



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:09 AM UTC

PDB ID : 6Z05 / pdb_00006z05
EMDB ID : EMD-11003
Title : Campylobacter jejuni serine protease HtrA
Authors : Grinzato, A.; Kandiah, E.; Zanotti, G.
Deposited on : 2020-05-07
Resolution : 5.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

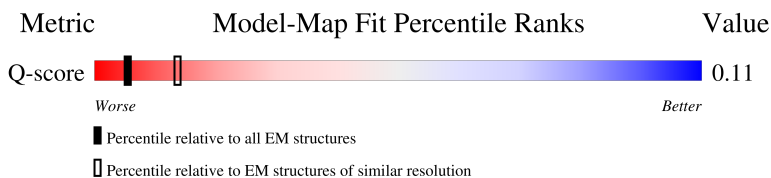
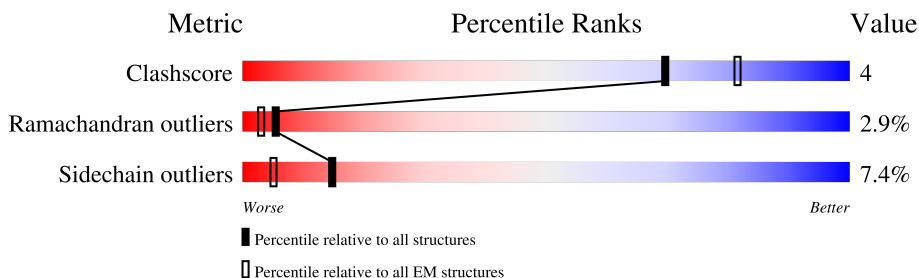
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 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.



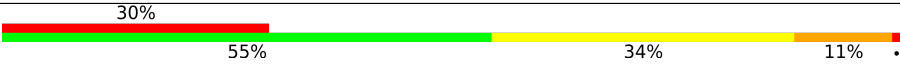
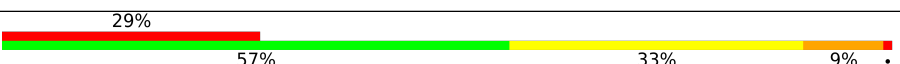
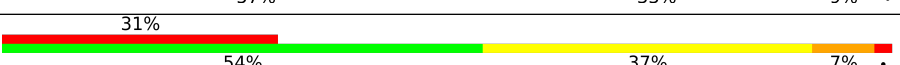
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	511 (5.30 - 6.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	434	32% 53% 37% 9% .
1	B	434	28% 54% 37% 9%
1	C	434	31% 56% 34% 9%
1	D	434	28% 57% 34% 7% .

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Mol	Chain	Length	Quality of chain
1	E	434	
1	F	434	
1	G	434	
1	H	434	
1	I	434	
1	J	434	
1	K	434	
1	L	434	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 39875 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

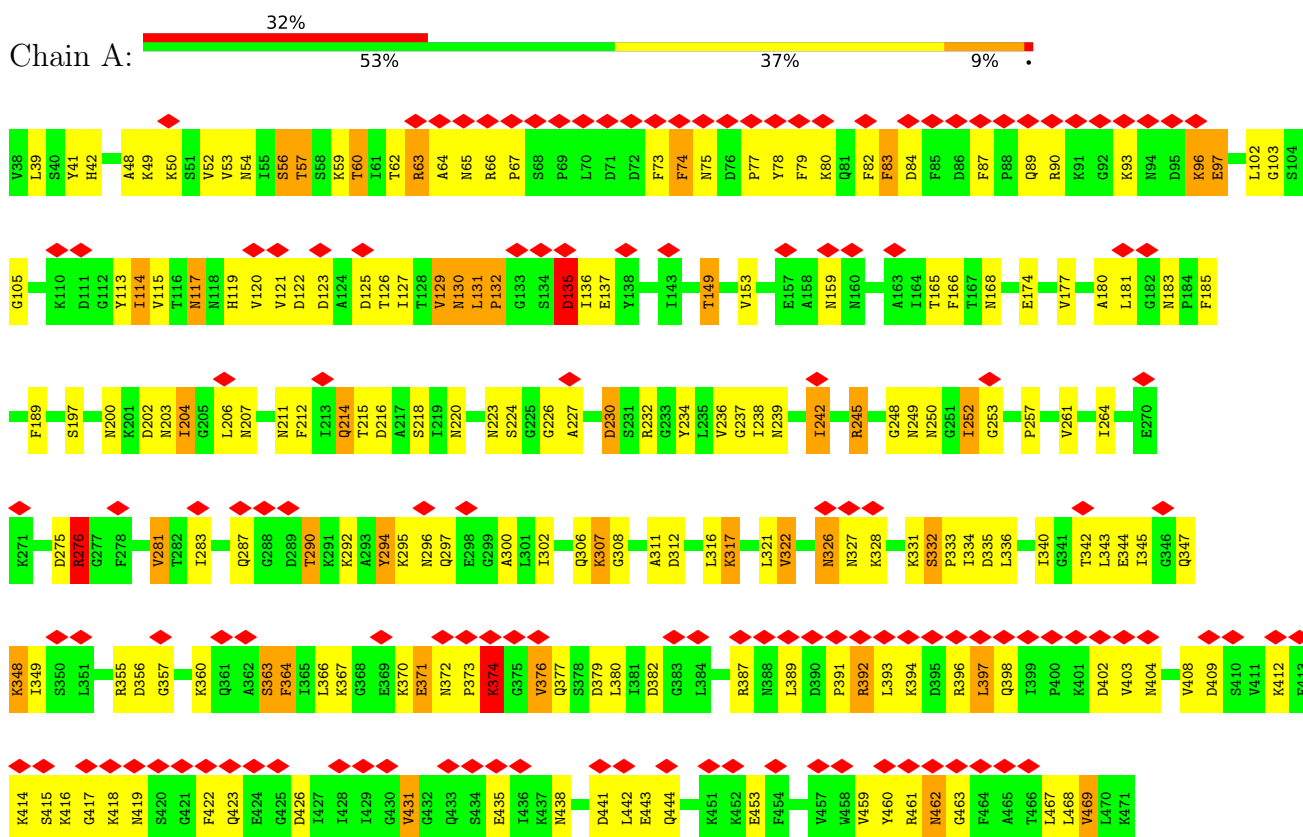
- Molecule 1 is a protein called DegQ family serine endoprotease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	B	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	C	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	D	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	E	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	F	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	G	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	H	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	I	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	J	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	K	434	Total 3323	C 2096	N 570	O 655	S 2	0	0
1	L	434	Total 3322	C 2096	N 570	O 654	S 2	0	0

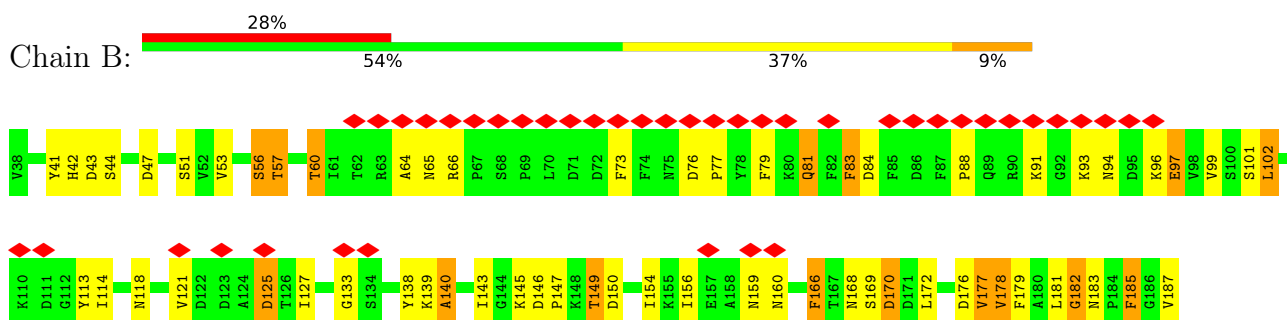
3 Residue-property plots

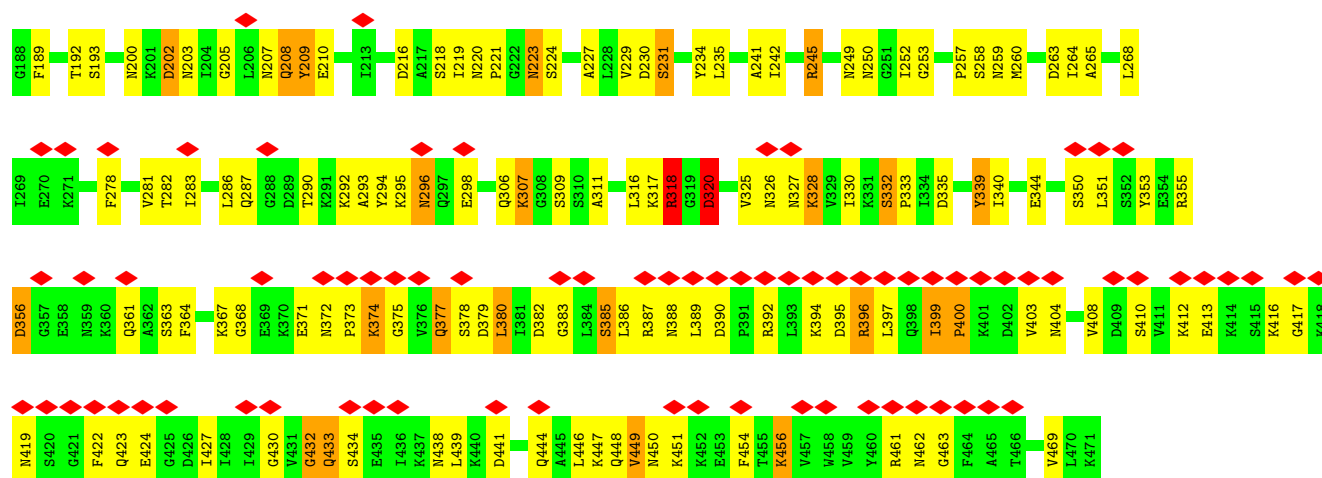
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DegQ family serine endoprotease

