12:LYS:HG2	1:C:222:TYR:CZ	2.39	0.57
1:K:80:HIS:CD2	1:K:137:TYR:OH	2.53	0.57
1:Q:118:THR:CG2	1:Q:121:GLU:H	2.17	0.57
1:B:151:LEU:HD12	1:B:208:VAL:HG11	1.86	0.57
1:E:347:SER:OG	1:E:348:SER:N	2.36	0.57
1:F:291:LEU:O	1:F:293:LYS:HG3	2.04	0.57
1:I:183:VAL:O	1:I:183:VAL:HG12	2.02	0.57
1:M:159:SER:O	1:M:163:ILE:HG13	2.04	0.57
1:M:224:GLU:OE1	1:M:224:GLU:N	2.34	0.57
1:O:3:ARG:O	1:O:4:PHE:C	2.47	0.57
1:P:118:THR:CG2	1:P:121:GLU:HB2	2.33	0.57
1:P:155:ASP:OD1	1:P:156:GLN:HG3	2.05	0.57
1:B:207:LYS:HD3	1:C:2:HIS:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:VAL:HG13	1:C:191:ILE:HG12	1.86	0.57
1:E:271:SER:HA	1:E:274:MET:HE1	1.86	0.57
1:I:284:ASN:OD1	1:I:340:GLY:HA2	2.05	0.57
1:L:219:HIS:O	1:L:220:HIS:HB2	2.04	0.57
1:P:77:ILE:HD13	1:P:146:LYS:HG3	1.86	0.57
1:H:9:GLN:HA	1:H:9:GLN:OE1	2.04	0.57
1:I:274:MET:HE3	1:I:279:ALA:CA	2.33	0.57
1:L:97:LEU:O	1:L:98:LYS:C	2.45	0.57
1:M:253:VAL:O	1:M:254:THR:C	2.43	0.57
1:O:271:SER:O	1:O:272:GLY:C	2.48	0.57
1:R:309:ALA:HB1	1:R:323:THR:CG2	2.33	0.57
1:B:298:SER:OG	1:B:299:PHE:N	2.34	0.57
1:C:147:TRP:HB2	1:C:173:TYR:CZ	2.40	0.57
1:I:118:THR:HG23	1:I:121:GLU:H	1.67	0.57
1:L:91:LYS:HD3	1:L:96:ILE:HG12	1.86	0.57
1:M:235:ALA:HB2	1:M:243:TYR:CE1	2.40	0.57
1:M:329:LYS:NZ	1:M:348:SER:HB2	2.20	0.57
1:A:44:GLN:HA	1:A:44:GLN:OE1	2.04	0.57
1:B:250:MET:HE1	1:B:291:LEU:HD11	1.86	0.57
1:E:203:TYR:OH	1:H:2:HIS:HA	2.03	0.57
1:I:80:HIS:HD2	1:I:137:TYR:OH	1.88	0.57
1:N:18:ILE:HD13	1:N:143:ASP:HB3	1.86	0.57
1:J:50:ASN:ND2	1:J:55:ARG:HH11	2.03	0.57
1:M:68:SER:C	1:M:70:ASN:H	2.13	0.57
1:M:71:GLN:NE2	3:M:501:HOH:O	1.63	0.57
1:M:106:ILE:O	1:M:106:ILE:HG23	2.04	0.57
1:O:230:PRO:HG3	1:O:267:ILE:HD13	1.85	0.57
1:P:8:THR:N	1:P:11:GLN:OE1	2.34	0.57
1:I:68:SER:HA	1:I:70:ASN:HD21	1.67	0.57
1:M:244:THR:HG23	1:M:247:GLN:CG	2.33	0.57
1:B:123:THR:HG21	1:B:165:GLU:OE2	2.04	0.56
1:B:155:ASP:O	1:B:156:GLN:HB2	2.04	0.56
1:C:54:ASN:O	1:C:55:ARG:C	2.48	0.56
1:G:219:HIS:O	1:G:220:HIS:HB2	2.05	0.56
1:L:220:HIS:CE1	3:L:407:HOH:O	2.53	0.56
1:L:335:CYS:O	1:L:339:LYS:HD2	2.05	0.56
1:O:1:ALA:H3	1:P:118:THR:HA	1.70	0.56
1:A:126:GLY:N	1:B:128:ASP:OD1	2.37	0.56
1:B:244:THR:HG23	1:B:246:GLU:N	2.20	0.56
1:C:2:HIS:O	1:D:156:GLN:OE1	2.23	0.56
1:I:232:MET:HE2	1:I:286:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:214:LYS:CG	1:K:214:LYS:HG2	2.36	0.56
1:M:313:TRP:O	1:M:315:GLY:N	2.38	0.56
1:N:2:HIS:CA	1:N:3:ARG:NH1	2.68	0.56
1:O:156:GLN:OE1	1:P:2:HIS:CB	2.49	0.56
1:B:87:ASP:O	1:B:88:SER:HB2	2.06	0.56
1:D:70:ASN:CB	1:D:71:GLN:N	2.67	0.56
1:E:244:THR:HG22	1:E:247:GLN:HG3	1.87	0.56
1:F:58:PHE:CE1	1:F:310:LEU:HD13	2.40	0.56
1:F:244:THR:HG23	1:F:247:GLN:H	1.69	0.56
1:G:244:THR:HG22	1:G:247:GLN:HG3	1.88	0.56
1:G:276:GLU:HB3	1:G:330:ARG:HH11	1.70	0.56
1:J:118:THR:HG23	1:J:121:GLU:H	1.70	0.56
1:K:244:THR:HG23	1:K:246:GLU:N	2.20	0.56
1:L:223:LEU:O	1:L:226:THR:HB	2.05	0.56
1:M:306:GLN:O	1:M:310:LEU:HB2	2.04	0.56
1:M:329:LYS:HZ1	1:M:348:SER:HB2	1.70	0.56
1:N:313:TRP:CH2	1:N:315:GLY:HA2	2.39	0.56
1:O:244:THR:HG23	1:O:246:GLU:N	2.19	0.56
1:O:244:THR:O	1:O:247:GLN:N	2.39	0.56
1:O:330:ARG:HA	1:O:330:ARG:NE	2.19	0.56
1:Q:244:THR:HG22	1:Q:247:GLN:HG3	1.88	0.56
1:C:271:SER:HB3	1:C:301:TYR:CD2	2.39	0.56
1:E:50:ASN:ND2	1:E:55:ARG:HD3	2.20	0.56
1:G:3:ARG:CD	1:H:156:GLN:HE22	2.18	0.56
1:I:50:ASN:HD21	1:I:55:ARG:HH11	1.52	0.56
1:P:118:THR:HG21	1:P:121:GLU:HB2	1.88	0.56
1:C:46:ILE:HG13	1:C:48:VAL:HG23	1.87	0.56
1:D:329:LYS:CE	1:D:347:SER:N	2.69	0.56
1:D:330:ARG:HA	1:D:330:ARG:NE	2.19	0.56
1:H:250:MET:CE	1:H:291:LEU:CD2	2.83	0.56
1:I:244:THR:HG22	1:I:247:GLN:CB	2.35	0.56
1:L:44:GLN:HA	1:L:44:GLN:OE1	2.06	0.56
1:M:118:THR:HG23	1:M:121:GLU:N	2.13	0.56
1:M:308:SER:CB	1:M:351:ALA:HB1	2.32	0.56
1:O:1:ALA:HB1	1:P:159:SER:HB3	1.87	0.56
1:P:276:GLU:CB	1:P:352:SER:HB3	2.36	0.56
1:Q:244:THR:HG22	1:Q:247:GLN:H	1.71	0.56
1:A:154:ALA:HB3	1:A:157:CYS:CB	2.33	0.56
1:E:88:SER:CA	1:E:89:GLN:HB3	2.12	0.56
1:E:233:VAL:CG2	1:E:252:THR:HA	2.36	0.56
1:F:190:VAL:H	1:F:231:ASN:HD22	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:THR:HG22	1:G:54:ASN:HB2	1.88	0.56
1:I:130:LEU:O	1:I:131:SER:C	2.48	0.56
1:I:272:GLY:HA2	1:I:303:ARG:NH1	2.21	0.56
1:J:352:SER:CB	3:J:503:HOH:O	2.53	0.56
1:Q:115:LEU:O	1:Q:118:THR:HB	2.05	0.56
1:D:277:GLU:OE2	1:D:344:HIS:ND1	2.38	0.56
1:D:313:TRP:CE2	1:D:315:GLY:HA2	2.41	0.56
1:I:118:THR:CG2	1:I:121:GLU:N	2.66	0.56
1:I:244:THR:HG22	1:I:247:GLN:N	2.21	0.56
1:N:197:ASP:C	1:N:197:ASP:OD1	2.47	0.56
1:O:308:SER:O	1:O:311:ALA:HB3	2.06	0.56
1:R:344:HIS:HD2	3:R:566:HOH:O	1.88	0.56
1:B:66:ASP:OD1	1:B:67:SER:N	2.39	0.56
1:B:281:LEU:CD2	1:B:344:HIS:ND1	2.62	0.56
1:D:319:ASN:O	1:D:320:LYS:C	2.49	0.56
1:O:118:THR:CG2	1:O:121:GLU:H	2.19	0.56
1:O:168:ASN:HB3	3:P:504:HOH:O	2.05	0.56
1:P:12:LYS:HD3	1:P:222:TYR:CE1	2.41	0.56
1:D:187:GLU:HG3	1:D:229:LYS:HB3	1.88	0.56
1:D:329:LYS:HD3	1:D:347:SER:CA	2.35	0.56
1:H:78:LEU:O	1:H:106:ILE:HD12	2.06	0.56
1:I:198:LEU:HD12	1:I:234:THR:HA	1.87	0.56
1:I:200:HIS:CE1	1:L:2:HIS:ND1	2.65	0.56
1:I:250:MET:CE	1:I:291:LEU:HD21	2.36	0.56
1:J:230:PRO:CG	1:J:267:ILE:HD12	2.31	0.56
1:J:352:SER:HB2	3:J:503:HOH:O	2.04	0.56
1:M:68:SER:CB	1:M:69:ILE:CD1	2.77	0.56
1:P:333:ALA:HB1	1:P:342:TYR:CE1	2.41	0.56
1:C:147:TRP:HB3	1:C:173:TYR:CE2	2.41	0.56
1:I:200:HIS:HE1	1:L:2:HIS:CE1	2.23	0.56
1:I:324:GLN:O	1:I:328:MET:HB2	2.05	0.56
1:J:329:LYS:HD3	1:J:347:SER:N	2.20	0.56
1:M:6:ALA:O	1:M:7:LEU:HD23	2.06	0.56
1:P:28:GLY:HA3	1:P:299:PHE:CE1	2.40	0.56
1:R:190:VAL:H	1:R:231:ASN:HD22	1.53	0.56
1:D:329:LYS:HD3	1:D:347:SER:HB2	1.87	0.55
1:F:200:HIS:HB2	3:F:467:HOH:O	2.06	0.55
1:F:344:HIS:CG	1:F:345:THR:N	2.73	0.55
1:G:128:ASP:HA	1:H:125:GLN:HE21	1.72	0.55
1:H:18:ILE:HD13	1:H:143:ASP:HB3	1.88	0.55
1:I:3:ARG:O	1:I:4:PHE:C	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:ASP:O	1:I:67:SER:CB	2.50	0.55
1:K:8:THR:OG1	1:K:11:GLN:HG3	2.06	0.55
1:L:244:THR:CG2	1:L:247:GLN:N	2.61	0.55
1:O:58:PHE:CZ	1:O:62:LEU:HD21	2.41	0.55
1:A:51:THR:CG2	1:A:53:GLU:N	2.69	0.55
1:A:303:ARG:HH21	1:A:359:ALA:CB	2.18	0.55
1:A:342:TYR:CZ	1:A:344:HIS:HB3	2.39	0.55
1:B:124:ILE:HG22	1:B:147:TRP:CZ2	2.41	0.55
1:F:244:THR:HG22	1:F:247:GLN:CB	2.35	0.55
1:G:65:VAL:HG12	1:G:324:GLN:HB3	1.89	0.55
1:H:66:ASP:O	1:H:67:SER:CB	2.54	0.55
1:I:123:THR:CG2	1:I:124:ILE:N	2.64	0.55
1:M:119:ASN:HB2	1:N:4:PHE:CZ	2.41	0.55
1:O:1:ALA:N	1:P:118:THR:HA	2.21	0.55
1:P:276:GLU:N	1:P:352:SER:HB3	2.21	0.55
1:R:244:THR:HG23	1:R:246:GLU:HB2	1.88	0.55
1:R:271:SER:HA	1:R:274:MET:HE3	1.89	0.55
1:B:151:LEU:CD1	1:B:208:VAL:HG11	2.37	0.55
1:C:322:ALA:O	1:C:325:GLU:HB2	2.06	0.55
1:F:329:LYS:HE2	1:F:347:SER:CA	2.05	0.55
1:I:2:HIS:HB3	1:J:156:GLN:CD	2.30	0.55
1:I:29:ILE:HB	1:I:300:SER:HA	1.87	0.55
1:I:58:PHE:CE1	1:I:310:LEU:HD13	2.41	0.55
1:M:2:HIS:CE1	1:P:203:TYR:HH	2.20	0.55
1:O:281:LEU:HD23	1:O:342:TYR:HE2	1.70	0.55
1:P:226:THR:HG23	3:P:520:HOH:O	2.00	0.55
1:A:303:ARG:HB3	1:A:357:PHE:CE1	2.41	0.55
1:E:3:ARG:O	1:E:3:ARG:HD2	2.07	0.55
1:J:214:LYS:HE3	1:J:218:ASP:OD1	2.06	0.55
1:M:1:ALA:H2	1:N:118:THR:CA	2.14	0.55
1:A:123:THR:HG22	1:A:124:ILE:H	1.72	0.55
1:H:253:VAL:CG1	1:H:291:LEU:HD23	2.35	0.55
1:I:244:THR:HG22	1:I:247:GLN:CG	2.36	0.55
1:L:118:THR:HG21	1:L:121:GLU:HB2	1.87	0.55
1:M:221:VAL:HG12	1:M:222:TYR:N	2.22	0.55
1:Q:126:GLY:H	1:R:128:ASP:CG	2.14	0.55
1:B:342:TYR:O	1:B:344:HIS:N	2.39	0.55
1:C:2:HIS:CD2	1:C:3:ARG:HH11	2.25	0.55
1:C:124:ILE:HG22	1:C:147:TRP:CZ2	2.42	0.55
1:J:272:GLY:HA2	1:J:303:ARG:NH1	2.22	0.55
1:K:347:SER:O	1:O:90:GLY:HA3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1:ALA:HB3	1:N:119:ASN:HB3	1.89	0.55
1:B:22:ILE:O	1:B:22:ILE:HG22	2.06	0.55
1:B:123:THR:CG2	1:B:165:GLU:HG3	2.30	0.55
1:H:59:ARG:HB3	1:H:63:PHE:CE1	2.42	0.55
1:J:123:THR:HG23	1:J:165:GLU:HG3	1.89	0.55
1:M:1:ALA:HB3	1:N:119:ASN:N	2.13	0.55
1:M:65:VAL:HG13	1:M:328:MET:SD	2.47	0.55
1:M:320:LYS:O	1:M:324:GLN:HG3	2.07	0.55
1:O:204:VAL:O	1:O:208:VAL:HG23	2.07	0.55
1:E:89:GLN:HA	3:E:504:HOH:O	2.07	0.55
1:E:271:SER:O	1:E:274:MET:CE	2.54	0.55
1:F:124:ILE:HG22	1:F:147:TRP:CZ2	2.42	0.55
1:G:50:ASN:HD21	1:G:55:ARG:HH11	1.54	0.55
1:I:128:ASP:OD1	1:J:125:GLN:HB3	2.06	0.55
1:K:115:LEU:HD13	1:K:123:THR:OG1	2.07	0.55
1:K:357:PHE:C	1:O:139:LYS:CE	2.80	0.55
1:P:115:LEU:HD22	1:P:122:THR:C	2.32	0.55
1:Q:93:PHE:O	1:Q:94:ARG:C	2.46	0.55
1:Q:159:SER:HB3	1:R:1:ALA:N	2.19	0.55
1:A:51:THR:HG23	1:A:53:GLU:H	1.71	0.55
1:A:66:ASP:C	1:A:66:ASP:OD1	2.50	0.55
1:A:154:ALA:O	1:A:155:ASP:C	2.47	0.55
1:H:320:LYS:O	1:H:324:GLN:HG3	2.06	0.55
1:K:120:LYS:HB2	1:K:152:ARG:HH12	1.72	0.55
1:K:150:VAL:HG13	1:K:191:ILE:HG13	1.89	0.55
1:D:277:GLU:OE2	1:D:344:HIS:CE1	2.60	0.55
1:G:28:GLY:HA3	1:G:299:PHE:CE1	2.41	0.55
1:G:229:LYS:HA	1:G:268:CYS:O	2.07	0.55
1:I:156:GLN:HE22	1:J:3:ARG:HG3	1.72	0.55
1:J:71:GLN:NE2	3:J:504:HOH:O	2.39	0.55
1:K:156:GLN:OE1	1:L:2:HIS:N	2.36	0.55
1:L:229:LYS:HA	1:L:268:CYS:O	2.07	0.55
1:M:150:VAL:HG13	1:M:191:ILE:HG12	1.89	0.55
1:M:349:GLY:C	1:M:351:ALA:H	2.15	0.55
1:L:187:GLU:HG3	1:L:229:LYS:O	2.08	0.54
1:L:271:SER:O	1:L:272:GLY:C	2.48	0.54
1:M:65:VAL:CG1	1:M:68:SER:HB2	2.37	0.54
1:N:58:PHE:CE1	1:N:310:LEU:HD13	2.42	0.54
1:O:118:THR:HA	1:P:1:ALA:H3	1.72	0.54
1:D:1:ALA:CB	1:D:2:HIS:ND1	2.70	0.54
1:E:2:HIS:O	1:F:156:GLN:OE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:GLU:OE1	1:I:159:SER:HB3	2.07	0.54
1:M:46:ILE:O	1:M:47:LYS:C	2.50	0.54
1:N:115:LEU:HD13	1:N:123:THR:OG1	2.07	0.54
1:O:223:LEU:O	1:O:226:THR:HB	2.06	0.54
1:C:58:PHE:CE1	1:C:310:LEU:HD13	2.42	0.54
1:C:125:GLN:HE21	1:D:129:GLY:H	1.55	0.54
1:H:277:GLU:OE2	1:H:345:THR:HA	2.07	0.54
1:I:149:ALA:HB1	1:I:166:ASN:OD1	2.07	0.54
1:J:349:GLY:O	1:J:350:ALA:C	2.51	0.54
1:M:159:SER:CB	1:N:1:ALA:HA	2.37	0.54
1:O:51:THR:HG23	1:O:54:ASN:H	1.71	0.54
1:B:244:THR:O	1:B:245:PRO:C	2.50	0.54
1:C:244:THR:HG23	1:C:246:GLU:N	2.22	0.54
1:D:51:THR:O	1:D:52:GLU:C	2.49	0.54
1:E:8:THR:O	1:E:12:LYS:HG3	2.07	0.54
1:G:51:THR:HG22	1:G:54:ASN:CB	2.37	0.54
1:H:86:LYS:CB	1:H:90:GLY:HA2	2.37	0.54
1:I:271:SER:HB2	1:I:274:MET:HE2	1.90	0.54
1:N:320:LYS:O	1:N:324:GLN:HG3	2.07	0.54
1:O:148:ARG:NH1	1:O:189:GLU:OE1	2.37	0.54
1:D:329:LYS:CD	1:D:347:SER:H	2.21	0.54
1:F:256:LEU:HD13	1:F:267:ILE:CD1	2.37	0.54
1:J:83:LEU:HG	1:J:83:LEU:O	2.08	0.54
1:M:124:ILE:HG21	1:M:147:TRP:NE1	2.22	0.54
1:B:207:LYS:NZ	1:C:2:HIS:HE2	2.06	0.54
1:E:219:HIS:O	1:E:220:HIS:HB2	2.08	0.54
1:I:65:VAL:CG1	1:I:69:ILE:HG21	2.38	0.54
1:I:171:ALA:HA	1:I:216:LEU:HD12	1.88	0.54
1:I:244:THR:HG22	1:I:247:GLN:HG3	1.90	0.54
1:I:258:ARG:HH11	1:L:224:GLU:CD	2.15	0.54
1:L:149:ALA:HB3	1:L:188:PRO:HA	1.90	0.54
1:L:233:VAL:O	1:L:248:VAL:HG13	2.07	0.54
1:M:117:GLY:O	1:N:3:ARG:HD3	2.07	0.54
1:R:29:ILE:HB	1:R:300:SER:HA	1.90	0.54
1:F:319:ASN:O	1:F:320:LYS:C	2.47	0.54
1:K:221:VAL:HG12	1:K:222:TYR:N	2.21	0.54
1:L:312:ALA:HB1	1:L:322:ALA:CB	2.38	0.54
1:M:303:ARG:HH11	1:M:303:ARG:HG3	1.72	0.54
1:B:146:LYS:HE2	1:B:187:GLU:OE1	2.07	0.54
1:D:329:LYS:HD3	1:D:347:SER:N	2.22	0.54
1:E:87:ASP:C	1:E:89:GLN:HB3	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1:ALA:N	1:N:118:THR:OG1	2.40	0.54
1:M:226:THR:HG23	3:M:509:HOH:O	2.08	0.54
1:N:8:THR:O	1:N:9:GLN:C	2.50	0.54
1:P:91:LYS:HD3	1:P:96:ILE:HG12	1.90	0.54
1:D:313:TRP:CZ2	1:D:315:GLY:HA2	2.42	0.54
1:E:319:ASN:O	1:E:320:LYS:C	2.48	0.54
1:M:4:PHE:CZ	1:N:119:ASN:HB2	2.42	0.54
1:N:276:GLU:HB3	1:N:330:ARG:NH1	2.23	0.54
1:Q:233:VAL:HG23	1:Q:252:THR:HA	1.89	0.54
1:Q:271:SER:O	1:Q:272:GLY:C	2.50	0.54
1:R:271:SER:HB3	1:R:301:TYR:CD2	2.42	0.54
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.43	0.54
1:B:202:GLN:O	1:B:206:GLU:N	2.36	0.54
1:H:63:PHE:O	1:H:100:LYS:NZ	2.41	0.54
1:I:190:VAL:H	1:I:231:ASN:HD22	1.55	0.54
1:I:330:ARG:HA	1:I:330:ARG:NE	2.20	0.54
1:J:67:SER:O	1:J:68:SER:C	2.51	0.54
1:J:226:THR:HG23	3:J:511:HOH:O	2.08	0.54
1:B:29:ILE:HB	1:B:300:SER:CB	2.37	0.53
1:C:3:ARG:N	1:C:3:ARG:HD3	2.22	0.53
1:C:53:GLU:OE1	1:C:53:GLU:HA	2.08	0.53
1:C:313:TRP:CE2	1:C:315:GLY:CA	2.88	0.53
1:F:244:THR:HG22	1:F:247:GLN:H	1.73	0.53
1:J:65:VAL:O	1:J:100:LYS:NZ	2.38	0.53
1:L:42:ARG:O	1:L:45:ARG:HB2	2.08	0.53
1:Q:22:ILE:HD11	1:Q:144:PHE:CD2	2.43	0.53
1:C:1:ALA:CB	1:C:4:PHE:CD1	2.92	0.53
1:C:244:THR:HG23	1:C:247:GLN:N	2.23	0.53
1:C:275:SER:O	1:C:276:GLU:C	2.48	0.53
1:C:295:TRP:O	1:C:296:LYS:C	2.50	0.53
1:E:8:THR:HG23	1:E:11:GLN:OE1	2.07	0.53
1:E:195:ASP:O	1:E:239:CYS:HB2	2.06	0.53
1:E:250:MET:HE1	1:E:291:LEU:HD13	1.89	0.53
1:E:351:ALA:O	1:E:352:SER:CB	2.50	0.53
1:F:71:GLN:CG	3:F:401:HOH:O	2.31	0.53
1:F:189:GLU:HG2	1:F:191:ILE:HD13	1.89	0.53
1:G:46:ILE:O	1:G:47:LYS:C	2.51	0.53
1:G:291:LEU:O	1:G:293:LYS:HG3	2.08	0.53
1:J:190:VAL:H	1:J:231:ASN:ND2	2.04	0.53
1:J:342:TYR:OH	1:J:345:THR:N	2.41	0.53
1:K:357:PHE:C	1:K:357:PHE:CD1	2.83	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:279:ALA:HB1	1:M:301:TYR:CE1	2.43	0.53
1:N:319:ASN:O	1:N:320:LYS:C	2.50	0.53
1:O:313:TRP:CE2	1:O:315:GLY:HA2	2.43	0.53
1:B:115:LEU:O	1:B:118:THR:HB	2.08	0.53
1:G:267:ILE:HG12	1:G:297:LEU:HD23	1.91	0.53
1:H:51:THR:O	1:H:52:GLU:C	2.48	0.53
1:H:124:ILE:CD1	3:H:426:HOH:O	2.56	0.53
1:H:276:GLU:H	1:H:352:SER:CB	2.22	0.53
1:H:329:LYS:HD2	1:H:347:SER:CB	2.38	0.53
1:I:277:GLU:HG3	1:I:281:LEU:HD11	1.91	0.53
1:J:2:HIS:O	1:J:3:ARG:O	2.26	0.53
1:N:224:GLU:OE2	1:O:258:ARG:HD3	2.09	0.53
1:A:244:THR:HG23	1:A:246:GLU:H	1.71	0.53
1:B:97:LEU:O	1:B:98:LYS:C	2.51	0.53
1:C:128:ASP:OD1	1:D:126:GLY:N	2.40	0.53
1:D:91:LYS:HG2	1:D:96:ILE:HG13	1.90	0.53
1:K:206:GLU:HG2	1:K:255:ALA:HA	1.90	0.53
1:L:13:LYS:O	1:L:17:GLU:HG3	2.08	0.53
1:A:95:ASN:O	1:A:99:GLU:HG3	2.09	0.53
1:B:66:ASP:OD1	1:B:66:ASP:C	2.52	0.53
1:C:301:TYR:HB3	1:C:304:ALA:HB3	1.91	0.53
1:D:67:SER:O	1:D:69:ILE:N	2.42	0.53
1:E:91:LYS:HD3	1:E:96:ILE:HG12	1.90	0.53
1:J:348:SER:OG	1:J:349:GLY:N	2.41	0.53
1:M:25:ASN:H	1:M:27:LYS:HG3	1.74	0.53
1:P:123:THR:CG2	1:P:124:ILE:H	2.12	0.53
1:B:245:PRO:HA	1:B:282:ASN:OD1	2.08	0.53
1:C:2:HIS:CD2	1:C:3:ARG:NH1	2.76	0.53
1:C:115:LEU:O	1:C:118:THR:HB	2.09	0.53
1:E:349:GLY:O	1:E:351:ALA:N	2.42	0.53
1:F:330:ARG:HE	1:F:347:SER:HB2	1.74	0.53
1:H:123:THR:HG23	1:H:165:GLU:HG3	1.91	0.53
1:H:354:GLN:HG2	1:H:356:LEU:HD21	1.89	0.53
1:L:244:THR:CG2	1:L:244:THR:O	2.56	0.53
1:P:345:THR:HG22	1:P:346:GLY:N	2.23	0.53
1:R:50:ASN:ND2	1:R:55:ARG:HH11	2.07	0.53
1:R:271:SER:CA	1:R:274:MET:HE3	2.38	0.53
1:E:172:ARG:NH2	1:E:176:ILE:HD11	2.23	0.53
1:G:313:TRP:CD2	1:G:315:GLY:HA2	2.43	0.53
1:I:66:ASP:O	1:I:67:SER:HB3	2.07	0.53
1:J:160:SER:O	1:J:164:GLN:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:124:ILE:HG22	1:M:147:TRP:CZ2	2.44	0.53
1:O:66:ASP:O	1:O:67:SER:C	2.50	0.53
1:P:354:GLN:O	1:P:355:SER:CB	2.56	0.53
1:Q:276:GLU:HB3	1:Q:330:ARG:HD3	1.90	0.53
1:R:198:LEU:CD1	1:R:234:THR:HA	2.39	0.53
1:A:294:PRO:HG2	1:A:295:TRP:CE2	2.43	0.53
1:B:3:ARG:O	1:B:4:PHE:C	2.51	0.53
1:B:65:VAL:CG2	1:B:324:GLN:HB3	2.39	0.53
1:B:228:LEU:O	1:B:267:ILE:HA	2.09	0.53
1:C:64:SER:O	1:C:65:VAL:C	2.51	0.53
1:E:68:SER:O	1:E:71:GLN:HB2	2.09	0.53
1:H:68:SER:O	1:H:71:GLN:HB2	2.09	0.53
1:I:41:ASN:O	1:I:44:GLN:HB3	2.08	0.53
1:J:199:GLU:HB2	3:J:534:HOH:O	2.09	0.53
1:K:22:ILE:HG22	1:K:22:ILE:O	2.08	0.53
1:M:123:THR:C	1:M:124:ILE:HD13	2.34	0.53
1:Q:291:LEU:O	1:Q:293:LYS:HG3	2.09	0.53
1:R:87:ASP:O	1:R:89:GLN:N	2.36	0.53
1:R:121:GLU:OE1	1:R:159:SER:HB3	2.09	0.53
1:C:244:THR:CG2	1:C:244:THR:O	2.57	0.53
1:D:189:GLU:CG	1:D:191:ILE:HD11	2.38	0.53
1:E:271:SER:CA	1:E:274:MET:CE	2.86	0.53
1:G:250:MET:HE1	1:G:291:LEU:HD21	1.91	0.53
1:H:250:MET:HE1	1:H:291:LEU:CD2	2.38	0.53
1:I:187:GLU:HG3	1:I:229:LYS:O	2.08	0.53
1:L:3:ARG:O	1:L:4:PHE:C	2.51	0.53
1:L:14:GLU:OE2	1:L:138:LYS:NZ	2.36	0.53
1:Q:137:TYR:O	1:Q:138:LYS:C	2.50	0.53
1:A:229:LYS:HG3	1:A:268:CYS:O	2.09	0.53
1:G:156:GLN:HB3	1:H:1:ALA:CA	2.39	0.53
1:M:137:TYR:O	1:M:138:LYS:C	2.51	0.53
1:N:313:TRP:CD2	1:N:315:GLY:CA	2.92	0.53
1:Q:92:LEU:O	1:Q:93:PHE:C	2.50	0.53
1:Q:148:ARG:HD2	3:Q:2008:HOH:O	2.09	0.53
1:R:65:VAL:HB	1:R:328:MET:HE1	1.90	0.53
1:B:89:GLN:C	1:B:91:LYS:N	2.67	0.52
1:F:12:LYS:HE2	1:F:222:TYR:CD1	2.44	0.52
1:K:212:VAL:O	1:K:215:ALA:HB3	2.09	0.52
1:L:62:LEU:O	1:L:65:VAL:HG13	2.09	0.52
1:M:198:LEU:CD1	1:M:234:THR:HA	2.39	0.52
1:P:150:VAL:HG13	1:P:191:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:271:SER:HA	1:Q:274:MET:CE	2.33	0.52
1:B:207:LYS:NZ	1:C:2:HIS:NE2	2.58	0.52
1:D:80:HIS:CD2	1:D:137:TYR:OH	2.62	0.52
1:D:271:SER:HB3	1:D:301:TYR:CD2	2.44	0.52
1:E:282:ASN:O	1:E:286:ILE:HG13	2.10	0.52
1:J:119:ASN:O	1:J:152:ARG:NH1	2.39	0.52
1:M:156:GLN:OE1	1:N:2:HIS:HB3	2.09	0.52
1:M:352:SER:HA	1:M:354:GLN:CB	2.40	0.52
1:R:254:THR:O	1:R:258:ARG:HG2	2.09	0.52
1:B:22:ILE:O	1:B:22:ILE:CG2	2.57	0.52
1:H:226:THR:HG21	3:H:421:HOH:O	2.06	0.52
1:I:119:ASN:HB2	1:J:4:PHE:CZ	2.44	0.52
1:J:330:ARG:NH1	1:J:347:SER:N	2.54	0.52
1:K:313:TRP:CE2	1:K:315:GLY:HA2	2.44	0.52
1:P:190:VAL:H	1:P:231:ASN:ND2	2.07	0.52
1:Q:275:SER:OG	1:Q:278:ASP:HB2	2.09	0.52
1:B:50:ASN:HD21	1:B:55:ARG:HH11	1.56	0.52
1:B:79:PHE:O	1:B:80:HIS:C	2.49	0.52
1:B:198:LEU:HD21	1:B:251:ALA:HB2	1.90	0.52
1:B:204:VAL:O	1:B:208:VAL:HG23	2.10	0.52
1:G:313:TRP:CH2	1:G:315:GLY:HA2	2.45	0.52
1:H:224:GLU:OE1	1:H:224:GLU:N	2.34	0.52
1:J:319:ASN:O	1:J:320:LYS:C	2.53	0.52
1:M:44:GLN:OE1	1:M:44:GLN:HA	2.09	0.52
1:D:121:GLU:OE1	1:D:159:SER:HB3	2.09	0.52
1:E:118:THR:CG2	1:E:121:GLU:H	2.21	0.52
1:F:276:GLU:HG3	1:F:352:SER:CB	2.40	0.52
1:H:191:ILE:N	1:H:191:ILE:CD1	2.71	0.52
1:K:191:ILE:HD13	1:K:192:PRO:HD2	1.91	0.52
1:K:347:SER:OG	1:K:348:SER:HA	2.08	0.52
1:L:65:VAL:O	1:L:100:LYS:NZ	2.33	0.52
1:Q:233:VAL:CG2	1:Q:252:THR:HA	2.40	0.52
1:A:147:TRP:HB2	1:A:173:TYR:CZ	2.45	0.52
1:A:199:GLU:HB2	3:A:566:HOH:O	2.08	0.52
1:G:80:HIS:HD2	1:G:137:TYR:OH	1.92	0.52
1:H:354:GLN:CG	1:H:356:LEU:HD23	2.39	0.52
1:I:12:LYS:HG2	1:I:222:TYR:CE2	2.44	0.52
1:N:42:ARG:CZ	1:N:303:ARG:HD3	2.40	0.52
1:O:106:ILE:HG22	1:O:142:VAL:HG11	1.91	0.52
1:O:155:ASP:O	1:O:156:GLN:HB2	2.10	0.52
1:A:91:LYS:HD3	1:A:96:ILE:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:LYS:NZ	1:F:99:GLU:OE1	2.42	0.52
1:F:231:ASN:ND2	1:F:231:ASN:H	2.06	0.52
1:I:119:ASN:N	1:J:1:ALA:H3	2.06	0.52
1:N:80:HIS:CD2	1:N:137:TYR:OH	2.59	0.52
1:O:172:ARG:HD2	3:O:510:HOH:O	2.09	0.52
1:R:33:ASP:O	1:R:107:LYS:HE2	2.10	0.52
1:B:179:GLN:HG2	3:B:403:HOH:O	2.09	0.52
1:C:161:LEU:O	1:C:162:ALA:C	2.52	0.52
1:F:344:HIS:CG	1:F:345:THR:H	2.28	0.52
1:G:275:SER:OG	1:G:278:ASP:HB2	2.10	0.52
1:K:190:VAL:H	1:K:231:ASN:ND2	2.08	0.52
1:L:27:LYS:HG2	1:L:72:SER:O	2.10	0.52
1:N:52:GLU:HB2	1:N:55:ARG:NH2	2.25	0.52
1:N:231:ASN:ND2	1:N:231:ASN:H	2.07	0.52
1:N:250:MET:CE	1:N:291:LEU:HD21	2.40	0.52
1:O:3:ARG:CG	1:O:4:PHE:H	2.12	0.52
1:O:76:VAL:HG23	1:O:102:ILE:HG21	1.92	0.52