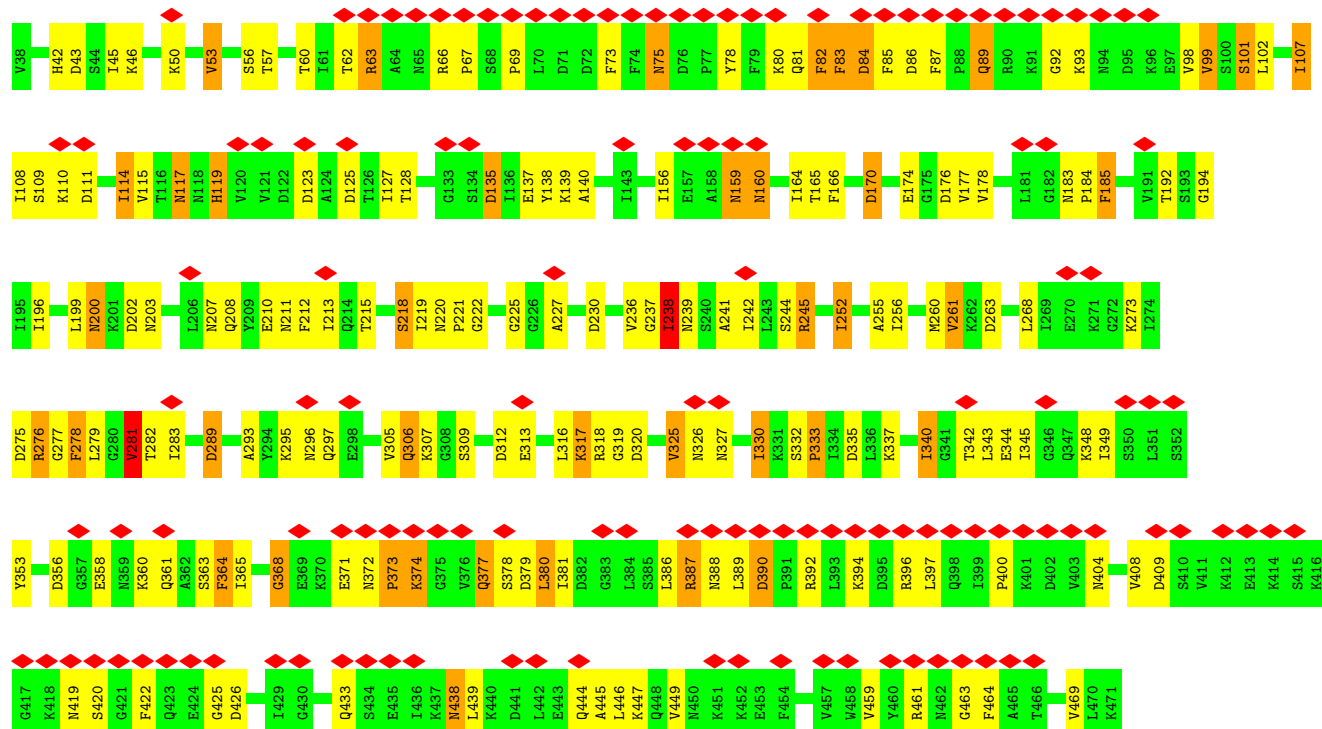


• Molecule 1: DegQ family serine endoprotease

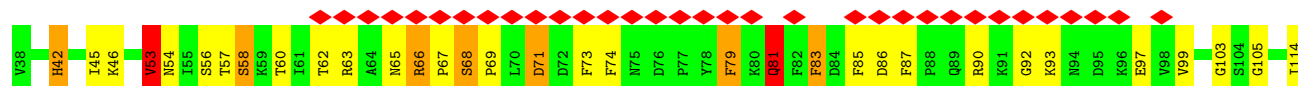


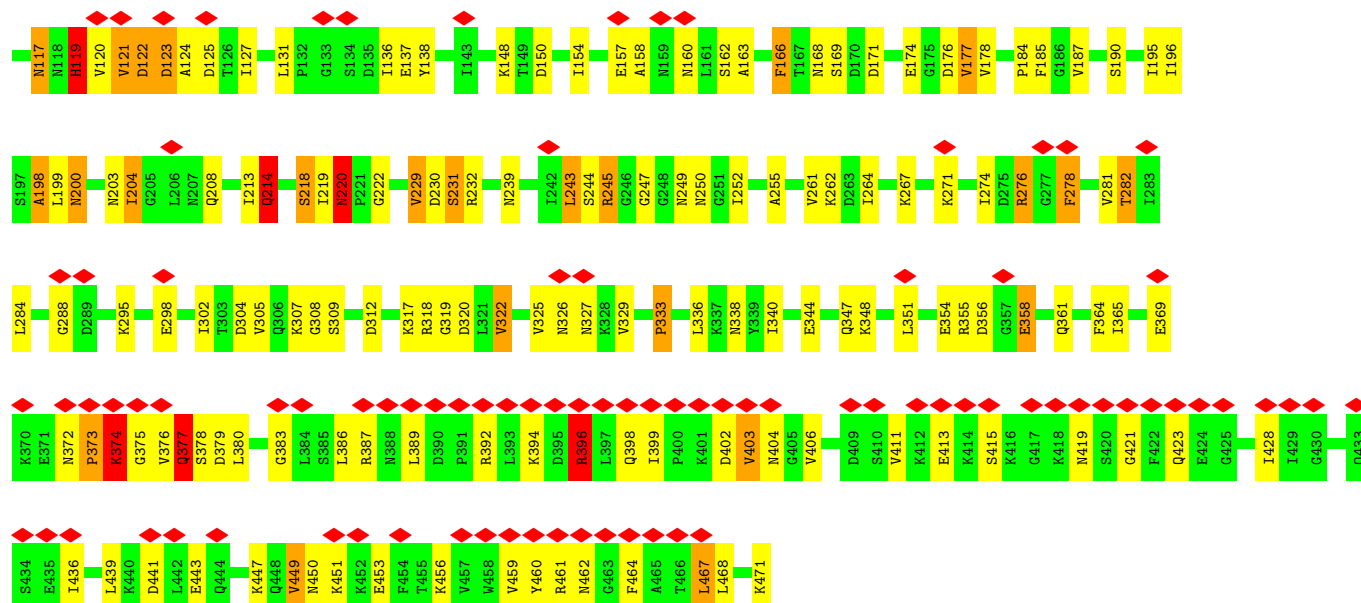


• Molecule 1: DegQ family serine endoprotease

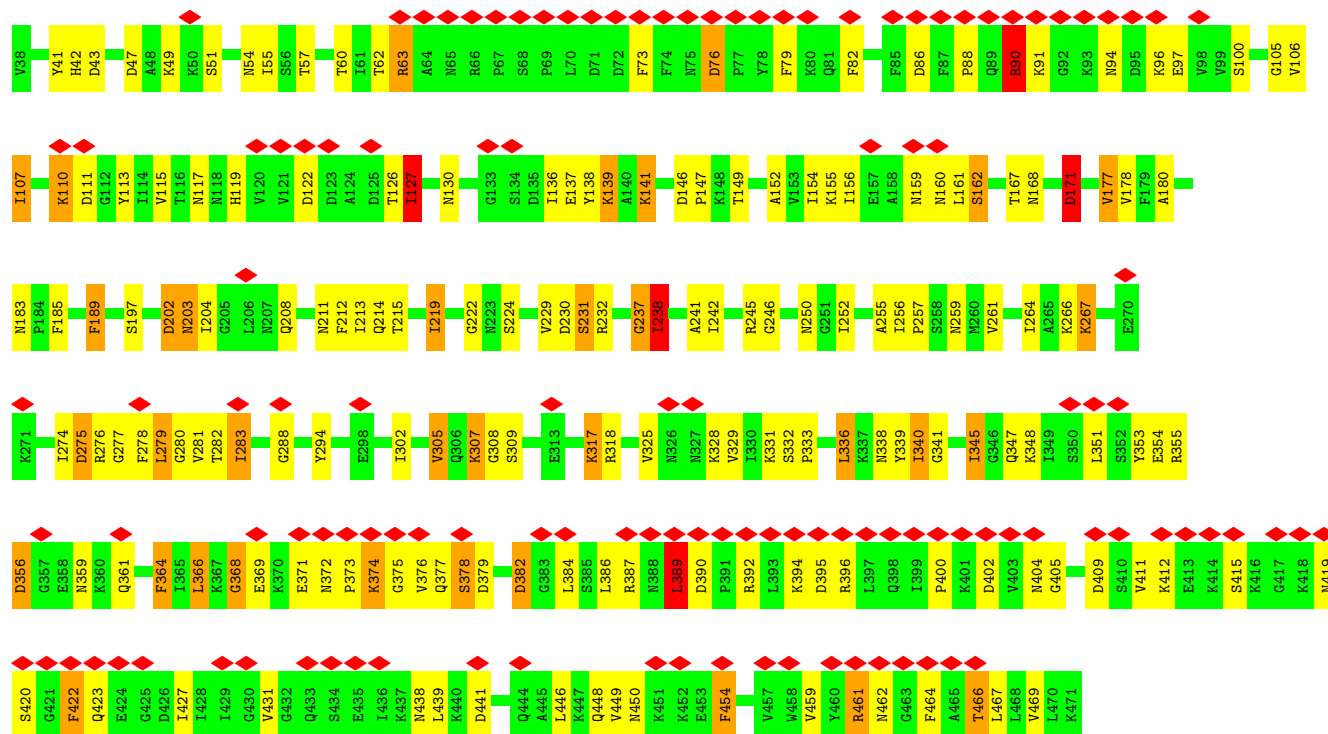


• Molecule 1: DegQ family serine endoprotease



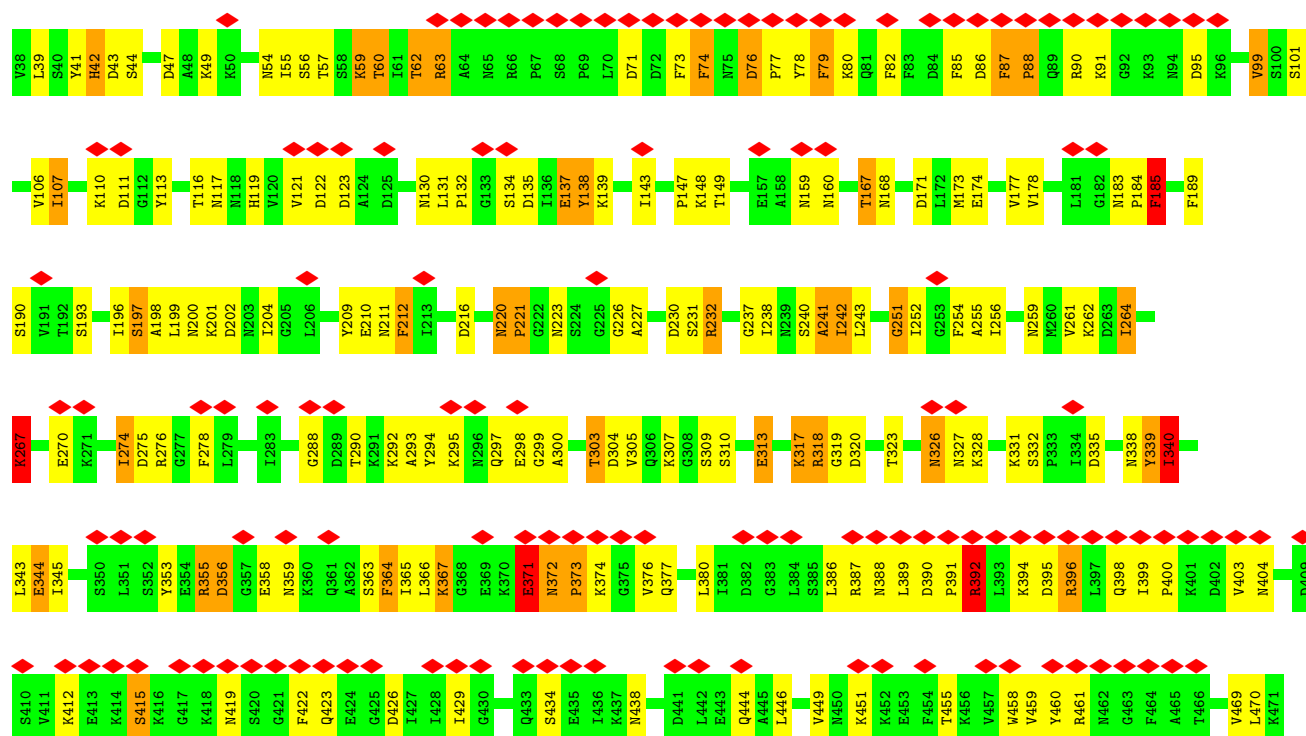


• Molecule 1: DegQ family serine endoprotease

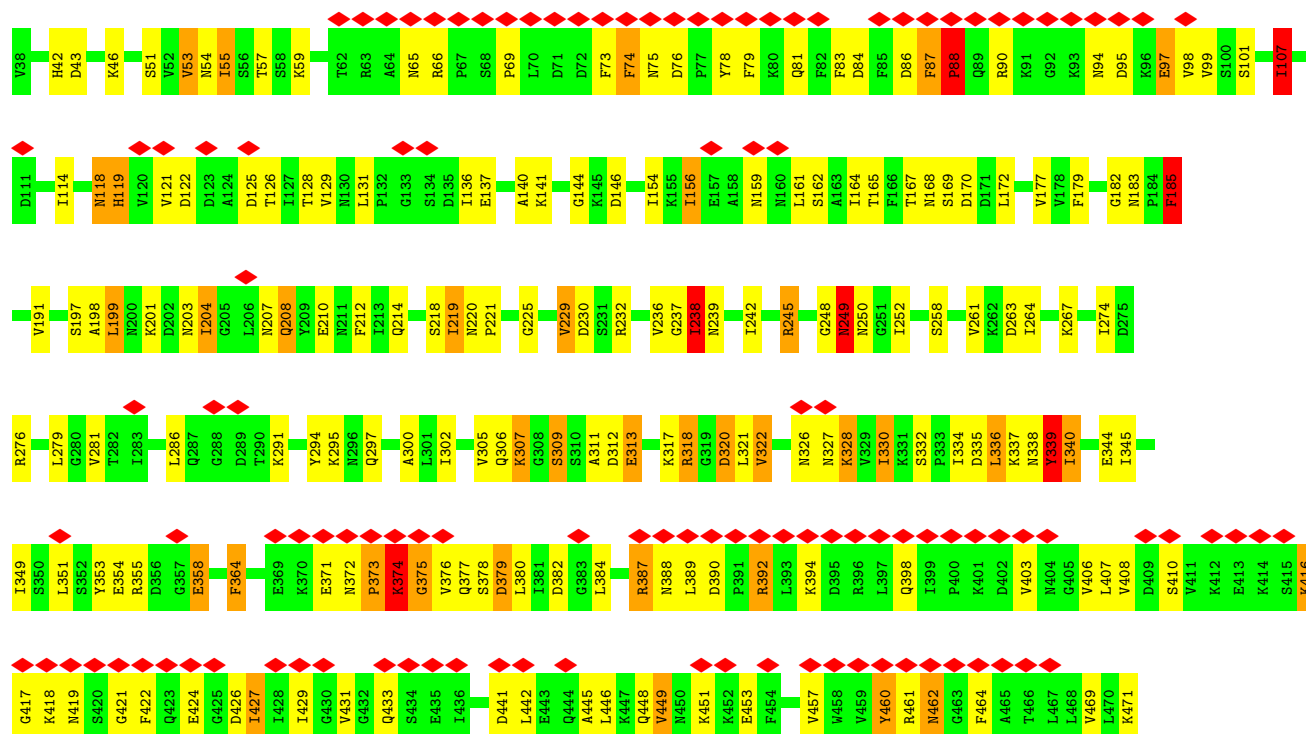


• Molecule 1: DegQ family serine endoprotease

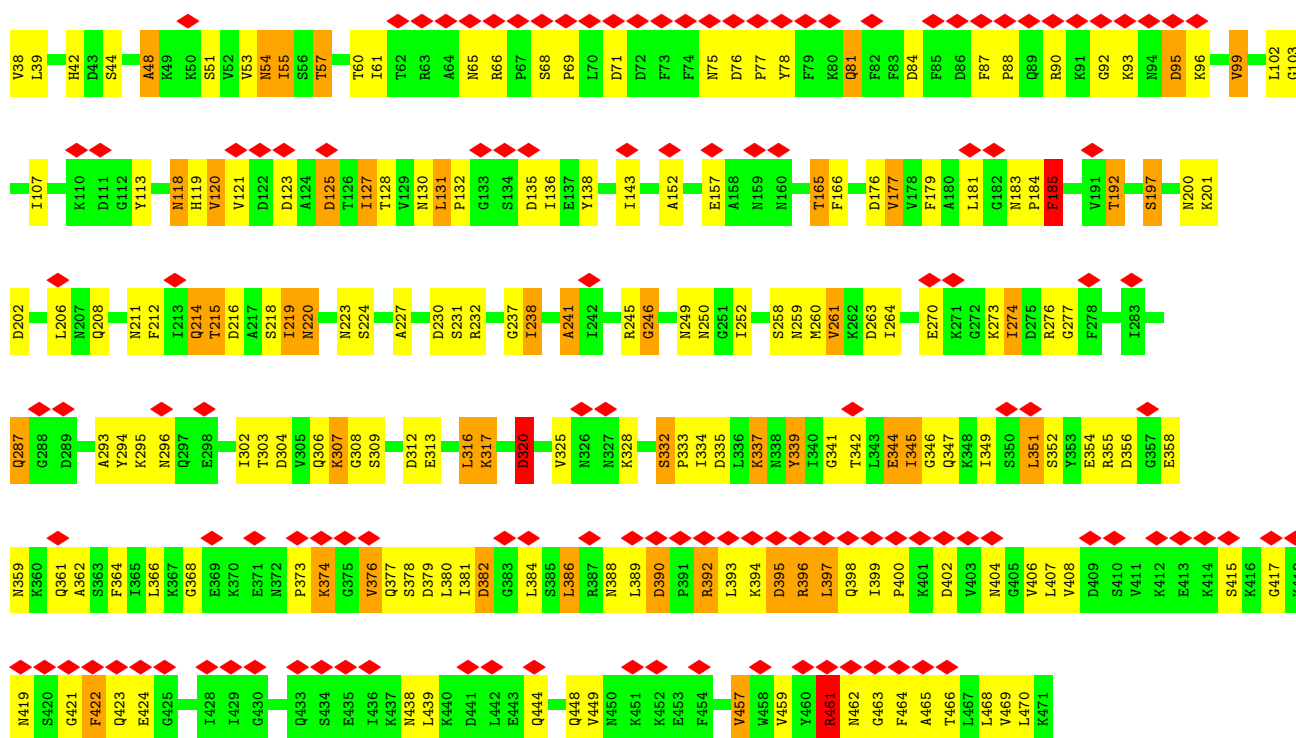




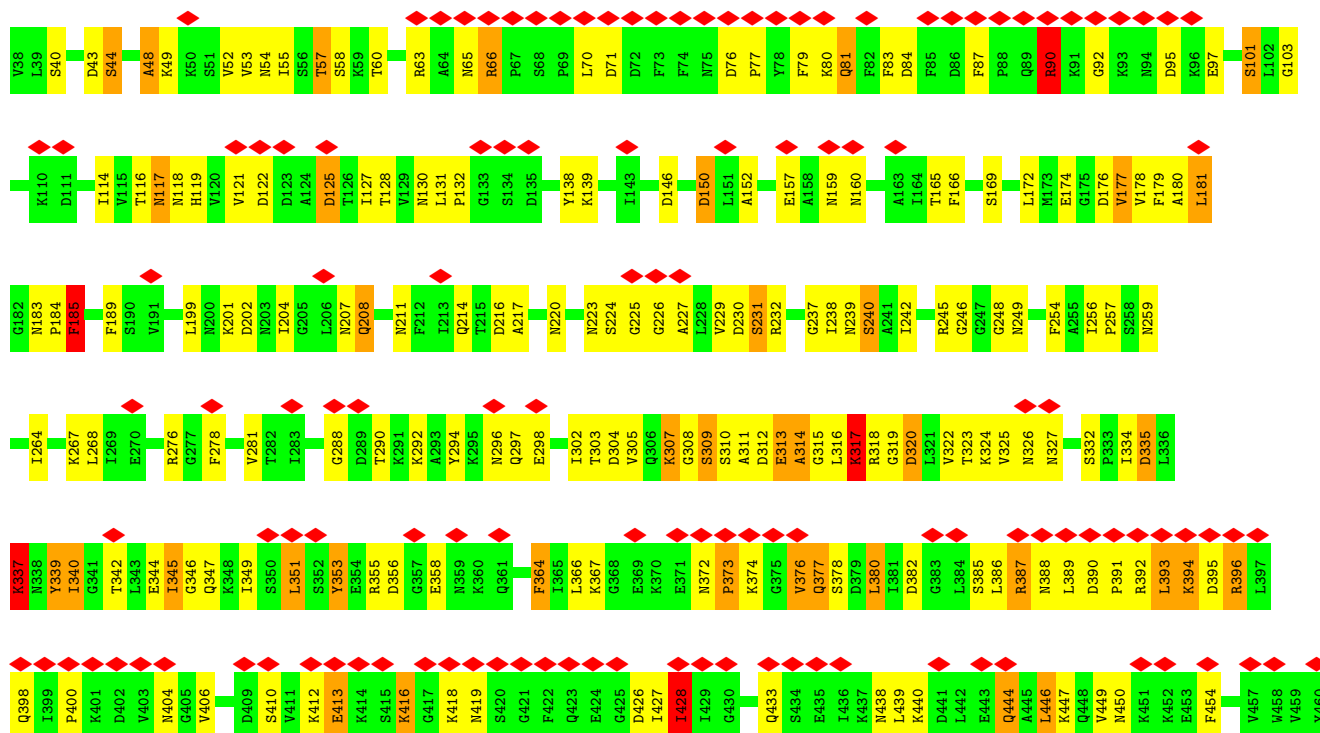
• Molecule 1: DegQ family serine endoprotease

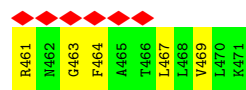


• Molecule 1: DegQ family serine endoprotease

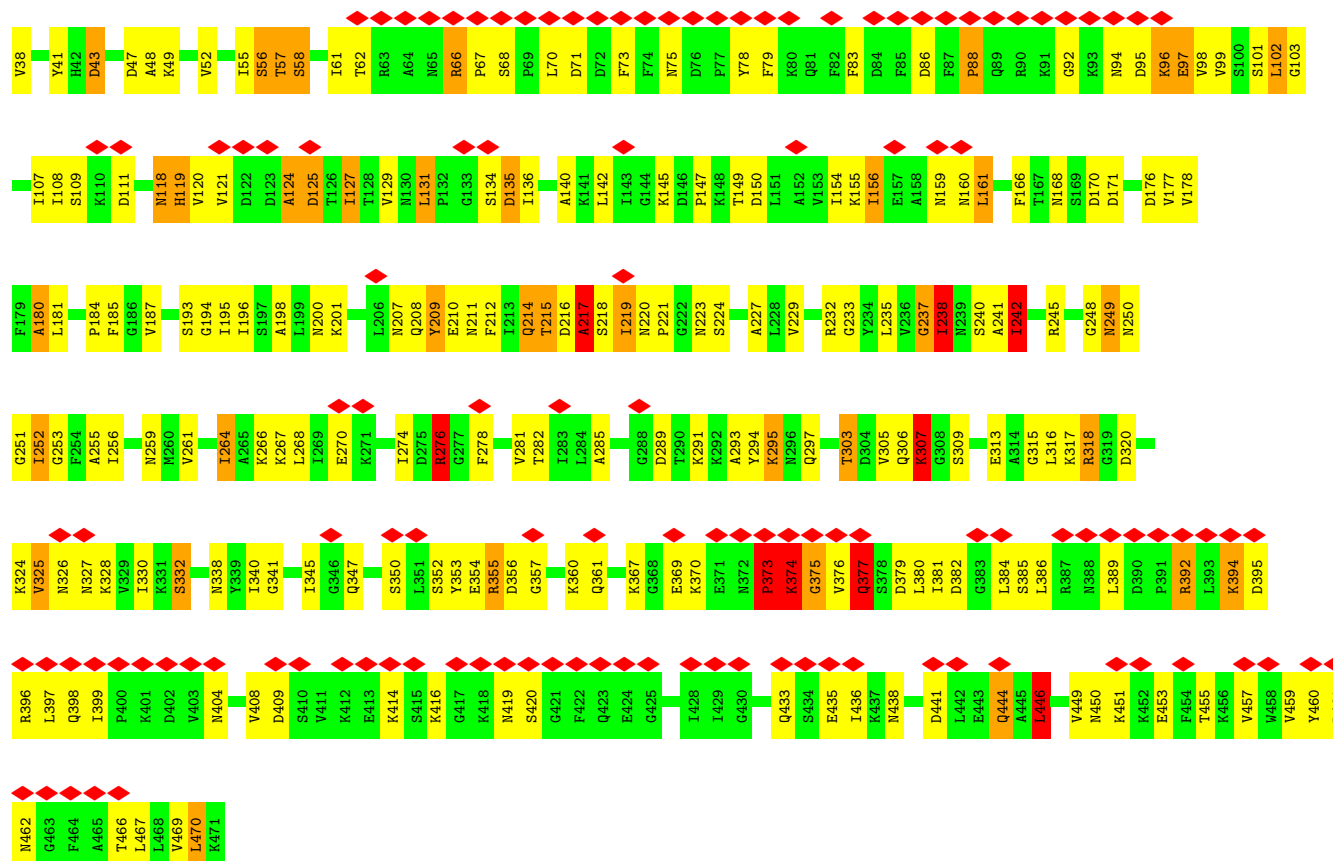


• Molecule 1: DegQ family serine endoprotease

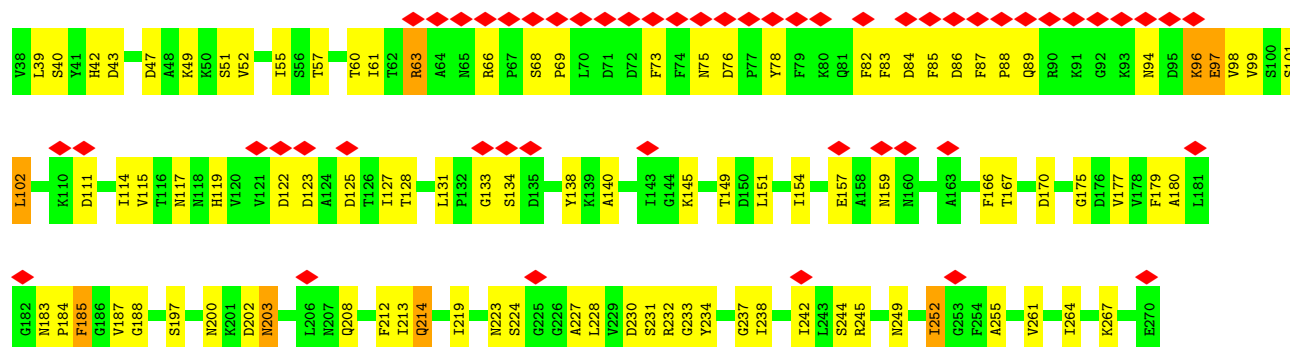




• Molecule 1: DegQ family serine endoprotease



• Molecule 1: DegQ family serine endoprotease





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	113843	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	328.30402, 328.30402, 328.30402	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.207, 1.207, 1.207	Depositor

5 Model quality

5.1 Standard geometry

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	0.58	0/3367	2.49	223/4532 (4.9%)
1	B	0.58	0/3367	2.47	222/4532 (4.9%)
1	C	0.57	0/3367	2.51	233/4532 (5.1%)
1	D	0.57	0/3367	2.49	215/4532 (4.7%)
1	E	0.57	0/3367	2.48	208/4532 (4.6%)
1	F	0.58	0/3367	2.55	254/4532 (5.6%)
1	G	0.57	0/3367	2.54	229/4532 (5.1%)
1	H	0.56	0/3367	2.53	228/4532 (5.0%)
1	I	0.57	0/3367	2.53	228/4532 (5.0%)
1	J	0.56	0/3367	2.51	238/4532 (5.3%)
1	K	0.56	0/3367	2.43	195/4532 (4.3%)
1	L	0.58	0/3366	2.49	229/4532 (5.1%)
All	All	0.57	0/40403	2.50	2702/54384 (5.0%)

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	14
1	B	0	19
1	C	0	19
1	D	0	17
1	E	0	12
1	F	0	16
1	G	0	18
1	H	0	16
1	I	0	17
1	J	0	21
1	K	0	21
1	L	0	15
All	All	0	205

There are no bond length outliers.

All (2702) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ARG	NE-CZ-NH2	14.76	132.49	119.20
1	C	183	ASN	OD1-CG-ND2	-13.72	108.88	122.60
1	B	200	ASN	CA-CB-CG	13.45	126.05	112.60
1	H	374	LYS	CA-C-N	13.09	145.27	121.70
1	H	374	LYS	C-N-CA	13.09	145.27	121.70
1	C	66	ARG	NE-CZ-NH2	13.01	130.91	119.20
1	H	259	ASN	CA-CB-CG	12.87	125.47	112.60
1	H	287	GLN	OE1-CD-NE2	-12.79	109.81	122.60
1	G	364	PHE	CA-CB-CG	12.55	126.35	113.80
1	E	372	ASN	OD1-CG-ND2	-12.54	110.06	122.60
1	K	426	ASP	CA-CB-CG	12.45	125.05	112.60
1	I	335	ASP	CA-CB-CG	12.13	124.73	112.60
1	J	398	GLN	OE1-CD-NE2	-12.02	110.58	122.60
1	B	375	GLY	N-CA-C	11.99	127.71	110.80
1	E	373	PRO	N-CA-C	11.88	127.03	114.68
1	A	166	PHE	CA-CB-CG	11.76	125.56	113.80
1	F	216	ASP	CA-CB-CG	11.50	124.10	112.60
1	H	220	ASN	OD1-CG-ND2	-11.49	111.11	122.60
1	E	232	ARG	NE-CZ-NH2	11.47	129.52	119.20
1	C	207	ASN	OD1-CG-ND2	-11.45	111.15	122.60
1	J	47	ASP	CA-CB-CG	11.44	124.04	112.60
1	I	207	ASN	OD1-CG-ND2	-11.43	111.17	122.60
1	L	335	ASP	CA-CB-CG	11.29	123.89	112.60
1	K	94	ASN	OD1-CG-ND2	-11.24	111.36	122.60
1	H	176	ASP	CA-CB-CG	11.18	123.78	112.60
1	G	377	GLN	N-CA-C	11.14	127.74	112.93
1	G	326	ASN	CA-CB-CG	11.04	123.64	112.60
1	I	119	HIS	CA-CB-CG	11.01	124.81	113.80
1	E	377	GLN	N-CA-C	10.97	126.42	111.71
1	I	326	ASN	OD1-CG-ND2	-10.85	111.75	122.60
1	G	354	GLU	CA-C-N	10.64	137.87	122.44
1	G	354	GLU	C-N-CA	10.64	137.87	122.44
1	I	347	GLN	OE1-CD-NE2	-10.57	112.03	122.60
1	A	63	ARG	NE-CZ-NH2	10.55	128.70	119.20
1	I	130	ASN	OD1-CG-ND2	-10.55	112.05	122.60
1	F	212	PHE	N-CA-C	10.37	123.72	110.24
1	G	320	ASP	CA-CB-CG	10.31	122.91	112.60
1	H	461	ARG	NE-CZ-NH2	-10.30	109.92	119.20
1	A	373	PRO	N-CA-C	10.30	127.23	113.84
1	B	364	PHE	CA-CB-CG	10.17	123.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	220	ASN	OD1-CG-ND2	-10.15	112.45	122.60
1	F	391	PRO	N-CA-CB	10.14	112.28	103.36
1	C	320	ASP	CA-CB-CG	10.11	122.71	112.60
1	E	464	PHE	O-C-N	-10.10	112.61	123.42
1	A	379	ASP	N-CA-C	10.06	122.89	108.00
1	A	398	GLN	OE1-CD-NE2	-10.05	112.55	122.60
1	J	161	LEU	CA-C-O	-10.04	110.83	121.87
1	H	320	ASP	CA-CB-CG	10.02	122.62	112.60
1	K	376	VAL	N-CA-C	10.00	125.45	108.95
1	I	159	ASN	N-CA-C	9.98	125.62	109.85
1	A	82	PHE	CA-CB-CG	9.97	123.77	113.80
1	K	378	SER	N-CA-C	9.85	123.94	111.24
1	D	326	ASN	CA-CB-CG	9.81	122.41	112.60
1	D	73	PHE	CA-CB-CG	9.80	123.60	113.80
1	H	77	PRO	N-CA-CB	9.80	111.98	103.36
1	I	202	ASP	CA-CB-CG	9.78	122.38	112.60
1	A	374	LYS	CA-C-N	9.77	139.29	121.70
1	A	374	LYS	C-N-CA	9.77	139.29	121.70
1	F	77	PRO	CB-CA-C	9.77	120.08	111.87
1	H	276	ARG	NE-CZ-NH2	9.77	127.99	119.20
1	C	373	PRO	N-CA-C	9.74	125.89	114.20
1	J	382	ASP	CA-CB-CG	9.72	122.32	112.60
1	C	117	ASN	CA-CB-CG	9.69	122.28	112.60
1	G	179	PHE	CA-CB-CG	9.66	123.46	113.80
1	J	450	ASN	OD1-CG-ND2	-9.65	112.95	122.60
1	K	131	LEU	CB-CA-C	9.64	119.12	110.44
1	A	203	ASN	CA-CB-CG	9.55	122.16	112.60
1	F	171	ASP	CA-CB-CG	9.55	122.15	112.60
1	J	295	LYS	N-CA-C	9.54	124.49	112.86
1	I	374	LYS	CA-C-N	9.51	138.81	121.70
1	I	374	LYS	C-N-CA	9.51	138.81	121.70
1	E	122	ASP	CA-CB-CG	9.48	122.08	112.60
1	H	287	GLN	CA-C-N	9.45	130.61	120.03
1	H	287	GLN	C-N-CA	9.45	130.61	120.03
1	D	150	ASP	N-CA-C	9.44	124.02	111.28
1	A	239	ASN	CA-CB-CG	9.43	122.03	112.60
1	D	105	GLY	O-C-N	-9.38	116.14	123.27
1	K	377	GLN	OE1-CD-NE2	-9.37	113.23	122.60
1	E	422	PHE	CA-CB-CG	9.37	123.17	113.80
1	C	377	GLN	N-CA-C	9.34	126.94	113.02
1	B	377	GLN	N-CA-C	9.34	122.72	108.52
1	D	392	ARG	NH1-CZ-NH2	-9.32	107.18	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	404	ASN	CB-CA-C	9.32	124.24	110.26
1	G	318	ARG	NE-CZ-NH2	9.31	127.58	119.20
1	L	216	ASP	CA-CB-CG	9.30	121.90	112.60
1	A	63	ARG	NH1-CZ-NH2	-9.30	107.21	119.30
1	I	426	ASP	CA-CB-CG	9.30	121.90	112.60
1	L	66	ARG	NE-CZ-NH2	9.27	127.54	119.20
1	K	185	PHE	CA-CB-CG	9.27	123.06	113.80
1	C	109	SER	CA-C-N	9.26	135.54	120.63
1	C	109	SER	C-N-CA	9.26	135.54	120.63
1	L	200	ASN	OD1-CG-ND2	-9.26	113.34	122.60
1	G	376	VAL	N-CA-C	9.22	122.19	108.46
1	D	239	ASN	OD1-CG-ND2	-9.21	113.39	122.60
1	F	259	ASN	CA-CB-CG	9.21	121.81	112.60
1	H	359	ASN	OD1-CG-ND2	-9.20	113.40	122.60
1	C	372	ASN	OD1-CG-ND2	-9.19	113.41	122.60
1	H	81	GLN	OE1-CD-NE2	-9.19	113.41	122.60
1	D	154	ILE	N-CA-CB	-9.18	99.33	111.82
1	L	327	ASN	CA-CB-CG	9.18	121.78	112.60
1	I	66	ARG	CB-CA-C	9.18	122.08	108.86
1	D	169	SER	N-CA-C	9.17	124.02	113.01
1	L	119	HIS	CB-CG-CD2	-9.15	119.30	131.20
1	K	320	ASP	CA-CB-CG	9.14	121.74	112.60
1	K	356	ASP	CA-CB-CG	9.14	121.74	112.60
1	D	245	ARG	NE-CZ-NH2	9.13	127.42	119.20
1	E	382	ASP	CA-CB-CG	9.12	121.72	112.60
1	E	47	ASP	CA-CB-CG	9.12	121.72	112.60
1	H	143	ILE	N-CA-C	-9.09	103.00	111.45
1	A	297	GLN	OE1-CD-NE2	-9.08	113.52	122.60
1	J	66	ARG	NE-CZ-NH2	9.08	127.37	119.20
1	B	183	ASN	OD1-CG-ND2	-9.04	113.56	122.60
1	B	185	PHE	CA-CB-CG	9.02	122.82	113.80
1	G	46	LYS	N-CA-C	9.02	121.19	111.36
1	I	103	GLY	N-CA-C	9.01	123.85	110.42
1	E	390	ASP	CA-CB-CG	9.00	121.60	112.60
1	D	166	PHE	CA-CB-CG	8.95	122.75	113.80
1	B	344	GLU	N-CA-C	8.94	122.82	109.95
1	F	394	LYS	O-C-N	-8.92	112.50	122.84
1	H	120	VAL	N-CA-C	8.90	120.77	110.62
1	F	230	ASP	CA-CB-CG	8.88	121.48	112.60
1	G	66	ARG	CD-NE-CZ	8.88	136.82	124.40
1	E	259	ASN	CA-CB-CG	8.87	121.47	112.60
1	I	116	THR	CA-C-N	8.86	133.39	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	116	THR	C-N-CA	8.86	133.39	120.90
1	H	218	SER	N-CA-C	8.85	122.39	108.67
1	G	79	PHE	CA-CB-CG	8.84	122.64	113.80
1	A	409	ASP	CA-C-N	8.83	137.56	122.37
1	A	409	ASP	C-N-CA	8.83	137.56	122.37
1	L	260	MET	CA-C-O	-8.81	111.75	121.00
1	D	117	ASN	CA-CB-CG	8.81	121.41	112.60
1	H	304	ASP	CB-CA-C	8.79	122.65	110.34
1	J	419	ASN	OD1-CG-ND2	-8.79	113.81	122.60
1	F	444	GLN	OE1-CD-NE2	-8.79	113.81	122.60
1	C	66	ARG	NE-CZ-NH1	-8.78	112.72	121.50
1	I	225	GLY	CA-C-N	8.76	128.42	120.10
1	I	225	GLY	C-N-CA	8.76	128.42	120.10
1	D	320	ASP	CA-CB-CG	8.73	121.33	112.60
1	E	379	ASP	CA-CB-CG	8.73	121.33	112.60
1	G	305	VAL	N-CA-CB	8.73	120.72	110.95
1	A	77	PRO	CB-CA-C	8.69	119.30	111.40
1	K	122	ASP	CA-CB-CG	8.66	121.26	112.60
1	L	388	ASN	CA-CB-CG	8.65	121.25	112.60
1	F	359	ASN	OD1-CG-ND2	-8.65	113.95	122.60
1	I	438	ASN	OD1-CG-ND2	-8.63	113.97	122.60
1	G	429	ILE	CA-CB-CG1	8.63	125.07	110.40
1	E	364	PHE	CA-CB-CG	8.61	122.41	113.80
1	G	398	GLN	OE1-CD-NE2	-8.61	113.99	122.60
1	J	119	HIS	CA-CB-CG	8.59	122.39	113.80
1	D	406	VAL	N-CA-C	8.59	119.68	108.35
1	E	336	LEU	N-CA-C	8.58	121.41	111.11
1	F	56	SER	CA-C-N	8.58	137.93	121.54
1	F	56	SER	C-N-CA	8.58	137.93	121.54
1	L	223	ASN	CA-CB-CG	8.58	121.18	112.60
1	J	171	ASP	CA-CB-CG	8.57	121.17	112.60
1	I	374	LYS	O-C-N	-8.56	112.92	123.44
1	K	306	GLN	CA-C-N	8.55	137.88	121.54
1	K	306	GLN	C-N-CA	8.55	137.88	121.54
1	D	171	ASP	CA-CB-CG	8.55	121.15	112.60
1	B	326	ASN	OD1-CG-ND2	-8.53	114.07	122.60
1	F	399	ILE	N-CA-C	8.52	116.94	109.02
1	L	318	ARG	NE-CZ-NH2	8.52	126.86	119.20
1	E	177	VAL	N-CA-C	8.51	120.13	108.89
1	K	404	ASN	OD1-CG-ND2	-8.51	114.09	122.60
1	C	202	ASP	CA-CB-CG	8.50	121.10	112.60
1	I	183	ASN	O-C-N	-8.49	111.55	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	214	GLN	OE1-CD-NE2	-8.49	114.11	122.60
1	F	372	ASN	N-CA-C	8.48	120.33	109.65
1	G	464	PHE	CA-CB-CG	8.47	122.27	113.80
1	E	159	ASN	CA-CB-CG	8.47	121.07	112.60
1	H	392	ARG	CB-CA-C	8.47	122.91	111.14
1	F	183	ASN	O-C-N	-8.46	113.73	121.42
1	A	374	LYS	O-C-N	-8.43	111.38	122.59
1	L	375	GLY	O-C-N	-8.43	111.74	122.70
1	G	159	ASN	CA-CB-CG	8.43	121.03	112.60
1	E	73	PHE	CA-CB-CG	8.42	122.22	113.80
1	G	387	ARG	NE-CZ-NH1	8.41	129.91	121.50
1	B	462	ASN	CA-CB-CG	8.40	121.00	112.60
1	I	54	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	D	203	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	L	372	ASN	CA-C-N	8.37	130.30	119.84
1	L	372	ASN	C-N-CA	8.37	130.30	119.84
1	G	239	ASN	OD1-CG-ND2	-8.33	114.27	122.60
1	E	438	ASN	CA-CB-CG	8.33	120.93	112.60
1	A	202	ASP	CA-CB-CG	8.33	120.93	112.60
1	A	402	ASP	CA-CB-CG	8.32	120.92	112.60
1	C	365	ILE	O-C-N	-8.30	113.69	122.57
1	C	208	GLN	OE1-CD-NE2	-8.29	114.31	122.60
1	E	347	GLN	OE1-CD-NE2	-8.29	114.31	122.60
1	L	171	ASP	CA-CB-CG	8.27	120.87	112.60
1	A	220	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	I	438	ASN	CA-C-N	8.25	131.69	120.38
1	I	438	ASN	C-N-CA	8.25	131.69	120.38
1	L	87	PHE	CA-C-N	8.25	127.91	119.82
1	L	87	PHE	C-N-CA	8.25	127.91	119.82
1	D	376	VAL	N-CA-C	8.24	119.25	107.88
1	L	159	ASN	CA-C-N	8.22	133.83	122.07
1	L	159	ASN	C-N-CA	8.22	133.83	122.07
1	H	249	ASN	CA-CB-CG	8.21	120.81	112.60
1	F	255	ALA	N-CA-C	8.21	121.90	108.52
1	F	461	ARG	NE-CZ-NH1	8.19	129.69	121.50
1	D	261	VAL	O-C-N	8.19	130.15	121.87
1	H	90	ARG	N-CA-C	8.19	120.49	110.41
1	I	372	ASN	OD1-CG-ND2	-8.19	114.41	122.60
1	C	378	SER	N-CA-C	8.19	123.05	109.46
1	L	212	PHE	N-CA-C	8.18	121.15	110.43
1	A	342	THR	N-CA-C	8.17	122.83	113.02
1	G	119	HIS	CA-CB-CG	8.17	121.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	GLY	N-CA-C	8.17	122.31	110.80
1	A	245	ARG	NE-CZ-NH2	8.15	126.53	119.20
1	L	76	ASP	CA-CB-CG	8.14	120.74	112.60
1	F	295	LYS	CA-C-N	8.14	136.46	123.93
1	F	295	LYS	C-N-CA	8.14	136.46	123.93
1	D	54	ASN	OD1-CG-ND2	-8.13	114.47	122.60
1	J	75	ASN	OD1-CG-ND2	-8.12	114.48	122.60
1	K	338	ASN	OD1-CG-ND2	-8.11	114.49	122.60
1	H	212	PHE	N-CA-C	8.10	121.37	110.35
1	I	77	PRO	N-CA-CB	8.10	111.50	102.67
1	I	90	ARG	NE-CZ-NH2	8.09	126.48	119.20
1	D	264	ILE	CA-C-N	8.08	130.94	120.44
1	D	264	ILE	C-N-CA	8.08	130.94	120.44
1	J	217	ALA	N-CA-C	8.08	121.66	110.35
1	E	152	ALA	CA-C-O	-8.08	110.34	120.28
1	I	184	PRO	N-CA-CB	8.06	110.34	103.17
1	A	73	PHE	CB-CA-C	8.04	121.18	111.22
1	F	376	VAL	CA-C-N	8.03	135.42	122.81
1	F	376	VAL	C-N-CA	8.03	135.42	122.81
1	B	43	ASP	CA-CB-CG	8.03	120.63	112.60
1	B	88	PRO	N-CA-C	8.01	124.26	113.84
1	C	348	LYS	CA-C-N	8.01	133.99	123.10
1	C	348	LYS	C-N-CA	8.01	133.99	123.10
1	D	378	SER	CA-C-N	8.01	136.84	121.54
1	D	378	SER	C-N-CA	8.01	136.84	121.54
1	B	377	GLN	CA-C-O	-8.00	111.79	120.75
1	F	238	ILE	CA-C-N	8.00	132.15	120.95
1	F	238	ILE	C-N-CA	8.00	132.15	120.95
1	J	394	LYS	CA-C-N	7.97	136.04	121.70
1	J	394	LYS	C-N-CA	7.97	136.04	121.70
1	F	295	LYS	N-CA-C	7.96	122.95	113.23
1	I	232	ARG	NH1-CZ-NH2	-7.95	108.96	119.30
1	G	165	THR	CA-C-N	7.95	133.10	122.06
1	G	165	THR	C-N-CA	7.95	133.10	122.06
1	F	117	ASN	CA-CB-CG	7.94	120.54	112.60
1	K	208	GLN	OE1-CD-NE2	-7.94	114.66	122.60
1	A	121	VAL	N-CA-C	7.92	120.51	112.90
1	B	56	SER	N-CA-C	7.92	123.05	113.23
1	F	299	GLY	CA-C-O	-7.92	113.06	121.38
1	D	137	GLU	CA-C-N	7.92	133.81	122.09
1	D	137	GLU	C-N-CA	7.92	133.81	122.09
1	E	107	ILE	N-CA-CB	7.92	119.82	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	GLY	CA-C-O	-7.91	114.36	121.64
1	J	131	LEU	CA-C-N	7.91	128.39	119.93
1	J	131	LEU	C-N-CA	7.91	128.39	119.93
1	C	327	ASN	CA-CB-CG	7.90	120.50	112.60
1	B	81	GLN	OE1-CD-NE2	-7.87	114.73	122.60
1	H	394	LYS	O-C-N	-7.86	113.49	122.68
1	I	220	ASN	OD1-CG-ND2	-7.86	114.75	122.60
1	L	377	GLN	N-CA-C	7.86	121.17	108.76
1	G	248	GLY	CA-C-O	-7.84	112.61	121.94
1	L	105	GLY	CA-C-O	-7.83	113.15	121.38
1	C	400	PRO	CA-C-N	7.83	131.81	120.38
1	C	400	PRO	C-N-CA	7.83	131.81	120.38
1	L	220	ASN	CA-CB-CG	7.83	120.43	112.60
1	H	131	LEU	CA-C-N	7.83	129.06	119.98
1	H	131	LEU	C-N-CA	7.83	129.06	119.98
1	G	390	ASP	CA-CB-CG	-7.82	104.78	112.60
1	K	306	GLN	OE1-CD-NE2	-7.82	114.78	122.60
1	C	99	VAL	CA-C-N	7.82	136.62	122.09
1	C	99	VAL	C-N-CA	7.82	136.62	122.09
1	E	127	ILE	CA-C-N	7.81	131.88	120.95
1	E	127	ILE	C-N-CA	7.81	131.88	120.95
1	I	292	LYS	N-CA-C	7.81	119.43	111.07
1	A	204	ILE	N-CA-C	-7.80	105.46	111.62
1	D	361	GLN	OE1-CD-NE2	-7.79	114.81	122.60
1	L	102	LEU	CA-C-N	7.79	131.62	120.56
1	L	102	LEU	C-N-CA	7.79	131.62	120.56
1	L	108	ILE	N-CA-C	7.79	118.58	110.72
1	C	388	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	L	249	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	J	150	ASP	CB-CA-C	7.77	122.77	111.73
1	I	388	ASN	OD1-CG-ND2	-7.77	114.83	122.60
1	A	426	ASP	CA-CB-CG	7.77	120.37	112.60
1	J	232	ARG	NE-CZ-NH2	7.77	126.19	119.20
1	I	121	VAL	O-C-N	-7.76	112.87	122.57
1	I	146	ASP	CA-CB-CG	-7.76	104.84	112.60
1	B	383	GLY	CA-C-O	7.76	129.34	120.03
1	K	89	GLN	CA-C-N	7.73	134.71	120.95
1	K	89	GLN	C-N-CA	7.73	134.71	120.95
1	K	290	THR	CA-CB-OG1	7.71	121.17	109.60
1	J	470	LEU	N-CA-C	7.70	120.95	108.63
1	D	404	ASN	CA-CB-CG	7.70	120.30	112.60
1	C	464	PHE	CA-CB-CG	7.70	121.50	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	74	PHE	CA-CB-CG	7.69	121.49	113.80
1	J	374	LYS	N-CA-C	7.69	127.18	110.80
1	E	400	PRO	CB-CA-C	-7.68	100.94	111.85
1	A	211	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	C	390	ASP	CA-C-N	7.67	129.43	119.84
1	C	390	ASP	C-N-CA	7.67	129.43	119.84
1	D	261	VAL	CA-C-O	-7.67	112.36	120.57
1	C	374	LYS	O-C-N	-7.67	112.39	122.59
1	D	441	ASP	CA-CB-CG	7.67	120.27	112.60
1	L	183	ASN	OD1-CG-ND2	-7.67	114.93	122.60
1	F	300	ALA	CA-C-N	7.66	133.61	121.66
1	F	300	ALA	C-N-CA	7.66	133.61	121.66
1	H	130	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	K	469	VAL	O-C-N	-7.65	113.01	122.57
1	A	462	ASN	OD1-CG-ND2	-7.65	114.95	122.60
1	K	119	HIS	CA-CB-CG	7.65	121.45	113.80
1	L	366	LEU	CA-C-N	7.65	133.72	122.86
1	L	366	LEU	C-N-CA	7.65	133.72	122.86
1	H	438	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	L	326	ASN	CA-CB-CG	7.64	120.24	112.60
1	F	237	GLY	CA-C-N	7.64	132.94	123.17
1	F	237	GLY	C-N-CA	7.64	132.94	123.17
1	G	65	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	F	392	ARG	NE-CZ-NH2	7.62	126.06	119.20
1	L	183	ASN	O-C-N	-7.61	114.49	121.42
1	C	438	ASN	CA-CB-CG	7.61	120.21	112.60
1	C	239	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	G	81	GLN	OE1-CD-NE2	-7.61	114.99	122.60
1	I	125	ASP	CA-CB-CG	7.61	120.21	112.60
1	I	398	GLN	OE1-CD-NE2	-7.61	115.00	122.60
1	G	107	ILE	CA-CB-CG1	7.60	123.33	110.40
1	G	327	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	K	281	VAL	CA-CB-CG1	7.59	123.31	110.40
1	L	126	THR	O-C-N	-7.59	112.50	122.59
1	I	208	GLN	OE1-CD-NE2	-7.59	115.01	122.60
1	I	376	VAL	N-CA-C	7.59	117.77	108.06
1	H	404	ASN	CA-CB-CG	7.58	120.18	112.60
1	L	382	ASP	CA-CB-CG	7.58	120.18	112.60
1	E	461	ARG	NE-CZ-NH1	7.57	129.07	121.50
1	H	258	SER	N-CA-CB	7.56	121.40	110.06
1	B	118	ASN	CA-CB-CG	-7.56	105.04	112.60
1	K	374	LYS	N-CA-C	7.56	126.90	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	392	ARG	NH1-CZ-NH2	-7.55	109.48	119.30
1	D	372	ASN	OD1-CG-ND2	-7.55	115.05	122.60
1	L	212	PHE	CA-C-N	7.55	132.84	123.10
1	L	212	PHE	C-N-CA	7.55	132.84	123.10
1	L	438	ASN	N-CA-C	7.54	117.84	107.73
1	D	396	ARG	CA-C-N	7.54	134.24	121.87
1	D	396	ARG	C-N-CA	7.54	134.24	121.87
1	H	54	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	L	404	ASN	OD1-CG-ND2	-7.53	115.07	122.60
1	G	426	ASP	CA-CB-CG	7.53	120.13	112.60
1	G	84	ASP	N-CA-C	7.53	120.29	110.43
1	C	178	VAL	O-C-N	7.52	131.60	122.58
1	D	398	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	C	343	LEU	CA-C-O	-7.51	111.30	120.54
1	K	60	THR	CA-C-O	7.51	128.39	119.60
1	H	57	THR	CA-CB-CG2	7.50	123.25	110.50
1	G	207	ASN	OD1-CG-ND2	-7.50	115.10	122.60
1	A	226	GLY	N-CA-C	7.50	121.81	112.14
1	I	119	HIS	CA-C-N	7.48	132.29	120.47
1	I	119	HIS	C-N-CA	7.48	132.29	120.47
1	C	374	LYS	N-CA-C	7.48	126.73	110.80
1	H	87	PHE	O-C-N	-7.47	112.06	121.70
1	I	179	PHE	CA-CB-CG	7.47	121.27	113.80
1	A	39	LEU	CA-C-O	7.47	129.24	120.58
1	G	382	ASP	CA-CB-CG	7.47	120.07	112.60
1	J	214	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	G	267	LYS	CA-C-O	-7.44	112.66	120.55
1	G	448	GLN	OE1-CD-NE2	-7.44	115.16	122.60
1	D	264	ILE	CB-CA-C	7.43	121.49	111.97
1	L	157	GLU	CB-CA-C	7.43	122.36	111.88
1	J	43	ASP	CA-CB-CG	7.42	120.02	112.60
1	D	333	PRO	CB-CA-C	-7.41	101.29	112.11
1	A	253	GLY	CA-C-O	-7.41	114.18	120.92
1	L	312	ASP	N-CA-C	7.41	119.43	111.36
1	D	404	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	A	64	ALA	CA-C-N	7.40	134.84	122.79
1	A	64	ALA	C-N-CA	7.40	134.84	122.79
1	F	220	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	B	172	LEU	CA-C-O	7.38	129.96	121.47
1	H	232	ARG	NE-CZ-NH2	7.38	125.84	119.20
1	K	304	ASP	CA-CB-CG	-7.38	105.22	112.60
1	L	281	VAL	O-C-N	-7.38	116.55	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	364	PHE	CA-C-N	7.38	130.61	120.35
1	H	364	PHE	C-N-CA	7.38	130.61	120.35
1	H	90	ARG	CA-C-O	-7.37	113.59	121.99
1	D	377	GLN	N-CA-C	7.37	119.58	108.46
1	G	339	TYR	CA-C-N	7.34	130.52	120.46
1	G	339	TYR	C-N-CA	7.34	130.52	120.46
1	I	174	GLU	O-C-N	-7.34	113.94	122.89
1	K	335	ASP	CA-C-N	7.34	130.11	120.28
1	K	335	ASP	C-N-CA	7.34	130.11	120.28