1:P:3:ARG:CD	1:P:4:PHE:N	2.66	0.52
1:P:45:ARG:NH1	1:P:356:LEU:HA	2.24	0.52
1:P:150:VAL:CG1	1:P:191:ILE:HG13	2.39	0.52
1:R:58:PHE:CE2	1:R:310:LEU:HD13	2.44	0.52
1:R:70:ASN:ND2	1:R:100:LYS:O	2.41	0.52
1:B:67:SER:C	1:B:68:SER:O	2.52	0.52
1:B:207:LYS:HZ3	1:C:2:HIS:CD2	2.28	0.52
1:B:291:LEU:HB3	1:B:292:PRO:CD	2.40	0.52
1:C:30:LEU:HD12	1:C:31:ALA:N	2.24	0.52
1:H:271:SER:HA	1:H:274:MET:CE	2.40	0.52
1:K:79:PHE:O	1:K:80:HIS:C	2.52	0.52
1:L:78:LEU:N	1:L:105:GLY:O	2.33	0.52
1:N:105:GLY:HA2	1:N:142:VAL:HG13	1.91	0.52
1:N:313:TRP:CD2	1:N:315:GLY:N	2.77	0.52
1:P:276:GLU:H	1:P:352:SER:CB	2.23	0.52
1:Q:112:GLY:HA2	1:Q:123:THR:O	2.09	0.52
1:A:187:GLU:HG2	1:A:187:GLU:O	2.09	0.52
1:G:126:GLY:H	1:H:128:ASP:CG	2.18	0.52
1:H:67:SER:O	1:H:70:ASN:HB2	2.10	0.52
1:I:118:THR:CB	1:J:1:ALA:N	2.73	0.52
1:I:263:ALA:HA	1:L:257:HIS:CD2	2.44	0.52
1:O:118:THR:HG23	1:O:121:GLU:HB2	1.91	0.52
1:A:8:THR:OG1	1:A:11:GLN:HG3	2.10	0.51
1:A:128:ASP:N	1:B:128:ASP:OD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:GLU:HG2	1:F:187:GLU:O	2.10	0.51
1:G:119:ASN:N	1:H:1:ALA:N	2.48	0.51
1:H:281:LEU:CD2	1:H:344:HIS:CE1	2.93	0.51
1:H:350:ALA:O	1:H:354:GLN:HB2	2.09	0.51
1:O:276:GLU:HB3	3:O:504:HOH:O	2.10	0.51
1:O:329:LYS:O	1:O:330:ARG:C	2.52	0.51
1:Q:231:ASN:HA	1:Q:270:LEU:HG	1.92	0.51
1:C:232:MET:HG2	1:C:286:ILE:HD11	1.91	0.51
1:E:250:MET:HE3	1:E:291:LEU:CD2	2.35	0.51
1:I:51:THR:CG2	1:I:53:GLU:N	2.62	0.51
1:I:51:THR:HG21	1:I:53:GLU:HB3	1.92	0.51
1:I:63:PHE:HB3	1:I:97:LEU:HD21	1.92	0.51
1:J:279:ALA:HB1	1:J:301:TYR:CE1	2.45	0.51
1:O:244:THR:HG23	1:O:246:GLU:OE1	2.10	0.51
1:P:298:SER:OG	1:P:299:PHE:N	2.43	0.51
1:A:45:ARG:NH2	1:A:358:THR:N	2.51	0.51
1:A:45:ARG:HH12	1:A:356:LEU:HA	1.75	0.51
1:B:198:LEU:CD1	1:B:234:THR:HA	2.40	0.51
1:C:285:ALA:O	1:C:286:ILE:C	2.53	0.51
1:E:244:THR:CG2	1:E:247:GLN:HG3	2.40	0.51
1:E:303:ARG:CG	1:E:303:ARG:NH1	2.73	0.51
1:F:226:THR:CG2	3:F:449:HOH:O	2.51	0.51
1:I:39:MET:O	1:I:40:GLY:C	2.53	0.51
1:I:189:GLU:HG3	1:I:270:LEU:CD2	2.40	0.51
1:K:123:THR:CG2	1:K:124:ILE:H	2.13	0.51
1:Q:313:TRP:CH2	1:Q:315:GLY:HA2	2.44	0.51
1:A:203:TYR:CE2	1:D:2:HIS:HD2	2.16	0.51
1:B:207:LYS:NZ	1:C:2:HIS:CD2	2.78	0.51
1:G:156:GLN:HB3	1:H:1:ALA:CB	2.41	0.51
1:H:276:GLU:CB	1:H:352:SER:HB3	2.40	0.51
1:K:244:THR:HG23	1:K:246:GLU:H	1.76	0.51
1:N:65:VAL:O	1:N:66:ASP:C	2.52	0.51
1:O:81:GLU:HG2	1:O:82:THR:N	2.25	0.51
1:O:231:ASN:ND2	1:O:231:ASN:H	2.08	0.51
1:Q:276:GLU:OE1	1:Q:308:SER:OG	2.19	0.51
1:R:173:TYR:CE1	1:R:177:CYS:SG	3.03	0.51
1:A:303:ARG:CB	1:A:357:PHE:HD1	2.24	0.51
1:B:56:ARG:HD2	1:B:86:LYS:O	2.11	0.51
1:C:237:HIS:ND1	3:C:403:HOH:O	2.34	0.51
1:E:148:ARG:NH1	1:E:189:GLU:OE1	2.42	0.51
1:E:271:SER:HB2	1:E:274:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:GLN:O	1:G:45:ARG:C	2.52	0.51
1:G:200:HIS:HB2	3:G:563:HOH:O	2.10	0.51
1:I:125:GLN:HE22	1:J:129:GLY:H	1.57	0.51
1:K:119:ASN:O	1:K:152:ARG:NH1	2.43	0.51
1:O:321:GLU:O	1:O:322:ALA:C	2.53	0.51
1:Q:123:THR:HG21	1:Q:165:GLU:OE2	2.11	0.51
1:Q:187:GLU:HG2	1:Q:187:GLU:O	2.10	0.51
1:A:67:SER:C	1:A:69:ILE:H	2.17	0.51
1:C:298:SER:OG	1:C:299:PHE:N	2.44	0.51
1:D:70:ASN:C	1:D:70:ASN:HB3	2.00	0.51
1:D:190:VAL:H	1:D:231:ASN:HD22	1.58	0.51
1:K:357:PHE:O	1:O:139:LYS:CE	2.55	0.51
1:L:61:ILE:HG22	1:L:324:GLN:HG2	1.93	0.51
1:M:277:GLU:O	1:M:278:ASP:C	2.50	0.51
1:O:244:THR:HG22	1:O:247:GLN:HG3	1.91	0.51
1:P:38:THR:HG23	1:P:358:THR:HG21	1.92	0.51
1:Q:161:LEU:O	1:Q:165:GLU:HB3	2.11	0.51
1:A:147:TRP:HB2	1:A:173:TYR:CE1	2.45	0.51
1:A:343:VAL:O	1:A:343:VAL:HG12	2.08	0.51
1:A:345:THR:O	1:A:346:GLY:C	2.50	0.51
1:C:80:HIS:HD2	1:C:137:TYR:OH	1.94	0.51
1:E:303:ARG:HG3	1:E:303:ARG:NH1	2.23	0.51
1:H:45:ARG:HH12	1:H:356:LEU:HA	1.74	0.51
1:H:121:GLU:OE2	1:H:158:PRO:HA	2.09	0.51
1:I:51:THR:HG22	1:I:54:ASN:N	2.25	0.51
1:M:115:LEU:HD22	1:M:122:THR:C	2.36	0.51
1:M:156:GLN:CD	1:N:2:HIS:HB3	2.36	0.51
1:Q:217:ASN:ND2	3:Q:2002:HOH:O	2.43	0.51
1:E:1:ALA:HA	1:E:220:HIS:CE1	2.46	0.51
1:F:108:LEU:HD22	1:F:130:LEU:HD11	1.92	0.51
1:H:284:ASN:HB2	1:H:337:ALA:HB1	1.92	0.51
1:H:354:GLN:CG	1:H:356:LEU:CD2	2.88	0.51
1:I:53:GLU:O	1:I:57:GLN:HB2	2.11	0.51
1:I:105:GLY:HA2	1:I:142:VAL:HG13	1.93	0.51
1:I:313:TRP:CE2	1:I:315:GLY:CA	2.91	0.51
1:L:94:ARG:NH1	1:L:140:ASP:HB3	2.26	0.51
1:M:118:THR:CG2	1:M:121:GLU:N	2.63	0.51
1:R:244:THR:HG23	1:R:246:GLU:N	2.26	0.51
1:A:45:ARG:NH2	1:A:357:PHE:HA	2.20	0.51
1:C:124:ILE:CG2	1:C:147:TRP:CZ2	2.94	0.51
1:C:313:TRP:CD2	1:C:315:GLY:HA2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:HIS:HD2	1:D:137:TYR:OH	1.94	0.51
1:E:2:HIS:O	1:E:4:PHE:CD1	2.63	0.51
1:G:146:LYS:HG2	1:G:147:TRP:N	2.26	0.51
1:I:244:THR:CG2	1:I:244:THR:O	2.59	0.51
1:I:244:THR:O	1:I:247:GLN:N	2.41	0.51
1:K:50:ASN:HD21	1:K:55:ARG:HH11	1.56	0.51
1:M:345:THR:HB	1:M:347:SER:OG	2.11	0.51
1:O:179:GLN:HG2	3:O:502:HOH:O	2.11	0.51
1:D:270:LEU:C	1:D:270:LEU:HD12	2.36	0.51
1:E:28:GLY:HA3	1:E:299:PHE:CE1	2.46	0.51
1:F:256:LEU:CD1	1:F:267:ILE:CD1	2.89	0.51
1:F:306:GLN:HA	3:F:414:HOH:O	2.11	0.51
1:G:18:ILE:CD1	1:G:143:ASP:HB3	2.35	0.51
1:H:284:ASN:HB2	1:H:337:ALA:CB	2.41	0.51
1:I:244:THR:CG2	1:I:247:GLN:N	2.74	0.51
1:L:146:LYS:HB2	1:L:185:ILE:HB	1.93	0.51
1:M:43:LEU:O	1:M:44:GLN:C	2.52	0.51
1:N:83:LEU:HD23	1:N:84:TYR:CZ	2.45	0.51
1:N:189:GLU:CG	1:N:191:ILE:HD12	2.40	0.51
1:P:244:THR:HG23	1:P:246:GLU:N	2.26	0.51
1:R:202:GLN:HB2	1:R:233:VAL:HG11	1.92	0.51
1:F:124:ILE:HD13	1:F:149:ALA:HA	1.93	0.50
1:I:272:GLY:HA2	1:I:303:ARG:HH12	1.76	0.50
1:L:52:GLU:HA	1:L:55:ARG:NH2	2.26	0.50
1:L:190:VAL:HB	1:L:231:ASN:ND2	2.26	0.50
1:L:284:ASN:O	1:L:285:ALA:C	2.54	0.50
1:A:244:THR:O	1:A:247:GLN:N	2.44	0.50
1:B:56:ARG:HB2	1:B:85:GLN:NE2	2.26	0.50
1:E:25:ASN:H	1:E:27:LYS:H	1.58	0.50
1:E:25:ASN:H	1:E:27:LYS:HG3	1.76	0.50
1:H:189:GLU:HG2	1:H:191:ILE:CD1	2.40	0.50
1:H:229:LYS:HA	1:H:268:CYS:O	2.10	0.50
1:J:94:ARG:HD3	1:J:140:ASP:O	2.11	0.50
1:L:256:LEU:HD22	1:L:267:ILE:CD1	2.42	0.50
1:L:256:LEU:HD22	1:L:267:ILE:HD12	1.92	0.50
1:L:283:LEU:HD11	1:L:297:LEU:O	2.11	0.50
1:O:1:ALA:O	1:O:2:HIS:HB2	2.11	0.50
1:O:215:ALA:O	1:O:218:ASP:HB2	2.11	0.50
1:O:336:GLN:HA	1:O:339:LYS:HD2	1.93	0.50
1:R:343:VAL:O	1:R:344:HIS:CB	2.58	0.50
1:B:65:VAL:HG13	1:B:66:ASP:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:GLU:OE2	1:B:307:ALA:HB3	2.11	0.50
1:D:86:LYS:HB3	1:D:90:GLY:HA2	1.93	0.50
1:D:119:ASN:O	1:D:120:LYS:HB2	2.10	0.50
1:D:155:ASP:O	1:D:156:GLN:HB2	2.10	0.50
1:D:233:VAL:N	1:D:252:THR:OG1	2.32	0.50
1:F:109:ASP:HA	1:F:147:TRP:CE3	2.47	0.50
1:F:213:TYR:OH	1:F:228:LEU:HD13	2.11	0.50
1:H:8:THR:HB	1:H:11:GLN:HG3	1.93	0.50
1:I:76:VAL:HG23	1:I:102:ILE:HG21	1.92	0.50
1:I:128:ASP:OD2	1:J:128:ASP:N	2.39	0.50
1:L:245:PRO:O	1:L:249:ALA:N	2.40	0.50
1:N:51:THR:HG22	1:N:53:GLU:N	2.27	0.50
1:P:119:ASN:O	1:P:119:ASN:CG	2.53	0.50
1:R:127:LEU:O	1:R:128:ASP:C	2.51	0.50
1:R:344:HIS:CD2	3:R:566:HOH:O	2.64	0.50
1:D:87:ASP:CB	1:D:89:GLN:O	2.59	0.50
1:E:51:THR:O	1:E:52:GLU:C	2.53	0.50
1:H:58:PHE:CE2	1:H:310:LEU:HD13	2.46	0.50
1:H:276:GLU:HB2	1:H:352:SER:HB3	1.93	0.50
1:H:313:TRP:CE2	1:H:315:GLY:HA2	2.47	0.50
1:I:36:VAL:HG13	1:I:55:ARG:CZ	2.42	0.50
1:I:326:ALA:O	1:I:327:PHE:C	2.49	0.50
1:J:271:SER:HB3	1:J:301:TYR:CD2	2.46	0.50
1:M:1:ALA:H2	1:N:118:THR:CB	2.23	0.50
1:P:232:MET:SD	1:P:274:MET:HE1	2.51	0.50
1:P:276:GLU:HG3	1:P:352:SER:CB	2.40	0.50
1:R:51:THR:CG2	1:R:54:ASN:H	1.99	0.50
1:A:50:ASN:ND2	1:A:50:ASN:C	2.67	0.50
1:A:207:LYS:CE	1:D:2:HIS:HE2	2.24	0.50
1:B:70:ASN:C	1:B:70:ASN:OD1	2.55	0.50
1:C:118:THR:HG22	1:C:121:GLU:H	1.70	0.50
1:D:276:GLU:OE2	1:D:307:ALA:HB3	2.11	0.50
1:H:158:PRO:O	1:H:158:PRO:HG2	2.12	0.50
1:I:46:ILE:HG13	1:I:48:VAL:HG23	1.94	0.50
1:I:211:ALA:O	1:I:212:VAL:C	2.52	0.50
1:J:313:TRP:CZ2	1:J:315:GLY:HA2	2.47	0.50
1:K:156:GLN:NE2	1:L:3:ARG:NE	2.59	0.50
1:L:118:THR:CG2	1:L:121:GLU:HB2	2.41	0.50
1:L:256:LEU:O	1:L:257:HIS:C	2.45	0.50
1:M:80:HIS:CD2	1:M:137:TYR:OH	2.64	0.50
1:R:44:GLN:OE1	1:R:44:GLN:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ILE:HG22	1:C:185:ILE:O	2.11	0.50
1:C:282:ASN:O	1:C:286:ILE:HG13	2.11	0.50
1:G:271:SER:HA	1:G:274:MET:HE3	1.93	0.50
1:H:250:MET:HE1	1:H:291:LEU:HD22	1.92	0.50
1:I:128:ASP:OD1	1:J:126:GLY:N	2.41	0.50
1:I:274:MET:CE	1:I:279:ALA:HA	2.42	0.50
1:I:337:ALA:C	1:I:339:LYS:N	2.68	0.50
1:M:3:ARG:NH1	1:N:156:GLN:HE21	2.06	0.50
1:O:196:HIS:O	1:O:239:CYS:HB2	2.11	0.50
1:Q:80:HIS:HD2	1:Q:137:TYR:OH	1.94	0.50
1:Q:147:TRP:HB3	1:Q:173:TYR:CE2	2.46	0.50
1:R:275:SER:O	1:R:276:GLU:C	2.52	0.50
1:A:313:TRP:CD2	1:A:315:GLY:HA2	2.46	0.50
1:C:189:GLU:CD	1:C:191:ILE:CD1	2.85	0.50
1:D:2:HIS:O	1:D:4:PHE:CD1	2.61	0.50
1:J:121:GLU:OE2	1:J:158:PRO:HA	2.12	0.50
1:O:220:HIS:CE1	3:O:528:HOH:O	2.56	0.50
1:O:244:THR:HB	1:O:247:GLN:OE1	2.11	0.50
1:Q:217:ASN:ND2	1:Q:217:ASN:C	2.70	0.50
1:A:79:PHE:O	1:A:80:HIS:C	2.52	0.50
1:A:121:GLU:OE2	1:A:158:PRO:HA	2.12	0.50
1:A:303:ARG:HB3	1:A:356:LEU:HD13	1.94	0.50
1:D:60:GLU:HB2	1:D:93:PHE:CE1	2.47	0.50
1:D:105:GLY:HA2	1:D:144:PHE:O	2.12	0.50
1:E:190:VAL:HB	1:E:231:ASN:ND2	2.26	0.50
1:I:75:GLY:HA2	1:I:103:VAL:O	2.12	0.50
1:N:299:PHE:CD1	1:N:299:PHE:N	2.78	0.50
1:B:132:GLU:O	1:B:133:ARG:C	2.50	0.50
1:F:343:VAL:O	1:F:344:HIS:C	2.55	0.50
1:K:222:TYR:O	1:K:223:LEU:C	2.54	0.50
1:N:61:ILE:HG22	1:N:324:GLN:HG2	1.92	0.50
1:O:79:PHE:O	1:O:80:HIS:C	2.55	0.50
1:A:222:TYR:CZ	1:A:224:GLU:HB2	2.47	0.49
1:B:343:VAL:O	1:B:345:THR:N	2.45	0.49
1:F:123:THR:CG2	1:F:165:GLU:CG	2.90	0.49
1:F:250:MET:HE3	1:F:291:LEU:HD21	1.93	0.49
1:G:3:ARG:HD2	3:G:574:HOH:O	2.12	0.49
1:G:249:ALA:HB1	1:G:286:ILE:HA	1.93	0.49
1:H:250:MET:HE3	1:H:291:LEU:HD22	1.92	0.49
1:J:161:LEU:O	1:J:165:GLU:HB3	2.12	0.49
1:K:123:THR:HG23	1:K:165:GLU:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:66:ASP:O	1:L:67:SER:C	2.53	0.49
1:M:65:VAL:CG1	1:M:328:MET:SD	3.00	0.49
1:P:303:ARG:NE	1:P:356:LEU:O	2.41	0.49
1:R:172:ARG:O	1:R:176:ILE:HG13	2.12	0.49
1:A:2:HIS:CB	1:A:3:ARG:HD2	2.22	0.49
1:A:303:ARG:HB3	1:A:357:PHE:HD1	1.77	0.49
1:C:244:THR:CG2	1:C:247:GLN:N	2.74	0.49
1:C:277:GLU:O	1:C:281:LEU:HG	2.11	0.49
1:I:38:THR:O	1:I:39:MET:C	2.55	0.49
1:I:226:THR:CG2	3:I:423:HOH:O	2.48	0.49
1:K:119:ASN:C	1:K:119:ASN:OD1	2.48	0.49
1:M:123:THR:HG22	1:M:124:ILE:N	2.19	0.49
1:N:244:THR:N	1:N:247:GLN:OE1	2.45	0.49
1:O:58:PHE:CE1	1:O:310:LEU:CD1	2.92	0.49
1:O:75:GLY:HA2	1:O:103:VAL:O	2.12	0.49
1:O:80:HIS:HD2	1:O:137:TYR:OH	1.95	0.49
1:O:198:LEU:CD1	1:O:234:THR:HA	2.43	0.49
1:R:214:LYS:HE3	1:R:218:ASP:OD1	2.12	0.49
1:C:1:ALA:HB1	1:C:4:PHE:HD1	1.77	0.49
1:E:123:THR:CG2	1:E:165:GLU:HG3	2.42	0.49
1:E:313:TRP:CZ2	1:E:315:GLY:HA2	2.47	0.49
1:F:123:THR:HG23	1:F:165:GLU:HG3	1.95	0.49
1:G:3:ARG:HG2	1:G:3:ARG:NH1	2.23	0.49
1:G:3:ARG:HE	1:H:156:GLN:HE21	1.59	0.49
1:H:106:ILE:O	1:H:106:ILE:HG23	2.11	0.49
1:O:244:THR:O	1:O:245:PRO:C	2.56	0.49
1:R:10:GLU:OE1	3:R:501:HOH:O	2.17	0.49
1:A:33:ASP:O	1:A:107:LYS:HE3	2.12	0.49
1:A:66:ASP:OD1	1:A:67:SER:HB2	2.12	0.49
1:B:44:GLN:O	1:B:45:ARG:C	2.53	0.49
1:B:95:ASN:O	1:B:96:ILE:C	2.54	0.49
1:B:333:ALA:O	1:B:336:GLN:HB2	2.13	0.49
1:C:232:MET:HG2	1:C:286:ILE:CD1	2.42	0.49
1:D:329:LYS:HE2	1:D:347:SER:N	2.27	0.49
1:H:220:HIS:CE1	3:H:407:HOH:O	2.62	0.49
1:H:349:GLY:HA2	1:H:353:THR:HG23	1.94	0.49
1:H:351:ALA:O	1:H:352:SER:HB2	2.12	0.49
1:J:231:ASN:ND2	1:J:231:ASN:H	2.11	0.49
1:J:329:LYS:HE2	1:J:346:GLY:O	2.11	0.49
1:K:12:LYS:O	1:K:13:LYS:C	2.52	0.49
1:K:154:ALA:O	1:K:155:ASP:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:ASP:OD1	1:L:156:GLN:HG3	2.12	0.49
1:M:342:TYR:OH	1:M:345:THR:OG1	2.28	0.49
1:P:115:LEU:O	1:P:118:THR:HB	2.13	0.49
1:Q:9:GLN:HG2	3:Q:2031:HOH:O	2.12	0.49
1:R:123:THR:HG23	1:R:165:GLU:HG3	1.94	0.49
1:B:66:ASP:O	1:B:68:SER:HB3	2.11	0.49
1:H:66:ASP:O	1:H:66:ASP:OD1	2.30	0.49
1:I:156:GLN:NE2	1:J:4:PHE:HE1	2.10	0.49
1:J:66:ASP:OD1	1:J:68:SER:HB2	2.13	0.49
1:K:276:GLU:HB3	1:K:330:ARG:HH11	1.78	0.49
1:L:282:ASN:O	1:L:286:ILE:HG13	2.12	0.49
1:N:3:ARG:NH1	1:O:203:TYR:CE2	2.80	0.49
1:N:9:GLN:CD	3:N:401:HOH:O	2.51	0.49
1:O:94:ARG:O	1:O:98:LYS:HB2	2.12	0.49
1:B:69:ILE:O	1:B:71:GLN:N	2.46	0.49
1:B:244:THR:HG23	1:B:247:GLN:H	1.70	0.49
1:C:80:HIS:CD2	1:C:137:TYR:OH	2.65	0.49
1:C:229:LYS:HG3	1:C:268:CYS:O	2.13	0.49
1:H:276:GLU:OE1	1:H:330:ARG:HD3	2.12	0.49
1:K:33:ASP:OD1	1:K:33:ASP:N	2.45	0.49
1:L:51:THR:CG2	1:L:54:ASN:N	2.59	0.49
1:M:189:GLU:CD	1:M:191:ILE:HD13	2.37	0.49
1:M:271:SER:HA	1:M:274:MET:HE3	1.95	0.49
1:P:51:THR:HG22	1:P:54:ASN:CB	2.43	0.49
1:A:51:THR:HG22	1:A:53:GLU:N	2.28	0.49
1:J:29:ILE:HB	1:J:300:SER:HA	1.94	0.49
1:K:65:VAL:HG12	1:K:324:GLN:HB3	1.94	0.49
1:K:119:ASN:HB2	1:L:4:PHE:CE1	2.48	0.49
1:K:229:LYS:HA	1:K:268:CYS:O	2.11	0.49
1:N:25:ASN:H	1:N:27:LYS:HG3	1.78	0.49
1:N:91:LYS:NZ	1:N:99:GLU:OE1	2.45	0.49
1:O:343:VAL:O	1:O:344:HIS:CG	2.66	0.49
1:R:257:HIS:HD2	1:R:292:PRO:HD2	1.73	0.49
1:A:8:THR:N	1:A:11:GLN:OE1	2.37	0.49
1:C:35:SER:O	1:C:36:VAL:C	2.55	0.49
1:D:293:LYS:HA	1:D:295:TRP:CZ3	2.47	0.49
1:G:3:ARG:CG	1:G:3:ARG:NH1	2.73	0.49
1:G:119:ASN:C	1:G:119:ASN:OD1	2.53	0.49
1:G:226:THR:CG2	3:G:506:HOH:O	2.61	0.49
1:J:112:GLY:HA2	1:J:123:THR:O	2.13	0.49
1:J:316:LYS:O	1:J:317:ALA:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:344:HIS:ND1	1:K:346:GLY:N	2.61	0.49
1:L:48:VAL:HG12	1:L:54:ASN:ND2	2.26	0.49
1:C:29:ILE:HB	1:C:300:SER:HA	1.93	0.49
1:C:270:LEU:C	1:C:270:LEU:HD12	2.38	0.49
1:D:66:ASP:OD2	1:D:68:SER:HB2	2.13	0.49
1:E:80:HIS:HD2	1:E:137:TYR:OH	1.95	0.49
1:G:250:MET:HG2	1:G:289:CYS:SG	2.53	0.49
1:I:38:THR:O	1:I:41:ASN:N	2.46	0.49
1:I:250:MET:HE3	1:I:291:LEU:HD21	1.95	0.49
1:I:313:TRP:CH2	1:I:315:GLY:HA2	2.48	0.49
1:J:253:VAL:O	1:J:254:THR:C	2.55	0.49
1:J:329:LYS:CD	1:J:347:SER:HA	2.36	0.49
1:J:350:ALA:O	1:J:351:ALA:C	2.55	0.49
1:K:271:SER:O	1:K:274:MET:HE3	2.12	0.49
1:M:329:LYS:HE3	1:M:348:SER:H	1.78	0.49
1:M:329:LYS:NZ	1:M:348:SER:N	2.57	0.49
1:O:335:CYS:SG	1:O:339:LYS:HE2	2.53	0.49
1:P:123:THR:HG22	1:P:124:ILE:N	2.23	0.49
1:Q:50:ASN:ND2	1:Q:55:ARG:HD3	2.20	0.49
1:R:62:LEU:O	1:R:65:VAL:HG13	2.13	0.49
1:C:42:ARG:O	1:C:45:ARG:HB2	2.13	0.49
1:D:354:GLN:HG2	1:D:356:LEU:HD21	1.95	0.49
1:F:118:THR:HG21	1:F:121:GLU:HB2	1.91	0.49
1:G:2:HIS:HB3	1:H:156:GLN:CD	2.38	0.49
1:G:33:ASP:CB	1:G:77:ILE:HG22	2.42	0.49
1:G:65:VAL:O	1:G:66:ASP:CB	2.59	0.49
1:J:199:GLU:CB	3:J:534:HOH:O	2.61	0.49
1:K:133:ARG:HH11	1:K:133:ARG:HD3	1.02	0.49
1:L:160:SER:O	1:L:161:LEU:C	2.52	0.49
1:L:294:PRO:HD2	1:L:295:TRP:CE2	2.48	0.49
1:M:86:LYS:HD3	1:M:90:GLY:HA2	1.95	0.49
1:N:113:ALA:HB2	1:N:125:GLN:HE21	1.78	0.49
1:Q:244:THR:HG22	1:Q:247:GLN:CB	2.43	0.49
1:A:8:THR:HG23	1:A:11:GLN:OE1	2.13	0.48
1:B:69:ILE:C	1:B:71:GLN:H	2.21	0.48
1:B:271:SER:O	1:B:272:GLY:C	2.56	0.48
1:B:329:LYS:HZ1	1:B:348:SER:HA	1.78	0.48
1:C:244:THR:HG21	1:C:247:GLN:HG3	1.93	0.48
1:E:23:VAL:HG23	1:E:296:LYS:HG3	1.94	0.48
1:F:95:ASN:O	1:F:99:GLU:HG3	2.13	0.48
1:F:291:LEU:O	1:F:292:PRO:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:322:ALA:O	1:G:325:GLU:HB2	2.12	0.48
1:J:80:HIS:HD2	1:J:137:TYR:OH	1.95	0.48
1:N:244:THR:HG22	1:N:247:GLN:CB	2.42	0.48
1:N:254:THR:O	1:N:258:ARG:HG2	2.13	0.48
1:O:4:PHE:CE1	1:P:119:ASN:HB2	2.48	0.48
1:P:254:THR:O	1:P:258:ARG:HG2	2.13	0.48
1:Q:256:LEU:CD1	1:Q:267:ILE:HD11	2.43	0.48
1:R:51:THR:O	1:R:52:GLU:C	2.56	0.48
1:R:60:GLU:OE1	1:R:87:ASP:HB2	2.12	0.48
1:R:131:SER:HB2	3:R:554:HOH:O	2.12	0.48
1:A:3:ARG:CD	1:B:156:GLN:HE22	2.27	0.48
1:A:12:LYS:HG2	1:A:222:TYR:CZ	2.49	0.48
1:A:125:GLN:HE22	1:B:129:GLY:N	1.96	0.48
1:A:343:VAL:O	1:A:344:HIS:C	2.54	0.48
1:C:123:THR:CG2	1:C:124:ILE:N	2.72	0.48
1:D:146:LYS:HE2	1:D:187:GLU:OE1	2.12	0.48
1:D:160:SER:O	1:D:161:LEU:C	2.56	0.48
1:D:244:THR:CG2	1:D:246:GLU:HB2	2.44	0.48
1:D:343:VAL:CG1	1:D:344:HIS:N	2.76	0.48
1:F:256:LEU:HD13	1:F:267:ILE:HD13	1.96	0.48
1:F:276:GLU:HB2	1:F:352:SER:HB3	1.95	0.48
1:H:231:ASN:ND2	1:H:231:ASN:H	2.11	0.48
1:I:118:THR:CA	1:J:1:ALA:H2	2.15	0.48
1:J:124:ILE:HG22	1:J:147:TRP:CZ2	2.48	0.48
1:K:28:GLY:HA3	1:K:299:PHE:CZ	2.48	0.48
1:K:118:THR:HG23	1:K:121:GLU:H	1.77	0.48
1:K:144:PHE:HB2	1:K:183:VAL:O	2.12	0.48
1:L:313:TRP:HB2	1:L:323:THR:OG1	2.13	0.48
1:P:313:TRP:CG	1:P:315:GLY:H	2.32	0.48
1:A:66:ASP:OD1	1:A:67:SER:N	2.45	0.48
1:B:87:ASP:O	1:B:88:SER:CB	2.58	0.48
1:B:313:TRP:HB2	1:B:323:THR:OG1	2.13	0.48
1:E:244:THR:HG23	1:E:246:GLU:OE1	2.12	0.48
1:G:164:GLN:O	1:G:168:ASN:ND2	2.47	0.48
1:I:337:ALA:C	1:I:339:LYS:H	2.21	0.48
1:K:268:CYS:HB3	1:K:300:SER:HB2	1.96	0.48
1:M:329:LYS:HE3	1:M:348:SER:N	2.28	0.48
1:O:128:ASP:OD1	1:P:125:GLN:HB3	2.12	0.48
1:O:278:ASP:O	1:O:280:THR:N	2.47	0.48
1:Q:123:THR:HG23	1:Q:165:GLU:HG3	1.94	0.48
1:B:118:THR:CG2	1:B:121:GLU:N	2.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:THR:CG2	3:D:541:HOH:O	2.48	0.48
1:H:277:GLU:CG	1:H:345:THR:HG23	2.37	0.48
1:I:68:SER:O	1:I:70:ASN:ND2	2.46	0.48
1:O:1:ALA:CB	1:P:159:SER:HB3	2.44	0.48
1:C:244:THR:HG23	1:C:246:GLU:H	1.77	0.48
1:F:25:ASN:H	1:F:27:LYS:H	1.61	0.48
1:F:65:VAL:HG22	1:F:328:MET:SD	2.54	0.48
1:F:352:SER:HA	1:F:354:GLN:HB3	1.96	0.48
1:G:187:GLU:HG3	1:G:229:LYS:CG	2.42	0.48
1:H:276:GLU:CG	1:H:352:SER:HB3	2.43	0.48
1:H:350:ALA:HA	1:H:353:THR:OG1	2.13	0.48
1:K:229:LYS:HG3	1:K:268:CYS:O	2.12	0.48
1:K:291:LEU:O	1:K:293:LYS:HG3	2.14	0.48
1:L:66:ASP:O	1:L:68:SER:N	2.47	0.48
1:L:174:ALA:O	1:L:175:SER:C	2.53	0.48
1:O:187:GLU:HG3	1:O:229:LYS:HG2	1.95	0.48
1:P:290:PRO:C	1:P:291:LEU:HG	2.35	0.48
1:Q:334:ASN:O	1:Q:338:ALA:N	2.41	0.48
1:A:3:ARG:HD3	1:B:156:GLN:HE22	1.75	0.48
1:D:67:SER:O	1:D:70:ASN:N	2.44	0.48
1:E:352:SER:HA	1:E:354:GLN:H	1.79	0.48
1:G:32:ALA:HB1	3:G:510:HOH:O	2.13	0.48
1:G:137:TYR:O	1:G:138:LYS:C	2.53	0.48
1:H:354:GLN:HA	3:H:435:HOH:O	2.13	0.48
1:I:271:SER:HB3	1:I:301:TYR:CD2	2.48	0.48
1:L:58:PHE:CE2	1:L:62:LEU:HD21	2.49	0.48
1:M:303:ARG:HD2	1:M:356:LEU:CB	2.43	0.48
1:N:218:ASP:HA	3:N:403:HOH:O	2.13	0.48
1:O:144:PHE:HB2	1:O:183:VAL:O	2.14	0.48
1:P:291:LEU:HB3	1:P:292:PRO:HD2	1.96	0.48
1:R:50:ASN:HD21	1:R:55:ARG:HD3	1.77	0.48
1:R:250:MET:O	1:R:250:MET:HG3	2.12	0.48
1:A:6:ALA:O	1:A:7:LEU:HD23	2.13	0.48
1:A:163:ILE:O	1:A:164:GLN:C	2.57	0.48
1:C:87:ASP:OD2	1:C:91:LYS:HB3	2.13	0.48
1:F:51:THR:HG22	1:F:54:ASN:N	2.22	0.48
1:G:112:GLY:HA2	1:G:123:THR:O	2.13	0.48
1:I:36:VAL:HG13	1:I:55:ARG:NH1	2.29	0.48
1:L:159:SER:O	1:L:160:SER:C	2.55	0.48
1:M:123:THR:CG2	1:M:124:ILE:N	2.77	0.48
1:N:58:PHE:CE1	1:N:310:LEU:HD12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:118:THR:HG23	1:N:121:GLU:HB2	1.96	0.48
1:O:58:PHE:CE2	1:O:62:LEU:HD11	2.49	0.48
1:Q:267:ILE:HD13	1:Q:267:ILE:HG21	1.57	0.48
1:A:28:GLY:HA3	1:A:299:PHE:CE1	2.49	0.48
1:A:58:PHE:CE1	1:A:310:LEU:HD13	2.49	0.48
2:A:402:SO4:O1	1:D:12:LYS:NZ	2.46	0.48
1:B:191:ILE:HA	1:B:191:ILE:HD13	1.41	0.48
1:D:28:GLY:O	1:D:74:GLY:N	2.38	0.48
1:D:329:LYS:NZ	1:D:347:SER:CA	2.72	0.48
1:E:244:THR:HG23	1:E:246:GLU:N	2.27	0.48
1:F:240:THR:O	1:F:242:LYS:HE3	2.14	0.48
1:G:67:SER:O	1:G:70:ASN:HB2	2.13	0.48
1:H:275:SER:O	1:H:276:GLU:C	2.57	0.48
1:I:78:LEU:O	1:I:106:ILE:HD12	2.13	0.48
1:J:191:ILE:HG23	1:J:191:ILE:HD12	1.56	0.48
1:M:78:LEU:O	1:M:106:ILE:HD12	2.14	0.48
1:O:7:LEU:HB3	1:O:11:GLN:HB2	1.95	0.48
1:Q:33:ASP:OD2	1:Q:107:LYS:HE3	2.14	0.48
1:H:25:ASN:HB3	3:H:414:HOH:O	2.14	0.48
1:H:67:SER:HA	1:H:100:LYS:HD3	1.94	0.48
1:J:118:THR:HG22	1:J:121:GLU:H	1.75	0.48
1:J:124:ILE:HG21	1:J:147:TRP:NE1	2.29	0.48
1:K:91:LYS:HD3	1:K:96:ILE:CG1	2.44	0.48
1:K:115:LEU:HD22	1:K:122:THR:C	2.39	0.48
1:M:352:SER:OG	1:M:354:GLN:HB3	2.13	0.48
1:N:78:LEU:O	1:N:106:ILE:HA	2.14	0.48
1:D:61:ILE:HG21	1:D:323:THR:HG21	1.95	0.48
1:D:305:LEU:HD23	1:D:330:ARG:HB3	1.94	0.48
1:I:204:VAL:O	1:I:207:LYS:N	2.45	0.48
1:J:93:PHE:N	3:J:506:HOH:O	2.46	0.48
1:K:128:ASP:HA	1:L:125:GLN:HE21	1.78	0.48
1:N:106:ILE:HG22	1:N:142:VAL:HG11	1.96	0.48
1:A:313:TRP:CZ2	1:A:315:GLY:HA2	2.48	0.47
1:B:285:ALA:O	1:B:286:ILE:C	2.55	0.47
1:E:160:SER:O	1:E:161:LEU:C	2.56	0.47
1:F:38:THR:O	1:F:42:ARG:HG2	2.14	0.47
1:G:3:ARG:O	1:G:4:PHE:C	2.57	0.47
1:L:46:ILE:HD12	1:L:48:VAL:HG23	1.95	0.47
1:L:337:ALA:O	1:L:339:LYS:N	2.47	0.47
1:N:298:SER:OG	1:N:299:PHE:N	2.47	0.47
1:Q:18:ILE:HD13	1:Q:143:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:LYS:NZ	1:C:99:GLU:OE1	2.47	0.47
1:C:171:ALA:HA	1:C:216:LEU:HD12	1.96	0.47
1:D:187:GLU:HG3	1:D:229:LYS:HG2	1.97	0.47
1:E:76:VAL:HG23	1:E:102:ILE:HG21	1.96	0.47
1:F:123:THR:HG23	1:F:165:GLU:CG	2.44	0.47
1:H:309:ALA:O	1:H:323:THR:HG23	2.13	0.47
1:I:123:THR:HG21	1:I:165:GLU:OE2	2.14	0.47
1:I:164:GLN:O	1:I:168:ASN:ND2	2.45	0.47
1:K:171:ALA:HA	1:K:216:LEU:HD12	1.94	0.47
1:M:156:GLN:OE1	1:N:2:HIS:CA	2.62	0.47
1:N:285:ALA:O	1:N:286:ILE:C	2.55	0.47
1:R:44:GLN:O	1:R:47:LYS:N	2.43	0.47
1:R:280:THR:HG21	1:R:333:ALA:HB1	1.96	0.47
1:A:83:LEU:O	1:A:83:LEU:HG	2.14	0.47
1:A:124:ILE:HD12	3:A:523:HOH:O	2.15	0.47
1:A:229:LYS:NZ	3:A:501:HOH:O	2.47	0.47
1:B:29:ILE:O	1:B:300:SER:HA	2.14	0.47
1:G:250:MET:CE	1:G:291:LEU:CD2	2.93	0.47
1:I:189:GLU:HG3	1:I:270:LEU:HD21	1.96	0.47
1:L:276:GLU:OE2	1:L:307:ALA:HB3	2.14	0.47
1:M:119:ASN:C	1:M:119:ASN:OD1	2.56	0.47
1:P:118:THR:CG2	1:P:121:GLU:H	2.27	0.47
1:Q:330:ARG:HA	1:Q:330:ARG:NE	2.29	0.47
1:C:2:HIS:O	1:C:3:ARG:HB2	2.15	0.47
1:C:133:ARG:O	1:C:134:CYS:C	2.53	0.47
1:D:44:GLN:O	1:D:45:ARG:C	2.54	0.47
1:E:87:ASP:O	1:E:89:GLN:HB2	2.14	0.47
1:G:121:GLU:OE2	1:G:158:PRO:HA	2.14	0.47
1:H:50:ASN:ND2	1:H:55:ARG:HH11	2.12	0.47
1:I:61:ILE:HG22	1:I:324:GLN:HG2	1.95	0.47
1:N:33:ASP:HB3	1:N:77:ILE:HG22	1.95	0.47
1:N:284:ASN:ND2	1:N:342:TYR:H	2.11	0.47
1:O:226:THR:CG2	1:O:227:LEU:N	2.77	0.47
1:Q:217:ASN:C	1:Q:217:ASN:HD22	2.23	0.47
1:R:191:ILE:HB	1:R:192:PRO:CD	2.44	0.47
1:A:249:ALA:HB1	1:A:286:ILE:HA	1.95	0.47
1:B:18:ILE:O	1:B:22:ILE:HD12	2.14	0.47
1:E:44:GLN:O	1:E:47:LYS:N	2.42	0.47
1:E:79:PHE:O	1:E:80:HIS:C	2.58	0.47
1:E:88:SER:C	1:E:89:GLN:NE2	2.72	0.47
1:E:260:VAL:HA	1:E:261:PRO:HD3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:THR:CG2	1:G:121:GLU:HB2	2.43	0.47
1:G:219:HIS:O	1:G:220:HIS:CB	2.62	0.47
1:I:17:GLU:O	1:I:18:ILE:C	2.55	0.47
1:K:349:GLY:O	1:K:352:SER:HB2	2.14	0.47
1:L:59:ARG:HB3	1:L:63:PHE:CE1	2.49	0.47
1:M:221:VAL:CG1	1:M:222:TYR:N	2.77	0.47
1:M:319:ASN:O	1:M:320:LYS:C	2.58	0.47
1:N:294:PRO:HD2	1:N:295:TRP:CH2	2.49	0.47
1:O:230:PRO:CG	1:O:267:ILE:CD1	2.92	0.47
1:Q:80:HIS:CD2	1:Q:137:TYR:OH	2.68	0.47
1:R:244:THR:CG2	1:R:247:GLN:HG3	2.44	0.47
1:D:163:ILE:O	1:D:164:GLN:C	2.55	0.47
1:E:229:LYS:HA	1:E:268:CYS:O	2.14	0.47
1:E:245:PRO:HA	1:E:282:ASN:OD1	2.14	0.47
1:H:42:ARG:HH11	1:H:42:ARG:HD2	1.24	0.47
1:I:106:ILE:HG22	1:I:142:VAL:HG11	1.94	0.47
1:J:50:ASN:HD21	1:J:55:ARG:HH11	1.62	0.47
1:M:69:ILE:CA	1:M:71:GLN:N	2.61	0.47
1:P:154:ALA:O	1:P:155:ASP:C	2.57	0.47
1:P:281:LEU:O	1:P:282:ASN:C	2.54	0.47
1:Q:228:LEU:HG	1:Q:230:PRO:HD3	1.96	0.47
1:R:118:THR:CG2	1:R:121:GLU:H	2.27	0.47
1:R:124:ILE:CD1	3:R:514:HOH:O	2.59	0.47
1:A:50:ASN:HD21	1:A:55:ARG:HD3	1.79	0.47
1:B:51:THR:HG23	1:B:54:ASN:H	1.69	0.47
1:B:58:PHE:CE2	1:B:62:LEU:HD11	2.49	0.47
1:B:233:VAL:O	1:B:248:VAL:HG13	2.15	0.47
1:B:256:LEU:HD13	1:B:267:ILE:HD11	1.97	0.47
1:C:51:THR:CG2	1:C:53:GLU:N	2.77	0.47
1:C:105:GLY:HA3	1:C:144:PHE:CZ	2.49	0.47
1:D:147:TRP:HB3	1:D:173:TYR:CE2	2.49	0.47
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.97	0.47
1:E:276:GLU:OE2	1:E:307:ALA:HB3	2.14	0.47
1:G:298:SER:OG	1:G:299:PHE:N	2.48	0.47
1:H:2:HIS:O	1:H:3:ARG:CB	2.56	0.47
1:H:105:GLY:HA3	1:H:144:PHE:CZ	2.50	0.47
1:H:242:LYS:HE2	1:H:242:LYS:HA	1.96	0.47
1:I:176:ILE:O	1:I:177:CYS:C	2.55	0.47
1:J:43:LEU:O	1:J:44:GLN:C	2.53	0.47
1:J:44:GLN:OE1	1:J:44:GLN:HA	2.14	0.47
1:J:120:LYS:HB2	1:J:152:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:330:ARG:NH1	1:J:346:GLY:CA	2.73	0.47
1:L:18:ILE:O	1:L:22:ILE:HG13	2.14	0.47
1:L:69:ILE:O	1:L:71:GLN:N	2.47	0.47
1:M:144:PHE:HB2	1:M:183:VAL:O	2.14	0.47
1:M:146:LYS:C	1:M:146:LYS:HD3	2.40	0.47
1:M:158:PRO:HG3	1:M:204:VAL:HG13	1.97	0.47
1:M:323:THR:O	1:M:324:GLN:C	2.58	0.47
1:M:343:VAL:O	1:M:344:HIS:HB2	2.14	0.47
1:O:121:GLU:OE1	1:P:1:ALA:HB2	2.14	0.47
1:P:8:THR:OG1	1:P:11:GLN:HG3	2.14	0.47
1:B:33:ASP:HB3	1:B:77:ILE:HG22	1.97	0.47
1:C:68:SER:O	1:C:71:GLN:HG3	2.15	0.47
1:D:29:ILE:HB	1:D:300:SER:HA	1.96	0.47
1:F:313:TRP:CZ2	1:F:315:GLY:HA2	2.50	0.47
1:F:329:LYS:CE	1:F:347:SER:CA	2.76	0.47
1:G:271:SER:O	1:G:272:GLY:C	2.57	0.47
1:K:18:ILE:O	1:K:19:ALA:C	2.56	0.47
1:L:80:HIS:CD2	1:L:137:TYR:OH	2.68	0.47
1:M:303:ARG:HB3	1:M:356:LEU:HD13	1.97	0.47
1:N:50:ASN:HD21	1:N:55:ARG:HD3	1.80	0.47
1:N:211:ALA:O	1:N:212:VAL:C	2.58	0.47
1:O:133:ARG:HH11	1:O:133:ARG:HD3	1.28	0.47
1:Q:244:THR:HG23	1:Q:247:GLN:H	1.77	0.47
1:A:244:THR:HG22	1:A:244:THR:O	2.14	0.47
1:B:118:THR:HG23	1:B:121:GLU:N	2.21	0.47
1:B:136:GLN:O	1:B:137:TYR:C	2.57	0.47
1:D:192:PRO:HD3	3:D:520:HOH:O	2.13	0.47
1:F:276:GLU:OE2	1:F:307:ALA:HB3	2.14	0.47
1:G:197:ASP:HA	1:G:235:ALA:HB1	1.96	0.47
1:H:339:LYS:NZ	3:H:403:HOH:O	2.40	0.47
1:J:342:TYR:OH	1:J:345:THR:HA	2.15	0.47
1:K:357:PHE:C	1:O:139:LYS:NZ	2.73	0.47
1:L:201:CYS:SG	1:L:233:VAL:HG13	2.54	0.47
1:L:271:SER:CA	1:L:274:MET:HE3	2.43	0.47
1:P:75:GLY:HA2	1:P:103:VAL:O	2.15	0.47
1:P:130:LEU:O	1:P:131:SER:C	2.56	0.47
1:P:165:GLU:O	1:P:166:ASN:C	2.57	0.47
1:Q:68:SER:O	1:Q:71:GLN:HB2	2.14	0.47
1:A:18:ILE:HD13	1:A:143:ASP:HB3	1.97	0.47
1:B:6:ALA:HB3	3:B:419:HOH:O	2.13	0.47
1:B:244:THR:CG2	1:B:244:THR:O	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ALA:O	1:B:329:LYS:HB3	2.14	0.47
1:D:118:THR:CG2	1:D:121:GLU:HB2	2.44	0.47
1:D:330:ARG:HH11	1:D:347:SER:HB2	1.79	0.47
1:D:330:ARG:HH11	1:D:347:SER:CB	2.28	0.47
1:D:339:LYS:NZ	3:D:506:HOH:O	2.48	0.47
1:E:320:LYS:HE3	1:E:324:GLN:NE2	2.30	0.47
1:I:4:PHE:CZ	1:J:119:ASN:HB2	2.50	0.47
1:I:18:ILE:HD13	1:I:143:ASP:HB3	1.97	0.47
1:J:80:HIS:CD2	1:J:137:TYR:OH	2.68	0.47
1:J:106:ILE:HG22	1:J:142:VAL:HG11	1.97	0.47
1:L:95:ASN:O	1:L:96:ILE:C	2.55	0.47
1:M:226:THR:CG2	3:M:509:HOH:O	2.62	0.47
1:N:133:ARG:O	1:N:134:CYS:C	2.55	0.47
1:P:25:ASN:H	1:P:27:LYS:HB2	1.80	0.47
1:A:229:LYS:NZ	1:A:300:SER:OG	2.48	0.46
1:B:207:LYS:HE2	1:C:2:HIS:NE2	2.29	0.46
1:C:343:VAL:HG12	1:C:344:HIS:N	2.30	0.46
1:E:33:ASP:OD1	1:E:33:ASP:N	2.48	0.46
1:F:27:LYS:HE2	3:F:424:HOH:O	2.15	0.46
1:G:119:ASN:N	1:H:1:ALA:H1	2.07	0.46
1:I:276:GLU:HG2	1:I:304:ALA:O	2.15	0.46
1:L:325:GLU:O	1:L:326:ALA:C	2.58	0.46
1:M:68:SER:HA	1:M:69:ILE:CG1	2.26	0.46
1:Q:231:ASN:ND2	1:Q:231:ASN:H	2.12	0.46
1:R:87:ASP:C	1:R:89:GLN:H	2.22	0.46
1:R:198:LEU:HD12	1:R:234:THR:HA	1.97	0.46
1:A:220:HIS:CE1	3:A:559:HOH:O	2.58	0.46
1:B:250:MET:CE	1:B:291:LEU:CD2	2.91	0.46
1:C:128:ASP:OD2	1:D:128:ASP:N	2.45	0.46
1:F:29:ILE:HG21	1:F:29:ILE:HD13	1.44	0.46
1:G:113:ALA:HA	1:G:114:PRO:HD2	1.60	0.46
1:H:202:GLN:HB2	1:H:233:VAL:HG11	1.96	0.46
1:J:230:PRO:CG	1:J:267:ILE:CD1	2.91	0.46
1:K:277:GLU:OE2	1:K:344:HIS:HD2	1.97	0.46
1:M:349:GLY:O	1:M:350:ALA:CB	2.63	0.46
1:N:173:TYR:CE1	1:N:177:CYS:SG	3.08	0.46
1:O:159:SER:HB3	1:P:1:ALA:HA	1.97	0.46
1:Q:156:GLN:NE2	1:R:3:ARG:CD	2.76	0.46
1:A:69:ILE:HD12	1:A:327:PHE:CE2	2.51	0.46
1:A:256:LEU:CD1	1:A:267:ILE:HD11	2.46	0.46
1:C:36:VAL:HG13	1:C:55:ARG:CZ	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ILE:HD12	1:F:191:ILE:HA	1.59	0.46
1:G:124:ILE:HG22	1:G:147:TRP:CZ2	2.51	0.46
1:H:12:LYS:HE2	1:H:222:TYR:CD1	2.50	0.46
1:H:224:GLU:HG3	1:H:263:ALA:HB1	1.97	0.46
1:I:53:GLU:CD	1:I:56:ARG:HE	2.23	0.46
1:O:48:VAL:HG21	1:O:315:GLY:HA3	1.97	0.46
1:O:201:CYS:O	1:O:202:GLN:C	2.57	0.46
1:P:196:HIS:O	1:P:239:CYS:HB2	2.16	0.46
1:P:252:THR:O	1:P:256:LEU:HG	2.15	0.46
1:A:277:GLU:CD	1:A:347:SER:CB	2.85	0.46
1:B:243:TYR:HA	1:B:247:GLN:OE1	2.15	0.46
1:E:61:ILE:CG2	1:E:324:GLN:HG2	2.45	0.46
1:G:119:ASN:HB2	1:H:4:PHE:CZ	2.51	0.46
1:H:29:ILE:HD13	1:H:29:ILE:HG21	1.77	0.46
1:M:29:ILE:HB	1:M:300:SER:HA	1.98	0.46
1:D:106:ILE:HD12	1:D:107:LYS:N	2.31	0.46
1:E:54:ASN:O	1:E:55:ARG:C	2.58	0.46
1:E:67:SER:C	1:E:69:ILE:H	2.21	0.46
1:F:105:GLY:HA2	1:F:144:PHE:O	2.15	0.46
1:F:270:LEU:HD12	1:F:270:LEU:O	2.15	0.46
1:F:276:GLU:CB	1:F:352:SER:HB3	2.46	0.46
1:H:115:LEU:HD13	1:H:123:THR:OG1	2.16	0.46
1:H:198:LEU:CD1	1:H:234:THR:HA	2.46	0.46
1:I:51:THR:HG22	1:I:53:GLU:CA	2.44	0.46
1:I:224:GLU:HG2	3:I:422:HOH:O	2.16	0.46
1:J:119:ASN:C	1:J:119:ASN:OD1	2.56	0.46
1:J:244:THR:HG23	1:J:246:GLU:OE1	2.15	0.46
1:M:8:THR:OG1	1:M:11:GLN:HG3	2.14	0.46
1:M:29:ILE:HD13	1:M:29:ILE:HG21	1.65	0.46
1:M:69:ILE:HG23	1:M:69:ILE:H	1.44	0.46
1:N:41:ASN:O	1:N:44:GLN:HB3	2.16	0.46
1:P:43:LEU:O	1:P:44:GLN:C	2.57	0.46
1:P:270:LEU:HD12	1:P:270:LEU:O	2.16	0.46
1:A:45:ARG:NH1	1:A:357:PHE:HA	2.27	0.46
1:A:51:THR:CG2	1:A:54:ASN:N	2.59	0.46
1:A:67:SER:C	1:A:69:ILE:N	2.72	0.46
1:A:277:GLU:OE1	1:A:347:SER:HB2	2.16	0.46
1:B:281:LEU:HD21	1:B:344:HIS:CE1	2.49	0.46
1:C:189:GLU:HB2	1:C:270:LEU:CD2	2.46	0.46
1:C:211:ALA:O	1:C:212:VAL:C	2.58	0.46
1:C:284:ASN:OD1	1:C:340:GLY:HA2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ILE:O	1:F:47:LYS:C	2.58	0.46
1:J:185:ILE:HD13	1:J:185:ILE:HG21	1.72	0.46
1:J:244:THR:HG23	1:J:246:GLU:N	2.31	0.46
1:K:9:GLN:O	1:K:10:GLU:C	2.57	0.46
1:L:313:TRP:CH2	1:L:315:GLY:HA2	2.50	0.46
1:M:3:ARG:CZ	1:N:156:GLN:HE22	2.28	0.46
1:M:124:ILE:HG21	1:M:147:TRP:CE2	2.51	0.46
1:M:256:LEU:HD13	1:M:267:ILE:HD13	1.98	0.46
1:M:267:ILE:HD13	1:M:267:ILE:HG21	1.69	0.46
1:M:312:ALA:O	1:M:319:ASN:HB3	2.16	0.46
1:O:173:TYR:CE1	1:O:177:CYS:SG	3.09	0.46
1:P:2:HIS:O	1:P:3:ARG:O	2.33	0.46
1:A:87:ASP:HB2	1:A:91:LYS:O	2.16	0.46
1:B:136:GLN:O	1:B:140:ASP:N	2.46	0.46
1:B:203:TYR:OH	1:C:2:HIS:ND1	2.27	0.46
1:C:108:LEU:O	1:C:109:ASP:C	2.59	0.46
1:C:159:SER:HB2	1:D:1:ALA:HB2	1.94	0.46
1:C:189:GLU:CG	1:C:191:ILE:CD1	2.94	0.46
1:D:343:VAL:O	1:D:344:HIS:C	2.57	0.46
1:L:49:GLU:O	1:L:51:THR:N	2.48	0.46
1:M:106:ILE:O	1:M:145:GLY:HA2	2.16	0.46
1:M:123:THR:HG21	1:M:165:GLU:OE2	2.16	0.46
1:M:277:GLU:OE2	1:M:342:TYR:OH	2.27	0.46
1:M:329:LYS:HZ1	1:M:348:SER:CB	2.28	0.46
1:N:91:LYS:HZ1	1:N:99:GLU:CD	2.23	0.46
1:C:34:GLU:HB3	1:C:38:THR:HB	1.97	0.46
1:C:51:THR:HG22	1:C:51:THR:O	2.15	0.46
1:F:92:LEU:O	1:F:95:ASN:N	2.47	0.46
1:G:62:LEU:O	1:G:65:VAL:HG22	2.16	0.46
1:H:51:THR:HG22	1:H:51:THR:O	2.16	0.46
1:H:191:ILE:HA	1:H:192:PRO:HD3	1.84	0.46
1:I:67:SER:OG	1:I:68:SER:N	2.10	0.46
1:I:250:MET:CE	1:I:291:LEU:CD2	2.94	0.46
1:J:329:LYS:CE	1:J:346:GLY:O	2.63	0.46
1:M:2:HIS:HE2	1:P:207:LYS:HE2	1.81	0.46
1:M:329:LYS:CE	1:M:347:SER:CB	2.86	0.46
1:N:244:THR:HG23	1:N:247:GLN:H	1.75	0.46
1:O:78:LEU:O	1:O:106:ILE:HD12	2.16	0.46
1:P:118:THR:HG23	1:P:121:GLU:H	1.81	0.46
1:P:154:ALA:HB3	1:P:157:CYS:HB2	1.96	0.46
1:Q:58:PHE:CE2	1:Q:310:LEU:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:172:ARG:NH2	1:R:176:ILE:HD11	2.30	0.46
1:A:231:ASN:H	1:A:231:ASN:ND2	2.14	0.46
1:C:189:GLU:CD	1:C:191:ILE:HD11	2.41	0.46
1:C:263:ALA:O	1:C:265:PRO:HD3	2.15	0.46
1:D:27:LYS:HB3	1:D:72:SER:O	2.15	0.46
1:D:215:ALA:O	1:D:216:LEU:C	2.57	0.46
1:E:65:VAL:HG21	1:E:69:ILE:HG12	1.97	0.46
1:E:146:LYS:HE2	1:E:187:GLU:OE1	2.15	0.46
1:G:50:ASN:HD21	1:G:55:ARG:HD3	1.81	0.46
1:H:276:GLU:OE2	1:H:307:ALA:HB3	2.15	0.46
1:I:87:ASP:OD1	1:I:89:GLN:HB3	2.15	0.46
1:I:156:GLN:O	1:J:1:ALA:HB1	2.16	0.46
1:I:244:THR:HG22	1:I:247:GLN:HB2	1.97	0.46
1:J:146:LYS:C	1:J:146:LYS:CD	2.89	0.46
1:K:116:ALA:N	3:K:501:HOH:O	2.43	0.46
1:N:83:LEU:O	1:N:83:LEU:HG	2.15	0.46
1:O:230:PRO:CG	1:O:267:ILE:HD13	2.46	0.46
1:P:106:ILE:HA	1:P:106:ILE:HD12	1.61	0.46
1:P:294:PRO:HG2	1:P:295:TRP:CE2	2.51	0.46
1:R:220:HIS:HE1	3:R:523:HOH:O	1.97	0.46
1:B:51:THR:CG2	1:B:54:ASN:N	2.59	0.46
1:B:133:ARG:O	1:B:134:CYS:C	2.58	0.46
1:C:83:LEU:HG	1:C:83:LEU:O	2.16	0.46
1:C:274:MET:HE2	1:C:274:MET:HB2	1.75	0.46
1:C:325:GLU:O	1:C:328:MET:HB3	2.16	0.46
1:D:12:LYS:O	1:D:13:LYS:C	2.58	0.46
1:D:106:ILE:HD12	1:D:107:LYS:H	1.81	0.46
1:G:55:ARG:NE	1:G:81:GLU:OE2	2.39	0.46
1:G:172:ARG:NH2	1:G:176:ILE:HD11	2.31	0.46
1:I:43:LEU:O	1:I:44:GLN:C	2.58	0.46
1:J:252:THR:O	1:J:256:LEU:HG	2.16	0.46
1:K:119:ASN:HB2	1:L:4:PHE:CD1	2.51	0.46
1:K:244:THR:HG23	1:K:246:GLU:HB2	1.97	0.46
1:L:29:ILE:HB	1:L:300:SER:HA	1.98	0.46
1:M:160:SER:O	1:M:164:GLN:HB3	2.16	0.46
1:M:279:ALA:HB1	1:M:301:TYR:CZ	2.52	0.46
1:B:191:ILE:HG23	1:B:191:ILE:HD12	1.68	0.45
1:C:1:ALA:N	1:D:121:GLU:OE1	2.49	0.45
1:D:87:ASP:HB2	1:D:91:LYS:O	2.17	0.45
1:D:121:GLU:OE2	1:D:158:PRO:HA	2.15	0.45
1:D:279:ALA:HB1	1:D:301:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:ASP:C	1:E:155:ASP:OD1	2.58	0.45
1:F:58:PHE:CE2	1:F:62:LEU:HD11	2.51	0.45
1:G:271:SER:HB3	1:G:301:TYR:CD2	2.51	0.45
1:J:87:ASP:HB2	1:J:88:SER:H	1.45	0.45
1:J:217:ASN:OD1	3:J:502:HOH:O	2.21	0.45
1:K:217:ASN:O	1:K:218:ASP:C	2.59	0.45
1:L:46:ILE:HD12	1:L:48:VAL:CG2	2.46	0.45
1:M:244:THR:HG23	1:M:247:GLN:CD	2.41	0.45
1:N:244:THR:O	1:N:247:GLN:N	2.48	0.45
1:N:335:CYS:O	1:N:339:LYS:HG3	2.15	0.45
1:P:83:LEU:HD23	1:P:84:TYR:CE1	2.51	0.45
1:P:103:VAL:CG1	1:P:143:ASP:HB2	2.45	0.45
1:R:121:GLU:OE1	1:R:159:SER:CB	2.64	0.45
1:A:33:ASP:HB3	1:A:77:ILE:HG22	1.98	0.45
1:B:226:THR:CG2	1:B:227:LEU:N	2.80	0.45
1:C:274:MET:HE3	1:C:279:ALA:HA	1.98	0.45
1:E:129:GLY:HA2	1:E:132:GLU:OE1	2.16	0.45
1:F:270:LEU:HD12	1:F:270:LEU:C	2.41	0.45
1:G:1:ALA:O	1:G:2:HIS:HB2	2.17	0.45
1:H:244:THR:HB	1:H:245:PRO:HD2	1.98	0.45
1:I:67:SER:HB3	1:I:69:ILE:H	1.82	0.45
1:I:78:LEU:O	1:I:106:ILE:HA	2.16	0.45
1:I:231:ASN:HA	1:I:270:LEU:HG	1.98	0.45
1:K:170:LEU:HD22	1:K:186:VAL:HG13	1.98	0.45
1:N:39:MET:O	1:N:40:GLY:C	2.55	0.45
1:N:51:THR:HG22	1:N:51:THR:O	2.16	0.45
1:Q:226:THR:HG23	3:Q:2024:HOH:O	2.09	0.45
1:Q:319:ASN:OD1	1:Q:319:ASN:N	2.46	0.45
1:R:80:HIS:CD2	1:R:137:TYR:OH	2.65	0.45
1:R:172:ARG:HH11	1:R:172:ARG:HD2	1.53	0.45
1:A:51:THR:HG23	1:A:53:GLU:N	2.32	0.45
1:A:65:VAL:HG23	1:A:324:GLN:HB3	1.98	0.45
1:A:83:LEU:HD23	1:A:84:TYR:CE1	2.51	0.45
1:A:87:ASP:HB2	1:A:91:LYS:H	1.80	0.45
1:A:87:ASP:OD2	1:A:91:LYS:HB3	2.16	0.45
1:B:25:ASN:H	1:B:27:LYS:HG3	1.81	0.45
1:E:306:GLN:O	1:E:307:ALA:C	2.59	0.45
1:G:2:HIS:HB3	1:H:156:GLN:OE1	2.17	0.45
1:G:12:LYS:HD3	1:G:222:TYR:CE1	2.51	0.45
1:H:60:GLU:OE1	1:H:87:ASP:HB2	2.16	0.45
1:H:348:SER:HB3	1:H:349:GLY:H	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:ASP:C	1:I:109:ASP:OD1	2.59	0.45
1:M:68:SER:O	1:M:69:ILE:CB	2.44	0.45
1:N:68:SER:C	1:N:70:ASN:N	2.73	0.45
1:O:61:ILE:HG12	1:O:320:LYS:HG3	1.99	0.45
1:O:303:ARG:HG3	1:O:303:ARG:HH11	1.81	0.45
1:Q:313:TRP:CD2	1:Q:315:GLY:HA2	2.51	0.45
1:R:129:GLY:O	1:R:130:LEU:C	2.58	0.45
1:A:3:ARG:HH21	1:B:156:GLN:NE2	2.15	0.45
1:C:144:PHE:HB2	1:C:183:VAL:O	2.16	0.45
1:D:89:GLN:HB2	1:D:89:GLN:HE21	1.53	0.45
1:D:244:THR:CG2	1:D:246:GLU:H	2.27	0.45
1:H:354:GLN:HG3	1:H:356:LEU:HD23	1.98	0.45
1:I:58:PHE:CE1	1:I:310:LEU:CD1	3.00	0.45
1:J:144:PHE:HB2	1:J:183:VAL:O	2.16	0.45
1:J:320:LYS:O	1:J:324:GLN:HG3	2.16	0.45
1:M:189:GLU:HG2	1:M:191:ILE:CD1	2.47	0.45
1:M:276:GLU:OE2	1:M:307:ALA:HB3	2.15	0.45
1:N:50:ASN:HD21	1:N:55:ARG:HH11	1.60	0.45
1:F:118:THR:HG23	1:F:121:GLU:H	1.81	0.45
1:I:14:GLU:O	1:I:18:ILE:HG13	2.16	0.45
1:I:229:LYS:NZ	1:I:300:SER:OG	2.36	0.45
1:I:244:THR:O	1:I:245:PRO:C	2.59	0.45
1:J:296:LYS:HA	1:J:296:LYS:HD2	1.74	0.45
1:L:144:PHE:HB2	1:L:183:VAL:O	2.17	0.45
1:M:189:GLU:CD	1:M:191:ILE:CD1	2.90	0.45
1:M:329:LYS:HD2	1:M:347:SER:CB	2.46	0.45
1:O:8:THR:OG1	1:O:11:GLN:HG3	2.16	0.45
1:O:28:GLY:HA3	1:O:299:PHE:CZ	2.51	0.45
1:P:51:THR:HG22	1:P:54:ASN:HB2	1.98	0.45
1:P:91:LYS:HD3	1:P:96:ILE:CG1	2.47	0.45
1:P:109:ASP:HB3	1:P:147:TRP:HA	1.99	0.45
1:Q:115:LEU:HD12	1:Q:115:LEU:HA	1.80	0.45
1:Q:152:ARG:HH11	1:Q:152:ARG:HD3	1.36	0.45
1:R:171:ALA:O	1:R:172:ARG:C	2.60	0.45
1:R:276:GLU:HB3	3:R:515:HOH:O	2.16	0.45
1:A:226:THR:HG21	3:A:536:HOH:O	2.09	0.45
1:B:87:ASP:O	1:B:88:SER:C	2.59	0.45
1:B:136:GLN:HE21	1:B:136:GLN:HB2	1.52	0.45
1:B:244:THR:HG22	1:B:244:THR:O	2.17	0.45
1:B:313:TRP:CH2	1:B:315:GLY:HA2	2.52	0.45
1:E:67:SER:C	1:E:69:ILE:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:ILE:HG21	1:E:191:ILE:HD13	1.25	0.45
1:G:69:ILE:O	1:G:71:GLN:N	2.49	0.45
1:G:244:THR:CG2	1:G:247:GLN:N	2.79	0.45
1:H:98:LYS:O	1:H:99:GLU:C	2.57	0.45
1:J:3:ARG:HB2	1:J:4:PHE:H	1.74	0.45
1:K:128:ASP:HA	1:L:125:GLN:NE2	2.32	0.45
1:K:335:CYS:SG	1:K:339:LYS:NZ	2.90	0.45
1:L:2:HIS:HB3	1:L:3:ARG:H	1.54	0.45
1:L:119:ASN:HB3	1:L:157:CYS:SG	2.56	0.45
1:M:222:TYR:CZ	1:M:224:GLU:HG2	2.51	0.45
1:N:28:GLY:HA3	1:N:299:PHE:CE1	2.52	0.45
1:N:284:ASN:ND2	1:N:340:GLY:CA	2.80	0.45
1:O:343:VAL:CG2	1:O:344:HIS:H	2.10	0.45
1:P:81:GLU:HG2	1:P:82:THR:N	2.31	0.45
1:P:276:GLU:CG	1:P:352:SER:HB2	2.47	0.45
1:Q:118:THR:CG2	1:Q:121:GLU:HB2	2.46	0.45
1:A:2:HIS:HA	1:D:203:TYR:OH	2.15	0.45
1:A:224:GLU:OE2	1:D:258:ARG:HD3	2.16	0.45
1:B:279:ALA:HB1	1:B:301:TYR:CZ	2.51	0.45
1:C:106:ILE:HG23	1:C:106:ILE:O	2.15	0.45
1:F:50:ASN:ND2	1:F:50:ASN:C	2.74	0.45
1:F:171:ALA:HA	1:F:216:LEU:HD12	1.98	0.45
1:F:271:SER:O	1:F:272:GLY:C	2.59	0.45
1:F:352:SER:HA	1:F:354:GLN:CB	2.47	0.45
1:I:274:MET:HE2	1:I:274:MET:HB2	1.66	0.45
1:M:119:ASN:H	1:N:1:ALA:CB	2.27	0.45
1:M:351:ALA:O	1:M:352:SER:HB2	2.16	0.45
1:O:87:ASP:OD2	1:O:91:LYS:N	2.45	0.45
1:P:86:LYS:HD3	1:P:90:GLY:HA2	1.99	0.45
1:P:236:GLY:O	1:P:237:HIS:C	2.58	0.45
1:Q:254:THR:O	1:Q:258:ARG:HG2	2.17	0.45
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.60	0.45
1:A:276:GLU:HG2	1:A:304:ALA:O	2.17	0.45
1:B:59:ARG:O	1:B:63:PHE:N	2.39	0.45
1:B:119:ASN:HB3	1:B:157:CYS:SG	2.56	0.45
1:C:36:VAL:O	1:C:36:VAL:CG1	2.64	0.45
1:D:118:THR:HG23	1:D:121:GLU:HB2	1.97	0.45
1:E:75:GLY:HA2	1:E:103:VAL:O	2.17	0.45
1:F:267:ILE:CG1	1:F:297:LEU:HD23	2.41	0.45