1	H	121	VAL	CA-C-O	-7.33	112.44	118.90
1	D	160	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	G	249	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	H	230	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	371	GLU	N-CA-C	7.33	123.60	112.54
1	J	198	ALA	N-CA-C	7.32	119.99	108.79
1	L	212	PHE	CA-CB-CG	7.32	121.11	113.80
1	L	121	VAL	CA-C-O	-7.30	112.20	119.20
1	G	94	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	I	87	PHE	CA-CB-CG	7.29	121.09	113.80
1	B	330	ILE	CA-C-N	7.29	133.23	122.08
1	B	330	ILE	C-N-CA	7.29	133.23	122.08
1	F	288	GLY	O-C-N	-7.29	114.45	122.68
1	H	238	ILE	CA-C-O	7.29	127.45	120.31
1	C	296	ASN	CA-C-O	7.28	130.01	120.98
1	A	129	VAL	N-CA-C	7.28	120.05	108.85
1	G	375	GLY	N-CA-C	7.28	125.56	111.66
1	H	87	PHE	CA-C-N	7.27	126.98	119.56
1	H	87	PHE	C-N-CA	7.27	126.98	119.56
1	D	249	ASN	CA-CB-CG	7.27	119.87	112.60
1	D	354	GLU	CA-C-N	7.27	132.98	122.44
1	D	354	GLU	C-N-CA	7.27	132.98	122.44
1	B	176	ASP	CA-CB-CG	7.27	119.87	112.60
1	B	388	ASN	CA-CB-CG	7.26	119.86	112.60
1	H	396	ARG	NE-CZ-NH2	7.25	125.73	119.20
1	D	372	ASN	N-CA-C	7.25	121.25	109.15
1	A	377	GLN	N-CA-C	7.24	121.82	112.12
1	L	263	ASP	CA-C-N	7.24	129.68	120.56
1	L	263	ASP	C-N-CA	7.24	129.68	120.56
1	L	373	PRO	N-CA-C	7.24	127.38	112.47
1	G	451	LYS	CA-C-O	-7.23	110.65	119.18
1	C	211	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	I	122	ASP	CA-CB-CG	7.23	119.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	427	ILE	O-C-N	-7.23	115.66	123.18
1	F	110	LYS	O-C-N	-7.22	112.82	122.43
1	L	117	ASN	CA-CB-CG	7.22	119.82	112.60
1	K	461	ARG	CD-NE-CZ	7.22	134.51	124.40
1	J	220	ASN	OD1-CG-ND2	-7.22	115.38	122.60
1	C	379	ASP	CA-C-O	-7.22	110.19	120.51
1	A	459	VAL	CA-C-O	7.22	127.38	120.31
1	J	316	LEU	CB-CA-C	7.22	121.60	109.84
1	C	183	ASN	O-C-N	-7.21	113.02	121.32
1	I	400	PRO	N-CA-CB	7.21	111.38	103.30
1	J	461	ARG	NE-CZ-NH1	7.21	128.72	121.50
1	I	220	ASN	CA-C-N	7.21	127.65	119.93
1	I	220	ASN	C-N-CA	7.21	127.65	119.93
1	B	146	ASP	CA-C-N	7.21	127.83	120.04
1	B	146	ASP	C-N-CA	7.21	127.83	120.04
1	B	182	GLY	CA-C-O	-7.21	115.93	120.91
1	I	332	SER	CA-C-N	7.21	126.70	118.85
1	I	332	SER	C-N-CA	7.21	126.70	118.85
1	F	232	ARG	NE-CZ-NH1	-7.20	114.30	121.50
1	B	283	ILE	O-C-N	-7.19	115.09	123.00
1	A	232	ARG	NH1-CZ-NH2	-7.19	109.96	119.30
1	B	311	ALA	O-C-N	7.19	129.56	122.09
1	C	255	ALA	CA-C-O	-7.18	113.07	120.54
1	G	225	GLY	O-C-N	-7.18	114.24	122.42
1	C	166	PHE	CA-CB-CG	7.17	120.97	113.80
1	C	221	PRO	N-CA-CB	7.17	109.56	103.25
1	A	469	VAL	N-CA-C	7.16	116.63	106.53
1	C	438	ASN	O-C-N	-7.16	115.33	122.99
1	H	65	ASN	OD1-CG-ND2	-7.16	115.44	122.60
1	H	378	SER	N-CA-C	7.16	126.05	110.80
1	A	226	GLY	CA-C-O	-7.15	114.18	121.90
1	H	382	ASP	CA-CB-CG	7.15	119.75	112.60
1	C	275	ASP	CA-CB-CG	7.14	119.74	112.60
1	C	73	PHE	CA-CB-CG	7.14	120.94	113.80
1	F	390	ASP	CA-C-N	7.14	127.40	119.90
1	F	390	ASP	C-N-CA	7.14	127.40	119.90
1	C	330	ILE	CA-C-N	7.14	132.90	121.98
1	C	330	ILE	C-N-CA	7.14	132.90	121.98
1	D	327	ASN	CA-CB-CG	7.14	119.74	112.60
1	J	409	ASP	CA-C-O	-7.14	113.33	120.82
1	H	88	PRO	N-CA-C	7.13	123.11	113.84
1	K	242	ILE	O-C-N	-7.13	115.50	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	75	ASN	CA-CB-CG	7.13	119.73	112.60
1	L	238	ILE	CA-CB-CG1	7.13	122.52	110.40
1	A	355	ARG	NE-CZ-NH2	7.12	125.61	119.20
1	C	358	GLU	CA-C-N	7.12	132.63	122.09
1	C	358	GLU	C-N-CA	7.12	132.63	122.09
1	C	374	LYS	CA-C-N	7.12	134.52	121.70
1	C	374	LYS	C-N-CA	7.12	134.52	121.70
1	D	218	SER	O-C-N	7.12	131.37	123.04
1	L	254	PHE	CA-C-N	7.11	132.82	123.00
1	L	254	PHE	C-N-CA	7.11	132.82	123.00
1	D	250	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	I	232	ARG	NE-CZ-NH2	7.11	125.60	119.20
1	L	387	ARG	CA-C-N	7.11	130.80	120.71
1	L	387	ARG	C-N-CA	7.11	130.80	120.71
1	K	227	ALA	CA-C-N	7.10	132.79	122.77
1	K	227	ALA	C-N-CA	7.10	132.79	122.77
1	E	454	PHE	O-C-N	-7.10	115.16	123.25
1	F	426	ASP	CA-CB-CG	7.10	119.70	112.60
1	L	218	SER	N-CA-C	7.09	120.02	109.59
1	A	87	PHE	CA-CB-CG	7.09	120.89	113.80
1	J	41	TYR	CB-CA-C	7.09	122.63	110.94
1	I	248	GLY	O-C-N	-7.08	118.11	123.35
1	L	166	PHE	CA-C-N	7.08	133.86	120.97
1	L	166	PHE	C-N-CA	7.08	133.86	120.97
1	B	220	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	C	444	GLN	OE1-CD-NE2	-7.08	115.52	122.60
1	H	208	GLN	OE1-CD-NE2	-7.07	115.53	122.60
1	B	374	LYS	CA-C-N	7.07	130.60	120.56
1	B	374	LYS	C-N-CA	7.07	130.60	120.56
1	A	276	ARG	CD-NE-CZ	7.07	134.29	124.40
1	A	331	LYS	N-CA-CB	-7.07	101.50	110.90
1	L	172	LEU	N-CA-C	7.06	121.54	110.17
1	G	297	GLN	CA-C-N	7.06	133.63	122.62
1	G	297	GLN	C-N-CA	7.06	133.63	122.62
1	D	250	ASN	CA-CB-CG	7.05	119.65	112.60
1	H	227	ALA	N-CA-C	7.05	120.45	110.50
1	I	165	THR	CA-C-O	7.05	128.59	120.98
1	A	96	LYS	CA-CB-CG	7.05	128.19	114.10
1	E	43	ASP	CA-CB-CG	7.04	119.64	112.60
1	I	382	ASP	CA-CB-CG	7.04	119.64	112.60
1	J	49	LYS	O-C-N	7.04	129.58	122.12
1	A	317	LYS	CA-CB-CG	7.03	128.17	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	270	GLU	CA-C-N	7.03	131.00	120.17
1	H	270	GLU	C-N-CA	7.03	131.00	120.17
1	A	374	LYS	N-CA-C	7.03	125.77	110.80
1	B	298	GLU	CA-C-N	7.03	130.97	121.83
1	B	298	GLU	C-N-CA	7.03	130.97	121.83
1	E	130	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	L	159	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	A	376	VAL	N-CA-C	7.03	117.62	108.35
1	G	42	HIS	CB-CG-CD2	-7.02	122.07	131.20
1	B	318	ARG	NE-CZ-NH2	7.01	125.51	119.20
1	G	125	ASP	CA-CB-CG	7.01	119.61	112.60
1	L	162	SER	N-CA-C	7.01	119.03	110.41
1	C	360	LYS	CA-C-O	-7.00	112.92	121.11
1	A	84	ASP	N-CA-C	7.00	120.82	110.46
1	B	372	ASN	N-CA-C	6.99	123.83	108.73
1	K	232	ARG	NH1-CZ-NH2	-6.99	110.21	119.30
1	F	130	ASN	CA-CB-CG	-6.99	105.61	112.60
1	C	236	VAL	CA-CB-CG2	6.99	122.28	110.40
1	I	87	PHE	CA-C-N	6.99	126.62	119.56
1	I	87	PHE	C-N-CA	6.99	126.62	119.56
1	C	107	ILE	CA-C-N	6.98	130.73	120.74
1	C	107	ILE	C-N-CA	6.98	130.73	120.74
1	C	75	ASN	CA-CB-CG	6.98	119.58	112.60
1	L	166	PHE	CA-CB-CG	6.98	120.78	113.80
1	C	110	LYS	CA-C-N	6.97	134.99	121.18
1	C	110	LYS	C-N-CA	6.97	134.99	121.18
1	A	90	ARG	NE-CZ-NH1	-6.97	114.53	121.50
1	E	355	ARG	NH1-CZ-NH2	-6.97	110.24	119.30
1	K	47	ASP	CA-CB-CG	6.97	119.57	112.60
1	L	212	PHE	O-C-N	-6.96	114.60	122.75
1	L	396	ARG	NE-CZ-NH1	-6.96	114.54	121.50
1	H	448	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	L	306	GLN	CA-C-N	6.95	134.82	121.54
1	L	306	GLN	C-N-CA	6.95	134.82	121.54
1	B	375	GLY	CA-C-O	-6.95	114.08	121.38
1	F	373	PRO	CA-C-N	6.95	134.81	121.54
1	F	373	PRO	C-N-CA	6.95	134.81	121.54
1	J	211	ASN	CA-C-N	6.95	130.69	120.90
1	J	211	ASN	C-N-CA	6.95	130.69	120.90
1	I	344	GLU	CA-C-N	6.93	130.87	120.75
1	I	344	GLU	C-N-CA	6.93	130.87	120.75
1	J	276	ARG	NE-CZ-NH1	6.93	128.43	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	ILE	N-CA-C	-6.93	104.10	110.82
1	F	292	LYS	CA-C-N	6.93	129.56	120.28
1	F	292	LYS	C-N-CA	6.93	129.56	120.28
1	J	159	ASN	CA-C-N	6.93	132.27	122.08
1	J	159	ASN	C-N-CA	6.93	132.27	122.08
1	A	248	GLY	CA-C-O	-6.92	115.15	120.76
1	H	406	VAL	N-CA-C	6.92	117.75	108.27
1	F	160	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	J	156	ILE	N-CA-CB	6.91	118.49	110.82
1	K	203	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	H	368	GLY	CA-C-N	6.91	131.66	120.60
1	H	368	GLY	C-N-CA	6.91	131.66	120.60
1	J	318	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	C	215	THR	CA-CB-OG1	6.91	119.96	109.60
1	I	454	PHE	CA-CB-CG	-6.91	106.89	113.80
1	J	438	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	H	419	ASN	CA-CB-CG	6.90	119.50	112.60
1	I	374	LYS	N-CA-C	6.89	120.89	108.48
1	J	227	ALA	CA-C-N	6.89	132.71	122.99
1	J	227	ALA	C-N-CA	6.89	132.71	122.99
1	E	372	ASN	N-CA-C	6.89	121.81	108.85
1	F	201	LYS	CA-C-O	6.89	127.67	120.30
1	L	369	GLU	CA-C-O	6.89	127.85	119.38
1	D	121	VAL	CA-C-O	-6.88	112.42	118.96
1	F	323	THR	CA-C-N	6.88	131.86	121.40
1	F	323	THR	C-N-CA	6.88	131.86	121.40
1	K	379	ASP	N-CA-C	6.88	125.46	110.80
1	B	91	LYS	N-CA-C	6.88	119.18	110.24
1	D	355	ARG	CA-C-N	6.88	134.68	121.54
1	D	355	ARG	C-N-CA	6.88	134.68	121.54
1	E	449	VAL	CA-C-O	-6.88	113.21	120.57
1	E	215	THR	N-CA-C	6.88	118.56	108.86
1	C	67	PRO	N-CA-CB	6.87	109.30	103.25
1	K	349	ILE	CB-CA-C	6.87	118.91	110.73
1	A	90	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	B	192	THR	CA-CB-OG1	6.87	119.90	109.60
1	E	448	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	K	326	ASN	N-CA-C	6.87	121.27	112.34
1	G	126	THR	CA-CB-CG2	6.86	122.17	110.50
1	G	311	ALA	N-CA-C	6.86	119.39	111.02
1	H	125	ASP	CA-CB-CG	6.86	119.45	112.60
1	I	63	ARG	NE-CZ-NH2	6.85	125.37	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	LYS	CA-C-N	6.85	129.46	120.28
1	B	412	LYS	C-N-CA	6.85	129.46	120.28
1	D	456	LYS	CA-C-O	6.85	131.47	122.63
1	E	208	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	G	182	GLY	CA-C-N	6.84	130.37	122.85
1	G	182	GLY	C-N-CA	6.84	130.37	122.85
1	J	97	GLU	N-CA-C	6.84	121.23	112.34
1	D	163	ALA	CB-CA-C	-6.84	105.85	114.40
1	F	451	LYS	CA-C-N	6.83	132.66	121.86
1	F	451	LYS	C-N-CA	6.83	132.66	121.86
1	L	241	ALA	N-CA-CB	-6.83	100.97	111.56
1	A	242	ILE	CA-CB-CG1	6.83	122.01	110.40
1	B	410	SER	N-CA-C	6.83	118.52	108.14
1	J	120	VAL	CA-C-O	6.83	127.09	119.92
1	C	263	ASP	CA-CB-CG	6.83	119.43	112.60
1	L	359	ASN	CA-CB-CG	-6.83	105.77	112.60
1	F	438	ASN	CB-CG-ND2	6.83	126.64	116.40
1	K	230	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	363	SER	CA-C-N	6.82	132.41	123.00
1	A	363	SER	C-N-CA	6.82	132.41	123.00
1	D	136	ILE	N-CA-C	6.82	117.30	106.32
1	B	127	ILE	CA-C-O	6.82	129.31	120.78
1	F	116	THR	CA-CB-CG2	6.82	122.09	110.50
1	K	389	LEU	CA-C-N	6.82	129.76	122.26
1	K	389	LEU	C-N-CA	6.82	129.76	122.26
1	F	43	ASP	CA-CB-CG	6.82	119.42	112.60
1	I	76	ASP	CB-CA-C	6.82	120.14	111.21
1	J	377	GLN	N-CA-C	6.82	119.22	108.79
1	J	404	ASN	CA-CB-CG	6.82	119.42	112.60
1	D	65	ASN	CB-CG-ND2	6.81	126.62	116.40
1	B	125	ASP	CA-CB-CG	6.81	119.41	112.60
1	E	42	HIS	ND1-CE1-NE2	6.81	115.21	108.40
1	I	80	LYS	CB-CG-CD	6.81	126.96	111.30
1	H	466	THR	CA-C-N	6.81	133.46	123.12
1	H	466	THR	C-N-CA	6.81	133.46	123.12
1	G	185	PHE	CA-CB-CG	6.80	120.61	113.80
1	H	362	ALA	CA-C-O	-6.80	110.78	120.51
1	E	441	ASP	CA-CB-CG	6.80	119.40	112.60
1	F	212	PHE	CA-C-N	6.80	132.88	122.68
1	F	212	PHE	C-N-CA	6.80	132.88	122.68
1	E	348	LYS	N-CA-C	6.79	120.56	109.76
1	G	128	THR	CA-CB-CG2	6.79	122.05	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	230	ASP	CA-CB-CG	6.79	119.39	112.60
1	C	447	LYS	CA-C-O	-6.79	113.22	120.42
1	D	406	VAL	O-C-N	-6.79	115.22	123.09
1	D	278	PHE	CA-C-O	-6.78	113.68	120.80
1	C	60	THR	CA-CB-CG2	6.78	122.03	110.50
1	F	47	ASP	N-CA-CB	6.77	120.18	110.16
1	B	424	GLU	CB-CG-CD	6.77	124.11	112.60
1	A	312	ASP	N-CA-CB	-6.77	100.14	110.16
1	E	378	SER	N-CA-C	6.76	125.20	110.80
1	G	87	PHE	CB-CA-C	6.76	119.02	108.88
1	K	212	PHE	N-CA-C	6.76	120.03	110.23
1	G	336	LEU	CA-C-N	6.76	130.18	120.79
1	G	336	LEU	C-N-CA	6.76	130.18	120.79
1	E	94	ASN	N-CA-C	6.75	119.48	107.80
1	K	223	ASN	CA-CB-CG	6.75	119.35	112.60
1	E	155	LYS	CB-CG-CD	6.75	126.82	111.30
1	B	356	ASP	N-CA-C	6.75	125.17	110.80
1	L	433	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	L	271	LYS	CA-C-O	-6.74	111.18	118.79
1	H	344	GLU	CA-C-N	6.74	129.72	120.35
1	H	344	GLU	C-N-CA	6.74	129.72	120.35
1	L	42	HIS	CB-CG-CD2	-6.73	122.45	131.20
1	B	99	VAL	CA-C-N	6.73	134.39	121.54
1	B	99	VAL	C-N-CA	6.73	134.39	121.54
1	K	167	THR	N-CA-C	6.73	119.25	110.43
1	B	44	SER	N-CA-CB	6.73	120.01	110.12
1	E	376	VAL	N-CA-C	6.72	118.17	108.48
1	F	167	THR	CA-CB-CG2	6.72	121.93	110.50
1	E	90	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	B	66	ARG	CA-C-N	6.72	126.68	119.76
1	B	66	ARG	C-N-CA	6.72	126.68	119.76
1	B	335	ASP	CA-CB-CG	6.72	119.32	112.60
1	E	97	GLU	O-C-N	-6.72	114.36	122.22
1	K	231	SER	CA-C-N	6.72	132.77	122.29
1	K	231	SER	C-N-CA	6.72	132.77	122.29
1	F	371	GLU	N-CA-C	6.71	125.10	110.80
1	I	325	VAL	CA-CB-CG2	6.71	121.81	110.40
1	K	233	GLY	CA-C-O	-6.71	110.94	119.13
1	K	373	PRO	CA-C-N	6.71	134.36	121.54
1	K	373	PRO	C-N-CA	6.71	134.36	121.54
1	D	168	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	F	264	ILE	CA-C-N	6.71	129.16	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	264	ILE	C-N-CA	6.71	129.16	120.44
1	K	448	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	A	349	ILE	CA-C-O	6.70	128.93	120.75
1	L	87	PHE	O-C-N	-6.70	113.49	121.39
1	E	178	VAL	N-CA-C	6.70	117.81	108.23
1	A	300	ALA	CA-C-N	6.69	132.10	121.66
1	A	300	ALA	C-N-CA	6.69	132.10	121.66
1	F	451	LYS	O-C-N	6.69	131.17	122.20
1	B	449	VAL	O-C-N	-6.69	115.11	121.87
1	C	215	THR	OG1-CB-CG2	-6.69	95.92	109.30
1	D	184	PRO	CA-C-N	6.69	132.10	122.40
1	D	184	PRO	C-N-CA	6.69	132.10	122.40
1	F	438	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	D	66	ARG	CD-NE-CZ	6.69	133.76	124.40
1	J	375	GLY	O-C-N	-6.68	115.53	123.61
1	E	294	TYR	CB-CA-C	6.68	119.44	111.22
1	F	54	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	G	168	ASN	CA-C-N	6.68	131.38	120.63
1	G	168	ASN	C-N-CA	6.68	131.38	120.63
1	D	208	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	E	160	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	J	376	VAL	N-CA-C	6.68	119.41	108.99
1	K	117	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	B	361	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	D	122	ASP	CA-CB-CG	6.67	119.27	112.60
1	H	55	ILE	CA-C-N	6.67	131.33	122.06
1	H	55	ILE	C-N-CA	6.67	131.33	122.06
1	L	297	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	A	122	ASP	CA-CB-CG	6.67	119.27	112.60
1	D	81	GLN	N-CA-C	6.67	120.77	112.24
1	K	55	ILE	CA-C-N	6.67	132.08	122.21
1	K	55	ILE	C-N-CA	6.67	132.08	122.21
1	D	86	ASP	CA-CB-CG	6.67	119.27	112.60
1	E	267	LYS	CA-C-N	6.67	130.44	120.31
1	E	267	LYS	C-N-CA	6.67	130.44	120.31
1	D	423	GLN	CA-C-O	6.66	128.79	121.06
1	F	355	ARG	NE-CZ-NH2	6.66	125.20	119.20
1	C	306	GLN	CA-C-N	6.65	134.24	121.54
1	C	306	GLN	C-N-CA	6.65	134.24	121.54
1	D	374	LYS	N-CA-C	6.65	124.96	110.80
1	L	438	ASN	CA-C-O	-6.65	114.03	120.94
1	A	306	GLN	OE1-CD-NE2	-6.64	115.95	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	192	THR	CA-C-N	6.64	133.49	122.73
1	C	192	THR	C-N-CA	6.64	133.49	122.73
1	F	41	TYR	CA-C-N	6.64	131.33	120.63
1	F	41	TYR	C-N-CA	6.64	131.33	120.63
1	G	230	ASP	CA-CB-CG	6.64	119.24	112.60
1	H	166	PHE	CA-CB-CG	6.64	120.44	113.80
1	B	220	ASN	CA-CB-CG	6.63	119.23	112.60
1	E	379	ASP	N-CA-C	6.63	118.39	108.31
1	D	394	LYS	CA-C-N	6.63	133.63	121.70
1	D	394	LYS	C-N-CA	6.63	133.63	121.70
1	H	66	ARG	NE-CZ-NH2	6.63	125.17	119.20
1	H	308	GLY	CA-C-N	6.63	132.75	120.95
1	H	308	GLY	C-N-CA	6.63	132.75	120.95
1	E	183	ASN	CA-CB-CG	6.63	119.23	112.60
1	D	121	VAL	O-C-N	6.62	128.94	122.25
1	C	82	PHE	CA-CB-CG	6.62	120.42	113.80
1	H	325	VAL	N-CA-C	-6.62	102.73	110.21
1	K	308	GLY	CA-C-N	6.62	132.80	121.29
1	K	308	GLY	C-N-CA	6.62	132.80	121.29
1	B	207	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	K	245	ARG	NE-CZ-NH2	6.62	125.15	119.20
1	A	54	ASN	CA-CB-CG	6.61	119.21	112.60
1	B	94	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	F	400	PRO	N-CA-C	6.61	122.57	113.65
1	G	203	ASN	CA-CB-CG	6.60	119.20	112.60
1	C	373	PRO	CA-C-N	6.59	134.14	121.54
1	C	373	PRO	C-N-CA	6.59	134.14	121.54
1	J	414	LYS	CA-C-O	-6.59	113.56	120.55
1	A	227	ALA	CA-C-N	6.58	132.05	122.77
1	A	227	ALA	C-N-CA	6.58	132.05	122.77
1	A	415	SER	CA-C-N	6.58	129.99	120.38
1	A	415	SER	C-N-CA	6.58	129.99	120.38
1	H	344	GLU	N-CA-CB	-6.58	99.93	110.46
1	I	394	LYS	O-C-N	-6.58	114.59	123.15
1	F	49	LYS	N-CA-C	6.58	120.41	112.38
1	J	436	ILE	O-C-N	-6.58	115.93	122.97
1	L	344	GLU	CA-C-N	6.58	129.32	120.50
1	L	344	GLU	C-N-CA	6.58	129.32	120.50
1	B	223	ASN	N-CA-C	-6.57	105.33	113.15
1	F	376	VAL	N-CA-C	6.57	118.25	108.46
1	D	451	LYS	CA-C-N	6.57	132.33	122.47
1	D	451	LYS	C-N-CA	6.57	132.33	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	244	SER	O-C-N	-6.57	113.84	122.97
1	G	374	LYS	CA-C-N	6.57	131.62	121.37
1	G	374	LYS	C-N-CA	6.57	131.62	121.37
1	B	417	GLY	CA-C-O	-6.57	114.29	121.05
1	B	449	VAL	N-CA-C	6.57	119.26	111.05
1	E	154	ILE	CA-C-O	-6.56	113.62	120.64
1	G	429	ILE	CB-CA-C	6.56	116.83	111.06
1	G	378	SER	N-CA-C	6.56	120.04	109.02
1	G	398	GLN	CA-CB-CG	-6.56	100.98	114.10
1	J	194	GLY	CA-C-N	6.56	132.11	123.06
1	J	194	GLY	C-N-CA	6.56	132.11	123.06
1	D	392	ARG	NE-CZ-NH2	6.56	125.10	119.20
1	A	149	THR	CA-C-N	6.55	132.07	122.63
1	A	149	THR	C-N-CA	6.55	132.07	122.63
1	G	162	SER	CA-C-O	-6.55	114.40	121.94
1	K	134	SER	N-CA-C	6.55	124.76	110.80
1	F	73	PHE	CA-CB-CG	6.55	120.35	113.80
1	L	43	ASP	CA-C-N	6.55	129.71	120.28
1	L	43	ASP	C-N-CA	6.55	129.71	120.28
1	I	172	LEU	CA-C-N	6.55	133.81	122.81
1	I	172	LEU	C-N-CA	6.55	133.81	122.81
1	E	361	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	F	86	ASP	CA-CB-CG	6.54	119.14	112.60
1	C	394	LYS	O-C-N	-6.54	115.14	122.86
1	J	444	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	J	466	THR	N-CA-C	6.53	119.55	108.90
1	B	379	ASP	N-CA-C	6.53	120.86	113.02
1	H	399	ILE	CA-C-N	6.53	126.22	119.56
1	H	399	ILE	C-N-CA	6.53	126.22	119.56
1	E	54	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	A	394	LYS	N-CA-C	6.53	119.14	110.53
1	C	297	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	F	415	SER	CA-C-N	6.52	129.90	120.38
1	F	415	SER	C-N-CA	6.52	129.90	120.38
1	B	250	ASN	CA-CB-CG	6.52	119.12	112.60
1	D	245	ARG	NH1-CZ-NH2	-6.52	110.83	119.30
1	F	87	PHE	CA-CB-CG	6.51	120.31	113.80
1	A	207	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	B	77	PRO	N-CA-CB	6.51	107.59	103.23
1	A	200	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	A	89	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	E	389	LEU	N-CA-C	6.51	119.07	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	252	ILE	CA-CB-CG1	6.51	121.46	110.40
1	F	398	GLN	OE1-CD-NE2	-6.50	116.09	122.60
1	J	185	PHE	CA-CB-CG	6.50	120.31	113.80
1	G	238	ILE	CA-C-N	6.50	130.61	121.24
1	G	238	ILE	C-N-CA	6.50	130.61	121.24
1	E	369	GLU	N-CA-CB	6.50	119.78	110.16
1	L	444	GLN	O-C-N	-6.50	115.37	122.07
1	B	150	ASP	N-CA-C	6.50	119.14	111.02
1	E	189	PHE	CA-CB-CG	6.50	120.30	113.80
1	A	119	HIS	CA-C-N	6.49	129.64	120.42
1	A	119	HIS	C-N-CA	6.49	129.64	120.42
1	L	53	VAL	O-C-N	-6.49	115.29	122.69
1	G	335	ASP	CA-CB-CG	6.49	119.08	112.60
1	A	79	PHE	CA-CB-CG	6.48	120.28	113.80
1	A	97	GLU	CA-C-N	6.48	130.75	121.55
1	A	97	GLU	C-N-CA	6.48	130.75	121.55
1	G	167	THR	OG1-CB-CG2	-6.48	96.34	109.30
1	B	114	ILE	CA-CB-CG1	6.48	121.41	110.40
1	B	332	SER	CA-C-N	6.48	125.91	118.85
1	B	332	SER	C-N-CA	6.48	125.91	118.85
1	B	400	PRO	CA-C-N	6.47	133.91	121.54
1	B	400	PRO	C-N-CA	6.47	133.91	121.54
1	D	358	GLU	N-CA-C	6.47	119.45	108.90
1	E	257	PRO	N-CA-CB	6.47	109.35	103.33
1	C	137	GLU	CB-CA-C	6.47	121.74	111.91
1	C	92	GLY	CA-C-N	6.46	128.84	120.44
1	C	92	GLY	C-N-CA	6.46	128.84	120.44
1	J	62	THR	N-CA-CB	6.46	117.59	110.35
1	K	289	ASP	CA-C-N	6.46	129.27	120.54
1	K	289	ASP	C-N-CA	6.46	129.27	120.54
1	J	200	ASN	CA-CB-CG	6.46	119.06	112.60
1	F	74	PHE	CA-CB-CG	6.46	120.26	113.80
1	J	256	ILE	N-CA-CB	6.46	116.08	110.08
1	G	264	ILE	CB-CA-C	-6.45	103.43	112.14
1	J	201	LYS	CA-C-O	6.45	128.70	120.57
1	L	189	PHE	CA-CB-CG	6.45	120.25	113.80
1	A	65	ASN	CA-C-N	6.45	129.35	120.39
1	A	65	ASN	C-N-CA	6.45	129.35	120.39
1	I	377	GLN	O-C-N	-6.45	115.69	123.10
1	K	394	LYS	N-CA-CB	-6.45	101.55	110.38
1	G	398	GLN	CG-CD-NE2	6.44	126.07	116.40
1	A	393	LEU	CA-C-O	-6.44	113.77	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	214	GLN	CA-C-N	6.44	133.64	122.82
1	H	214	GLN	C-N-CA	6.44	133.64	122.82
1	J	159	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	327	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	K	307	LYS	CA-CB-CG	6.44	126.98	114.10
1	L	135	ASP	N-CA-C	6.43	121.08	113.23
1	L	189	PHE	CA-C-O	-6.43	113.30	120.70
1	K	159	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	A	283	ILE	CA-C-N	6.43	132.64	122.36
1	A	283	ILE	C-N-CA	6.43	132.64	122.36
1	D	68	SER	CA-C-N	6.43	127.87	119.84
1	D	68	SER	C-N-CA	6.43	127.87	119.84
1	A	227	ALA	N-CA-C	6.42	119.01	110.53
1	J	218	SER	CA-C-N	6.42	132.08	122.58
1	J	218	SER	C-N-CA	6.42	132.08	122.58
1	F	276	ARG	CA-C-N	6.42	133.99	121.41
1	F	276	ARG	C-N-CA	6.42	133.99	121.41
1	J	166	PHE	CA-CB-CG	6.42	120.22	113.80
1	B	290	THR	CA-C-N	6.42	129.71	120.79
1	B	290	THR	C-N-CA	6.42	129.71	120.79
1	G	220	ASN	CA-CB-CG	6.42	119.02	112.60
1	G	349	ILE	N-CA-CB	-6.42	103.81	111.90
1	E	171	ASP	CA-CB-CG	6.42	119.02	112.60
1	J	315	GLY	CA-C-N	6.41	130.67	121.50
1	J	315	GLY	C-N-CA	6.41	130.67	121.50
1	K	335	ASP	CA-CB-CG	6.41	119.01	112.60
1	G	238	ILE	CA-CB-CG1	6.41	121.30	110.40
1	L	121	VAL	O-C-N	6.41	128.51	122.23
1	F	363	SER	O-C-N	6.40	131.19	123.13
1	L	82	PHE	CA-CB-CG	6.40	120.20	113.80
1	K	261	VAL	N-CA-CB	6.39	119.23	110.54
1	H	407	LEU	CD1-CG-CD2	-6.39	96.74	110.80
1	K	318	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	A	90	ARG	CA-C-N	6.39	129.91	120.90
1	A	90	ARG	C-N-CA	6.39	129.91	120.90
1	D	378	SER	N-CA-C	6.38	124.40	110.80
1	F	392	ARG	NH1-CZ-NH2	-6.38	111.00	119.30
1	D	419	ASN	CA-CB-CG	6.38	118.98	112.60
1	I	419	ASN	CA-CB-CG	6.38	118.98	112.60
1	C	210	GLU	CB-CG-CD	6.38	123.44	112.60
1	D	325	VAL	CB-CA-C	-6.38	104.31	111.45
1	G	250	ASN	CA-CB-CG	6.38	118.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	373	PRO	N-CA-C	6.37	125.60	112.47
1	L	356	ASP	CA-CB-CG	6.37	118.97	112.60
1	H	131	LEU	O-C-N	-6.37	116.07	121.23
1	K	203	ASN	CA-C-N	6.37	128.84	122.66
1	K	203	ASN	C-N-CA	6.37	128.84	122.66
1	G	445	ALA	O-C-N	-6.37	113.80	122.33
1	D	220	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	D	79	PHE	CA-CB-CG	6.36	120.16	113.80
1	C	83	PHE	CA-C-N	6.35	129.86	120.90
1	C	83	PHE	C-N-CA	6.35	129.86	120.90
1	I	297	GLN	O-C-N	-6.35	115.00	122.81
1	L	220	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	C	42	HIS	CA-C-N	6.35	128.69	120.44
1	C	42	HIS	C-N-CA	6.35	128.69	120.44
1	F	451	LYS	CA-C-O	-6.35	112.84	120.65
1	I	367	LYS	CA-C-O	-6.35	113.27	120.32
1	J	210	GLU	N-CA-CB	-6.35	99.81	111.37
1	B	351	LEU	CA-C-N	6.35	130.50	121.42
1	B	351	LEU	C-N-CA	6.35	130.50	121.42
1	D	125	ASP	CA-CB-CG	6.35	118.95	112.60
1	G	372	ASN	N-CA-C	6.34	118.68	109.04
1	E	392	ARG	NH1-CZ-NH2	-6.34	111.05	119.30
1	F	320	ASP	CA-CB-CG	6.34	118.94	112.60
1	F	459	VAL	CA-CB-CG2	6.34	121.18	110.40
1	K	249	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	G	300	ALA	CA-C-N	6.34	131.43	121.99
1	G	300	ALA	C-N-CA	6.34	131.43	121.99
1	I	446	LEU	CB-CA-C	6.34	122.84	110.67
1	L	234	TYR	O-C-N	-6.34	115.96	123.06
1	K	202	ASP	CA-CB-CG	6.33	118.93	112.60
1	D	163	ALA	N-CA-CB	-6.33	101.17	108.96
1	G	122	ASP	CA-C-N	6.33	132.41	122.78
1	G	122	ASP	C-N-CA	6.33	132.41	122.78
1	J	459	VAL	CA-C-O	-6.33	113.88	120.27
1	H	378	SER	O-C-N	-6.33	114.17	122.59
1	L	266	LYS	CB-CA-C	6.33	122.34	110.63
1	G	140	ALA	CA-C-N	6.33	131.11	122.19
1	G	140	ALA	C-N-CA	6.33	131.11	122.19
1	J	293	ALA	CA-C-N	6.33	132.57	122.83
1	J	293	ALA	C-N-CA	6.33	132.57	122.83
1	L	154	ILE	CA-C-N	6.33	131.18	122.77
1	L	154	ILE	C-N-CA	6.33	131.18	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	320	ASP	N-CA-C	6.33	118.88	110.53
1	A	216	ASP	CA-CB-CG	6.32	118.92	112.60
1	D	119	HIS	N-CA-C	6.32	118.98	111.71
1	C	43	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	418	LYS	N-CA-C	6.32	120.25	112.54
1	D	261	VAL	N-CA-C	6.32	118.95	111.05
1	G	387	ARG	NE-CZ-NH2	-6.32	113.51	119.20
1	B	133	GLY	O-C-N	6.32	129.72	122.33
1	H	55	ILE	CA-C-O	-6.32	113.89	120.27
1	H	334	ILE	O-C-N	-6.32	114.86	122.06
1	G	131	LEU	N-CA-CB	-6.31	102.15	110.17
1	H	388	ASN	CA-CB-CG	6.31	118.91	112.60
1	F	388	ASN	CA-CB-CG	6.31	118.91	112.60
1	J	255	ALA	N-CA-C	6.31	119.22	109.07
1	K	188	GLY	CA-C-O	-6.31	116.52	122.13
1	E	356	ASP	N-CA-C	6.31	124.23	110.80
1	G	264	ILE	CA-CB-CG2	6.31	121.22	110.50
1	B	282	THR	OG1-CB-CG2	-6.30	96.69	109.30
1	B	438	ASN	CA-C-N	6.30	129.02	120.38
1	B	438	ASN	C-N-CA	6.30	129.02	120.38
1	C	196	ILE	CA-C-N	6.30	132.12	122.29
1	C	196	ILE	C-N-CA	6.30	132.12	122.29
1	K	366	LEU	CA-C-O	-6.30	114.73	122.36
1	J	435	GLU	O-C-N	-6.30	115.57	123.01
1	K	462	ASN	CA-CB-CG	6.30	118.90	112.60
1	I	76	ASP	CA-CB-CG	6.30	118.90	112.60
1	E	423	GLN	OE1-CD-NE2	-6.29	116.31	122.60
1	F	304	ASP	CB-CA-C	6.29	119.83	110.14
1	K	344	GLU	N-CA-C	6.29	119.72	110.59
1	C	337	LYS	O-C-N	6.29	128.81	122.08
1	J	88	PRO	N-CD-CG	6.29	112.64	103.20
1	A	334	ILE	CA-C-O	-6.29	113.84	120.57
1	D	428	ILE	CA-C-O	-6.29	113.32	120.74
1	L	60	THR	N-CA-C	6.29	118.94	111.71
1	L	438	ASN	CA-C-N	6.29	129.33	120.28
1	L	438	ASN	C-N-CA	6.29	129.33	120.28
1	A	80	LYS	O-C-N	-6.28	115.14	122.87
1	D	348	LYS	CA-C-N	6.28	131.90	122.98
1	D	348	LYS	C-N-CA	6.28	131.90	122.98
1	J	327	ASN	N-CA-CB	-6.28	101.41	110.65
1	F	373	PRO	CA-N-CD	-6.28	103.21	112.00
1	G	136	ILE	CA-C-O	-6.28	113.35	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	318	ARG	CA-C-O	-6.28	113.82	121.36
1	I	128	THR	CA-CB-OG1	-6.28	100.18	109.60
1	B	231	SER	N-CA-C	6.28	120.40	112.87
1	B	292	LYS	N-CA-CB	-6.28	100.89	110.12
1	I	267	LYS	CA-C-N	6.28	129.21	120.29
1	I	267	LYS	C-N-CA	6.28	129.21	120.29
1	E	105	GLY	O-C-N	-6.28	116.64	123.29
1	I	90	ARG	NE-CZ-NH1	-6.28	115.22	121.50
1	J	453	GLU	CA-C-N	6.27	132.41	122.62
1	J	453	GLU	C-N-CA	6.27	132.41	122.62
1	B	64	ALA	N-CA-C	6.27	119.41	111.69
1	G	55	ILE	CA-C-O	6.27	126.91	120.39
1	D	436	ILE	CA-C-O	-6.27	115.28	121.67
1	B	245	ARG	CA-C-N	6.27	133.69	121.41
1	B	245	ARG	C-N-CA	6.27	133.69	121.41
1	E	377	GLN	N-CA-CB	-6.27	101.88	111.66
1	E	402	ASP	CA-CB-CG	6.27	118.87	112.60
1	F	294	TYR	CB-CA-C	6.27	119.85	111.14
1	H	227	ALA	N-CA-CB	-6.27	101.14	110.17
1	F	469	VAL	O-C-N	6.26	130.40	122.57
1	D	449	VAL	O-C-N	-6.26	113.84	122.05
1	K	63	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	K	321	LEU	N-CA-C	6.26	119.11	108.90
1	C	409	ASP	CA-CB-CG	-6.26	106.34	112.60
1	F	470	LEU	CA-C-N	6.26	132.97	121.70
1	F	470	LEU	C-N-CA	6.26	132.97	121.70
1	I	81	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	D	439	LEU	N-CA-CB	6.26	120.02	110.14
1	I	349	ILE	N-CA-CB	-6.26	104.13	111.39
1	K	175	GLY	CA-C-N	6.26	130.37	121.42
1	K	175	GLY	C-N-CA	6.26	130.37	121.42
1	F	196	ILE	CA-CB-CG2	6.25	121.13	110.50
1	D	415	SER	CA-C-O	6.25	128.18	121.05
1	B	339	TYR	O-C-N	-6.25	115.63	122.07
1	D	220	ASN	CA-CB-CG	6.25	118.85	112.60
1	E	450	ASN	N-CA-C	-6.25	106.03	113.21
1	B	448	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	D	373	PRO	N-CA-C	6.25	125.34	112.47
1	I	52	VAL	CA-C-N	6.25	128.87	120.50
1	I	52	VAL	C-N-CA	6.25	128.87	120.50
1	E	245	ARG	N-CA-C	6.24	120.60	112.92
1	F	274	ILE	CB-CG1-CD1	6.24	126.91	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	264	ILE	CB-CA-C	6.24	119.92	111.87
1	L	298	GLU	N-CA-C	6.24	119.72	108.48
1	A	237	GLY	N-CA-C	6.24	120.92	110.56
1	K	404	ASN	CA-CB-CG	6.24	118.84	112.60
1	L	396	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	B	44	SER	CA-C-N	6.24	130.53	120.30
1	B	44	SER	C-N-CA	6.24	130.53	120.30
1	J	259	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	B	327	ASN	N-CA-C	6.24	121.95	113.97
1	L	168	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	G	208	GLN	OE1-CD-NE2	-6.23	116.37	122.60
1	A	97	GLU	O-C-N	-6.23	114.14	122.43
1	B	200	ASN	CA-C-N	6.23	131.96	123.11
1	B	200	ASN	C-N-CA	6.23	131.96	123.11
1	K	203	ASN	N-CA-C	6.23	120.22	112.24
1	F	138	TYR	CD1-CG-CD2	6.22	127.44	118.10
1	I	288	GLY	CA-C-O	-6.22	114.10	120.45
1	J	462	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	B	419	ASN	CA-C-N	6.22	131.95	122.37
1	B	419	ASN	C-N-CA	6.22	131.95	122.37
1	J	398	GLN	CG-CD-NE2	6.22	125.73	116.40
1	B	235	LEU	N-CA-C	6.22	118.73	109.59
1	C	419	ASN	CA-C-N	6.22	132.53	122.14
1	C	419	ASN	C-N-CA	6.22	132.53	122.14
1	H	358	GLU	O-C-N	-6.22	116.14	123.41
1	I	412	LYS	CA-C-N	6.22	129.46	120.38
1	I	412	LYS	C-N-CA	6.22	129.46	120.38
1	A	364	PHE	CA-CB-CG	6.22	120.02	113.80
1	I	276	ARG	CA-C-N	6.22	133.59	121.41
1	I	276	ARG	C-N-CA	6.22	133.59	121.41
1	B	118	ASN	CA-C-O	-6.21	112.82	119.97
1	H	462	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	K	96	LYS	N-CA-C	6.21	118.85	111.71
1	L	73	PHE	CA-CB-CG	6.21	120.01	113.80
1	C	199	LEU	CA-C-N	6.21	133.40	121.54
1	C	199	LEU	C-N-CA	6.21	133.40	121.54
1	L	294	TYR	CA-C-N	6.21	130.94	122.19
1	L	294	TYR	C-N-CA	6.21	130.94	122.19
1	L	119	HIS	CB-CG-ND1	6.21	132.01	122.70
1	L	408	VAL	N-CA-C	6.20	116.31	106.88
1	D	83	PHE	N-CA-CB	-6.20	102.75	111.00
1	F	185	PHE	CA-CB-CG	6.20	120.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	351	LEU	N-CA-CB	-6.20	101.25	110.17
1	F	458	TRP	CA-C-O	-6.20	113.50	120.32
1	L	99	VAL	CA-CB-CG1	6.20	120.93	110.40
1	E	368	GLY	CA-C-N	6.19	129.08	120.29
1	E	368	GLY	C-N-CA	6.19	129.08	120.29
1	A	215	THR	OG1-CB-CG2	-6.19	96.92	109.30
1	A	252	ILE	CA-CB-CG1	6.19	120.92	110.40
1	B	227	ALA	CA-C-N	6.19	131.50	122.77
1	B	227	ALA	C-N-CA	6.19	131.50	122.77
1	C	140	ALA	CA-C-N	6.19	130.89	122.84
1	C	140	ALA	C-N-CA	6.19	130.89	122.84
1	H	252	ILE	CA-CB-CG1	6.19	120.92	110.40
1	D	461	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	E	446	LEU	CA-C-N	6.19	132.75	122.54
1	E	446	LEU	C-N-CA	6.19	132.75	122.54
1	K	114	ILE	CA-CB-CG1	6.18	120.91	110.40
1	D	60	THR	CA-CB-OG1	-6.18	100.33	109.60
1	G	421	GLY	O-C-N	-6.18	115.64	122.50
1	I	319	GLY	CA-C-N	6.18	131.24	122.09
1	I	319	GLY	C-N-CA	6.18	131.24	122.09
1	L	387	ARG	NH1-CZ-NH2	-6.18	111.26	119.30
1	K	128	THR	CA-CB-CG2	6.18	121.00	110.50
1	L	350	SER	O-C-N	6.17	130.43	122.71
1	H	103	GLY	N-CA-C	6.17	119.50	110.80
1	F	82	PHE	CA-CB-CG	6.17	119.97	113.80
1	K	398	GLN	OE1-CD-NE2	-6.17	116.44	122.60
1	E	372	ASN	CB-CG-ND2	6.16	125.65	116.40
1	L	171	ASP	O-C-N	-6.16	114.39	122.59
1	B	394	LYS	CA-C-N	6.16	132.79	121.70
1	B	394	LYS	C-N-CA	6.16	132.79	121.70
1	D	60	THR	CA-C-N	6.16	131.48	123.10
1	D	60	THR	C-N-CA	6.16	131.48	123.10
1	I	79	PHE	CB-CA-C	6.16	119.94	109.53
1	A	165	THR	O-C-N	-6.16	114.32	122.57
1	A	250	ASN	CA-CB-CG	6.16	118.76	112.60
1	C	268	LEU	CA-C-N	6.16	128.32	120.56
1	C	268	LEU	C-N-CA	6.16	128.32	120.56
1	K	332	SER	N-CA-C	6.15	115.22	108.14
1	L	185	PHE	CA-C-O	6.15	128.68	121.54
1	C	256	ILE	CA-C-N	6.15	126.17	119.90
1	C	256	ILE	C-N-CA	6.15	126.17	119.90
1	F	355	ARG	NH1-CZ-NH2	-6.15	111.30	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	253	GLY	O-C-N	-6.15	117.20	123.35
1	A	67	PRO	N-CA-CB	6.15	108.78	103.31
1	E	464	PHE	N-CA-C	6.14	118.19	108.79
1	G	43	ASP	CA-CB-CG	6.14	118.75	112.60
1	K	145	LYS	N-CA-C	6.14	118.52	109.24
1	C	276	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	K	337	LYS	CA-C-N	6.14	130.98	120.72
1	K	337	LYS	C-N-CA	6.14	130.98	120.72
1	E	294	TYR	CA-C-N	6.14	130.85	122.19
1	E	294	TYR	C-N-CA	6.14	130.85	122.19
1	E	395	ASP	CA-C-N	6.14	133.27	121.54
1	E	395	ASP	C-N-CA	6.14	133.27	121.54
1	L	409	ASP	CA-C-O	-6.14	114.38	120.82
1	E	76	ASP	CA-CB-CG	6.14	118.74	112.60
1	K	63	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	B	378	SER	O-C-N	-6.13	114.43	122.59
1	C	422	PHE	CA-CB-CG	6.13	119.93	113.80
1	K	449	VAL	N-CA-C	6.13	120.72	111.89
1	B	91	LYS	CA-C-O	-6.13	114.82	121.44
1	H	339	TYR	CB-CG-CD2	-6.13	111.61	120.80
1	E	438	ASN	CA-C-N	6.13	128.49	120.28
1	E	438	ASN	C-N-CA	6.13	128.49	120.28
1	F	344	GLU	O-C-N	-6.13	114.90	123.11
1	I	216	ASP	CA-CB-CG	6.13	118.73	112.60
1	I	223	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	K	75	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	C	283	ILE	CA-C-N	6.12	131.91	121.87
1	C	283	ILE	C-N-CA	6.12	131.91	121.87
1	E	392	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	F	149	THR	CA-C-O	6.12	126.47	119.18
1	G	462	ASN	CA-C-N	6.12	133.41	121.41
1	G	462	ASN	C-N-CA	6.12	133.41	121.41
1	H	277	GLY	CA-C-N	6.12	132.73	122.20
1	H	277	GLY	C-N-CA	6.12	132.73	122.20
1	D	468	LEU	N-CA-C	6.12	118.71	109.41
1	G	305	VAL	O-C-N	6.12	129.68	122.83
1	C	377	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	E	229	VAL	O-C-N	-6.12	116.11	123.02
1	D	204	ILE	N-CA-C	-6.11	96.62	109.34
1	G	355	ARG	CB-CA-C	-6.11	101.69	110.62
1	H	461	ARG	NE-CZ-NH1	6.11	127.61	121.50
1	A	103	GLY	O-C-N	6.11	131.14	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ILE	O-C-N	-6.11	117.27	122.65
1	C	327	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	F	363	SER	CA-C-O	-6.11	113.92	120.46
1	D	304	ASP	CB-CA-C	6.11	120.21	109.89
1	C	184	PRO	CA-C-N	6.11	131.07	122.46
1	C	184	PRO	C-N-CA	6.11	131.07	122.46
1	G	286	LEU	N-CA-C	-6.11	101.89	110.50
1	E	415	SER	N-CA-C	6.11	119.44	110.59
1	J	215	THR	CA-C-N	6.11	132.41	121.66
1	J	215	THR	C-N-CA	6.11	132.41	121.66
1	L	157	GLU	N-CA-CB	-6.11	102.76	110.45
1	E	411	VAL	CA-C-N	6.10	129.43	120.82
1	E	411	VAL	C-N-CA	6.10	129.43	120.82
1	H	394	LYS	CA-C-N	6.10	132.69	121.70
1	H	394	LYS	C-N-CA	6.10	132.69	121.70
1	B	294	TYR	CB-CA-C	6.10	121.37	110.81
1	F	340	ILE	O-C-N	-6.10	115.71	121.87
1	L	88	PRO	CB-CA-C	-6.10	102.71	111.62
1	F	339	TYR	CA-C-O	-6.10	114.42	120.82
1	H	53	VAL	CA-CB-CG1	6.10	120.77	110.40
1	I	214	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	C	89	GLN	OE1-CD-NE2	-6.09	116.50	122.60
1	F	343	LEU	N-CA-C	6.09	118.67	109.23
1	G	43	ASP	N-CA-C	6.09	118.70	111.33
1	H	261	VAL	CA-CB-CG2	6.09	120.75	110.40