1:H:187:GLU:HG3	1:H:229:LYS:HG2	1.99	0.45
1:N:284:ASN:HD22	1:N:340:GLY:CA	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:320:LYS:O	1:O:323:THR:HB	2.17	0.45
1:P:23:VAL:CG2	1:P:296:LYS:HG3	2.47	0.45
1:R:131:SER:O	1:R:132:GLU:C	2.60	0.45
1:A:42:ARG:HH11	1:A:357:PHE:C	2.24	0.45
1:B:76:VAL:HG23	1:B:102:ILE:HG21	1.99	0.45
1:B:291:LEU:HB3	1:B:292:PRO:HD2	1.99	0.45
1:D:250:MET:CE	1:D:291:LEU:CD2	2.94	0.45
1:G:51:THR:CG2	1:G:54:ASN:N	2.72	0.45
1:G:184:PRO:HD2	1:G:225:GLY:O	2.17	0.45
1:H:154:ALA:O	1:H:155:ASP:C	2.59	0.45
1:I:12:LYS:HG2	1:I:222:TYR:CD1	2.52	0.45
1:J:227:LEU:HD23	1:J:227:LEU:HA	1.72	0.45
1:J:354:GLN:HB3	3:J:501:HOH:O	2.17	0.45
1:K:172:ARG:HH11	1:K:172:ARG:HD2	1.50	0.45
1:L:83:LEU:HB3	1:L:84:TYR:CD1	2.52	0.45
1:M:352:SER:HA	1:M:354:GLN:N	2.32	0.45
1:N:83:LEU:HD23	1:N:84:TYR:CE1	2.52	0.45
1:O:61:ILE:HG22	1:O:324:GLN:HG2	1.99	0.45
1:O:65:VAL:HG21	1:O:328:MET:HE2	1.99	0.45
1:O:65:VAL:HB	1:O:328:MET:CE	2.47	0.45
1:Q:289:CYS:SG	1:Q:291:LEU:HD22	2.57	0.45
1:A:80:HIS:CD2	1:A:137:TYR:OH	2.68	0.45
1:A:213:TYR:O	1:A:214:LYS:C	2.59	0.45
1:B:108:LEU:HB3	1:B:130:LEU:HD11	2.00	0.45
1:C:12:LYS:O	1:C:13:LYS:C	2.59	0.45
1:C:121:GLU:OE2	1:C:157:CYS:HB3	2.17	0.45
1:E:223:LEU:HD11	3:E:555:HOH:O	2.17	0.45
1:F:118:THR:HG23	1:F:121:GLU:CB	2.40	0.45
1:J:226:THR:CG2	3:J:511:HOH:O	2.65	0.45
1:M:244:THR:O	1:M:245:PRO:C	2.60	0.45
1:N:3:ARG:N	1:N:3:ARG:HH11	2.14	0.45
1:P:2:HIS:O	1:P:3:ARG:C	2.59	0.45
1:P:80:HIS:CD2	1:P:137:TYR:OH	2.58	0.45
1:P:330:ARG:HH11	1:P:330:ARG:HD3	0.92	0.45
1:R:245:PRO:HD2	1:R:246:GLU:OE1	2.17	0.45
1:A:123:THR:CG2	1:A:124:ILE:H	2.30	0.44
1:B:75:GLY:HA2	1:B:103:VAL:O	2.16	0.44
1:F:50:ASN:HD22	1:F:51:THR:N	2.15	0.44
1:F:215:ALA:O	1:F:216:LEU:C	2.60	0.44
1:G:250:MET:O	1:G:250:MET:HE3	2.17	0.44
1:N:240:THR:O	1:N:242:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:LYS:HA	1:O:91:LYS:O	2.17	0.44
1:O:97:LEU:O	1:O:98:LYS:C	2.58	0.44
1:Q:191:ILE:HA	1:Q:191:ILE:HD13	1.46	0.44
1:B:13:LYS:O	1:B:14:GLU:C	2.54	0.44
1:B:49:GLU:O	1:B:54:ASN:ND2	2.25	0.44
1:B:56:ARG:NH1	1:B:56:ARG:HG2	2.31	0.44
1:B:69:ILE:C	1:B:71:GLN:N	2.75	0.44
1:C:41:ASN:O	1:C:44:GLN:HB3	2.18	0.44
1:C:94:ARG:HD3	1:C:140:ASP:O	2.16	0.44
1:D:329:LYS:HZ3	1:D:347:SER:CA	2.27	0.44
1:E:44:GLN:OE1	1:E:44:GLN:HA	2.17	0.44
1:E:349:GLY:O	1:E:350:ALA:C	2.59	0.44
1:F:58:PHE:CE1	1:F:310:LEU:CD1	3.00	0.44
1:G:65:VAL:CG1	1:G:324:GLN:HB3	2.47	0.44
1:H:3:ARG:HD3	1:H:3:ARG:C	2.39	0.44
1:H:12:LYS:HB3	1:H:222:TYR:CZ	2.52	0.44
1:H:61:ILE:CG2	1:H:324:GLN:HG2	2.48	0.44
1:H:277:GLU:HG2	1:H:345:THR:CG2	2.40	0.44
1:H:342:TYR:OH	1:H:346:GLY:N	2.51	0.44
1:J:86:LYS:HB3	1:J:90:GLY:HA2	1.99	0.44
1:K:355:SER:O	1:K:356:LEU:HD23	2.17	0.44
1:L:61:ILE:CG2	1:L:324:GLN:HG2	2.47	0.44
1:L:76:VAL:HG23	1:L:102:ILE:HG21	1.98	0.44
1:L:248:VAL:O	1:L:249:ALA:C	2.59	0.44
1:M:75:GLY:HA2	1:M:103:VAL:O	2.17	0.44
1:M:272:GLY:HA2	1:M:303:ARG:HH12	1.82	0.44
1:N:193:ASP:N	1:N:193:ASP:OD1	2.51	0.44
1:C:164:GLN:O	1:C:168:ASN:ND2	2.47	0.44
1:D:12:LYS:HG2	1:D:222:TYR:CZ	2.52	0.44
1:D:75:GLY:CA	1:D:103:VAL:O	2.65	0.44
1:F:224:GLU:HB3	3:F:425:HOH:O	2.16	0.44
1:F:313:TRP:CE2	1:F:315:GLY:HA2	2.52	0.44
1:H:233:VAL:CG2	1:H:252:THR:HA	2.48	0.44
1:H:267:ILE:HG12	1:H:297:LEU:HD23	1.98	0.44
1:I:201:CYS:SG	1:I:233:VAL:HG13	2.57	0.44
1:J:12:LYS:HE2	1:J:222:TYR:CD1	2.53	0.44
1:L:8:THR:O	1:L:9:GLN:C	2.57	0.44
1:L:80:HIS:HD2	1:L:137:TYR:OH	2.01	0.44
1:M:68:SER:CA	1:M:69:ILE:HD12	2.32	0.44
1:M:155:ASP:O	1:M:156:GLN:HB2	2.17	0.44
1:M:352:SER:HA	1:M:354:GLN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:337:ALA:C	1:O:339:LYS:N	2.74	0.44
1:P:44:GLN:OE1	1:P:44:GLN:HA	2.13	0.44
1:Q:335:CYS:O	1:Q:336:GLN:C	2.58	0.44
1:A:29:ILE:HB	1:A:300:SER:HA	1.99	0.44
1:B:148:ARG:HA	1:B:187:GLU:HB3	2.00	0.44
1:D:250:MET:HE1	1:D:291:LEU:HD22	1.99	0.44
1:D:260:VAL:O	1:D:261:PRO:C	2.60	0.44
1:E:125:GLN:HE21	1:F:128:ASP:HA	1.83	0.44
1:E:324:GLN:O	1:E:328:MET:HB2	2.18	0.44
1:F:148:ARG:HD3	3:F:458:HOH:O	2.17	0.44
1:F:191:ILE:HA	1:F:192:PRO:HD3	1.71	0.44
1:G:29:ILE:HD13	1:G:29:ILE:HG21	1.71	0.44
1:H:1:ALA:CB	1:H:4:PHE:CD1	3.01	0.44
1:H:319:ASN:O	1:H:320:LYS:C	2.60	0.44
1:J:24:ALA:HA	3:J:543:HOH:O	2.17	0.44
1:K:28:GLY:HA3	1:K:299:PHE:CE1	2.52	0.44
1:L:244:THR:O	1:L:247:GLN:HB2	2.18	0.44
1:M:2:HIS:O	1:M:3:ARG:O	2.35	0.44
1:M:29:ILE:O	1:M:300:SER:HA	2.17	0.44
1:N:22:ILE:HD11	1:N:144:PHE:CD2	2.53	0.44
1:N:274:MET:HE3	1:N:279:ALA:CA	2.44	0.44
1:O:325:GLU:O	1:O:326:ALA:C	2.60	0.44
1:R:196:HIS:O	1:R:239:CYS:HB2	2.18	0.44
1:A:12:LYS:HG2	1:A:222:TYR:CE2	2.52	0.44
1:A:40:GLY:HA2	1:A:50:ASN:HB2	1.98	0.44
1:B:257:HIS:CD2	1:C:263:ALA:HA	2.52	0.44
1:D:279:ALA:HB1	1:D:301:TYR:CZ	2.52	0.44
1:E:4:PHE:HA	1:E:5:PRO:HD2	1.77	0.44
1:F:250:MET:CE	1:F:291:LEU:CD2	2.95	0.44
1:G:80:HIS:CD2	1:G:137:TYR:OH	2.70	0.44
1:J:62:LEU:O	1:J:65:VAL:HG13	2.17	0.44
1:K:326:ALA:O	1:K:327:PHE:C	2.60	0.44
1:M:154:ALA:O	1:M:155:ASP:C	2.59	0.44
1:M:190:VAL:H	1:M:231:ASN:ND2	2.16	0.44
1:N:184:PRO:O	1:N:184:PRO:HG2	2.18	0.44
1:O:296:LYS:N	1:O:296:LYS:HD2	2.32	0.44
1:O:342:TYR:CD2	1:O:342:TYR:C	2.92	0.44
1:Q:109:ASP:OD1	1:Q:109:ASP:C	2.60	0.44
1:B:68:SER:C	1:B:70:ASN:N	2.72	0.44
1:D:4:PHE:HA	1:D:5:PRO:HD2	1.76	0.44
1:D:119:ASN:C	1:D:119:ASN:OD1	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ILE:CG2	1:E:147:TRP:CZ2	2.99	0.44
1:E:163:ILE:HG22	1:E:164:GLN:N	2.31	0.44
1:F:248:VAL:O	1:F:249:ALA:C	2.55	0.44
1:I:69:ILE:HD11	1:I:327:PHE:CE2	2.52	0.44
1:I:214:LYS:HE3	1:I:218:ASP:OD1	2.17	0.44
1:J:120:LYS:HB2	1:J:152:ARG:NH1	2.33	0.44
1:J:352:SER:CA	3:J:503:HOH:O	2.64	0.44
1:N:161:LEU:O	1:N:162:ALA:C	2.60	0.44
1:O:44:GLN:OE1	1:O:44:GLN:HA	2.17	0.44
1:P:65:VAL:O	1:P:100:LYS:NZ	2.43	0.44
1:P:133:ARG:HH11	1:P:133:ARG:HD3	1.27	0.44
1:Q:253:VAL:HG23	1:Q:286:ILE:HG23	1.98	0.44
1:R:50:ASN:HD21	1:R:55:ARG:HH11	1.64	0.44
1:R:64:SER:O	1:R:65:VAL:C	2.58	0.44
1:R:154:ALA:O	1:R:155:ASP:C	2.60	0.44
1:R:313:TRP:CH2	1:R:315:GLY:HA2	2.52	0.44
1:B:7:LEU:HD21	1:B:178:GLN:HB3	1.99	0.44
1:B:186:VAL:O	1:B:228:LEU:HD12	2.18	0.44
1:C:110:GLN:N	1:C:125:GLN:O	2.49	0.44
1:C:244:THR:O	1:C:247:GLN:HB2	2.18	0.44
1:E:115:LEU:HD12	1:E:115:LEU:HA	1.78	0.44
1:F:45:ARG:HH12	1:F:356:LEU:HA	1.82	0.44
1:G:311:ALA:O	1:G:312:ALA:C	2.58	0.44
1:H:350:ALA:O	1:H:351:ALA:C	2.60	0.44
1:I:51:THR:HG22	1:I:51:THR:O	2.18	0.44
1:I:51:THR:CG2	1:I:53:GLU:HB3	2.47	0.44
1:I:202:GLN:HB2	1:I:233:VAL:HG11	2.00	0.44
1:J:207:LYS:HD3	3:K:570:HOH:O	2.17	0.44
1:M:67:SER:C	1:M:69:ILE:HG13	2.43	0.44
1:M:271:SER:HB3	1:M:301:TYR:CD2	2.53	0.44
1:N:244:THR:HG23	1:N:246:GLU:CA	2.47	0.44
1:P:23:VAL:HG23	1:P:296:LYS:HG3	1.99	0.44
1:Q:232:MET:HE2	1:Q:286:ILE:HD12	2.00	0.44
1:A:117:GLY:HA2	1:B:4:PHE:O	2.17	0.44
1:A:119:ASN:OD1	1:A:119:ASN:C	2.54	0.44
1:D:154:ALA:O	1:D:155:ASP:C	2.61	0.44
1:D:252:THR:O	1:D:256:LEU:HG	2.18	0.44
1:E:309:ALA:O	1:E:323:THR:HG23	2.18	0.44
1:F:60:GLU:HG3	1:F:93:PHE:HE1	1.83	0.44
1:G:51:THR:HG22	1:G:54:ASN:N	2.28	0.44
1:I:66:ASP:OD1	1:I:67:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:GLN:O	1:I:168:ASN:N	2.50	0.44
1:K:244:THR:HG22	1:K:247:GLN:CB	2.48	0.44
1:L:256:LEU:HD13	1:L:267:ILE:HD11	1.99	0.44
1:L:333:ALA:O	1:L:336:GLN:HB2	2.18	0.44
1:N:322:ALA:O	1:N:323:THR:C	2.61	0.44
1:O:104:VAL:HG12	1:O:105:GLY:N	2.33	0.44
1:O:159:SER:O	1:O:160:SER:C	2.59	0.44
1:O:191:ILE:CD1	1:O:192:PRO:HD2	2.48	0.44
1:O:295:TRP:CD2	1:O:295:TRP:N	2.85	0.44
1:P:173:TYR:CD2	1:P:174:ALA:N	2.86	0.44
1:P:268:CYS:HB3	1:P:300:SER:HB2	1.98	0.44
1:A:2:HIS:C	1:A:4:PHE:N	2.71	0.44
1:B:296:LYS:HA	1:B:296:LYS:HD2	1.75	0.44
1:C:191:ILE:HA	1:C:191:ILE:HD12	1.21	0.44
1:E:28:GLY:HA3	1:E:299:PHE:CE2	2.53	0.44
1:E:224:GLU:OE2	1:H:258:ARG:NH1	2.34	0.44
1:E:329:LYS:CD	1:E:347:SER:OG	2.61	0.44
1:F:244:THR:HG22	1:F:247:GLN:CG	2.48	0.44
1:J:81:GLU:HG2	1:J:82:THR:N	2.32	0.44
1:J:191:ILE:HD13	1:J:192:PRO:HD3	2.00	0.44
1:J:244:THR:H	1:J:247:GLN:HE21	1.61	0.44
1:K:119:ASN:O	1:K:120:LYS:HB2	2.18	0.44
1:L:53:GLU:OE2	1:L:57:GLN:HG3	2.17	0.44
1:L:191:ILE:HG22	1:L:193:ASP:H	1.82	0.44
1:N:28:GLY:HA3	1:N:299:PHE:CZ	2.53	0.44
1:N:148:ARG:HB2	1:N:187:GLU:OE1	2.18	0.44
1:N:189:GLU:HB2	1:N:270:LEU:CD2	2.48	0.44
1:N:276:GLU:HB3	1:N:330:ARG:HH11	1.83	0.44
1:O:14:GLU:OE2	1:O:138:LYS:NZ	2.45	0.44
1:O:275:SER:O	1:O:276:GLU:C	2.60	0.44
1:P:67:SER:C	1:P:69:ILE:N	2.75	0.44
1:A:30:LEU:HB3	1:A:76:VAL:HG22	1.99	0.43
1:D:53:GLU:HG3	1:D:57:GLN:NE2	2.32	0.43
1:D:286:ILE:HG22	1:D:297:LEU:HD13	2.00	0.43
1:D:316:LYS:O	1:D:317:ALA:C	2.61	0.43
1:K:130:LEU:HD12	1:K:130:LEU:HA	1.77	0.43
1:L:244:THR:O	1:L:245:PRO:C	2.61	0.43
1:M:81:GLU:HG2	1:M:82:THR:N	2.32	0.43
1:O:223:LEU:HD23	1:O:223:LEU:HA	1.70	0.43
1:R:8:THR:HG21	3:R:501:HOH:O	2.18	0.43
1:A:190:VAL:H	1:A:231:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:TYR:CE1	1:B:177:CYS:SG	3.10	0.43
1:C:106:ILE:HA	1:C:106:ILE:HD12	1.78	0.43
1:D:189:GLU:CD	1:D:191:ILE:HD11	2.44	0.43
1:F:50:ASN:C	1:F:50:ASN:HD22	2.25	0.43
1:G:306:GLN:O	1:G:307:ALA:C	2.59	0.43
1:H:192:PRO:O	1:H:193:ASP:C	2.61	0.43
1:I:44:GLN:O	1:I:47:LYS:N	2.48	0.43
1:K:30:LEU:HD22	1:K:327:PHE:CZ	2.53	0.43
1:K:118:THR:CG2	1:K:121:GLU:HB2	2.48	0.43
1:K:226:THR:HG21	3:K:512:HOH:O	2.11	0.43
1:K:313:TRP:CZ2	1:K:315:GLY:HA2	2.53	0.43
1:N:25:ASN:C	1:N:27:LYS:N	2.76	0.43
1:P:244:THR:HG23	1:P:246:GLU:H	1.82	0.43
1:R:112:GLY:HA2	1:R:123:THR:O	2.18	0.43
1:B:70:ASN:ND2	1:B:100:LYS:O	2.40	0.43
1:B:274:MET:HE3	1:B:279:ALA:CB	2.46	0.43
1:B:330:ARG:NE	1:B:330:ARG:CA	2.72	0.43
1:D:343:VAL:O	1:D:345:THR:HG23	2.18	0.43
1:H:121:GLU:OE1	1:H:159:SER:OG	2.32	0.43
1:I:58:PHE:CE2	1:I:310:LEU:HD13	2.54	0.43
1:J:61:ILE:HG21	1:J:323:THR:CG2	2.48	0.43
1:J:108:LEU:HD12	1:J:145:GLY:HA3	2.00	0.43
1:J:233:VAL:CG2	1:J:252:THR:HA	2.47	0.43
1:K:118:THR:HG21	1:K:121:GLU:HB2	2.00	0.43
1:Q:244:THR:HG23	1:Q:246:GLU:H	1.82	0.43
1:R:267:ILE:HG21	1:R:267:ILE:HD13	1.43	0.43
1:A:45:ARG:CZ	1:A:357:PHE:CA	2.74	0.43
1:A:197:ASP:HB2	1:A:243:TYR:OH	2.18	0.43
1:B:38:THR:O	1:B:41:ASN:N	2.51	0.43
1:B:174:ALA:O	1:B:175:SER:C	2.59	0.43
1:E:51:THR:HG23	1:E:54:ASN:H	1.79	0.43
1:F:25:ASN:N	1:F:27:LYS:H	2.16	0.43
1:F:275:SER:O	1:F:276:GLU:C	2.61	0.43
1:G:3:ARG:H	1:G:4:PHE:HD1	1.65	0.43
1:G:118:THR:HG23	1:G:119:ASN:N	2.34	0.43
1:H:276:GLU:H	1:H:352:SER:HB3	1.83	0.43
1:I:124:ILE:CG2	1:I:147:TRP:CZ2	3.00	0.43
1:N:36:VAL:HG13	1:N:55:ARG:NH1	2.33	0.43
1:N:43:LEU:O	1:N:44:GLN:C	2.61	0.43
1:N:64:SER:O	1:N:65:VAL:C	2.60	0.43
1:N:270:LEU:C	1:N:270:LEU:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:191:ILE:HA	1:O:191:ILE:HD13	1.26	0.43
1:Q:109:ASP:HB3	1:Q:147:TRP:CD2	2.53	0.43
1:Q:128:ASP:HA	1:R:125:GLN:HE21	1.83	0.43
1:A:244:THR:CG2	1:A:244:THR:O	2.65	0.43
1:B:8:THR:HG1	1:B:11:GLN:HG3	1.77	0.43
1:C:198:LEU:CD1	1:C:234:THR:HA	2.48	0.43
1:C:244:THR:N	1:C:247:GLN:OE1	2.40	0.43
1:C:303:ARG:HG3	1:C:303:ARG:NH1	2.25	0.43
1:D:69:ILE:O	1:D:69:ILE:HG13	2.17	0.43
1:E:94:ARG:HD2	1:E:140:ASP:O	2.18	0.43
1:G:217:ASN:ND2	1:G:217:ASN:C	2.75	0.43
1:H:8:THR:HG22	1:H:10:GLU:N	2.19	0.43
1:L:43:LEU:O	1:L:46:ILE:HG13	2.18	0.43
1:L:45:ARG:C	1:L:47:LYS:H	2.27	0.43
1:L:158:PRO:CG	1:L:163:ILE:HD11	2.49	0.43
1:M:1:ALA:HB3	1:N:119:ASN:CB	2.48	0.43
1:M:115:LEU:O	1:M:118:THR:CG2	2.66	0.43
1:O:164:GLN:HG2	1:O:165:GLU:N	2.32	0.43
1:P:263:ALA:O	1:P:265:PRO:HD3	2.19	0.43
1:P:313:TRP:C	1:P:315:GLY:N	2.76	0.43
1:R:8:THR:O	1:R:9:GLN:C	2.59	0.43
1:R:289:CYS:O	1:R:293:LYS:CE	2.62	0.43
1:C:51:THR:O	1:C:52:GLU:C	2.59	0.43
1:C:215:ALA:O	1:C:216:LEU:C	2.60	0.43
1:D:250:MET:HE3	1:D:254:THR:OG1	2.19	0.43
1:E:154:ALA:O	1:E:155:ASP:C	2.59	0.43
1:F:12:LYS:HD3	1:F:222:TYR:CE1	2.53	0.43
1:F:110:GLN:HG3	1:F:126:GLY:HA2	2.01	0.43
1:F:330:ARG:NH1	3:F:411:HOH:O	2.47	0.43
1:H:42:ARG:NH1	1:H:303:ARG:HG3	2.33	0.43
1:I:270:LEU:HD12	1:I:271:SER:N	2.33	0.43
1:L:232:MET:HE2	1:L:286:ILE:HD12	2.01	0.43
1:M:119:ASN:N	1:N:1:ALA:HB3	2.27	0.43
1:N:118:THR:CG2	1:N:121:GLU:N	2.78	0.43
1:Q:58:PHE:CE1	1:Q:310:LEU:HD13	2.54	0.43
1:Q:87:ASP:HB2	1:Q:91:LYS:N	2.34	0.43
1:A:3:ARG:CD	1:B:156:GLN:NE2	2.82	0.43
1:B:313:TRP:CD2	1:B:315:GLY:HA2	2.53	0.43
1:C:147:TRP:CB	1:C:173:TYR:CE2	3.02	0.43
1:F:197:ASP:C	1:F:197:ASP:OD1	2.61	0.43
1:F:233:VAL:CG2	1:F:252:THR:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:PHE:O	1:J:117:GLY:HA2	2.19	0.43
1:J:33:ASP:HB3	1:J:77:ILE:HG22	2.00	0.43
1:N:244:THR:HG21	1:N:247:GLN:HG3	1.96	0.43
1:O:121:GLU:OE2	1:O:158:PRO:HA	2.18	0.43
1:R:254:THR:HG21	2:R:402:SO4:O4	2.19	0.43
1:A:86:LYS:HD3	1:A:90:GLY:HA2	2.01	0.43
1:C:66:ASP:O	1:C:68:SER:N	2.52	0.43
1:C:147:TRP:CB	1:C:173:TYR:CZ	3.02	0.43
1:C:172:ARG:HH11	1:C:172:ARG:HD2	1.54	0.43
1:D:121:GLU:HG3	1:D:157:CYS:SG	2.59	0.43
1:D:329:LYS:CD	1:D:347:SER:N	2.81	0.43
1:E:46:ILE:O	1:E:48:VAL:HG23	2.18	0.43
1:F:195:ASP:HB3	1:F:238:ALA:CB	2.48	0.43
1:G:46:ILE:HG13	1:G:48:VAL:HG23	2.01	0.43
1:J:193:ASP:OD1	1:J:193:ASP:N	2.52	0.43
1:K:44:GLN:O	1:K:45:ARG:C	2.58	0.43
1:L:65:VAL:HG23	1:L:69:ILE:HB	2.01	0.43
1:M:229:LYS:HA	1:M:268:CYS:O	2.19	0.43
1:N:60:GLU:HB2	1:N:93:PHE:CZ	2.53	0.43
1:N:147:TRP:HB3	1:N:173:TYR:CE2	2.54	0.43
1:P:146:LYS:CE	3:P:557:HOH:O	2.66	0.43
1:P:191:ILE:HA	1:P:191:ILE:HD13	1.68	0.43
1:P:223:LEU:HD23	1:P:223:LEU:HA	1.74	0.43
1:R:12:LYS:HB3	1:R:222:TYR:CZ	2.53	0.43
1:R:79:PHE:O	1:R:80:HIS:C	2.62	0.43
1:R:191:ILE:HG21	1:R:191:ILE:HD13	1.32	0.43
1:R:271:SER:O	1:R:274:MET:HE3	2.19	0.43
1:B:184:PRO:HD2	1:B:225:GLY:O	2.18	0.43
1:B:224:GLU:OE2	1:C:258:ARG:NH1	2.43	0.43
1:E:184:PRO:HD2	1:E:225:GLY:O	2.19	0.43
1:E:267:ILE:HG23	1:E:267:ILE:HD13	1.75	0.43
1:G:136:GLN:O	1:G:137:TYR:C	2.60	0.43
1:G:190:VAL:H	1:G:231:ASN:HD22	1.65	0.43
1:H:29:ILE:HB	1:H:300:SER:HA	2.00	0.43
1:H:329:LYS:HE2	1:H:347:SER:HA	2.00	0.43
1:I:270:LEU:HD12	1:I:270:LEU:C	2.44	0.43
1:I:337:ALA:O	1:I:339:LYS:N	2.52	0.43
1:J:235:ALA:HB2	1:J:243:TYR:CE1	2.54	0.43
1:J:240:THR:C	1:J:241:LYS:O	2.60	0.43
1:K:61:ILE:HG12	1:K:320:LYS:HG3	2.00	0.43
1:K:319:ASN:O	1:K:320:LYS:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:35:SER:O	1:L:36:VAL:C	2.60	0.43
1:L:67:SER:C	1:L:69:ILE:N	2.73	0.43
1:M:128:ASP:OD2	1:N:128:ASP:N	2.36	0.43
1:P:184:PRO:HD2	1:P:225:GLY:O	2.18	0.43
1:A:14:GLU:O	1:A:18:ILE:HG13	2.19	0.43
1:A:254:THR:HG21	2:A:402:SO4:O3	2.19	0.43
1:C:219:HIS:O	1:C:220:HIS:C	2.61	0.43
1:C:244:THR:HG22	1:C:247:GLN:CD	2.44	0.43
1:D:259:THR:O	1:D:261:PRO:HD3	2.19	0.43
1:E:126:GLY:H	1:F:128:ASP:CG	2.27	0.43
1:E:352:SER:HA	1:E:354:GLN:HG2	2.01	0.43
1:F:252:THR:O	1:F:256:LEU:HG	2.19	0.43
1:H:3:ARG:HB3	1:H:4:PHE:CD1	2.54	0.43
1:H:80:HIS:CD2	1:H:137:TYR:OH	2.60	0.43
1:H:299:PHE:HB2	1:H:301:TYR:CD1	2.53	0.43
1:I:2:HIS:HA	1:L:203:TYR:OH	2.19	0.43
1:I:109:ASP:HA	1:I:147:TRP:CE3	2.53	0.43
1:I:115:LEU:HD11	1:I:165:GLU:HG2	2.00	0.43
1:J:105:GLY:HA2	1:J:144:PHE:O	2.19	0.43
1:J:229:LYS:HA	1:J:268:CYS:O	2.19	0.43
1:L:28:GLY:HA3	1:L:299:PHE:CZ	2.54	0.43
1:L:46:ILE:HG21	1:L:310:LEU:O	2.19	0.43
1:L:107:LYS:HB2	1:L:107:LYS:HE2	1.96	0.43
1:M:1:ALA:HB1	1:N:156:GLN:CB	2.48	0.43
1:M:124:ILE:CG2	1:M:147:TRP:CE2	3.01	0.43
1:N:3:ARG:HD2	1:N:220:HIS:CD2	2.54	0.43
1:P:330:ARG:NH1	3:P:506:HOH:O	2.50	0.43
1:Q:97:LEU:O	1:Q:98:LYS:C	2.61	0.43
1:Q:244:THR:CG2	1:Q:247:GLN:N	2.79	0.43
1:A:149:ALA:HB3	1:A:188:PRO:HA	2.00	0.42
1:A:256:LEU:HD13	1:A:267:ILE:CD1	2.49	0.42
1:B:88:SER:O	1:B:89:GLN:CB	2.62	0.42
1:B:106:ILE:CG2	1:B:142:VAL:HG11	2.48	0.42
1:B:118:THR:HG23	1:B:121:GLU:HG3	2.00	0.42
1:C:128:ASP:HB2	1:D:128:ASP:OD2	2.19	0.42
1:D:82:THR:HG21	3:D:529:HOH:O	2.19	0.42
1:D:92:LEU:O	1:D:93:PHE:C	2.60	0.42
1:G:123:THR:CG2	1:G:165:GLU:HG3	2.43	0.42
1:H:15:LEU:O	1:H:16:SER:C	2.62	0.42
1:I:60:GLU:OE1	1:I:87:ASP:HB2	2.18	0.42
1:J:28:GLY:HA3	1:J:299:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:191:ILE:HA	1:J:192:PRO:HD3	1.83	0.42
1:K:88:SER:O	1:K:89:GLN:HG2	2.16	0.42
1:K:344:HIS:CE1	1:K:348:SER:HB2	2.54	0.42
1:M:98:LYS:HE3	1:M:141:GLY:HA3	2.01	0.42
1:N:123:THR:HG21	1:N:165:GLU:OE2	2.18	0.42
1:O:226:THR:HG23	1:O:227:LEU:N	2.34	0.42
1:P:224:GLU:OE1	1:P:224:GLU:N	2.47	0.42
1:A:298:SER:OG	1:A:299:PHE:N	2.50	0.42
1:B:58:PHE:CD1	1:B:310:LEU:CD1	3.02	0.42
1:C:330:ARG:NE	1:C:330:ARG:HA	2.34	0.42
1:D:267:ILE:HG21	1:D:267:ILE:HD13	1.57	0.42
1:D:350:ALA:O	1:D:354:GLN:N	2.52	0.42
1:E:326:ALA:O	1:E:327:PHE:C	2.60	0.42
1:G:123:THR:O	1:G:124:ILE:HD12	2.19	0.42
1:G:148:ARG:HD2	3:G:516:HOH:O	2.19	0.42
1:G:148:ARG:HA	1:G:187:GLU:HB3	2.01	0.42
1:H:303:ARG:HB3	1:H:356:LEU:CD1	2.49	0.42
1:L:211:ALA:O	1:L:212:VAL:C	2.61	0.42
1:N:119:ASN:C	1:N:119:ASN:OD1	2.60	0.42
1:O:264:VAL:O	1:O:295:TRP:HB3	2.19	0.42
1:P:58:PHE:CE1	1:P:310:LEU:HD13	2.54	0.42
1:P:187:GLU:O	1:P:187:GLU:HG2	2.18	0.42
1:P:275:SER:O	1:P:276:GLU:C	2.60	0.42
1:Q:270:LEU:C	1:Q:270:LEU:HD12	2.44	0.42
1:A:203:TYR:OH	1:D:2:HIS:HA	2.19	0.42
1:C:204:VAL:O	1:C:205:THR:C	2.60	0.42
1:D:354:GLN:HG2	1:D:356:LEU:CD2	2.50	0.42
1:F:109:ASP:HA	1:F:147:TRP:CZ3	2.53	0.42
1:H:172:ARG:HH22	1:H:176:ILE:HD11	1.81	0.42
1:I:177:CYS:HB3	1:I:182:LEU:HB2	2.01	0.42
1:J:209:LEU:HA	1:J:209:LEU:HD23	1.72	0.42
1:K:22:ILE:O	1:K:22:ILE:CG2	2.66	0.42
1:K:244:THR:CG2	1:K:247:GLN:HG3	2.49	0.42
1:L:91:LYS:HD3	1:L:96:ILE:HG13	2.01	0.42
1:O:58:PHE:HE2	1:O:62:LEU:HD11	1.84	0.42
1:P:106:ILE:CG2	1:P:142:VAL:HG11	2.50	0.42
1:R:152:ARG:HH11	1:R:152:ARG:HD3	1.56	0.42
1:A:42:ARG:HD2	1:A:357:PHE:CG	2.53	0.42
1:A:184:PRO:HD2	1:A:225:GLY:O	2.18	0.42
1:A:207:LYS:CE	1:D:2:HIS:NE2	2.69	0.42
1:C:3:ARG:O	1:C:4:PHE:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:CG2	1:C:121:GLU:CB	2.98	0.42
1:C:152:ARG:HH11	1:C:152:ARG:HD3	1.28	0.42
1:E:130:LEU:O	1:E:131:SER:C	2.61	0.42
1:F:201:CYS:SG	1:F:233:VAL:HG13	2.59	0.42
1:H:86:LYS:HD3	1:H:90:GLY:HA2	2.02	0.42
1:J:67:SER:O	1:J:69:ILE:N	2.53	0.42
1:J:75:GLY:HA2	1:J:103:VAL:O	2.20	0.42
1:J:144:PHE:CE1	1:J:185:ILE:HD11	2.54	0.42
1:K:106:ILE:HD12	1:K:107:LYS:H	1.84	0.42
1:K:330:ARG:HA	1:K:330:ARG:HE	1.84	0.42
1:K:344:HIS:CE1	1:K:346:GLY:HA2	2.54	0.42
1:L:48:VAL:HG12	1:L:54:ASN:HD22	1.85	0.42
1:N:1:ALA:O	1:N:3:ARG:NH2	2.52	0.42
1:N:123:THR:CG2	1:N:124:ILE:N	2.53	0.42
1:N:267:ILE:HG21	1:N:267:ILE:HD13	1.39	0.42
1:O:68:SER:C	1:O:70:ASN:N	2.76	0.42
1:R:213:TYR:OH	1:R:228:LEU:HD13	2.19	0.42
1:A:256:LEU:HD13	1:A:267:ILE:HD11	2.01	0.42
1:A:279:ALA:HB1	1:A:301:TYR:CZ	2.55	0.42
1:B:29:ILE:HD13	1:B:29:ILE:HG21	1.73	0.42
1:B:89:GLN:C	1:B:91:LYS:H	2.27	0.42
1:F:8:THR:OG1	1:F:11:GLN:HG3	2.19	0.42
1:I:108:LEU:O	1:I:109:ASP:C	2.58	0.42
1:I:121:GLU:OE1	1:J:1:ALA:HB2	2.20	0.42
1:I:206:GLU:HG2	1:I:255:ALA:HA	2.01	0.42
1:I:313:TRP:HA	1:I:319:ASN:CB	2.50	0.42
1:J:198:LEU:CD1	1:J:234:THR:HA	2.50	0.42
1:K:29:ILE:HG21	1:K:29:ILE:HD13	1.76	0.42
1:L:3:ARG:HB2	1:L:4:PHE:H	1.59	0.42
1:L:295:TRP:O	1:L:296:LYS:C	2.61	0.42