1	J	125	ASP	CA-CB-CG	6.09	118.69	112.60
1	L	160	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	H	202	ASP	CA-CB-CG	6.08	118.68	112.60
1	J	399	ILE	CA-CB-CG1	6.08	120.73	110.40
1	B	84	ASP	CA-C-N	6.08	133.14	121.54
1	B	84	ASP	C-N-CA	6.08	133.14	121.54
1	H	376	VAL	N-CA-C	6.08	117.11	108.42
1	A	344	GLU	CA-C-N	6.07	129.73	120.13
1	A	344	GLU	C-N-CA	6.07	129.73	120.13
1	F	275	ASP	CA-C-O	6.07	126.89	120.33
1	A	392	ARG	N-CA-CB	6.07	117.32	110.35
1	G	373	PRO	N-CA-C	6.07	124.96	112.47
1	K	60	THR	O-C-N	-6.07	113.75	122.36
1	F	106	VAL	N-CA-C	6.06	116.85	108.12
1	F	423	GLN	O-C-N	-6.06	115.27	123.15
1	H	376	VAL	CA-CB-CG2	6.06	120.70	110.40
1	B	385	SER	CA-C-O	6.06	127.52	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	200	ASN	CA-CB-CG	6.06	118.66	112.60
1	C	371	GLU	CA-C-N	6.05	130.21	122.64
1	C	371	GLU	C-N-CA	6.05	130.21	122.64
1	A	227	ALA	CA-C-O	-6.05	114.85	121.87
1	G	167	THR	CA-CB-CG2	6.05	120.78	110.50
1	H	69	PRO	N-CA-CB	6.05	109.60	103.25
1	H	99	VAL	CA-C-N	6.05	132.14	122.10
1	H	99	VAL	C-N-CA	6.05	132.14	122.10
1	H	328	LYS	CG-CD-CE	-6.05	97.39	111.30
1	J	57	THR	O-C-N	-6.05	115.01	122.57
1	J	156	ILE	CA-C-N	6.05	133.46	122.27
1	J	156	ILE	C-N-CA	6.05	133.46	122.27
1	L	47	ASP	N-CA-CB	6.05	119.30	110.47
1	A	49	LYS	N-CA-C	6.05	119.49	111.75
1	I	337	LYS	O-C-N	-6.04	115.80	122.09
1	J	268	LEU	CA-C-O	-6.04	113.27	120.10
1	F	79	PHE	N-CA-C	-6.04	100.34	109.95
1	G	229	VAL	CA-CB-CG1	6.04	120.67	110.40
1	J	392	ARG	CB-CA-C	6.04	121.01	112.07
1	L	372	ASN	CA-CB-CG	6.04	118.64	112.60
1	F	198	ALA	CA-C-O	-6.04	114.25	120.89
1	A	223	ASN	CA-CB-CG	6.04	118.64	112.60
1	G	311	ALA	CA-C-N	6.04	128.28	120.44
1	G	311	ALA	C-N-CA	6.04	128.28	120.44
1	L	360	LYS	O-C-N	6.04	131.04	123.19
1	E	62	THR	OG1-CB-CG2	-6.03	97.23	109.30
1	F	298	GLU	N-CA-C	6.03	118.24	107.80
1	G	382	ASP	N-CA-C	6.03	118.95	109.96
1	J	375	GLY	N-CA-C	6.03	119.94	111.19
1	D	406	VAL	CA-C-N	6.03	131.04	122.72
1	D	406	VAL	C-N-CA	6.03	131.04	122.72
1	F	313	GLU	CA-CB-CG	6.03	126.16	114.10
1	H	250	ASN	CB-CG-ND2	6.03	125.44	116.40
1	E	282	THR	CA-CB-OG1	6.03	118.64	109.60
1	L	358	GLU	N-CA-C	6.03	118.21	108.32
1	B	203	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	C	387	ARG	N-CA-C	6.03	118.45	108.99
1	D	177	VAL	N-CA-C	6.03	118.03	108.87
1	A	114	ILE	CA-CB-CG1	6.02	120.64	110.40
1	C	185	PHE	CA-CB-CG	6.02	119.82	113.80
1	D	56	SER	CA-C-N	6.02	130.93	122.08
1	D	56	SER	C-N-CA	6.02	130.93	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	204	ILE	N-CA-C	6.02	116.66	110.82
1	G	457	VAL	CA-CB-CG1	6.02	120.64	110.40
1	J	66	ARG	NH1-CZ-NH2	-6.02	111.47	119.30
1	A	74	PHE	CA-C-N	6.02	133.04	121.54
1	A	74	PHE	C-N-CA	6.02	133.04	121.54
1	E	88	PRO	N-CA-CB	6.02	109.57	103.25
1	D	288	GLY	N-CA-C	6.02	119.95	112.73
1	J	441	ASP	CA-CB-CG	6.02	118.62	112.60
1	L	324	LYS	N-CA-C	6.02	117.86	107.93
1	E	149	THR	CA-C-N	6.01	131.52	122.68
1	E	149	THR	C-N-CA	6.01	131.52	122.68
1	J	215	THR	CA-CB-CG2	6.01	120.72	110.50
1	I	353	TYR	O-C-N	-6.01	116.54	123.33
1	E	146	ASP	CA-C-N	6.01	127.35	119.84
1	E	146	ASP	C-N-CA	6.01	127.35	119.84
1	I	447	LYS	CA-C-O	-6.01	113.06	119.97
1	J	305	VAL	N-CA-C	-6.01	101.79	109.30
1	A	468	LEU	N-CA-C	6.00	118.30	109.24
1	E	419	ASN	CA-CB-CG	6.00	118.60	112.60
1	F	200	ASN	N-CA-C	6.00	119.52	111.24
1	G	98	VAL	CA-C-N	6.00	132.77	121.97
1	G	98	VAL	C-N-CA	6.00	132.77	121.97
1	B	76	ASP	O-C-N	-6.00	115.59	121.17
1	B	209	TYR	O-C-N	-6.00	116.30	123.31
1	D	443	GLU	CB-CG-CD	6.00	122.79	112.60
1	A	204	ILE	CA-C-N	5.99	133.15	121.41
1	A	204	ILE	C-N-CA	5.99	133.15	121.41
1	F	202	ASP	CA-CB-CG	5.99	118.59	112.60
1	L	381	ILE	CA-CB-CG1	5.99	120.58	110.40
1	D	122	ASP	CA-C-O	-5.99	115.25	120.88
1	H	376	VAL	O-C-N	-5.99	116.41	123.00
1	E	412	LYS	CA-C-N	5.99	128.30	120.28
1	E	412	LYS	C-N-CA	5.99	128.30	120.28
1	C	326	ASN	CA-CB-CG	5.98	118.58	112.60
1	A	136	ILE	N-CA-C	5.98	115.22	106.55
1	D	196	ILE	O-C-N	5.98	129.13	122.61
1	E	42	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	L	108	ILE	CA-CB-CG1	5.98	120.56	110.40
1	F	71	ASP	CA-CB-CG	5.98	118.58	112.60
1	K	412	LYS	CA-C-N	5.97	128.61	120.54
1	K	412	LYS	C-N-CA	5.97	128.61	120.54
1	A	348	LYS	N-CA-C	5.97	118.02	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	232	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	E	168	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	B	335	ASP	N-CA-CB	5.97	118.62	109.91
1	F	55	ILE	CA-C-N	5.97	132.02	122.83
1	F	55	ILE	C-N-CA	5.97	132.02	122.83
1	A	131	LEU	O-C-N	5.97	128.18	121.32
1	C	128	THR	CA-CB-CG2	5.97	120.64	110.50
1	E	96	LYS	CA-C-N	5.97	128.87	120.28
1	E	96	LYS	C-N-CA	5.97	128.87	120.28
1	G	154	ILE	N-CA-CB	-5.97	103.71	111.82
1	B	363	SER	CA-C-O	-5.96	114.08	120.46
1	H	61	ILE	CB-CA-C	5.96	118.51	111.59
1	A	397	LEU	N-CA-C	5.96	117.27	108.86
1	A	409	ASP	O-C-N	-5.96	114.95	122.17
1	J	266	LYS	N-CA-C	5.96	117.45	111.07
1	G	263	ASP	CA-C-N	5.96	128.62	120.46
1	G	263	ASP	C-N-CA	5.96	128.62	120.46
1	L	207	ASN	N-CA-CB	5.96	120.56	110.49
1	I	211	ASN	CA-CB-CG	5.96	118.56	112.60
1	J	460	TYR	CB-CA-C	5.95	119.42	109.89
1	E	462	ASN	CA-CB-CG	5.95	118.55	112.60
1	F	403	VAL	CB-CA-C	5.95	117.47	110.93
1	G	388	ASN	CA-CB-CG	5.95	118.55	112.60
1	H	107	ILE	CA-CB-CG1	5.95	120.52	110.40
1	L	62	THR	OG1-CB-CG2	-5.95	97.40	109.30
1	A	377	GLN	CA-C-O	-5.95	112.24	119.61
1	I	296	ASN	CA-C-O	-5.95	111.80	119.59
1	D	348	LYS	N-CA-C	5.94	119.74	110.17
1	D	369	GLU	CA-C-N	5.94	132.16	122.65
1	D	369	GLU	C-N-CA	5.94	132.16	122.65
1	H	400	PRO	CA-C-N	5.94	128.52	120.38
1	H	400	PRO	C-N-CA	5.94	128.52	120.38
1	B	250	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	D	447	LYS	CA-C-N	5.94	132.12	121.66
1	D	447	LYS	C-N-CA	5.94	132.12	121.66
1	F	356	ASP	CA-CB-CG	5.94	118.54	112.60
1	H	136	ILE	CA-CB-CG1	5.94	120.50	110.40
1	L	411	VAL	O-C-N	-5.94	116.91	123.03
1	A	120	VAL	N-CA-C	-5.94	104.72	110.72
1	K	125	ASP	CA-CB-CG	5.94	118.54	112.60
1	E	307	LYS	CA-C-N	5.94	133.05	121.41
1	E	307	LYS	C-N-CA	5.94	133.05	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	55	ILE	CA-C-N	5.94	131.98	122.83
1	I	55	ILE	C-N-CA	5.94	131.98	122.83
1	L	180	ALA	CB-CA-C	5.94	119.64	110.14
1	I	339	TYR	CA-CB-CG	5.94	124.59	113.90
1	F	101	SER	CA-C-N	5.93	131.84	122.94
1	F	101	SER	C-N-CA	5.93	131.84	122.94
1	F	90	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	G	338	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	B	83	PHE	CA-C-N	5.92	129.70	120.75
1	B	83	PHE	C-N-CA	5.92	129.70	120.75
1	F	60	THR	CA-C-O	5.92	126.23	119.18
1	F	168	ASN	CA-C-O	5.92	126.70	120.36
1	J	267	LYS	CA-C-N	5.92	128.81	120.28
1	J	267	LYS	C-N-CA	5.92	128.81	120.28
1	K	159	ASN	N-CA-C	5.92	118.87	109.81
1	F	318	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	L	218	SER	CA-C-N	5.92	130.75	122.23
1	L	218	SER	C-N-CA	5.92	130.75	122.23
1	C	261	VAL	CA-C-N	5.92	128.53	120.54
1	C	261	VAL	C-N-CA	5.92	128.53	120.54
1	D	411	VAL	N-CA-CB	-5.92	103.95	111.64
1	K	43	ASP	N-CA-C	5.92	118.21	111.11
1	K	61	ILE	N-CA-CB	-5.92	106.32	112.06
1	L	428	ILE	CA-C-N	5.92	129.33	122.35
1	L	428	ILE	C-N-CA	5.92	129.33	122.35
1	A	189	PHE	CA-C-N	5.91	132.18	121.89
1	A	189	PHE	C-N-CA	5.91	132.18	121.89
1	J	373	PRO	CA-C-N	5.91	132.83	121.54
1	J	373	PRO	C-N-CA	5.91	132.83	121.54
1	L	178	VAL	CG1-CB-CG2	-5.91	97.79	110.80
1	A	326	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	C	445	ALA	CA-C-O	-5.91	113.68	120.24
1	F	223	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	L	373	PRO	N-CD-CG	5.91	112.06	103.20
1	G	328	LYS	O-C-N	-5.91	116.18	123.33
1	C	62	THR	O-C-N	-5.91	114.15	122.06
1	B	264	ILE	CA-CB-CG1	5.90	120.44	110.40
1	E	275	ASP	CA-C-N	5.90	131.31	122.99
1	E	275	ASP	C-N-CA	5.90	131.31	122.99
1	H	392	ARG	CD-NE-CZ	5.90	132.66	124.40
1	J	355	ARG	CA-C-N	5.90	132.82	121.54
1	J	355	ARG	C-N-CA	5.90	132.82	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	VAL	N-CA-C	5.90	117.59	108.44
1	H	346	GLY	CA-C-N	5.90	129.50	120.82
1	H	346	GLY	C-N-CA	5.90	129.50	120.82
1	I	324	LYS	CA-C-N	5.90	130.64	121.85
1	I	324	LYS	C-N-CA	5.90	130.64	121.85
1	L	162	SER	N-CA-CB	-5.90	102.29	110.38
1	C	218	SER	CA-C-N	5.90	131.21	122.71
1	C	218	SER	C-N-CA	5.90	131.21	122.71
1	K	42	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	K	457	VAL	CA-C-O	5.90	128.16	120.78
1	A	370	LYS	CA-CB-CG	5.90	125.90	114.10
1	A	168	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	F	387	ARG	CD-NE-CZ	5.90	132.66	124.40
1	J	207	ASN	CA-CB-CG	5.90	118.50	112.60
1	E	404	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	D	392	ARG	NE-CZ-NH1	5.89	127.39	121.50
1	J	328	LYS	O-C-N	-5.89	116.20	123.33
1	E	283	ILE	CA-CB-CG2	5.89	120.51	110.50
1	B	290	THR	CB-CA-C	-5.89	100.67	110.68
1	K	381	ILE	CA-CB-CG1	5.88	120.40	110.40
1	K	435	GLU	O-C-N	-5.88	115.71	122.89
1	B	57	THR	N-CA-C	5.88	119.66	111.90
1	B	295	LYS	CA-C-N	5.88	132.77	121.54
1	B	295	LYS	C-N-CA	5.88	132.77	121.54
1	F	270	GLU	CA-C-N	5.88	130.29	120.70
1	F	270	GLU	C-N-CA	5.88	130.29	120.70
1	I	347	GLN	CG-CD-NE2	5.88	125.22	116.40
1	F	422	PHE	CA-CB-CG	5.88	119.68	113.80
1	C	256	ILE	CA-CB-CG1	5.88	120.39	110.40
1	G	379	ASP	N-CA-CB	5.88	120.42	110.49
1	J	147	PRO	N-CA-C	5.88	124.58	112.47
1	K	179	PHE	CA-CB-CG	5.88	119.68	113.80
1	H	245	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	D	329	VAL	O-C-N	-5.87	116.70	122.93
1	H	399	ILE	CA-C-O	-5.87	112.08	119.95
1	L	81	GLN	N-CA-C	5.87	121.72	113.56
1	E	372	ASN	CA-C-N	5.87	126.82	120.83
1	E	372	ASN	C-N-CA	5.87	126.82	120.83
1	H	48	ALA	CA-C-N	5.87	128.15	120.28
1	H	48	ALA	C-N-CA	5.87	128.15	120.28
1	I	180	ALA	N-CA-CB	-5.87	101.49	110.65
1	C	119	HIS	N-CA-C	5.87	118.46	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	PRO	N-CA-CB	5.87	109.41	103.25
1	E	141	LYS	O-C-N	-5.87	116.36	123.29
1	F	76	ASP	CA-CB-CG	5.87	118.47	112.60
1	J	435	GLU	CA-C-N	5.87	132.25	122.57
1	J	435	GLU	C-N-CA	5.87	132.25	122.57
1	K	402	ASP	CA-CB-CG	5.87	118.47	112.60
1	D	119	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	E	55	ILE	CA-C-N	5.87	132.04	123.12
1	E	55	ILE	C-N-CA	5.87	132.04	123.12
1	F	267	LYS	CB-CG-CD	5.87	124.79	111.30
1	C	183	ASN	CA-C-N	5.87	127.17	119.84
1	C	183	ASN	C-N-CA	5.87	127.17	119.84
1	F	256	ILE	CA-CB-CG1	5.87	120.37	110.40
1	K	345	ILE	CA-CB-CG1	5.87	120.37	110.40
1	B	328	LYS	N-CA-C	5.86	119.03	109.06
1	L	130	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	A	132	PRO	N-CA-CB	5.86	108.38	103.17
1	C	263	ASP	CA-C-O	-5.85	113.74	120.24
1	B	382	ASP	CA-C-O	-5.85	114.83	120.92
1	J	252	ILE	O-C-N	-5.85	115.25	122.57
1	A	417	GLY	O-C-N	5.85	127.81	122.19
1	F	178	VAL	CA-CB-CG1	5.85	120.34	110.40
1	H	312	ASP	CA-CB-CG	5.85	118.45	112.60
1	H	51	SER	CA-CB-OG	-5.84	99.41	111.10
1	J	209	TYR	CB-CG-CD1	-5.84	112.04	120.80
1	A	402	ASP	CA-C-O	5.84	125.81	119.15
1	L	458	TRP	CG-CD2-CE3	5.84	139.74	133.90
1	B	444	GLN	O-C-N	-5.84	115.78	122.09
1	K	234	TYR	O-C-N	-5.84	116.39	123.10
1	B	168	ASN	CA-CB-CG	-5.84	106.76	112.60
1	E	203	ASN	N-CA-C	5.84	119.71	112.47
1	E	238	ILE	CA-C-N	5.84	129.40	120.82
1	E	238	ILE	C-N-CA	5.84	129.40	120.82
1	G	375	GLY	CA-C-N	5.84	131.05	122.94
1	G	375	GLY	C-N-CA	5.84	131.05	122.94
1	K	469	VAL	CA-C-O	5.84	128.08	120.78
1	G	419	ASN	CA-C-N	5.83	131.35	122.08
1	G	419	ASN	C-N-CA	5.83	131.35	122.08
1	D	377	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	J	180	ALA	O-C-N	-5.83	115.81	123.21
1	D	250	ASN	CA-C-N	5.82	130.90	120.77
1	D	250	ASN	C-N-CA	5.82	130.90	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	326	ASN	N-CA-C	5.82	118.41	111.71
1	J	223	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	J	94	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	H	462	ASN	CB-CG-ND2	5.82	125.13	116.40
1	J	107	ILE	CA-CB-CG1	5.82	120.29	110.40
1	D	208	GLN	CB-CG-CD	5.82	122.49	112.60
1	J	129	VAL	CA-C-N	5.82	133.10	122.92
1	J	129	VAL	C-N-CA	5.82	133.10	122.92
1	K	264	ILE	CA-CB-CG1	5.82	120.29	110.40
1	I	66	ARG	N-CA-C	-5.82	102.27	110.29
1	C	295	LYS	N-CA-C	5.81	119.68	112.24
1	B	430	GLY	CA-C-O	-5.81	116.51	121.57
1	E	420	SER	N-CA-C	5.81	122.33	113.61
1	A	75	ASN	CA-CB-CG	-5.81	106.79	112.60
1	L	232	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	I	390	ASP	CA-C-N	5.81	126.29	120.14
1	I	390	ASP	C-N-CA	5.81	126.29	120.14
1	L	188	GLY	N-CA-C	-5.81	103.91	111.52
1	F	242	ILE	N-CA-C	5.80	116.01	108.35
1	G	313	GLU	CA-C-N	5.80	131.34	122.23
1	G	313	GLU	C-N-CA	5.80	131.34	122.23
1	A	211	ASN	CB-CG-ND2	5.80	125.10	116.40
1	H	423	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	E	266	LYS	CA-C-N	5.80	128.05	120.28
1	E	266	LYS	C-N-CA	5.80	128.05	120.28
1	A	275	ASP	N-CA-C	5.80	118.25	107.99
1	H	211	ASN	CA-CB-CG	5.80	118.40	112.60
1	G	453	GLU	O-C-N	5.79	128.26	122.12
1	I	249	ASN	CA-CB-CG	5.79	118.39	112.60
1	I	396	ARG	CD-NE-CZ	5.79	132.51	124.40
1	J	52	VAL	CB-CA-C	5.79	119.28	112.68
1	B	350	SER	CA-C-N	5.79	129.06	120.95
1	B	350	SER	C-N-CA	5.79	129.06	120.95
1	G	460	TYR	CB-CA-C	5.79	120.44	110.77
1	J	125	ASP	CA-C-O	5.79	128.79	120.51
1	I	226	GLY	CA-C-N	5.79	130.66	120.87
1	I	226	GLY	C-N-CA	5.79	130.66	120.87
1	L	88	PRO	N-CA-CB	5.79	109.02	103.52
1	D	232	ARG	NH1-CZ-NH2	-5.79	111.78	119.30
1	G	431	VAL	CA-CB-CG2	5.79	120.24	110.40
1	F	174	GLU	CA-C-N	5.78	132.75	121.41
1	F	174	GLU	C-N-CA	5.78	132.75	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	419	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	L	121	VAL	CA-C-N	5.78	130.58	121.56
1	L	121	VAL	C-N-CA	5.78	130.58	121.56
1	C	194	GLY	CA-C-N	5.78	130.98	122.94
1	C	194	GLY	C-N-CA	5.78	130.98	122.94
1	C	208	GLN	CG-CD-NE2	5.78	125.07	116.40
1	F	461	ARG	NH1-CZ-NH2	-5.78	111.78	119.30
1	A	345	ILE	CA-C-N	5.78	132.16	122.16
1	A	345	ILE	C-N-CA	5.78	132.16	122.16
1	L	120	VAL	CA-CB-CG1	5.78	120.22	110.40
1	G	462	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	E	387	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	I	310	SER	N-CA-C	5.77	118.35	111.71
1	C	373	PRO	O-C-N	-5.77	112.53	122.17
1	G	267	LYS	CA-CB-CG	5.77	125.64	114.10
1	K	396	ARG	NH1-CZ-NH2	-5.77	111.80	119.30
1	A	367	LYS	N-CA-C	5.77	118.20	107.99
1	I	378	SER	N-CA-C	5.77	123.09	110.80
1	B	454	PHE	CA-C-O	-5.77	115.00	121.40
1	E	345	ILE	CB-CA-C	5.77	119.24	111.28
1	F	210	GLU	CB-CG-CD	5.77	122.41	112.60
1	I	239	ASN	CA-CB-CG	-5.77	106.83	112.60
1	D	264	ILE	N-CA-CB	-5.77	103.80	110.55
1	E	279	LEU	CA-C-N	5.77	132.72	121.41
1	E	279	LEU	C-N-CA	5.77	132.72	121.41
1	I	207	ASN	CA-CB-CG	5.77	118.37	112.60
1	B	450	ASN	CA-C-O	5.77	127.53	119.80
1	D	249	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	J	170	ASP	CB-CA-C	5.76	120.46	110.72
1	E	139	LYS	CA-C-N	5.76	131.64	122.59
1	E	139	LYS	C-N-CA	5.76	131.64	122.59
1	E	237	GLY	N-CA-C	5.76	119.50	110.91
1	A	391	PRO	N-CA-C	5.76	120.33	111.57
1	C	63	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	H	422	PHE	CA-CB-CG	5.76	119.56	113.80
1	L	217	ALA	N-CA-C	5.76	118.58	110.23
1	C	62	THR	CA-C-O	5.75	127.51	119.80
1	H	464	PHE	N-CA-CB	-5.75	102.30	111.62
1	E	97	GLU	CA-C-N	5.75	130.34	121.19
1	E	97	GLU	C-N-CA	5.75	130.34	121.19
1	F	110	LYS	CA-C-N	5.75	129.81	120.60
1	F	110	LYS	C-N-CA	5.75	129.81	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	373	PRO	CA-C-O	-5.75	115.05	122.13
1	J	198	ALA	CA-C-O	-5.75	115.07	121.23
1	C	281	VAL	N-CA-C	5.75	117.35	108.44
1	C	282	THR	CA-CB-OG1	5.75	118.23	109.60
1	F	290	THR	N-CA-CB	5.75	118.69	110.06
1	G	81	GLN	N-CA-C	5.75	119.60	112.58
1	G	336	LEU	CA-C-O	-5.75	114.42	120.63
1	C	438	ASN	CA-C-N	5.75	128.25	120.38
1	C	438	ASN	C-N-CA	5.75	128.25	120.38
1	I	428	ILE	N-CA-CB	5.75	117.39	110.95
1	L	97	GLU	CA-C-N	5.75	129.73	120.82
1	L	97	GLU	C-N-CA	5.75	129.73	120.82
1	L	200	ASN	CA-C-N	5.75	130.93	123.00
1	L	200	ASN	C-N-CA	5.75	130.93	123.00
1	L	312	ASP	N-CA-CB	-5.75	101.66	110.16
1	I	297	GLN	CA-C-N	5.74	130.77	122.44
1	I	297	GLN	C-N-CA	5.74	130.77	122.44
1	J	102	LEU	CB-CA-C	5.74	120.65	109.33
1	A	408	VAL	N-CA-C	5.74	115.87	107.37
1	G	429	ILE	N-CA-C	-5.74	107.22	112.96
1	J	379	ASP	CA-CB-CG	-5.74	106.86	112.60
1	J	455	THR	OG1-CB-CG2	-5.74	97.82	109.30
1	F	135	ASP	CA-CB-CG	5.74	118.34	112.60
1	E	107	ILE	O-C-N	-5.73	116.41	122.83
1	H	119	HIS	N-CA-C	5.73	117.53	111.28
1	L	268	LEU	CA-C-O	-5.73	113.38	119.97
1	D	120	VAL	N-CA-C	-5.73	104.93	110.72
1	D	198	ALA	N-CA-CB	-5.73	102.33	111.62
1	L	156	ILE	N-CA-C	5.73	116.83	108.58
1	H	184	PRO	N-CA-CB	5.73	109.27	103.25
1	H	260	MET	CA-C-O	-5.73	114.98	121.00
1	K	261	VAL	O-C-N	-5.73	116.31	121.87
1	A	42	HIS	CA-C-N	5.73	128.53	120.28
1	A	42	HIS	C-N-CA	5.73	128.53	120.28
1	D	53	VAL	N-CA-C	5.73	117.41	109.45
1	G	172	LEU	N-CA-CB	5.73	119.75	110.41
1	E	438	ASN	O-C-N	-5.73	116.86	122.99
1	F	132	PRO	CA-N-CD	-5.72	103.99	112.00
1	F	147	PRO	N-CA-CB	5.72	108.64	103.20
1	I	469	VAL	CB-CA-C	5.72	120.68	111.29
1	C	139	LYS	CA-C-O	-5.72	115.48	121.55
1	C	160	ASN	OD1-CG-ND2	-5.72	116.88	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	444	GLN	N-CA-C	-5.72	104.95	111.07
1	F	429	ILE	CA-CB-CG1	5.72	120.12	110.40
1	D	322	VAL	CA-CB-CG1	5.72	120.12	110.40
1	J	285	ALA	CA-C-O	-5.72	114.34	120.92
1	B	353	TYR	CG-CD1-CE1	-5.71	112.63	121.20
1	B	397	LEU	N-CA-C	5.71	115.78	108.24
1	C	53	VAL	CG1-CB-CG2	-5.71	98.23	110.80
1	C	306	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	H	127	ILE	CB-CA-C	5.71	120.66	111.29
1	I	391	PRO	CB-CA-C	5.71	118.80	110.63
1	B	423	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	G	83	PHE	CA-C-N	5.71	130.52	120.87
1	G	83	PHE	C-N-CA	5.71	130.52	120.87
1	D	92	GLY	CA-C-N	5.71	127.86	120.44
1	D	92	GLY	C-N-CA	5.71	127.86	120.44
1	B	91	LYS	O-C-N	5.71	130.12	122.82
1	B	432	GLY	CA-C-N	5.71	132.44	121.54
1	B	432	GLY	C-N-CA	5.71	132.44	121.54
1	D	99	VAL	CA-C-N	5.71	132.44	121.54
1	D	99	VAL	C-N-CA	5.71	132.44	121.54
1	E	375	GLY	CA-C-N	5.71	130.94	123.06
1	E	375	GLY	C-N-CA	5.71	130.94	123.06
1	D	344	GLU	CA-C-N	5.70	129.14	120.13
1	D	344	GLU	C-N-CA	5.70	129.14	120.13
1	F	373	PRO	N-CA-C	5.70	122.90	114.80
1	F	438	ASN	O-C-N	-5.70	116.14	122.75
1	K	134	SER	CA-C-O	5.70	128.67	120.51
1	C	273	LYS	CA-C-O	-5.70	115.35	121.45
1	D	399	ILE	CA-CB-CG2	5.70	120.19	110.50
1	A	174	GLU	CA-C-O	-5.70	114.88	121.15
1	G	88	PRO	O-C-N	-5.70	114.95	122.64
1	J	291	LYS	CA-C-N	5.70	128.19	120.44
1	J	291	LYS	C-N-CA	5.70	128.19	120.44
1	I	160	ASN	CB-CG-ND2	5.70	124.94	116.40
1	F	77	PRO	O-C-N	-5.69	118.69	122.73
1	B	114	ILE	CA-C-N	5.69	130.25	123.19
1	B	114	ILE	C-N-CA	5.69	130.25	123.19
1	B	456	LYS	CB-CG-CD	5.69	124.39	111.30
1	D	222	GLY	O-C-N	-5.69	116.49	122.52
1	L	96	LYS	N-CA-C	5.69	119.70	112.87
1	H	374	LYS	O-C-N	-5.69	115.02	122.59
1	H	215	THR	CA-CB-CG2	5.69	120.17	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	211	ASN	CA-C-N	5.69	129.87	120.94
1	I	211	ASN	C-N-CA	5.69	129.87	120.94
1	B	374	LYS	N-CA-C	5.69	122.91	110.80
1	I	97	GLU	CB-CA-C	5.69	121.31	110.27
1	L	375	GLY	CA-C-N	5.69	131.00	122.58
1	L	375	GLY	C-N-CA	5.69	131.00	122.58
1	B	404	ASN	CB-CA-C	5.68	119.92	109.46
1	C	177	VAL	CA-C-N	5.68	130.96	123.17
1	C	177	VAL	C-N-CA	5.68	130.96	123.17
1	E	63	ARG	CB-CA-C	5.68	118.57	109.02
1	C	278	PHE	CA-CB-CG	-5.68	108.12	113.80
1	D	131	LEU	CA-C-O	-5.68	113.86	119.49
1	I	323	THR	CA-CB-OG1	5.68	118.12	109.60
1	H	347	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	K	327	ASN	CA-CB-CG	5.68	118.28	112.60
1	B	350	SER	CB-CA-C	5.68	121.14	112.00
1	D	387	ARG	O-C-N	-5.68	116.91	123.33
1	E	305	VAL	CB-CA-C	5.68	120.60	111.29
1	K	166	PHE	CA-CB-CG	5.68	119.48	113.80
1	H	119	HIS	CA-C-O	5.68	126.57	120.55
1	I	254	PHE	CA-C-N	5.68	131.45	122.94
1	I	254	PHE	C-N-CA	5.68	131.45	122.94
1	F	138	TYR	CG-CD1-CE1	-5.67	112.69	121.20
1	H	332	SER	CA-C-N	5.67	125.04	118.85
1	H	332	SER	C-N-CA	5.67	125.04	118.85
1	J	212	PHE	CA-CB-CG	-5.67	108.12	113.80
1	L	387	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	F	227	ALA	CA-C-N	5.67	130.99	123.05
1	F	227	ALA	C-N-CA	5.67	130.99	123.05
1	F	438	ASN	CA-C-O	5.67	126.84	120.94
1	B	450	ASN	N-CA-C	-5.67	106.96	112.97
1	C	213	ILE	O-C-N	-5.67	116.94	123.00
1	G	65	ASN	CB-CA-C	5.67	121.70	110.42
1	I	117	ASN	CA-C-O	-5.67	114.92	121.15
1	D	229	VAL	CA-CB-CG1	5.67	120.03	110.40
1	A	290	THR	CA-C-O	-5.66	114.51	120.63
1	B	96	LYS	N-CA-C	5.66	119.67	112.87
1	C	425	GLY	CA-C-O	-5.66	113.04	119.04
1	G	312	ASP	N-CA-CB	-5.66	101.80	110.01
1	H	224	SER	CB-CA-C	5.66	120.23	110.77
1	E	404	ASN	N-CA-CB	5.66	118.38	109.83
1	J	57	THR	CA-C-N	5.66	132.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	57	THR	C-N-CA	5.66	132.35	121.54
1	C	212	PHE	CA-CB-CG	5.66	119.46	113.80
1	A	336	LEU	CA-C-N	5.66	130.19	121.19
1	A	336	LEU	C-N-CA	5.66	130.19	121.19
1	C	45	ILE	CA-C-N	5.66	128.12	120.65
1	C	45	ILE	C-N-CA	5.66	128.12	120.65
1	C	123	ASP	CA-C-N	5.66	132.35	121.54
1	C	123	ASP	C-N-CA	5.66	132.35	121.54
1	G	198	ALA	CA-C-N	5.66	131.69	122.81
1	G	198	ALA	C-N-CA	5.66	131.69	122.81
1	E	359	ASN	CA-CB-CG	5.66	118.26	112.60
1	I	225	GLY	O-C-N	-5.66	114.98	122.28
1	J	370	LYS	CB-CA-C	5.66	120.13	111.02
1	A	87	PHE	CA-C-N	5.65	126.91	119.84
1	A	87	PHE	C-N-CA	5.65	126.91	119.84
1	A	347	GLN	CA-C-N	5.65	129.94	122.42
1	A	347	GLN	C-N-CA	5.65	129.94	122.42
1	L	470	LEU	CA-C-O	5.65	127.09	120.98
1	B	306	GLN	CA-C-N	5.65	132.34	121.54
1	B	306	GLN	C-N-CA	5.65	132.34	121.54
1	G	208	GLN	N-CA-CB	-5.65	100.94	110.49
1	F	79	PHE	CA-CB-CG	5.65	119.45	113.80
1	H	95	ASP	CA-CB-CG	5.65	118.25	112.60
1	I	95	ASP	N-CA-CB	-5.65	102.90	111.15
1	F	338	ASN	CA-CB-CG	5.65	118.25	112.60
1	K	184	PRO	N-CA-CB	5.65	107.82	103.30
1	F	395	ASP	CA-CB-CG	5.64	118.24	112.60
1	D	383	GLY	CA-C-O	5.64	126.47	119.25
1	F	326	ASN	CA-C-N	5.64	130.41	121.44
1	F	326	ASN	C-N-CA	5.64	130.41	121.44
1	K	234	TYR	CA-C-O	5.64	127.94	121.28
1	F	159	ASN	CB-CG-ND2	5.64	124.86	116.40
1	C	227	ALA	CA-C-N	5.63	130.72	122.77
1	C	227	ALA	C-N-CA	5.63	130.72	122.77
1	E	338	ASN	CA-CB-CG	-5.63	106.97	112.60
1	H	263	ASP	CA-CB-CG	5.63	118.23	112.60
1	J	381	ILE	CA-CB-CG1	5.63	119.98	110.40
1	L	134	SER	CA-C-O	-5.63	112.45	120.51
1	C	244	SER	CA-C-O	-5.63	115.00	121.82
1	G	340	ILE	CA-C-O	-5.63	115.09	120.95
1	F	44	SER	N-CA-CB	5.63	118.50	110.16
1	G	274	ILE	CA-C-N	5.63	130.71	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	274	ILE	C-N-CA	5.63	130.71	122.77
1	L	436	ILE	CB-CA-C	5.63	119.70	110.69
1	C	212	PHE	N-CA-C	5.63	117.81	110.43
1	E	461	ARG	NH1-CZ-NH2	-5.63	111.98	119.30
1	F	131	LEU	CA-C-N	5.63	126.88	119.84
1	F	131	LEU	C-N-CA	5.63	126.88	119.84
1	H	444	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	B	79	PHE	CA-CB-CG	5.63	119.43	113.80
1	I	281	VAL	CA-CB-CG1	5.62	119.96	110.40
1	D	428	ILE	O-C-N	5.62	129.13	122.83
1	I	376	VAL	O-C-N	-5.62	117.79	123.19
1	L	46	LYS	CA-C-O	-5.62	114.46	120.42
1	G	355	ARG	CA-C-O	5.62	127.33	120.25
1	J	282	THR	CA-C-O	-5.62	114.20	120.66
1	F	107	ILE	CA-CB-CG1	5.61	119.94	110.40
1	K	55	ILE	CA-C-O	5.61	125.94	120.27
1	E	162	SER	N-CA-C	5.61	118.09	110.35
1	J	178	VAL	CA-CB-CG2	5.61	119.93	110.40
1	A	326	ASN	CA-C-N	5.61	131.30	122.11
1	A	326	ASN	C-N-CA	5.61	131.30	122.11
1	H	276	ARG	NH1-CZ-NH2	-5.61	112.01	119.30
1	I	79	PHE	CA-CB-CG	5.61	119.41	113.80
1	C	419	ASN	O-C-N	-5.60	115.66	122.22
1	L	65	ASN	CA-CB-CG	-5.60	107.00	112.60
1	C	342	THR	CA-C-N	5.60	131.80	121.94
1	C	342	THR	C-N-CA	5.60	131.80	121.94
1	D	203	ASN	CB-CA-C	5.60	118.99	111.82
1	G	433	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	A	332	SER	O-C-N	-5.60	114.88	121.32
1	B	447	LYS	CA-CB-CG	5.60	125.30	114.10
1	F	134	SER	CA-C-N	5.60	131.35	122.61
1	F	134	SER	C-N-CA	5.60	131.35	122.61
1	L	140	ALA	CA-C-N	5.60	130.08	122.19
1	L	140	ALA	C-N-CA	5.60	130.08	122.19
1	C	84	ASP	N-CA-C	5.60	118.13	110.24
1	D	54	ASN	CB-CG-ND2	5.60	124.80	116.40
1	G	358	GLU	N-CA-C	5.60	118.53	109.40
1	C	114	ILE	CA-C-O	5.59	127.10	120.72
1	E	115	VAL	CB-CA-C	5.59	119.11	110.50
1	E	373	PRO	CB-CA-C	-5.59	102.91	110.52
1	D	423	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	H	439	LEU	CA-C-O	-5.59	113.94	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	43	ASP	CA-C-N	5.59	128.23	120.29
1	F	43	ASP	C-N-CA	5.59	128.23	120.29
1	G	136	ILE	CA-CB-CG1	5.59	119.90	110.40
1	B	281	VAL	N-CA-C	5.58	117.10	108.44
1	C	361	GLN	O-C-N	-5.58	116.74	123.27
1	E	355	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	E	283	ILE	CA-C-N	5.58	130.99	122.11
1	E	283	ILE	C-N-CA	5.58	130.99	122.11
1	H	381	ILE	CA-CB-CG1	5.58	119.89	110.40
1	B	209	TYR	CA-C-N	5.58	131.76	121.94
1	B	209	TYR	C-N-CA	5.58	131.76	121.94
1	C	333	PRO	CA-C-N	5.58	129.45	120.30
1	C	333	PRO	C-N-CA	5.58	129.45	120.30
1	J	124	ALA	N-CA-C	5.58	122.68	110.80
1	L	461	ARG	N-CA-C	5.58	117.16	109.29
1	C	469	VAL	CB-CA-C	5.58	120.44	111.29
1	D	62	THR	CA-CB-CG2	5.58	119.98	110.50
1	H	107	ILE	CA-CB-CG2	-5.58	101.02	110.50
1	J	338	ASN	N-CA-C	-5.58	106.48	113.28
1	K	51	SER	O-C-N	-5.58	115.44	122.19
1	C	377	GLN	O-C-N	-5.57	115.18	122.20
1	H	395	ASP	CA-CB-CG	5.57	118.17	112.60
1	J	369	GLU	CA-C-N	5.57	131.53	122.67
1	J	369	GLU	C-N-CA	5.57	131.53	122.67
1	D	298	GLU	CA-C-O	-5.57	114.14	120.32
1	D	187	VAL	N-CA-C	5.57	120.92	109.34
1	C	439	LEU	N-CA-C	5.57	118.07	111.33
1	H	398	GLN	O-C-N	5.57	129.56	122.04
1	F	117	ASN	CA-C-N	5.57	128.19	120.29
1	F	117	ASN	C-N-CA	5.57	128.19	120.29
1	H	465	ALA	CA-C-O	5.57	126.14	120.24
1	L	259	ASN	CA-CB-CG	5.57	118.17	112.60
1	C	459	VAL	CA-C-O	5.56	125.76	120.31
1	D	239	ASN	CB-CG-ND2	5.56	124.74	116.40
1	E	212	PHE	N-CA-C	5.56	118.42	110.24
1	F	423	GLN	CA-C-N	5.56	128.74	120.90
1	F	423	GLN	C-N-CA	5.56	128.74	120.90
1	L	249	ASN	CB-CA-C	5.56	119.16	109.65
1	C	170	ASP	CB-CG-OD1	5.56	131.19	118.40
1	D	462	ASN	CA-C-O	-5.56	113.97	120.20
1	I	132	PRO	N-CA-CB	5.56	107.75	103.30
1	F	317	LYS	CB-CG-CD	5.56	124.08	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	416	LYS	CA-C-N	5.56	126.27	119.99
1	B	416	LYS	C-N-CA	5.56	126.27	119.99
1	G	101	SER	CA-C-O	5.55	127.33	121.33
1	B	265	ALA	CA-C-N	5.55	127.66	120.44
1	B	265	ALA	C-N-CA	5.55	127.66	120.44
1	H	303	THR	N-CA-C	-5.55	106.18	113.12
1	L	279	LEU	CA-C-O	5.55	125.48	119.15
1	A	343	LEU	O-C-N	-5.55	115.97	123.19
1	E	237	GLY	CA-C-O	-5.55	115.57	121.29
1	F	62	THR	O-C-N	-5.55	115.27	122.37
1	G	164	ILE	CB-CA-C	5.55	119.22	111.34
1	I	185	PHE	CB-CG-CD2	-5.55	111.26	120.70
1	G	322	VAL	CA-C-O	-5.55	114.52	120.85
1	K	119	HIS	CB-CG-CD2	-5.55	123.99	131.20
1	C	372	ASN	N-CA-C	5.55	120.71	108.73
1	H	354	GLU	N-CA-C	5.55	118.61	109.85
1	K	214	GLN	CA-C-O	5.55	126.48	120.32
1	E	394	LYS	CA-C-N	5.54	131.68	121.70
1	E	394	LYS	C-N-CA	5.54	131.68	121.70
1	G	69	PRO	CA-C-N	5.54	131.44	122.29
1	G	69	PRO	C-N-CA	5.54	131.44	122.29
1	J	450	ASN	N-CA-C	-5.54	106.72	112.93
1	F	446	LEU	CB-CA-C	5.54	121.48	110.17
1	G	418	LYS	N-CA-C	-5.54	106.02	112.89
1	I	464	PHE	CA-CB-CG	5.54	119.34	113.80
1	C	184	PRO	O-C-N	-5.54	115.16	122.64
1	I	166	PHE	CB-CA-C	5.54	121.44	110.42
1	J	249	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	B	427	ILE	O-C-N	-5.54	117.42	123.18
1	F	99	VAL	CA-C-N	5.54	132.87	122.84
1	F	99	VAL	C-N-CA	5.54	132.87	122.84
1	J	136	ILE	CB-CG1-CD1	-5.54	102.17	113.80
1	E	232	ARG	CA-C-N	5.54	130.57	122.10
1	E	232	ARG	C-N-CA	5.54	130.57	122.10
1	F	200	ASN	CB-CG-ND2	5.54	124.70	116.40
1	G	121	VAL	N-CA-C	5.54	117.43	112.17
1	A	404	ASN	CA-C-O	-5.53	115.45	121.87
1	G	377	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	F	148	LYS	CA-C-N	5.53	132.34	122.06
1	F	148	LYS	C-N-CA	5.53	132.34	122.06
1	H	211	ASN	CA-C-O	5.53	126.95	121.20
1	J	374	LYS	CA-C-N	5.53	129.52	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	374	LYS	C-N-CA	5.53	129.52	120.51
1	E	333	PRO	CA-C-N	5.53	130.21	121.09
1	E	333	PRO	C-N-CA	5.53	130.21	121.09
1	G	76	ASP	N-CA-C	5.53	119.30	110.73
1	G	165	THR	OG1-CB-CG2	-5.53	98.25	109.30
1	B	51	SER	CB-CA-C	5.52	118.75	110.08
1	G	372	ASN	CA-CB-CG	5.52	118.12	112.60
1	J	195	ILE	CB-CA-C	5.52	118.85	110.62
1	J	196	ILE	CA-CB-CG1	5.52	119.79	110.40
1	J	118	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	F	190	SER	CA-C-O	-5.52	114.66	121.06
1	G	65	ASN	CA-CB-CG	5.52	118.12	112.60
1	G	161	LEU	CA-C-O	-5.52	115.12	121.19
1	E	369	GLU	CA-C-N	5.52	133.32	122.61
1	E	369	GLU	C-N-CA	5.52	133.32	122.61
1	I	393	LEU	CA-C-N	5.52	131.25	122.59
1	I	393	LEU	C-N-CA	5.52	131.25	122.59
1	I	439	LEU	O-C-N	-5.52	116.27	122.12
1	C	312	ASP	N-CA-C	5.52	117.73	111.11
1	C	337	LYS	CA-C-O	-5.51	115.00	121.07
1	J	88	PRO	N-CA-CB	5.51	109.04	103.25
1	L	42	HIS	CB-CG-ND1	5.51	130.97	122.70
1	E	250	ASN	O-C-N	-5.51	115.52	122.19
1	H	165	THR	CA-CB-OG1	5.51	117.87	109.60
1	L	126	THR	CA-C-O	5.51	128.39	120.51
1	J	356	ASP	CA-C-N	5.51	132.21	121.41
1	J	356	ASP	C-N-CA	5.51	132.21	121.41
1	K	457	VAL	N-CA-CB	5.51	120.32	111.23
1	L	169	SER	CA-C-O	5.51	125.80	119.35
1	A	292	LYS	CA-C-N	5.51	127.93	120.44
1	A	292	LYS	C-N-CA	5.51	127.93	120.44
1	A	414	LYS	CB-CA-C	5.51	121.94	110.32
1	F	373	PRO	CB-CA-C	5.51	117.37	110.27
1	J	99	VAL	CA-CB-CG1	5.51	119.76	110.40
1	E	469	VAL	CB-CA-C	5.50	120.32	111.29
1	K	55	ILE	CB-CA-C	5.50	117.85	110.42
1	D	123	ASP	O-C-N	-5.50	115.27	122.59
1	F	293	ALA	N-CA-CB	-5.50	102.03	110.12
1	C	279	LEU	CA-C-O	5.50	126.44	119.95
1	J	325	VAL	CA-C-N	5.50	128.41	120.38
1	J	325	VAL	C-N-CA	5.50	128.41	120.38
1	F	458	TRP	CZ3-CH2-CZ2	-5.50	114.35	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	342	THR	CA-CB-CG2	5.50	119.84	110.50
1	G	218	SER	CA-C-O	5.50	126.95	120.69
1	C	319	GLY	CA-C-N	5.49	130.22	122.09
1	C	319	GLY	C-N-CA	5.49	130.22	122.09
1	I	119	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	L	126	THR	OG1-CB-CG2	-5.49	98.31	109.30
1	B	143	ILE	N-CA-C	-5.49	104.61	112.35
1	G	199	LEU	CA-C-N	5.49	130.75	122.68
1	G	199	LEU	C-N-CA	5.49	130.75	122.68
1	J	470	LEU	CA-C-N	5.49	131.59	121.70
1	J	470	LEU	C-N-CA	5.49	131.59	121.70
1	I	450	ASN	N-CA-C	-5.49	106.78	112.93
1	J	315	GLY	O-C-N	-5.49	115.91	122.33
1	L	339	TYR	N-CA-C	5.49	118.02	111.71
1	F	137	GLU	CB-CA-C	5.49	121.88	112.44
1	H	337	LYS	CA-C-N	5.49	129.89	120.72
1	H	337	LYS	C-N-CA	5.49	129.89	120.72
1	E	208	GLN	CG-CD-NE2	5.49	124.63	116.40
1	A	93	LYS	N-CA-CB	-5.49	100.80	110.34
1	B	293	ALA	CA-C-N	5.48	131.75	122.65
1	B	293	ALA	C-N-CA	5.48	131.75	122.65
1	C	230	ASP	CA-CB-CG	5.48	118.08	112.60
1	G	183	ASN	N-CA-CB	-5.48	103.67	110.79
1	K	333	PRO	O-C-N	5.48	129.08	122.23
1	D	338	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	E	111	ASP	CA-CB-CG	5.48	118.08	112.60
1	H	219	ILE	CA-CB-CG2	5.48	119.81	110.50
1	K	426	ASP	N-CA-C	5.48	117.40	110.33
1	A	60	THR	N-CA-C	5.48	119.68	112.89
1	B	241	ALA	O-C-N	-5.48	117.56	123.42
1	F	412	LYS	O-C-N	-5.48	116.55	123.01
1	B	101	SER	O-C-N	-5.47	116.92	123.27
1	C	282	THR	CA-C-O	-5.47	114.91	120.71
1	F	223	ASN	CB-CG-ND2	5.47	124.61	116.40
1	A	397	LEU	O-C-N	-5.47	115.50	122.78
1	C	108	ILE	CB-CG1-CD1	5.47	125.29	113.80
1	K	82	PHE	CA-CB-CG	5.47	119.27	113.80
1	B	60	THR	CB-CA-C	5.47	121.85	110.32
1	C	135	ASP	N-CA-C	5.47	119.90	113.23
1	F	426	ASP	N-CA-C	5.47	117.13	110.41
1	I	217	ALA	CA-C-O	-5.47	114.69	120.92
1	D	199	LEU	CA-C-N	5.46	131.98	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	LEU	C-N-CA	5.46	131.98	121.54
1	D	230	ASP	CA-CB-CG	5.46	118.06	112.60
1	L	398	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	F	110	LYS	CA-C-O	5.46	125.98	119.10
1	K	261	VAL	N-CA-C	-5.46	105.05	110.62
1	C	238	ILE	CA-CB-CG1	5.46	119.68	110.40
1	A	102	LEU	CB-CA-C	5.46	119.70	109.71
1	B	423	GLN	O-C-N	-5.46	116.05	123.15
1	E	317	LYS	CB-CG-CD	5.46	123.86	111.30
1	J	370	LYS	CA-C-O	-5.46	113.51	119.95
1	B	216	ASP	CA-C-N	5.46	128.51	120.82
1	B	216	ASP	C-N-CA	5.46	128.51	120.82
1	F	434	SER	CA-C-O	-5.46	114.81	120.70
1	G	408	VAL	CA-CB-CG1	5.46	119.67	110.40
1	G	471	LYS	CB-CG-CD	5.46	123.85	111.30
1	I	48	ALA	CA-C-O	-5.46	115.28	120.90
1	I	138	TYR	O-C-N	-5.46	116.86	123.03
1	L	275	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	386	LEU	CA-C-O	-5.45	114.95	121.11
1	J	218	SER	CA-CB-OG	-5.45	100.20	111.10
1	D	123	ASP	CA-CB-CG	5.45	118.05	112.60
1	L	203	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	G	330	ILE	CA-CB-CG2	-5.45	101.24	110.50
1	G	419	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	H	39	LEU	O-C-N	5.45	129.90	122.82
1	G	42	HIS	CA-C-N	5.45	127.84	120.38
1	G	42	HIS	C-N-CA	5.45	127.84	120.38
1	I	416	LYS	N-CA-CB	-5.44	100.41	110.32
1	D	373	PRO	O-C-N	-5.44	115.30	122.64
1	I	345	ILE	N-CA-C	5.44	117.03	109.80
1	L	114	ILE	CA-CB-CG1	5.44	119.65	110.40
1	D	176	ASP	CA-CB-CG	5.44	118.04	112.60
1	G	90	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	L	333	PRO	N-CA-CB	5.44	108.96	103.25
1	A	387	ARG	CA-C-N	5.44	130.06	120.87
1	A	387	ARG	C-N-CA	5.44	130.06	120.87
1	B	318	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	D	464	PHE	N-CA-CB	-5.44	101.88	111.39
1	K	249	ASN	CB-CG-ND2	5.44	124.56	116.40
1	A	453	GLU	CA-C-N	5.43	131.01	122.21
1	A	453	GLU	C-N-CA	5.43	131.01	122.21
1	B	283	ILE	CA-C-O	5.43	126.79	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	ASP	N-CA-CB	-5.43	101.28	110.46
1	F	372	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	E	450	ASN	CA-CB-CG	5.43	118.03	112.60
1	H	177	VAL	CA-C-N	5.43	130.05	122.23
1	H	177	VAL	C-N-CA	5.43	130.05	122.23
1	E	464	PHE	CA-CB-CG	5.43	119.23	113.80
1	F	305	VAL	CA-CB-CG1	5.43	119.63	110.40