1:O:4:PHE:CZ	1:P:119:ASN:HB2	2.54	0.42
1:P:3:ARG:CD	1:P:4:PHE:H	2.08	0.42
1:Q:44:GLN:OE1	1:Q:44:GLN:HA	2.18	0.42
1:R:119:ASN:O	1:R:152:ARG:NH1	2.36	0.42
1:C:4:PHE:CE1	1:D:119:ASN:HB2	2.54	0.42
1:D:214:LYS:HA	1:D:214:LYS:HD3	1.81	0.42
1:F:33:ASP:CB	1:F:77:ILE:HG22	2.47	0.42
1:F:171:ALA:HA	1:F:216:LEU:CD1	2.49	0.42
1:F:278:ASP:O	1:F:279:ALA:C	2.61	0.42
1:I:8:THR:OG1	1:I:11:GLN:HG3	2.19	0.42
1:I:240:THR:HB	1:N:240:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:VAL:O	1:J:212:VAL:HG23	2.20	0.42
1:K:349:GLY:H	1:O:86:LYS:NZ	2.17	0.42
1:M:172:ARG:O	1:M:176:ILE:HG13	2.19	0.42
1:N:259:THR:O	1:N:261:PRO:HD3	2.20	0.42
1:O:128:ASP:HA	1:P:125:GLN:NE2	2.30	0.42
1:Q:121:GLU:OE2	1:Q:158:PRO:HA	2.20	0.42
1:Q:174:ALA:O	1:Q:178:GLN:HG3	2.19	0.42
1:R:191:ILE:HB	1:R:192:PRO:HD2	2.01	0.42
1:B:48:VAL:HG12	1:B:54:ASN:ND2	2.34	0.42
1:B:284:ASN:OD1	1:B:340:GLY:HA2	2.20	0.42
1:B:330:ARG:HH21	1:B:333:ALA:CB	2.32	0.42
1:C:147:TRP:HB2	1:C:173:TYR:CE1	2.54	0.42
1:C:171:ALA:HB1	1:C:219:HIS:CG	2.55	0.42
1:E:213:TYR:OH	1:E:228:LEU:HD13	2.20	0.42
1:F:250:MET:CE	1:F:291:LEU:HD21	2.49	0.42
1:G:9:GLN:O	1:G:10:GLU:C	2.61	0.42
1:H:44:GLN:OE1	1:H:44:GLN:HA	2.20	0.42
1:K:29:ILE:HB	1:K:300:SER:HA	2.00	0.42
1:N:171:ALA:HB1	1:N:219:HIS:CG	2.54	0.42
1:N:216:LEU:HB3	1:N:221:VAL:HB	2.00	0.42
1:O:231:ASN:HA	1:O:270:LEU:HG	2.01	0.42
1:O:287:ASN:O	1:O:293:LYS:NZ	2.53	0.42
1:P:123:THR:HG21	1:P:165:GLU:OE2	2.19	0.42
1:P:299:PHE:HB2	1:P:301:TYR:CD2	2.55	0.42
1:Q:165:GLU:HB2	3:Q:2003:HOH:O	2.19	0.42
1:R:244:THR:HG23	1:R:246:GLU:OE1	2.20	0.42
1:A:344:HIS:ND1	1:A:344:HIS:N	2.65	0.42
1:B:1:ALA:N	1:B:220:HIS:HE1	2.18	0.42
1:B:320:LYS:O	1:B:324:GLN:HG3	2.20	0.42
1:D:354:GLN:HB3	1:D:355:SER:H	1.56	0.42
1:E:231:ASN:HA	1:E:270:LEU:HG	2.01	0.42
1:G:93:PHE:O	1:G:94:ARG:C	2.59	0.42
1:L:294:PRO:HD2	1:L:295:TRP:CZ2	2.55	0.42
1:L:320:LYS:O	1:L:324:GLN:HG3	2.20	0.42
1:M:2:HIS:O	1:M:4:PHE:HD1	2.02	0.42
1:N:294:PRO:HD2	1:N:295:TRP:CZ2	2.55	0.42
1:O:105:GLY:HA2	1:O:144:PHE:O	2.20	0.42
1:Q:33:ASP:O	1:Q:107:LYS:HE3	2.19	0.42
1:R:118:THR:HG23	1:R:121:GLU:H	1.85	0.42
1:B:12:LYS:O	1:B:13:LYS:C	2.60	0.42
1:C:94:ARG:O	1:C:98:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:GLU:OE1	3:F:402:HOH:O	2.21	0.42
1:F:259:THR:O	1:F:261:PRO:HD3	2.19	0.42
1:G:69:ILE:C	1:G:71:GLN:H	2.28	0.42
1:H:83:LEU:HG	1:H:83:LEU:O	2.20	0.42
1:I:85:GLN:O	1:I:92:LEU:HD23	2.20	0.42
1:K:156:GLN:O	1:L:1:ALA:HB2	2.20	0.42
1:L:22:ILE:O	1:L:22:ILE:HG22	2.20	0.42
1:L:201:CYS:O	1:L:202:GLN:C	2.62	0.42
1:M:1:ALA:HA	1:N:159:SER:HB3	2.01	0.42
1:M:187:GLU:O	1:M:187:GLU:HG2	2.19	0.42
1:N:106:ILE:HD12	1:N:106:ILE:HA	1.82	0.42
1:N:325:GLU:O	1:N:328:MET:HB3	2.19	0.42
1:O:77:ILE:HG21	1:O:77:ILE:HD13	1.74	0.42
1:P:115:LEU:HD12	1:P:115:LEU:HA	1.94	0.42
1:Q:43:LEU:HD23	1:Q:43:LEU:HA	1.86	0.42
1:Q:130:LEU:O	1:Q:133:ARG:HB2	2.20	0.42
1:A:51:THR:O	1:A:52:GLU:C	2.60	0.42
1:A:80:HIS:O	1:A:81:GLU:C	2.61	0.42
1:A:118:THR:HG23	1:A:121:GLU:HB2	2.00	0.42
1:A:172:ARG:NH2	1:A:176:ILE:HD11	2.35	0.42
1:B:325:GLU:O	1:B:326:ALA:C	2.62	0.42
1:E:9:GLN:HA	1:E:9:GLN:NE2	2.35	0.42
1:G:65:VAL:O	1:G:66:ASP:HB3	2.20	0.42
1:G:250:MET:CE	1:G:291:LEU:HD22	2.50	0.42
1:H:189:GLU:CD	1:H:191:ILE:HD11	2.45	0.42
1:H:306:GLN:O	1:H:307:ALA:C	2.61	0.42
1:I:66:ASP:OD1	1:I:67:SER:CA	2.68	0.42
1:J:44:GLN:O	1:J:47:LYS:N	2.45	0.42
1:J:345:THR:O	1:J:345:THR:HG23	2.19	0.42
1:M:4:PHE:CE1	1:N:119:ASN:HB2	2.55	0.42
1:N:59:ARG:HB3	1:N:63:PHE:CE1	2.55	0.42
1:N:249:ALA:HB1	1:N:286:ILE:HA	2.02	0.42
1:N:321:GLU:O	1:N:322:ALA:C	2.59	0.42
1:P:87:ASP:OD2	1:P:91:LYS:HB3	2.20	0.42
1:P:222:TYR:O	1:P:223:LEU:C	2.63	0.42
1:P:332:MET:HG2	3:P:552:HOH:O	2.19	0.42
1:Q:87:ASP:HB3	1:Q:89:GLN:H	1.84	0.42
1:R:28:GLY:HA3	1:R:299:PHE:CZ	2.55	0.42
1:R:271:SER:O	1:R:272:GLY:C	2.63	0.42
1:B:18:ILE:HB	1:B:183:VAL:HG23	2.02	0.41
1:B:194:GLY:O	1:B:238:ALA:N	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:HG22	1:B:253:VAL:N	2.25	0.41
1:B:320:LYS:O	1:B:321:GLU:C	2.61	0.41
1:C:240:THR:O	1:C:242:LYS:HE3	2.19	0.41
1:D:50:ASN:ND2	1:D:50:ASN:C	2.78	0.41
1:D:84:TYR:OH	1:D:140:ASP:OD2	2.28	0.41
1:E:329:LYS:CE	1:E:346:GLY:O	2.56	0.41
1:F:147:TRP:CD1	1:F:170:LEU:HD23	2.55	0.41
1:H:324:GLN:O	1:H:325:GLU:C	2.62	0.41
1:H:329:LYS:NZ	1:H:347:SER:O	2.46	0.41
1:I:12:LYS:O	1:I:13:LYS:C	2.63	0.41
1:I:115:LEU:HD13	1:I:123:THR:OG1	2.20	0.41
1:I:152:ARG:HH11	1:I:152:ARG:HD3	1.33	0.41
1:K:146:LYS:HE2	1:K:187:GLU:OE1	2.19	0.41
1:L:33:ASP:OD2	1:L:107:LYS:HB2	2.20	0.41
1:L:229:LYS:NZ	1:L:300:SER:OG	2.21	0.41
1:M:117:GLY:O	1:N:3:ARG:CD	2.67	0.41
1:N:3:ARG:CD	1:N:3:ARG:H	2.32	0.41
1:N:324:GLN:O	1:N:328:MET:HB2	2.20	0.41
1:O:8:THR:O	1:O:9:GLN:C	2.60	0.41
1:P:216:LEU:HD12	1:P:216:LEU:HA	1.68	0.41
1:R:123:THR:HG22	1:R:124:ILE:H	1.85	0.41
1:R:313:TRP:CE2	1:R:315:GLY:HA2	2.54	0.41
1:A:4:PHE:CE1	1:B:119:ASN:HB2	2.55	0.41
1:B:28:GLY:HA3	1:B:299:PHE:CE2	2.55	0.41
1:B:42:ARG:HH11	1:B:42:ARG:HD2	1.54	0.41
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.73	0.41
1:C:255:ALA:O	1:C:256:LEU:C	2.63	0.41
1:C:267:ILE:HG21	1:C:267:ILE:HD13	1.47	0.41
1:F:17:GLU:O	1:F:18:ILE:C	2.60	0.41
1:G:15:LEU:HD23	1:G:15:LEU:HA	1.85	0.41
1:G:197:ASP:OD1	1:G:197:ASP:C	2.63	0.41
1:H:244:THR:HG23	1:H:247:GLN:CD	2.45	0.41
1:H:276:GLU:HG3	1:H:352:SER:HB3	2.03	0.41
1:I:72:SER:HB3	1:I:331:ALA:O	2.20	0.41
1:I:160:SER:O	1:I:161:LEU:C	2.62	0.41
1:J:69:ILE:O	1:J:69:ILE:HG13	2.21	0.41
1:J:244:THR:O	1:J:245:PRO:C	2.61	0.41
1:K:227:LEU:HD23	1:K:227:LEU:HA	1.95	0.41
1:M:79:PHE:O	1:M:80:HIS:C	2.63	0.41
1:O:294:PRO:HD2	1:O:295:TRP:CZ2	2.55	0.41
1:Q:131:SER:O	1:Q:132:GLU:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:147:TRP:CD1	1:Q:147:TRP:C	2.97	0.41
1:Q:156:GLN:HE22	1:R:3:ARG:HE	1.40	0.41
1:R:244:THR:N	1:R:247:GLN:OE1	2.53	0.41
1:B:138:LYS:NZ	1:B:143:ASP:OD1	2.40	0.41
1:D:158:PRO:HG3	1:D:204:VAL:HG13	2.03	0.41
1:F:306:GLN:O	1:F:307:ALA:C	2.62	0.41
1:G:3:ARG:CG	1:H:156:GLN:HE22	2.32	0.41
1:H:187:GLU:HG3	1:H:229:LYS:O	2.21	0.41
1:H:250:MET:HE3	1:H:291:LEU:CD2	2.50	0.41
1:I:118:THR:HG22	1:I:121:GLU:H	1.78	0.41
1:I:156:GLN:CB	1:J:1:ALA:HB1	2.47	0.41
1:J:107:LYS:HB2	1:J:107:LYS:HE2	1.79	0.41
1:K:244:THR:CG2	1:K:246:GLU:HB2	2.50	0.41
1:M:44:GLN:O	1:M:45:ARG:C	2.61	0.41
1:M:176:ILE:O	1:M:177:CYS:C	2.64	0.41
1:M:191:ILE:HA	1:M:192:PRO:HD3	1.84	0.41
1:N:66:ASP:OD1	1:N:67:SER:N	2.54	0.41
1:O:335:CYS:O	1:O:339:LYS:HD2	2.20	0.41
1:P:79:PHE:O	1:P:80:HIS:C	2.62	0.41
1:P:166:ASN:O	1:P:167:ALA:C	2.63	0.41
1:Q:224:GLU:HB3	3:Q:2026:HOH:O	2.19	0.41
1:A:3:ARG:NH2	1:B:156:GLN:NE2	2.69	0.41
1:B:207:LYS:HD3	1:C:2:HIS:CE1	2.56	0.41
1:B:232:MET:HE2	1:B:286:ILE:CD1	2.49	0.41
1:B:280:THR:O	1:B:281:LEU:C	2.59	0.41
1:C:102:ILE:HG21	1:C:102:ILE:HD13	1.82	0.41
1:C:148:ARG:HH21	1:C:148:ARG:HD3	1.67	0.41
1:D:182:LEU:HD23	1:D:182:LEU:HA	1.82	0.41
1:D:203:TYR:O	1:D:204:VAL:C	2.62	0.41
1:F:144:PHE:HB2	1:F:183:VAL:O	2.21	0.41
1:I:2:HIS:NE2	1:L:200:HIS:CE1	2.89	0.41
1:I:66:ASP:OD1	1:I:67:SER:N	2.53	0.41
1:J:92:LEU:O	1:J:93:PHE:C	2.64	0.41
1:L:3:ARG:HG2	1:L:3:ARG:NH1	2.35	0.41
1:N:78:LEU:HA	1:N:78:LEU:HD23	1.89	0.41
1:Q:18:ILE:HD13	1:Q:18:ILE:HG21	1.79	0.41
1:R:3:ARG:HB2	1:R:4:PHE:H	1.68	0.41
1:A:42:ARG:O	1:A:45:ARG:HB2	2.21	0.41
1:A:44:GLN:O	1:A:45:ARG:C	2.63	0.41
1:B:186:VAL:O	1:B:186:VAL:HG12	2.20	0.41
1:C:106:ILE:O	1:C:107:LYS:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ARG:HD2	1:C:172:ARG:HA	1.81	0.41
1:D:18:ILE:O	1:D:19:ALA:C	2.62	0.41
1:D:326:ALA:O	1:D:327:PHE:C	2.61	0.41
1:E:286:ILE:HG22	1:E:297:LEU:HD13	2.03	0.41
1:F:123:THR:HG21	1:F:165:GLU:HG3	2.02	0.41
1:F:354:GLN:HG2	1:F:355:SER:O	2.21	0.41
1:G:322:ALA:O	1:G:323:THR:C	2.63	0.41
1:H:228:LEU:HG	1:H:230:PRO:HD3	2.02	0.41
1:I:4:PHE:CE1	1:J:119:ASN:HB2	2.55	0.41
1:I:119:ASN:HB2	1:J:4:PHE:CE1	2.56	0.41
1:J:93:PHE:HA	1:J:96:ILE:HD12	2.03	0.41
1:K:51:THR:HG22	1:K:54:ASN:CB	2.50	0.41
1:K:106:ILE:HG23	1:K:108:LEU:HG	2.01	0.41
1:K:191:ILE:HD12	1:K:191:ILE:HG23	1.80	0.41
1:M:87:ASP:OD1	1:M:87:ASP:C	2.63	0.41
1:M:105:GLY:HA2	1:M:144:PHE:O	2.21	0.41
1:N:63:PHE:O	1:N:100:LYS:NZ	2.53	0.41
1:P:231:ASN:ND2	3:P:505:HOH:O	2.53	0.41
1:R:70:ASN:HD22	1:R:70:ASN:HA	1.38	0.41
1:B:312:ALA:HB1	1:B:322:ALA:HB1	2.02	0.41
1:C:61:ILE:CG2	1:C:324:GLN:HG2	2.50	0.41
1:C:324:GLN:O	1:C:328:MET:HB2	2.21	0.41
1:D:121:GLU:CG	1:D:157:CYS:SG	3.08	0.41
1:E:36:VAL:HG13	1:E:55:ARG:NH1	2.36	0.41
1:G:250:MET:HE1	1:G:291:LEU:CD2	2.50	0.41
1:H:8:THR:O	1:H:9:GLN:C	2.64	0.41
1:H:123:THR:CG2	1:H:165:GLU:HG3	2.50	0.41
1:H:158:PRO:O	1:H:158:PRO:CG	2.69	0.41
1:I:184:PRO:HD2	1:I:225:GLY:O	2.20	0.41
1:K:106:ILE:HD12	1:K:106:ILE:HA	1.74	0.41
1:K:187:GLU:HB2	1:K:229:LYS:HB3	2.01	0.41
1:K:249:ALA:HB1	1:K:286:ILE:HA	2.02	0.41
1:L:267:ILE:HD12	1:L:267:ILE:HG21	1.82	0.41
1:N:195:ASP:O	1:N:196:HIS:C	2.63	0.41
1:N:306:GLN:O	1:N:309:ALA:HB3	2.20	0.41
1:O:294:PRO:HD2	1:O:295:TRP:CE2	2.54	0.41
1:P:121:GLU:OE2	1:P:158:PRO:HA	2.21	0.41
1:P:276:GLU:HB2	1:P:352:SER:CB	2.46	0.41
1:Q:123:THR:CG2	1:Q:165:GLU:HG3	2.51	0.41
1:Q:129:GLY:N	1:R:125:GLN:HE22	1.96	0.41
1:R:208:VAL:O	1:R:212:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:213:TYR:O	1:R:214:LYS:C	2.63	0.41
1:A:144:PHE:HB2	1:A:183:VAL:O	2.21	0.41
1:A:280:THR:HG22	1:A:342:TYR:CD2	2.55	0.41
1:C:1:ALA:CB	1:D:119:ASN:H	2.33	0.41
1:D:49:GLU:O	1:D:51:THR:N	2.52	0.41
1:D:106:ILE:HG23	1:D:108:LEU:HG	2.03	0.41
1:D:230:PRO:O	1:D:270:LEU:HG	2.20	0.41
1:D:335:CYS:O	1:D:338:ALA:HB3	2.21	0.41
1:E:275:SER:O	1:E:276:GLU:C	2.58	0.41
1:F:86:LYS:HG3	1:F:92:LEU:HD23	2.02	0.41
1:I:65:VAL:HG12	1:I:69:ILE:HG21	2.02	0.41
1:I:67:SER:HB3	1:I:68:SER:H	0.83	0.41
1:J:20:GLN:HG2	3:J:563:HOH:O	2.20	0.41
1:L:56:ARG:O	1:L:56:ARG:HG2	2.20	0.41
1:L:58:PHE:O	1:L:59:ARG:C	2.61	0.41
1:O:172:ARG:HD2	1:O:172:ARG:HH11	1.68	0.41
1:P:51:THR:HG23	1:P:53:GLU:N	2.35	0.41
1:P:191:ILE:HG22	1:P:193:ASP:HB2	2.02	0.41
1:P:227:LEU:HD23	1:P:227:LEU:HA	1.96	0.41
1:Q:77:ILE:HD13	1:Q:77:ILE:HG21	1.66	0.41
1:Q:144:PHE:HB2	1:Q:183:VAL:O	2.20	0.41
1:A:123:THR:C	1:A:124:ILE:HG13	2.46	0.41
1:A:129:GLY:H	1:B:125:GLN:HE22	1.68	0.41
1:A:192:PRO:O	1:A:193:ASP:C	2.63	0.41
1:B:207:LYS:CD	1:C:2:HIS:NE2	2.80	0.41
3:B:408:HOH:O	1:C:258:ARG:HD2	2.20	0.41
1:C:12:LYS:HG2	1:C:222:TYR:CD1	2.56	0.41
1:C:123:THR:HG23	1:C:165:GLU:HG3	2.01	0.41
1:D:17:GLU:O	1:D:18:ILE:C	2.59	0.41
1:D:346:GLY:O	1:D:347:SER:C	2.64	0.41
1:E:36:VAL:HG22	1:E:55:ARG:NH2	2.36	0.41
1:F:138:LYS:NZ	1:F:181:GLY:O	2.39	0.41
1:I:8:THR:HG23	1:I:11:GLN:OE1	2.21	0.41
1:J:223:LEU:O	1:J:226:THR:CG2	2.68	0.41
1:J:342:TYR:OH	1:J:345:THR:CA	2.69	0.41
1:L:244:THR:HG23	1:L:246:GLU:N	2.36	0.41
1:M:106:ILE:O	1:M:106:ILE:CG2	2.68	0.41
1:N:183:VAL:O	1:N:183:VAL:HG12	2.18	0.41
1:O:24:ALA:O	1:O:25:ASN:CB	2.60	0.41
1:Q:244:THR:O	1:Q:245:PRO:C	2.64	0.41
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:HG23	1:A:191:ILE:HD13	1.78	0.41
1:B:26:GLY:HA3	1:B:339:LYS:HD2	2.03	0.41
1:B:39:MET:O	1:B:39:MET:HG3	2.20	0.41
1:B:324:GLN:O	1:B:328:MET:HB2	2.21	0.41
1:C:1:ALA:HB3	1:D:119:ASN:N	2.36	0.41
1:C:75:GLY:HA2	1:C:103:VAL:O	2.20	0.41
1:C:143:ASP:O	1:C:182:LEU:HA	2.21	0.41
1:C:244:THR:CG2	1:C:247:GLN:CG	2.82	0.41
1:C:249:ALA:HB1	1:C:286:ILE:HA	2.03	0.41
1:E:244:THR:O	1:E:245:PRO:C	2.62	0.41
1:F:43:LEU:CD1	1:F:50:ASN:HA	2.51	0.41
1:G:58:PHE:CE2	1:G:310:LEU:HD13	2.56	0.41
1:H:86:LYS:CG	1:H:90:GLY:HA2	2.50	0.41
1:H:87:ASP:OD1	1:H:96:ILE:HD11	2.20	0.41
1:H:233:VAL:O	1:H:248:VAL:HG13	2.21	0.41
1:H:237:HIS:NE2	1:H:357:PHE:CD2	2.89	0.41
1:H:354:GLN:HG2	1:H:356:LEU:HD23	1.98	0.41
1:I:155:ASP:O	1:I:156:GLN:HB2	2.21	0.41
1:J:171:ALA:HA	1:J:216:LEU:HD12	2.02	0.41
1:J:223:LEU:HD23	1:J:223:LEU:HA	1.88	0.41
1:J:228:LEU:HD23	1:J:267:ILE:HD12	2.02	0.41
1:K:50:ASN:HD21	1:K:55:ARG:HD3	1.85	0.41
1:K:154:ALA:HB3	1:K:157:CYS:HB2	2.03	0.41
1:K:276:GLU:HB3	1:K:330:ARG:HD3	2.03	0.41
1:L:104:VAL:O	1:L:142:VAL:HG13	2.21	0.41
1:L:121:GLU:OE2	1:L:158:PRO:HA	2.20	0.41
1:L:154:ALA:O	1:L:155:ASP:C	2.63	0.41
1:L:217:ASN:ND2	1:L:217:ASN:C	2.78	0.41
1:L:256:LEU:HD13	1:L:267:ILE:CD1	2.51	0.41
1:L:276:GLU:HG2	1:L:304:ALA:O	2.21	0.41
1:M:81:GLU:O	1:M:85:GLN:HG3	2.21	0.41
1:M:125:GLN:NE2	1:N:129:GLY:H	2.19	0.41
1:M:129:GLY:O	1:M:130:LEU:C	2.64	0.41
1:M:150:VAL:HG13	1:M:191:ILE:CG1	2.51	0.41
1:M:174:ALA:O	1:M:178:GLN:HG3	2.21	0.41
1:M:244:THR:CG2	1:M:247:GLN:HG3	2.47	0.41
1:N:203:TYR:OH	1:O:2:HIS:HA	2.20	0.41
1:O:119:ASN:HB3	1:O:157:CYS:SG	2.61	0.41
1:P:51:THR:HG23	1:P:53:GLU:H	1.86	0.41
1:P:153:ILE:HG12	1:P:204:VAL:HG21	2.02	0.41
1:Q:73:ILE:HD13	1:Q:73:ILE:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:244:THR:HG22	1:Q:247:GLN:HB2	2.02	0.41
1:R:276:GLU:OE1	1:R:330:ARG:HD2	2.21	0.41
1:A:12:LYS:HG2	1:A:222:TYR:CE1	2.56	0.41
1:A:274:MET:HA	3:A:509:HOH:O	2.20	0.41
1:C:22:ILE:HD13	1:C:22:ILE:HG21	1.91	0.41
1:C:28:GLY:O	1:C:74:GLY:N	2.50	0.41
1:C:61:ILE:HG23	1:C:324:GLN:CG	2.51	0.41
1:C:115:LEU:HD22	1:C:122:THR:C	2.46	0.41
1:C:156:GLN:HE22	1:D:3:ARG:CD	2.31	0.41
1:C:244:THR:O	1:C:247:GLN:N	2.47	0.41
1:C:313:TRP:HA	1:C:323:THR:OG1	2.20	0.41
1:C:313:TRP:CH2	1:C:315:GLY:HA2	2.52	0.41
1:D:244:THR:HG23	1:D:246:GLU:N	2.29	0.41
1:E:118:THR:HG23	1:E:121:GLU:H	1.84	0.41
1:G:18:ILE:HD13	1:G:18:ILE:HG21	1.83	0.41
1:H:12:LYS:HG2	1:H:222:TYR:CE1	2.56	0.41
1:H:152:ARG:HH11	1:H:152:ARG:HD3	1.49	0.41
1:I:28:GLY:HA3	1:I:299:PHE:CE1	2.56	0.41
1:I:156:GLN:HE22	1:J:3:ARG:CG	2.32	0.41
1:J:142:VAL:HG12	1:J:143:ASP:N	2.36	0.41
1:K:39:MET:O	1:K:40:GLY:C	2.60	0.41
1:M:4:PHE:O	1:N:117:GLY:HA2	2.21	0.41
1:M:223:LEU:O	1:M:226:THR:HB	2.21	0.41
1:M:224:GLU:OE2	1:P:258:ARG:NH1	2.44	0.41
1:N:172:ARG:O	1:N:173:TYR:C	2.62	0.41
1:N:339:LYS:O	1:N:341:GLN:HG3	2.20	0.41
1:P:281:LEU:H	1:P:281:LEU:HG	1.69	0.41
1:A:3:ARG:HD2	1:A:3:ARG:N	2.32	0.40
1:A:94:ARG:HD2	1:A:140:ASP:O	2.20	0.40
1:C:78:LEU:O	1:C:106:ILE:HD12	2.21	0.40
1:C:198:LEU:HD22	1:C:243:TYR:CD2	2.56	0.40
1:D:321:GLU:O	1:D:322:ALA:C	2.60	0.40
1:F:244:THR:HA	1:F:245:PRO:HD3	1.98	0.40
1:G:313:TRP:CE2	1:G:315:GLY:CA	3.01	0.40
1:G:313:TRP:CD2	1:G:315:GLY:CA	3.04	0.40
1:H:89:GLN:HB2	1:H:89:GLN:HE21	1.70	0.40
1:H:273:GLY:CA	1:H:357:PHE:HA	2.51	0.40
1:I:66:ASP:O	1:I:69:ILE:HG22	2.20	0.40
1:I:124:ILE:HG21	1:I:147:TRP:CE2	2.55	0.40
1:J:349:GLY:O	1:J:351:ALA:N	2.53	0.40
1:O:138:LYS:HD2	3:O:505:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:264:VAL:HA	1:P:265:PRO:HD2	1.84	0.40
1:R:2:HIS:O	1:R:4:PHE:HD1	2.03	0.40
1:B:137:TYR:O	1:B:138:LYS:C	2.63	0.40
1:C:128:ASP:OD2	1:D:128:ASP:HB2	2.21	0.40
1:D:216:LEU:HD12	1:D:216:LEU:HA	1.66	0.40
1:D:249:ALA:HB2	1:D:285:ALA:HB3	2.02	0.40
1:E:18:ILE:HD13	1:E:143:ASP:HB3	2.03	0.40
1:H:285:ALA:O	1:H:286:ILE:C	2.64	0.40
1:I:294:PRO:HD2	1:I:295:TRP:CE2	2.55	0.40
1:J:184:PRO:HD2	1:J:225:GLY:O	2.22	0.40
1:K:58:PHE:CE2	1:K:310:LEU:HD13	2.55	0.40
1:N:36:VAL:HG13	1:N:55:ARG:CZ	2.51	0.40
1:O:43:LEU:O	1:O:44:GLN:C	2.65	0.40
1:O:78:LEU:O	1:O:106:ILE:HA	2.21	0.40
1:P:343:VAL:O	1:P:344:HIS:HB3	2.20	0.40
1:Q:156:GLN:HB3	1:R:1:ALA:HA	2.01	0.40
1:Q:191:ILE:HG22	1:Q:193:ASP:HB2	2.02	0.40
1:R:86:LYS:HD3	1:R:90:GLY:HA2	2.03	0.40
1:A:116:ALA:HB3	3:A:507:HOH:O	2.20	0.40
1:B:51:THR:HG22	1:B:54:ASN:CA	2.49	0.40
1:B:166:ASN:O	1:B:167:ALA:C	2.60	0.40
1:B:192:PRO:O	1:B:193:ASP:C	2.64	0.40
1:D:130:LEU:O	1:D:131:SER:C	2.61	0.40
1:E:65:VAL:O	1:E:66:ASP:C	2.61	0.40
1:F:95:ASN:O	1:F:96:ILE:C	2.62	0.40
1:F:118:THR:CG2	1:F:121:GLU:H	2.35	0.40
1:G:244:THR:HG22	1:G:247:GLN:CG	2.51	0.40
1:G:260:VAL:HA	1:G:261:PRO:HD3	1.86	0.40
1:I:240:THR:O	1:I:242:LYS:HE3	2.22	0.40
1:J:277:GLU:O	1:J:278:ASP:C	2.59	0.40
1:K:226:THR:HG23	3:K:512:HOH:O	2.08	0.40
1:L:196:HIS:O	1:L:239:CYS:HB2	2.21	0.40
1:O:73:ILE:HD13	1:O:73:ILE:HA	1.86	0.40
1:O:337:ALA:O	1:O:338:ALA:C	2.64	0.40
1:P:33:ASP:O	1:P:34:GLU:C	2.62	0.40
1:P:198:LEU:HD22	1:P:243:TYR:CD2	2.56	0.40
1:Q:189:GLU:HB2	1:Q:270:LEU:CD2	2.51	0.40
1:R:299:PHE:HB2	1:R:301:TYR:CD1	2.56	0.40
1:B:214:LYS:O	1:B:215:ALA:C	2.63	0.40
1:C:155:ASP:OD1	1:C:156:GLN:HG3	2.21	0.40
1:D:250:MET:O	1:D:254:THR:OG1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:LEU:HD23	1:F:227:LEU:HA	1.84	0.40
1:F:344:HIS:CD2	1:F:345:THR:N	2.89	0.40
1:G:161:LEU:HD11	1:H:219:HIS:CE1	2.56	0.40
1:H:25:ASN:H	1:H:27:LYS:H	1.69	0.40
1:H:276:GLU:HG2	1:H:304:ALA:O	2.21	0.40
1:I:1:ALA:HB2	1:J:159:SER:HB3	2.03	0.40
1:J:354:GLN:O	1:J:354:GLN:HG2	2.20	0.40
1:K:120:LYS:CB	1:K:152:ARG:HH12	2.33	0.40
1:L:118:THR:CG2	1:L:121:GLU:CB	2.99	0.40
1:L:118:THR:HG21	1:L:121:GLU:CB	2.51	0.40
1:L:136:GLN:HE21	1:L:136:GLN:HB2	1.61	0.40
1:M:18:ILE:HG21	1:M:18:ILE:HD13	1.79	0.40
1:M:21:SER:OG	1:M:22:ILE:N	2.55	0.40
1:N:187:GLU:HG3	1:N:229:LYS:O	2.21	0.40
1:N:231:ASN:HA	1:N:270:LEU:HG	2.02	0.40
1:O:4:PHE:CD1	1:P:119:ASN:HB2	2.56	0.40
1:O:174:ALA:O	1:O:175:SER:C	2.65	0.40
1:P:133:ARG:O	1:P:137:TYR:CD2	2.75	0.40
1:R:216:LEU:O	1:R:217:ASN:C	2.62	0.40
1:A:229:LYS:HA	1:A:268:CYS:O	2.21	0.40
1:B:28:GLY:CA	1:B:299:PHE:CZ	3.05	0.40
1:B:58:PHE:HE2	1:B:62:LEU:HD11	1.85	0.40
1:E:12:LYS:HE2	1:E:222:TYR:CD1	2.56	0.40
1:E:163:ILE:O	1:E:164:GLN:C	2.64	0.40
1:E:223:LEU:HD23	1:E:223:LEU:HA	1.69	0.40
1:F:349:GLY:O	1:F:350:ALA:C	2.65	0.40
1:G:119:ASN:N	1:H:1:ALA:H3	2.14	0.40
1:G:330:ARG:HA	1:G:330:ARG:NE	2.34	0.40
1:H:69:ILE:C	1:H:71:GLN:H	2.30	0.40
1:I:49:GLU:O	1:I:51:THR:N	2.54	0.40
1:I:66:ASP:OD1	1:I:67:SER:CB	2.70	0.40
1:J:267:ILE:HD13	1:J:267:ILE:HG21	1.85	0.40
1:K:63:PHE:CD2	1:K:63:PHE:N	2.87	0.40
1:N:250:MET:O	1:N:254:THR:OG1	2.23	0.40
1:O:163:ILE:HD13	1:O:163:ILE:HG21	1.87	0.40
1:O:271:SER:HB2	1:O:274:MET:HE3	2.03	0.40
1:Q:118:THR:HG23	1:Q:119:ASN:N	2.35	0.40
1:R:89:GLN:O	1:R:89:GLN:HG3	2.22	0.40
1:R:147:TRP:HB3	1:R:173:TYR:CE2	2.56	0.40
1:R:192:PRO:O	1:R:193:ASP:C	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	358/363 (99%)	324 (90%)	27 (8%)	7 (2%)	6	10
1	B	346/363 (95%)	300 (87%)	35 (10%)	11 (3%)	3	4
1	C	343/363 (94%)	317 (92%)	22 (6%)	4 (1%)	10	20
1	D	354/363 (98%)	319 (90%)	24 (7%)	11 (3%)	3	5
1	E	344/363 (95%)	308 (90%)	25 (7%)	11 (3%)	3	4
1	F	351/363 (97%)	315 (90%)	25 (7%)	11 (3%)	3	5
1	G	342/363 (94%)	311 (91%)	25 (7%)	6 (2%)	6	12
1	H	355/363 (98%)	319 (90%)	22 (6%)	14 (4%)	2	3
1	I	342/363 (94%)	300 (88%)	34 (10%)	8 (2%)	5	8
1	J	354/363 (98%)	320 (90%)	24 (7%)	10 (3%)	4	6
1	K	352/363 (97%)	325 (92%)	22 (6%)	5 (1%)	9	17
1	L	342/363 (94%)	307 (90%)	30 (9%)	5 (2%)	8	16
1	M	358/363 (99%)	318 (89%)	29 (8%)	11 (3%)	3	5
1	N	342/363 (94%)	307 (90%)	29 (8%)	6 (2%)	6	12
1	O	342/363 (94%)	305 (89%)	33 (10%)	4 (1%)	10	20
1	P	358/363 (99%)	328 (92%)	23 (6%)	7 (2%)	6	10
1	Q	342/363 (94%)	319 (93%)	18 (5%)	5 (2%)	8	16
1	R	342/363 (94%)	316 (92%)	23 (7%)	3 (1%)	14	27
All	All	6267/6534 (96%)	5658 (90%)	470 (8%)	139 (2%)	5	9

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	3	ARG
1	A	87	ASP
1	A	357	PHE

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Mol	Chain	Res	Type
1	B	69	ILE
1	B	342	TYR
1	B	345	THR
1	C	272	GLY
1	D	89	GLN
1	D	90	GLY
1	D	354	GLN
1	E	2	HIS
1	E	89	GLN
1	E	196	HIS
1	E	345	THR
1	E	350	ALA
1	E	352	SER
1	F	345	THR
1	F	352	SER
1	F	353	THR
1	F	355	SER
1	H	3	ARG
1	H	89	GLN
1	H	90	GLY
1	H	344	HIS
1	H	345	THR
1	H	346	GLY
1	H	347	SER
1	H	350	ALA
1	H	354	GLN
1	I	3	ARG
1	I	67	SER
1	I	69	ILE
1	I	272	GLY
1	J	3	ARG
1	J	196	HIS
1	J	345	THR
1	J	351	ALA
1	K	346	GLY
1	L	3	ARG
1	L	272	GLY
1	M	3	ARG
1	M	67	SER
1	M	68	SER
1	M	70	ASN
1	M	344	HIS

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Mol	Chain	Res	Type
1	M	353	THR
1	O	2	HIS
1	O	272	GLY
1	O	343	VAL
1	P	2	HIS
1	P	3	ARG
1	Q	87	ASP
1	R	3	ARG
1	A	154	ALA
1	A	344	HIS
1	B	68	SER
1	B	70	ASN
1	B	90	GLY
1	B	272	GLY
1	B	346	GLY
1	B	347	SER
1	C	3	ARG
1	C	87	ASP
1	C	344	HIS
1	D	70	ASN
1	D	87	ASP
1	D	346	GLY
1	D	347	SER
1	D	355	SER
1	E	67	SER
1	E	347	SER
1	F	70	ASN
1	F	272	GLY
1	G	2	HIS
1	G	65	VAL
1	G	67	SER
1	G	70	ASN
1	G	272	GLY
1	H	2	HIS
1	H	67	SER
1	H	272	GLY
1	H	355	SER
1	J	68	SER
1	J	272	GLY
1	J	347	SER
1	J	348	SER
1	K	89	GLN

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Mol	Chain	Res	Type
1	K	348	SER
1	M	272	GLY
1	M	352	SER
1	N	3	ARG
1	N	65	VAL
1	N	69	ILE
1	N	87	ASP
1	N	272	GLY
1	O	320	LYS
1	Q	3	ARG
1	Q	272	GLY
1	R	272	GLY
1	B	67	SER
1	B	89	GLN
1	D	3	ARG
1	F	351	ALA
1	G	66	ASP
1	K	347	SER
1	M	345	THR
1	M	355	SER
1	P	355	SER
1	Q	2	HIS
1	D	344	HIS
1	F	350	ALA
1	I	80	HIS
1	I	224	GLU
1	P	87	ASP
1	P	230	PRO
1	R	196	HIS
1	D	188	PRO
1	E	164	GLN
1	F	274	MET
1	H	196	HIS
1	J	355	SER
1	L	70	ASN
1	N	4	PHE
1	F	188	PRO
1	L	320	LYS
1	F	191	ILE
1	A	230	PRO
1	E	188	PRO
1	I	4	PHE

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Mol	Chain	Res	Type
1	I	343	VAL
1	L	46	ILE
1	Q	188	PRO
1	E	163	ILE
1	K	230	PRO
1	P	188	PRO
1	J	343	VAL
1	P	272	GLY
1	M	314	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/290 (99%)	245 (85%)	42 (15%)	3	6
1	B	279/290 (96%)	237 (85%)	42 (15%)	3	5
1	C	277/290 (96%)	231 (83%)	46 (17%)	2	4
1	D	284/290 (98%)	248 (87%)	36 (13%)	4	9
1	E	282/290 (97%)	244 (86%)	38 (14%)	4	8
1	F	282/290 (97%)	236 (84%)	46 (16%)	2	4
1	G	276/290 (95%)	234 (85%)	42 (15%)	3	5
1	H	285/290 (98%)	241 (85%)	44 (15%)	2	5
1	I	276/290 (95%)	231 (84%)	45 (16%)	2	4
1	J	284/290 (98%)	247 (87%)	37 (13%)	4	8
1	K	283/290 (98%)	246 (87%)	37 (13%)	4	8
1	L	276/290 (95%)	234 (85%)	42 (15%)	3	5
1	M	287/290 (99%)	249 (87%)	38 (13%)	4	8
1	N	276/290 (95%)	240 (87%)	36 (13%)	4	8
1	O	276/290 (95%)	234 (85%)	42 (15%)	3	5
1	P	287/290 (99%)	250 (87%)	37 (13%)	4	9
1	Q	276/290 (95%)	241 (87%)	35 (13%)	4	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	276/290 (95%)	241 (87%)	35 (13%)	4	9
All	All	5049/5220 (97%)	4329 (86%)	720 (14%)	3	6

All (720) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	10	GLU
1	A	25	ASN
1	A	45	ARG
1	A	51	THR
1	A	65	VAL
1	A	69	ILE
1	A	81	GLU
1	A	87	ASP
1	A	89	GLN
1	A	94	ARG
1	A	100	LYS
1	A	106	ILE
1	A	115	LEU
1	A	118	THR
1	A	123	THR
1	A	124	ILE
1	A	131	SER
1	A	146	LYS
1	A	152	ARG
1	A	160	SER
1	A	191	ILE
1	A	199	GLU
1	A	216	LEU
1	A	226	THR
1	A	230	PRO
1	A	237	HIS
1	A	244	THR
1	A	257	HIS
1	A	258	ARG
1	A	267	ILE
1	A	291	LEU
1	A	295	TRP
1	A	303	ARG
1	A	310	LEU
1	A	316	LYS

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Mol	Chain	Res	Type
1	A	321	GLU
1	A	325	GLU
1	A	328	MET
1	A	330	ARG
1	A	348	SER
1	A	355	SER
1	B	3	ARG
1	B	7	LEU
1	B	9	GLN
1	B	10	GLU
1	B	25	ASN
1	B	27	LYS
1	B	45	ARG
1	B	51	THR
1	B	61	ILE
1	B	65	VAL
1	B	67	SER
1	B	71	GLN
1	B	94	ARG
1	B	118	THR
1	B	123	THR
1	B	124	ILE
1	B	132	GLU
1	B	139	LYS
1	B	164	GLN
1	B	176	ILE
1	B	183	VAL
1	B	199	GLU
1	B	226	THR
1	B	227	LEU
1	B	230	PRO
1	B	233	VAL
1	B	242	LYS
1	B	244	THR
1	B	258	ARG
1	B	267	ILE
1	B	270	LEU
1	B	291	LEU
1	B	295	TRP
1	B	296	LYS
1	B	303	ARG
1	B	310	LEU

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Mol	Chain	Res	Type
1	B	316	LYS
1	B	325	GLU
1	B	330	ARG
1	B	339	LYS
1	B	344	HIS
1	B	345	THR
1	C	2	HIS
1	C	3	ARG
1	C	9	GLN
1	C	10	GLU
1	C	16	SER
1	C	27	LYS
1	C	30	LEU
1	C	44	GLN
1	C	51	THR
1	C	53	GLU
1	C	69	ILE
1	C	81	GLU
1	C	89	GLN
1	C	94	ARG
1	C	100	LYS
1	C	110	GLN
1	C	115	LEU
1	C	118	THR
1	C	123	THR
1	C	131	SER
1	C	132	GLU
1	C	146	LYS
1	C	152	ARG
1	C	157	CYS
1	C	160	SER
1	C	164	GLN
1	C	179	GLN
1	C	183	VAL
1	C	185	ILE
1	C	191	ILE
1	C	199	GLU
1	C	207	LYS
1	C	216	LEU
1	C	224	GLU
1	C	226	THR
1	C	228	LEU

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Mol	Chain	Res	Type
1	C	231	ASN
1	C	234	THR
1	C	237	HIS
1	C	257	HIS
1	C	274	MET
1	C	291	LEU
1	C	295	TRP
1	C	303	ARG
1	C	316	LYS
1	C	325	GLU
1	D	30	LEU
1	D	44	GLN
1	D	51	THR
1	D	65	VAL
1	D	68	SER
1	D	70	ASN
1	D	77	ILE
1	D	81	GLU
1	D	106	ILE
1	D	118	THR
1	D	123	THR
1	D	125	GLN
1	D	132	GLU
1	D	139	LYS
1	D	146	LYS
1	D	193	ASP
1	D	199	GLU
1	D	207	LYS
1	D	216	LEU
1	D	217	ASN
1	D	226	THR
1	D	231	ASN
1	D	237	HIS
1	D	244	THR
1	D	250	MET
1	D	257	HIS
1	D	258	ARG
1	D	291	LEU
1	D	295	TRP
1	D	303	ARG
1	D	310	LEU
1	D	316	LYS

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Mol	Chain	Res	Type
1	D	325	GLU
1	D	328	MET
1	D	347	SER
1	D	348	SER
1	E	2	HIS
1	E	10	GLU
1	E	12	LYS
1	E	44	GLN
1	E	45	ARG
1	E	51	THR
1	E	67	SER
1	E	69	ILE
1	E	72	SER
1	E	107	LYS
1	E	115	LEU
1	E	118	THR
1	E	123	THR
1	E	131	SER
1	E	132	GLU
1	E	148	ARG
1	E	160	SER
1	E	173	TYR
1	E	183	VAL
1	E	193	ASP
1	E	216	LEU
1	E	226	THR
1	E	230	PRO
1	E	237	HIS
1	E	244	THR
1	E	257	HIS
1	E	267	ILE
1	E	293	LYS
1	E	295	TRP
1	E	303	ARG
1	E	310	LEU
1	E	316	LYS
1	E	321	GLU
1	E	325	GLU
1	E	328	MET
1	E	345	THR
1	E	348	SER
1	E	352	SER

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Mol	Chain	Res	Type
1	F	16	SER
1	F	51	THR
1	F	68	SER
1	F	69	ILE
1	F	71	GLN
1	F	89	GLN
1	F	94	ARG
1	F	98	LYS
1	F	100	LYS
1	F	107	LYS
1	F	110	GLN
1	F	115	LEU
1	F	118	THR
1	F	120	LYS
1	F	123	THR
1	F	124	ILE
1	F	131	SER
1	F	139	LYS
1	F	151	LEU
1	F	164	GLN
1	F	173	TYR
1	F	183	VAL
1	F	191	ILE
1	F	199	GLU
1	F	216	LEU
1	F	217	ASN
1	F	226	THR
1	F	231	ASN
1	F	242	LYS
1	F	245	PRO
1	F	257	HIS
1	F	258	ARG
1	F	267	ILE
1	F	274	MET
1	F	291	LEU
1	F	295	TRP
1	F	310	LEU
1	F	316	LYS
1	F	321	GLU
1	F	325	GLU
1	F	328	MET
1	F	329	LYS

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Mol	Chain	Res	Type
1	F	330	ARG
1	F	345	THR
1	F	352	SER
1	F	353	THR
1	G	16	SER
1	G	51	THR
1	G	70	ASN
1	G	72	SER
1	G	87	ASP
1	G	89	GLN
1	G	94	ARG
1	G	98	LYS
1	G	115	LEU
1	G	118	THR
1	G	123	THR
1	G	131	SER
1	G	139	LYS
1	G	153	ILE
1	G	164	GLN
1	G	173	TYR
1	G	179	GLN
1	G	191	ILE
1	G	195	ASP
1	G	198	LEU
1	G	199	GLU
1	G	207	LYS
1	G	214	LYS
1	G	216	LEU
1	G	217	ASN
1	G	224	GLU
1	G	226	THR
1	G	231	ASN
1	G	232	MET
1	G	242	LYS
1	G	244	THR
1	G	250	MET
1	G	257	HIS
1	G	258	ARG
1	G	267	ILE
1	G	274	MET
1	G	291	LEU
1	G	295	TRP

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Mol	Chain	Res	Type
1	G	303	ARG
1	G	310	LEU
1	G	321	GLU
1	G	330	ARG
1	H	3	ARG
1	H	9	GLN
1	H	10	GLU
1	H	45	ARG
1	H	51	THR
1	H	67	SER
1	H	70	ASN
1	H	81	GLU
1	H	115	LEU
1	H	118	THR
1	H	123	THR
1	H	124	ILE
1	H	131	SER
1	H	132	GLU
1	H	139	LYS
1	H	151	LEU
1	H	158	PRO
1	H	160	SER
1	H	161	LEU
1	H	164	GLN
1	H	185	ILE
1	H	191	ILE
1	H	195	ASP
1	H	199	GLU
1	H	216	LEU
1	H	226	THR
1	H	237	HIS
1	H	239	CYS
1	H	244	THR
1	H	246	GLU
1	H	257	HIS
1	H	258	ARG
1	H	267	ILE
1	H	291	LEU
1	H	295	TRP
1	H	296	LYS
1	H	303	ARG
1	H	310	LEU

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Mol	Chain	Res	Type
1	H	316	LYS
1	H	321	GLU
1	H	325	GLU
1	H	329	LYS
1	H	352	SER
1	H	356	LEU
1	I	3	ARG
1	I	7	LEU
1	I	10	GLU
1	I	16	SER
1	I	34	GLU
1	I	42	ARG
1	I	44	GLN
1	I	51	THR
1	I	57	GLN
1	I	59	ARG
1	I	65	VAL
1	I	69	ILE
1	I	76	VAL
1	I	81	GLU
1	I	88	SER
1	I	89	GLN
1	I	94	ARG
1	I	118	THR
1	I	123	THR
1	I	124	ILE
1	I	163	ILE
1	I	164	GLN
1	I	170	LEU
1	I	183	VAL
1	I	195	ASP
1	I	199	GLU
1	I	207	LYS
1	I	216	LEU
1	I	217	ASN
1	I	224	GLU
1	I	226	THR
1	I	231	ASN
1	I	245	PRO
1	I	257	HIS
1	I	258	ARG
1	I	274	MET

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Mol	Chain	Res	Type
1	I	291	LEU
1	I	295	TRP
1	I	300	SER
1	I	303	ARG
1	I	310	LEU
1	I	316	LYS
1	I	321	GLU
1	I	325	GLU
1	I	329	LYS
1	J	2	HIS
1	J	3	ARG
1	J	30	LEU
1	J	51	THR
1	J	67	SER
1	J	68	SER
1	J	72	SER
1	J	81	GLU
1	J	94	ARG
1	J	115	LEU
1	J	118	THR
1	J	123	THR
1	J	131	SER
1	J	173	TYR
1	J	193	ASP
1	J	199	GLU
1	J	207	LYS
1	J	214	LYS
1	J	216	LEU
1	J	224	GLU
1	J	226	THR
1	J	231	ASN
1	J	244	THR
1	J	245	PRO
1	J	257	HIS
1	J	258	ARG
1	J	267	ILE
1	J	291	LEU
1	J	295	TRP
1	J	303	ARG
1	J	310	LEU
1	J	316	LYS
1	J	321	GLU

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Mol	Chain	Res	Type
1	J	325	GLU
1	J	328	MET
1	J	345	THR
1	J	355	SER
1	K	10	GLU
1	K	25	ASN
1	K	44	GLN
1	K	51	THR
1	K	68	SER
1	K	81	GLU
1	K	94	ARG
1	K	99	GLU
1	K	106	ILE
1	K	109	ASP
1	K	115	LEU
1	K	118	THR
1	K	123	THR
1	K	131	SER
1	K	139	LYS
1	K	146	LYS
1	K	152	ARG
1	K	199	GLU
1	K	207	LYS
1	K	216	LEU
1	K	226	THR
1	K	237	HIS
1	K	244	THR
1	K	257	HIS
1	K	258	ARG
1	K	270	LEU
1	K	291	LEU
1	K	295	TRP
1	K	298	SER
1	K	303	ARG
1	K	308	SER
1	K	310	LEU
1	K	316	LYS
1	K	325	GLU
1	K	348	SER
1	K	353	THR
1	K	354	GLN
1	L	3	ARG

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Mol	Chain	Res	Type
1	L	9	GLN
1	L	10	GLU
1	L	20	GLN
1	L	21	SER
1	L	25	ASN
1	L	44	GLN
1	L	51	THR
1	L	69	ILE
1	L	87	ASP
1	L	89	GLN
1	L	94	ARG
1	L	107	LYS
1	L	115	LEU
1	L	118	THR
1	L	123	THR
1	L	146	LYS
1	L	151	LEU
1	L	153	ILE
1	L	164	GLN
1	L	173	TYR
1	L	176	ILE
1	L	191	ILE
1	L	199	GLU
1	L	207	LYS
1	L	226	THR
1	L	237	HIS
1	L	250	MET
1	L	258	ARG
1	L	267	ILE
1	L	270	LEU
1	L	291	LEU
1	L	295	TRP
1	L	303	ARG
1	L	310	LEU
1	L	316	LYS
1	L	325	GLU
1	L	329	LYS
1	L	330	ARG
1	L	339	LYS
1	L	343	VAL
1	L	344	HIS
1	M	2	HIS

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Mol	Chain	Res	Type
1	M	9	GLN
1	M	25	ASN
1	M	51	THR
1	M	69	ILE
1	M	70	ASN
1	M	77	ILE
1	M	81	GLU
1	M	89	GLN
1	M	109	ASP
1	M	115	LEU
1	M	118	THR
1	M	123	THR
1	M	160	SER
1	M	164	GLN
1	M	191	ILE
1	M	195	ASP
1	M	199	GLU
1	M	216	LEU
1	M	224	GLU
1	M	226	THR
1	M	240	THR
1	M	244	THR
1	M	245	PRO
1	M	257	HIS
1	M	291	LEU
1	M	295	TRP
1	M	303	ARG
1	M	316	LYS
1	M	321	GLU
1	M	325	GLU
1	M	328	MET
1	M	345	THR
1	M	352	SER
1	M	353	THR
1	M	354	GLN
1	M	355	SER
1	M	356	LEU
1	N	3	ARG
1	N	10	GLU
1	N	16	SER
1	N	44	GLN
1	N	51	THR

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Mol	Chain	Res	Type
1	N	53	GLU
1	N	65	VAL
1	N	69	ILE
1	N	81	GLU
1	N	82	THR
1	N	89	GLN
1	N	94	ARG
1	N	100	LYS
1	N	118	THR
1	N	152	ARG
1	N	179	GLN
1	N	183	VAL
1	N	191	ILE
1	N	195	ASP
1	N	199	GLU
1	N	216	LEU
1	N	217	ASN
1	N	224	GLU
1	N	226	THR
1	N	234	THR
1	N	237	HIS
1	N	257	HIS
1	N	258	ARG
1	N	267	ILE
1	N	291	LEU
1	N	295	TRP
1	N	310	LEU
1	N	316	LYS
1	N	321	GLU
1	N	325	GLU
1	N	328	MET
1	O	3	ARG
1	O	7	LEU
1	O	9	GLN
1	O	10	GLU
1	O	25	ASN
1	O	27	LYS
1	O	30	LEU
1	O	44	GLN
1	O	45	ARG
1	O	51	THR
1	O	67	SER

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Mol	Chain	Res	Type
1	O	70	ASN
1	O	81	GLU
1	O	98	LYS
1	O	107	LYS
1	O	118	THR
1	O	123	THR
1	O	131	SER
1	O	132	GLU
1	O	146	LYS
1	O	164	GLN
1	O	173	TYR
1	O	176	ILE
1	O	182	LEU
1	O	183	VAL
1	O	191	ILE
1	O	199	GLU
1	O	226	THR
1	O	244	THR
1	O	245	PRO
1	O	258	ARG
1	O	267	ILE
1	O	270	LEU
1	O	291	LEU
1	O	295	TRP
1	O	296	LYS
1	O	303	ARG
1	O	310	LEU
1	O	316	LYS
1	O	325	GLU
1	O	330	ARG
1	O	339	LYS
1	P	9	GLN
1	P	44	GLN
1	P	45	ARG
1	P	49	GLU
1	P	51	THR
1	P	67	SER
1	P	81	GLU
1	P	82	THR
1	P	87	ASP
1	P	94	ARG
1	P	109	ASP

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Mol	Chain	Res	Type
1	P	115	LEU
1	P	118	THR
1	P	123	THR
1	P	146	LYS
1	P	152	ARG
1	P	164	GLN
1	P	199	GLU
1	P	216	LEU
1	P	226	THR
1	P	230	PRO
1	P	244	THR
1	P	257	HIS
1	P	258	ARG
1	P	267	ILE
1	P	295	TRP
1	P	303	ARG
1	P	310	LEU
1	P	321	GLU
1	P	325	GLU
1	P	343	VAL
1	P	348	SER
1	P	352	SER
1	P	354	GLN
1	P	355	SER
1	P	356	LEU
1	P	358	THR
1	Q	7	LEU
1	Q	16	SER
1	Q	51	THR
1	Q	88	SER
1	Q	89	GLN
1	Q	98	LYS
1	Q	107	LYS
1	Q	115	LEU
1	Q	118	THR
1	Q	123	THR
1	Q	125	GLN
1	Q	131	SER
1	Q	146	LYS
1	Q	161	LEU
1	Q	164	GLN
1	Q	165	GLU

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Mol	Chain	Res	Type
1	Q	173	TYR
1	Q	191	ILE
1	Q	199	GLU
1	Q	216	LEU
1	Q	217	ASN
1	Q	224	GLU
1	Q	226	THR
1	Q	231	ASN
1	Q	250	MET
1	Q	257	HIS
1	Q	258	ARG
1	Q	267	ILE
1	Q	291	LEU
1	Q	295	TRP
1	Q	303	ARG
1	Q	310	LEU
1	Q	316	LYS
1	Q	325	GLU
1	Q	344	HIS
1	R	3	ARG
1	R	42	ARG
1	R	45	ARG
1	R	51	THR
1	R	69	ILE
1	R	70	ASN
1	R	81	GLU
1	R	98	LYS
1	R	107	LYS
1	R	115	LEU
1	R	118	THR
1	R	123	THR
1	R	131	SER
1	R	132	GLU
1	R	139	LYS
1	R	146	LYS
1	R	156	GLN
1	R	164	GLN
1	R	173	TYR
1	R	199	GLU
1	R	214	LYS
1	R	216	LEU
1	R	226	THR

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Mol	Chain	Res	Type
1	R	230	PRO
1	R	237	HIS
1	R	244	THR
1	R	245	PRO
1	R	257	HIS
1	R	290	PRO
1	R	291	LEU
1	R	295	TRP
1	R	310	LEU
1	R	316	LYS
1	R	325	GLU
1	R	344	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (221) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	80	HIS
1	A	125	GLN
1	A	136	GLN
1	A	168	ASN
1	A	220	HIS
1	A	231	ASN
1	A	336	GLN
1	A	341	GLN
1	A	354	GLN
1	B	9	GLN
1	B	50	ASN
1	B	57	GLN
1	B	80	HIS
1	B	89	GLN
1	B	125	GLN
1	B	136	GLN
1	B	156	GLN
1	B	179	GLN
1	B	219	HIS
1	B	220	HIS
1	B	231	ASN
1	B	287	ASN
1	C	50	ASN
1	C	57	GLN
1	C	70	ASN

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Mol	Chain	Res	Type
1	C	80	HIS
1	C	125	GLN
1	C	179	GLN
1	C	200	HIS
1	C	231	ASN
1	C	282	ASN
1	C	287	ASN
1	C	324	GLN
1	D	50	ASN
1	D	57	GLN
1	D	70	ASN
1	D	80	HIS
1	D	85	GLN
1	D	89	GLN
1	D	125	GLN
1	D	136	GLN
1	D	179	GLN
1	D	220	HIS
1	D	231	ASN
1	D	287	ASN
1	E	2	HIS
1	E	9	GLN
1	E	50	ASN
1	E	57	GLN
1	E	80	HIS
1	E	125	GLN
1	E	136	GLN
1	E	168	ASN
1	E	200	HIS
1	E	220	HIS
1	E	231	ASN
1	E	287	ASN
1	E	324	GLN
1	E	344	HIS
1	F	50	ASN
1	F	80	HIS
1	F	110	GLN
1	F	125	GLN
1	F	136	GLN
1	F	166	ASN
1	F	180	ASN
1	F	200	HIS

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Mol	Chain	Res	Type
1	F	217	ASN
1	F	231	ASN
1	F	287	ASN
1	F	336	GLN
1	G	50	ASN
1	G	57	GLN
1	G	70	ASN
1	G	80	HIS
1	G	125	GLN
1	G	136	GLN
1	G	200	HIS
1	G	217	ASN
1	G	220	HIS
1	G	231	ASN
1	G	247	GLN
1	G	287	ASN
1	H	50	ASN
1	H	57	GLN
1	H	70	ASN
1	H	80	HIS
1	H	110	GLN
1	H	125	GLN
1	H	136	GLN
1	H	179	GLN
1	H	200	HIS
1	H	220	HIS
1	H	231	ASN
1	H	287	ASN
1	H	336	GLN
1	I	50	ASN
1	I	70	ASN
1	I	80	HIS
1	I	89	GLN
1	I	125	GLN
1	I	136	GLN
1	I	179	GLN
1	I	200	HIS
1	I	217	ASN
1	I	231	ASN
1	I	287	ASN
1	J	2	HIS
1	J	20	GLN

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Mol	Chain	Res	Type
1	J	50	ASN
1	J	57	GLN
1	J	80	HIS
1	J	125	GLN
1	J	136	GLN
1	J	166	ASN
1	J	179	GLN
1	J	180	ASN
1	J	202	GLN
1	J	217	ASN
1	J	220	HIS
1	J	231	ASN
1	J	247	GLN
1	K	20	GLN
1	K	50	ASN
1	K	80	HIS
1	K	85	GLN
1	K	125	GLN
1	K	136	GLN
1	K	166	ASN
1	K	168	ASN
1	K	179	GLN
1	K	200	HIS
1	K	231	ASN
1	K	287	ASN
1	K	336	GLN
1	L	50	ASN
1	L	80	HIS
1	L	89	GLN
1	L	125	GLN
1	L	136	GLN
1	L	179	GLN
1	L	200	HIS
1	L	217	ASN
1	L	220	HIS
1	L	231	ASN
1	L	287	ASN
1	L	336	GLN
1	M	50	ASN
1	M	70	ASN
1	M	80	HIS
1	M	89	GLN

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Mol	Chain	Res	Type
1	M	125	GLN
1	M	136	GLN
1	M	166	ASN
1	M	179	GLN
1	M	231	ASN
1	M	287	ASN
1	M	341	GLN
1	M	344	HIS
1	M	354	GLN
1	N	50	ASN
1	N	57	GLN
1	N	80	HIS
1	N	136	GLN
1	N	156	GLN
1	N	166	ASN
1	N	179	GLN
1	N	200	HIS
1	N	217	ASN
1	N	231	ASN
1	N	282	ASN
1	N	284	ASN
1	N	287	ASN
1	N	336	GLN
1	N	344	HIS
1	O	50	ASN
1	O	70	ASN
1	O	80	HIS
1	O	85	GLN
1	O	125	GLN
1	O	164	GLN
1	O	168	ASN
1	O	200	HIS
1	O	220	HIS
1	O	231	ASN
1	O	287	ASN
1	O	324	GLN
1	P	50	ASN
1	P	80	HIS
1	P	125	GLN
1	P	136	GLN
1	P	168	ASN
1	P	179	GLN

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Mol	Chain	Res	Type
1	P	231	ASN
1	P	287	ASN
1	P	341	GLN
1	Q	50	ASN
1	Q	80	HIS
1	Q	125	GLN
1	Q	136	GLN
1	Q	156	GLN
1	Q	164	GLN
1	Q	168	ASN
1	Q	179	GLN
1	Q	217	ASN
1	Q	220	HIS
1	Q	231	ASN
1	Q	287	ASN
1	Q	336	GLN
1	R	50	ASN
1	R	57	GLN
1	R	70	ASN
1	R	80	HIS
1	R	89	GLN
1	R	125	GLN
1	R	136	GLN
1	R	179	GLN
1	R	220	HIS
1	R	231	ASN
1	R	287	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	401	-	4,4,4	0.77	0	6,6,6	1.06	0
2	SO4	G	401	-	4,4,4	1.25	1 (25%)	6,6,6	0.42	0
2	SO4	G	403	-	4,4,4	0.63	0	6,6,6	0.73	0
2	SO4	K	400	-	4,4,4	1.18	1 (25%)	6,6,6	1.27	0
2	SO4	O	401	-	4,4,4	0.73	0	6,6,6	0.72	0
2	SO4	D	400	-	4,4,4	1.50	1 (25%)	6,6,6	3.07	3 (50%)
2	SO4	E	400	-	4,4,4	0.97	0	6,6,6	0.40	0
2	SO4	J	400	-	4,4,4	0.88	0	6,6,6	0.64	0
2	SO4	P	402	-	4,4,4	0.54	0	6,6,6	0.54	0
2	SO4	R	402	-	4,4,4	0.66	0	6,6,6	1.04	0
2	SO4	G	402	-	4,4,4	0.81	0	6,6,6	0.93	0
2	SO4	M	401	-	4,4,4	0.72	0	6,6,6	1.13	0
2	SO4	R	401	-	4,4,4	1.05	0	6,6,6	1.50	1 (16%)
2	SO4	A	402	-	4,4,4	0.95	0	6,6,6	1.18	1 (16%)
2	SO4	P	401	-	4,4,4	1.03	0	6,6,6	1.21	1 (16%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	SO4	O2-S	2.26	1.58	1.44
2	D	400	SO4	O1-S	2.23	1.58	1.44
2	K	400	SO4	O2-S	2.18	1.57	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	SO4	O4-S-O1	6.32	142.60	109.56
2	D	400	SO4	O4-S-O2	-2.95	94.16	109.56
2	D	400	SO4	O4-S-O3	-2.55	94.46	108.54
2	R	401	SO4	O4-S-O3	2.54	122.56	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	SO4	O4-S-O1	-2.47	96.66	109.56
2	P	401	SO4	O3-S-O2	2.32	121.67	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	2	0
2	R	402	SO4	1	0
2	A	402	SO4	2	0

5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.