1	I	249	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	B	355	ARG	CA-C-O	-5.43	114.42	120.66
1	J	168	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	E	136	ILE	N-CA-C	5.42	116.00	108.84
1	E	377	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	C	73	PHE	CA-C-N	5.42	131.07	121.80
1	C	73	PHE	C-N-CA	5.42	131.07	121.80
1	B	450	ASN	CA-C-N	5.42	131.19	122.14
1	B	450	ASN	C-N-CA	5.42	131.19	122.14
1	C	53	VAL	CA-CB-CG2	5.42	119.61	110.40
1	L	435	GLU	O-C-N	-5.42	116.87	122.94
1	A	412	LYS	N-CA-CB	-5.42	102.00	109.97
1	C	159	ASN	CA-CB-CG	5.42	118.02	112.60
1	G	54	ASN	O-C-N	-5.42	116.91	123.03
1	J	108	ILE	CA-CB-CG1	5.42	119.61	110.40
1	J	367	LYS	CA-C-N	5.42	128.10	121.06
1	J	367	LYS	C-N-CA	5.42	128.10	121.06
1	K	187	VAL	CA-C-O	-5.42	114.62	120.47
1	F	461	ARG	CD-NE-CZ	5.42	131.98	124.40
1	G	97	GLU	CA-C-N	5.42	127.96	121.84
1	G	97	GLU	C-N-CA	5.42	127.96	121.84
1	I	225	GLY	CA-C-O	5.42	124.78	119.04
1	K	457	VAL	O-C-N	-5.42	115.80	122.57
1	B	433	GLN	CA-C-N	5.41	129.16	121.42
1	B	433	GLN	C-N-CA	5.41	129.16	121.42
1	F	374	LYS	CA-C-N	5.41	132.02	121.41
1	F	374	LYS	C-N-CA	5.41	132.02	121.41
1	I	340	ILE	CA-CB-CG2	5.41	119.70	110.50
1	E	439	LEU	O-C-N	-5.41	116.38	122.12
1	G	460	TYR	N-CA-C	5.41	117.06	108.67
1	J	127	ILE	CA-C-N	5.41	128.53	120.90
1	J	127	ILE	C-N-CA	5.41	128.53	120.90
1	J	264	ILE	CA-CB-CG1	5.41	119.59	110.40
1	L	79	PHE	CA-CB-CG	5.41	119.21	113.80
1	F	256	ILE	CA-C-O	-5.40	114.63	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ILE	O-C-N	-5.40	116.07	122.77
1	A	404	ASN	CA-CB-CG	5.40	118.00	112.60
1	B	65	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	B	193	SER	CA-C-O	-5.40	114.53	120.69
1	C	164	ILE	N-CA-C	5.40	115.89	108.12
1	F	300	ALA	CA-C-O	-5.40	114.60	120.81
1	F	355	ARG	CA-C-N	5.40	131.85	121.54
1	F	355	ARG	C-N-CA	5.40	131.85	121.54
1	G	191	VAL	CA-C-O	-5.40	115.56	121.28
1	I	231	SER	CA-CB-OG	5.40	121.89	111.10
1	L	420	SER	CA-CB-OG	5.40	121.89	111.10
1	L	459	VAL	CA-C-O	5.40	126.00	120.39
1	G	59	LYS	CB-CA-C	5.39	119.23	110.22
1	H	84	ASP	CA-C-N	5.39	130.68	121.29
1	H	84	ASP	C-N-CA	5.39	130.68	121.29
1	H	238	ILE	O-C-N	-5.39	117.80	123.03
1	J	420	SER	N-CA-CB	-5.39	102.97	111.39
1	K	289	ASP	CA-CB-CG	5.39	117.99	112.60
1	I	290	THR	CA-C-N	5.39	128.28	120.79
1	I	290	THR	C-N-CA	5.39	128.28	120.79
1	C	220	ASN	O-C-N	-5.39	117.35	121.55
1	B	42	HIS	CB-CG-CD2	-5.39	124.20	131.20
1	B	56	SER	CA-C-O	5.39	125.57	119.27
1	B	372	ASN	CA-C-O	-5.39	113.94	119.49
1	G	416	LYS	N-CA-C	5.39	119.47	113.01
1	H	42	HIS	CB-CG-CD2	-5.39	124.20	131.20
1	H	273	LYS	CA-C-N	5.38	130.49	123.06
1	H	273	LYS	C-N-CA	5.38	130.49	123.06
1	J	103	GLY	CA-C-O	5.38	126.44	121.38
1	L	268	LEU	CA-C-N	5.38	128.06	120.42
1	L	268	LEU	C-N-CA	5.38	128.06	120.42
1	B	367	LYS	O-C-N	-5.38	116.02	123.12
1	I	314	ALA	CA-C-O	5.38	125.49	119.41
1	A	376	VAL	CA-C-O	-5.38	115.14	120.90
1	B	413	GLU	CA-C-O	-5.38	114.85	120.55
1	I	410	SER	CA-C-O	-5.38	114.97	120.99
1	J	196	ILE	CA-C-N	5.38	130.68	122.24
1	J	196	ILE	C-N-CA	5.38	130.68	122.24
1	L	402	ASP	N-CA-C	-5.38	105.94	112.88
1	A	431	VAL	CA-C-N	5.38	131.95	121.41
1	A	431	VAL	C-N-CA	5.38	131.95	121.41
1	G	118	ASN	CB-CA-C	5.38	119.71	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	317	LYS	CA-C-N	5.38	131.78	122.64
1	I	317	LYS	C-N-CA	5.38	131.78	122.64
1	E	232	ARG	NH1-CZ-NH2	-5.38	112.31	119.30
1	I	165	THR	CA-C-N	5.38	131.81	121.54
1	I	165	THR	C-N-CA	5.38	131.81	121.54
1	C	176	ASP	N-CA-CB	5.37	117.94	110.04
1	F	54	ASN	CB-CA-C	5.37	118.58	109.50
1	D	124	ALA	N-CA-C	5.37	118.91	111.55
1	D	178	VAL	CA-C-N	5.37	131.25	122.81
1	D	178	VAL	C-N-CA	5.37	131.25	122.81
1	E	63	ARG	O-C-N	-5.37	116.43	122.34
1	F	455	THR	N-CA-C	5.37	117.27	108.52
1	J	98	VAL	CA-CB-CG2	5.37	119.53	110.40
1	B	399	ILE	CA-CB-CG2	5.37	119.62	110.50
1	G	141	LYS	O-C-N	-5.37	117.10	123.22
1	G	392	ARG	CD-NE-CZ	5.37	131.91	124.40
1	J	135	ASP	N-CA-C	5.37	118.99	111.74
1	K	66	ARG	N-CA-CB	-5.37	102.80	110.04
1	K	214	GLN	O-C-N	-5.37	117.03	123.31
1	F	123	ASP	CB-CA-C	5.37	119.35	111.73
1	I	387	ARG	NH1-CZ-NH2	-5.36	112.33	119.30
1	I	150	ASP	CB-CA-C	5.36	119.05	111.86
1	H	216	ASP	CA-CB-CG	5.36	117.96	112.60
1	J	233	GLY	CA-C-N	5.36	129.16	121.50
1	J	233	GLY	C-N-CA	5.36	129.16	121.50
1	L	160	ASN	CB-CG-ND2	5.36	124.44	116.40
1	B	145	LYS	CA-C-O	5.36	127.45	121.40
1	E	119	HIS	N-CA-C	5.36	117.81	111.33
1	L	147	PRO	N-CA-CB	5.36	107.80	102.17
1	A	236	VAL	CA-CB-CG2	5.36	119.51	110.40
1	F	331	LYS	CA-C-N	5.36	131.68	123.96
1	F	331	LYS	C-N-CA	5.36	131.68	123.96
1	K	328	LYS	CA-C-N	5.36	129.68	122.93
1	K	328	LYS	C-N-CA	5.36	129.68	122.93
1	L	83	PHE	CA-C-N	5.36	129.29	121.31
1	L	83	PHE	C-N-CA	5.36	129.29	121.31
1	A	250	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	B	159	ASN	N-CA-C	5.36	117.66	109.95
1	E	177	VAL	CA-CB-CG2	5.36	119.50	110.40
1	F	197	SER	CA-CB-OG	5.36	121.81	111.10
1	G	212	PHE	N-CA-C	5.36	118.21	110.28
1	H	361	GLN	O-C-N	5.36	129.49	123.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	307	LYS	CA-CB-CG	5.36	124.81	114.10
1	L	402	ASP	CB-CA-C	5.36	119.77	110.72
1	B	94	ASN	CA-CB-CG	5.35	117.95	112.60
1	H	128	THR	CA-C-N	5.35	128.60	120.95
1	H	128	THR	C-N-CA	5.35	128.60	120.95
1	H	404	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	H	333	PRO	N-CA-CB	5.35	109.43	103.44
1	C	212	PHE	N-CA-CB	-5.35	102.61	110.26
1	F	338	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	F	419	ASN	O-C-N	-5.35	116.10	122.20
1	L	146	ASP	CA-CB-CG	-5.35	107.25	112.60
1	G	417	GLY	CA-C-N	5.35	130.50	121.14
1	G	417	GLY	C-N-CA	5.35	130.50	121.14
1	H	93	LYS	CA-C-N	5.35	130.65	122.95
1	H	93	LYS	C-N-CA	5.35	130.65	122.95
1	K	154	ILE	O-C-N	-5.35	117.42	123.20
1	J	320	ASP	CA-CB-CG	5.35	117.95	112.60
1	E	329	VAL	CB-CA-C	5.34	117.54	110.91
1	F	297	GLN	CA-C-N	5.34	130.19	122.44
1	F	297	GLN	C-N-CA	5.34	130.19	122.44
1	G	321	LEU	N-CA-C	5.34	117.61	108.90
1	J	88	PRO	CA-N-CD	-5.34	104.52	112.00
1	J	249	ASN	CB-CG-ND2	5.34	124.42	116.40
1	H	152	ALA	N-CA-CB	-5.34	102.39	111.69
1	B	293	ALA	N-CA-CB	-5.34	102.26	110.16
1	F	243	LEU	CD1-CG-CD2	-5.34	99.05	110.80
1	H	176	ASP	CA-C-N	5.34	128.25	120.98
1	H	176	ASP	C-N-CA	5.34	128.25	120.98
1	I	296	ASN	O-C-N	5.34	128.68	122.00
1	C	364	PHE	CD1-CG-CD2	-5.34	110.59	118.60
1	I	327	ASN	N-CA-CB	-5.34	103.51	110.88
1	J	79	PHE	CA-CB-CG	5.34	119.14	113.80
1	L	283	ILE	O-C-N	5.34	127.61	122.97
1	J	327	ASN	CB-CA-C	5.34	118.52	109.55
1	B	326	ASN	CA-C-N	5.33	130.86	122.11
1	B	326	ASN	C-N-CA	5.33	130.86	122.11
1	H	120	VAL	CG1-CB-CG2	-5.33	99.06	110.80
1	H	468	LEU	O-C-N	-5.33	115.21	122.36
1	J	240	SER	CB-CA-C	-5.33	102.18	109.28
1	C	349	ILE	N-CA-CB	-5.33	105.70	112.15
1	F	211	ASN	CB-CG-ND2	5.33	124.40	116.40
1	H	349	ILE	CB-CA-C	5.33	118.29	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	119	HIS	CA-C-N	5.33	129.09	120.82
1	J	119	HIS	C-N-CA	5.33	129.09	120.82
1	L	422	PHE	O-C-N	-5.33	117.14	123.22
1	B	259	ASN	N-CA-C	5.33	118.00	111.82
1	B	367	LYS	CA-C-N	5.33	129.16	121.54
1	B	367	LYS	C-N-CA	5.33	129.16	121.54
1	G	422	PHE	N-CA-CB	-5.33	102.01	110.06
1	K	302	ILE	CB-CG1-CD1	5.33	125.00	113.80
1	E	366	LEU	CA-C-N	5.33	130.17	122.44
1	E	366	LEU	C-N-CA	5.33	130.17	122.44
1	G	261	VAL	N-CA-CB	5.33	119.76	110.65
1	C	381	ILE	CA-CB-CG1	5.33	119.46	110.40
1	F	131	LEU	CB-CA-C	5.33	115.23	110.44
1	L	347	GLN	CA-C-O	-5.33	115.75	121.56
1	A	238	ILE	CB-CG1-CD1	5.33	124.98	113.80
1	C	174	GLU	CA-CB-CG	5.33	124.75	114.10
1	D	160	ASN	CA-CB-CG	-5.33	107.27	112.60
1	E	73	PHE	O-C-N	-5.33	115.77	123.07
1	K	138	TYR	CA-C-O	-5.32	114.88	121.11
1	K	464	PHE	N-CA-CB	-5.32	103.31	111.56
1	B	227	ALA	N-CA-C	5.32	117.56	110.53
1	G	318	ARG	NH1-CZ-NH2	-5.32	112.38	119.30
1	I	178	VAL	CA-C-O	-5.32	116.36	121.63
1	B	81	GLN	N-CA-CB	-5.32	103.83	111.70
1	B	242	ILE	O-C-N	-5.32	116.91	123.03
1	D	336	LEU	CA-C-N	5.32	128.19	120.79
1	D	336	LEU	C-N-CA	5.32	128.19	120.79
1	E	282	THR	N-CA-C	-5.32	100.57	109.24
1	K	400	PRO	CA-C-N	5.32	128.15	120.38
1	K	400	PRO	C-N-CA	5.32	128.15	120.38
1	G	394	LYS	CB-CG-CD	5.32	123.53	111.30
1	H	39	LEU	CB-CA-C	5.32	119.65	110.77
1	E	404	ASN	CA-C-O	-5.32	115.34	121.19
1	H	232	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	H	465	ALA	CA-C-N	5.32	131.43	122.87
1	H	465	ALA	C-N-CA	5.32	131.43	122.87
1	F	119	HIS	CA-CB-CG	5.32	119.12	113.80
1	G	137	GLU	CB-CA-C	5.32	121.00	110.42
1	G	214	GLN	CB-CG-CD	5.32	121.64	112.60
1	L	444	GLN	CA-C-O	5.32	126.40	120.82
1	A	60	THR	CA-CB-CG2	5.31	119.53	110.50
1	D	255	ALA	CA-C-N	5.31	130.00	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	ALA	C-N-CA	5.31	130.00	120.59
1	I	240	SER	CA-CB-OG	5.31	121.73	111.10
1	B	93	LYS	N-CA-C	5.31	116.88	111.14
1	C	202	ASP	CB-CA-C	5.31	121.92	113.37
1	H	386	LEU	N-CA-CB	-5.31	102.00	111.08
1	I	440	LYS	CB-CA-C	5.31	119.36	110.92
1	J	216	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	249	ASN	N-CA-C	5.31	117.92	110.23
1	E	202	ASP	CB-CA-C	5.31	120.98	110.42
1	C	140	ALA	CA-C-O	-5.30	115.02	121.28
1	F	39	LEU	CA-C-O	-5.30	114.61	120.60
1	G	305	VAL	CA-C-O	-5.30	114.48	120.74
1	L	213	ILE	O-C-N	-5.30	117.73	123.14
1	G	242	ILE	CA-CB-CG1	5.30	119.41	110.40
1	J	270	GLU	N-CA-C	5.30	118.53	111.75
1	A	431	VAL	CA-CB-CG2	5.30	119.41	110.40
1	E	431	VAL	O-C-N	-5.30	117.57	123.03
1	G	371	GLU	CA-CB-CG	5.30	124.70	114.10
1	H	388	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	J	58	SER	CA-C-N	5.30	129.94	122.09
1	J	58	SER	C-N-CA	5.30	129.94	122.09
1	J	56	SER	CA-C-N	5.30	129.93	122.46
1	J	56	SER	C-N-CA	5.30	129.93	122.46
1	K	98	VAL	CA-CB-CG1	5.30	119.41	110.40
1	B	177	VAL	CA-C-N	5.30	129.45	122.51
1	B	177	VAL	C-N-CA	5.30	129.45	122.51
1	J	98	VAL	N-CA-C	5.30	115.96	110.82
1	B	257	PRO	N-CA-C	5.29	119.40	111.14
1	C	212	PHE	CB-CG-CD1	-5.29	111.70	120.70
1	I	177	VAL	CA-C-N	5.29	130.21	122.69
1	I	177	VAL	C-N-CA	5.29	130.21	122.69
1	K	364	PHE	CA-CB-CG	5.29	119.09	113.80
1	K	390	ASP	CA-C-N	-5.29	115.14	120.85
1	K	390	ASP	C-N-CA	-5.29	115.14	120.85
1	B	234	TYR	CA-CB-CG	5.29	123.42	113.90
1	G	73	PHE	O-C-N	-5.29	116.30	122.96
1	L	235	LEU	CB-CA-C	5.29	118.35	109.89
1	A	119	HIS	O-C-N	-5.29	115.34	122.43
1	A	135	ASP	CB-CA-C	5.29	118.94	111.86
1	E	288	GLY	N-CA-C	5.29	119.04	112.64
1	H	354	GLU	CA-C-N	5.29	130.88	122.74
1	H	354	GLU	C-N-CA	5.29	130.88	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	402	ASP	N-CA-CB	-5.29	102.84	110.56
1	C	50	LYS	N-CA-C	5.29	118.83	112.38
1	H	201	LYS	N-CA-C	5.29	117.52	108.90
1	H	307	LYS	CA-CB-CG	5.29	124.67	114.10
1	K	330	ILE	CA-C-N	5.29	130.17	122.08
1	K	330	ILE	C-N-CA	5.29	130.17	122.08
1	B	403	VAL	CA-C-O	-5.28	114.18	120.78
1	C	46	LYS	N-CA-C	5.28	116.73	110.97
1	E	404	ASN	CA-CB-CG	5.28	117.88	112.60
1	E	404	ASN	CB-CA-C	5.28	118.49	109.72
1	I	298	GLU	CA-C-N	5.28	128.06	120.56
1	I	298	GLU	C-N-CA	5.28	128.06	120.56
1	B	170	ASP	N-CA-CB	-5.28	102.73	111.49
1	I	204	ILE	CB-CA-C	5.28	117.62	111.55
1	K	282	THR	CA-CB-OG1	5.28	117.52	109.60
1	A	183	ASN	CA-C-O	-5.28	114.06	120.08
1	E	364	PHE	O-C-N	-5.28	117.02	123.30
1	J	185	PHE	CB-CA-C	5.28	119.96	111.36
1	K	69	PRO	N-CA-CB	5.28	108.79	103.25
1	D	365	ILE	CA-C-O	-5.28	116.16	121.59
1	D	421	GLY	CA-C-O	-5.27	112.58	119.44
1	I	313	GLU	N-CA-C	5.27	119.46	113.19
1	B	241	ALA	N-CA-C	5.27	116.86	108.79
1	J	433	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	403	VAL	CA-CB-CG2	5.27	119.36	110.40
1	A	443	GLU	CA-C-N	5.27	127.29	120.44
1	A	443	GLU	C-N-CA	5.27	127.29	120.44
1	D	213	ILE	O-C-N	-5.27	116.68	122.69
1	E	371	GLU	N-CA-C	5.27	120.58	113.21
1	I	346	GLY	CA-C-N	5.27	128.19	120.71
1	I	346	GLY	C-N-CA	5.27	128.19	120.71
1	L	161	LEU	O-C-N	5.27	129.07	122.86
1	J	176	ASP	CA-C-N	5.27	128.46	120.77
1	J	176	ASP	C-N-CA	5.27	128.46	120.77
1	K	283	ILE	N-CA-C	5.27	116.60	108.44
1	C	305	VAL	N-CA-CB	5.26	116.54	110.49
1	D	413	GLU	N-CA-C	5.26	117.43	111.11
1	E	341	GLY	O-C-N	-5.26	115.86	122.70
1	I	268	LEU	CA-C-O	-5.26	114.84	120.42
1	K	123	ASP	CB-CA-C	5.26	119.20	111.73
1	K	428	ILE	N-CA-C	5.26	115.92	107.98
1	G	53	VAL	N-CA-CB	5.26	120.73	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	144	GLY	CA-C-N	5.26	131.41	122.37
1	G	144	GLY	C-N-CA	5.26	131.41	122.37
1	H	424	GLU	CA-C-N	5.26	131.21	120.80
1	H	424	GLU	C-N-CA	5.26	131.21	120.80
1	A	214	GLN	O-C-N	-5.26	117.16	123.31
1	E	318	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	K	52	VAL	CA-C-O	5.26	126.03	120.51
1	K	232	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	C	46	LYS	CG-CD-CE	-5.25	99.21	111.30
1	L	152	ALA	N-CA-CB	-5.25	102.23	110.69
1	C	293	ALA	CA-C-N	5.25	130.92	122.83
1	C	293	ALA	C-N-CA	5.25	130.92	122.83
1	H	220	ASN	CB-CG-OD1	5.25	131.30	120.80
1	H	457	VAL	O-C-N	5.25	127.95	122.54
1	G	159	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	A	54	ASN	CA-C-O	-5.25	115.23	121.16
1	I	259	ASN	N-CA-C	-5.25	106.14	112.54
1	B	390	ASP	N-CA-C	-5.24	97.41	108.73
1	F	189	PHE	CA-C-N	5.24	130.94	122.29
1	F	189	PHE	C-N-CA	5.24	130.94	122.29
1	F	303	THR	N-CA-C	-5.24	105.96	112.93
1	H	382	ASP	O-C-N	-5.24	116.35	122.96
1	I	101	SER	O-C-N	-5.24	116.98	123.33
1	I	160	ASN	N-CA-C	5.24	118.82	111.90
1	I	239	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	I	304	ASP	CA-CB-CG	5.24	117.84	112.60
1	J	136	ILE	CB-CA-C	5.24	117.36	111.80
1	C	183	ASN	CB-CG-ND2	5.24	124.26	116.40
1	I	157	GLU	CA-C-N	5.24	130.97	122.53
1	I	157	GLU	C-N-CA	5.24	130.97	122.53
1	J	176	ASP	O-C-N	-5.24	116.04	123.01
1	K	111	ASP	N-CA-C	5.24	119.30	113.01
1	H	51	SER	N-CA-CB	-5.24	102.41	110.42
1	I	400	PRO	CA-C-N	5.24	131.55	121.54
1	I	400	PRO	C-N-CA	5.24	131.55	121.54
1	J	352	SER	N-CA-C	5.24	118.02	109.59
1	L	196	ILE	CA-C-O	-5.24	115.60	121.36
1	L	223	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	435	GLU	N-CA-C	5.24	118.26	110.14
1	G	441	ASP	CA-CB-CG	5.24	117.84	112.60
1	E	211	ASN	N-CA-CB	5.24	118.07	111.79
1	E	332	SER	CA-C-N	5.24	124.74	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	332	SER	C-N-CA	5.24	124.74	119.19
1	F	367	LYS	CB-CA-C	-5.24	102.08	110.14
1	H	68	SER	CA-C-N	5.24	126.38	119.84
1	H	68	SER	C-N-CA	5.24	126.38	119.84
1	I	404	ASN	CA-CB-CG	5.23	117.83	112.60
1	L	156	ILE	CA-C-N	5.23	129.93	122.08
1	L	156	ILE	C-N-CA	5.23	129.93	122.08
1	F	76	ASP	CA-C-O	-5.23	112.99	120.16
1	F	211	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	J	285	ALA	N-CA-C	5.23	118.75	109.96
1	L	100	SER	O-C-N	-5.23	117.60	123.04
1	D	169	SER	CB-CA-C	5.23	120.83	110.17
1	A	257	PRO	CA-C-N	5.23	127.81	120.28
1	A	257	PRO	C-N-CA	5.23	127.81	120.28
1	K	398	GLN	CA-C-O	-5.23	114.23	120.55
1	J	361	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	F	241	ALA	CA-C-N	5.22	130.45	122.25
1	F	241	ALA	C-N-CA	5.22	130.45	122.25
1	I	169	SER	CB-CA-C	5.22	118.32	109.55
1	J	433	GLN	O-C-N	-5.22	115.64	122.59
1	K	228	LEU	N-CA-C	-5.22	99.77	108.34
1	A	438	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	C	203	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	H	309	SER	CA-C-N	5.22	127.53	120.38
1	H	309	SER	C-N-CA	5.22	127.53	120.38
1	I	181	LEU	O-C-N	-5.22	116.36	123.15
1	K	426	ASP	CA-C-N	5.22	130.39	122.98
1	K	426	ASP	C-N-CA	5.22	130.39	122.98
1	F	359	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	345	ILE	CB-CA-C	5.22	117.75	111.13
1	F	160	ASN	CA-C-O	5.22	127.28	120.81
1	H	316	LEU	N-CA-C	5.21	117.23	109.25
1	I	364	PHE	CA-CB-CG	5.21	119.01	113.80
1	K	49	LYS	CG-CD-CE	5.21	123.29	111.30
1	D	74	PHE	CB-CA-C	5.21	121.44	111.48
1	L	348	LYS	O-C-N	5.21	129.44	123.29
1	L	449	VAL	O-C-N	-5.21	116.12	122.06
1	E	266	LYS	N-CA-CB	-5.21	102.45	110.16
1	F	204	ILE	CA-C-N	5.21	130.51	120.66
1	F	204	ILE	C-N-CA	5.21	130.51	120.66
1	F	251	GLY	O-C-N	-5.21	115.93	122.70
1	G	219	ILE	CA-CB-CG2	5.21	119.36	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	155	LYS	CA-C-O	-5.21	115.35	120.98
1	A	119	HIS	CB-CG-ND1	5.21	130.51	122.70
1	F	386	LEU	CA-C-N	5.21	131.07	121.85
1	F	386	LEU	C-N-CA	5.21	131.07	121.85
1	H	296	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	K	303	THR	OG1-CB-CG2	-5.21	98.89	109.30
1	L	91	LYS	CB-CG-CD	5.21	123.27	111.30
1	A	308	GLY	N-CA-C	-5.20	105.84	114.48
1	L	195	ILE	O-C-N	-5.20	117.57	123.03
1	G	54	ASN	CA-CB-CG	5.20	117.80	112.60
1	D	459	VAL	CB-CA-C	5.20	117.44	110.42
1	B	325	VAL	O-C-N	-5.20	116.58	122.72
1	G	355	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	H	421	GLY	N-CA-C	5.20	122.49	115.32
1	J	253	GLY	CA-C-O	-5.20	116.90	121.58
1	B	353	TYR	O-C-N	-5.20	117.86	123.42
1	E	147	PRO	N-CA-CB	5.20	108.71	103.25
1	J	48	ALA	N-CA-C	5.20	117.85	111.82
1	B	439	LEU	O-C-N	-5.20	116.61	122.12
1	J	49	LYS	CA-C-O	-5.20	115.04	120.55
1	J	278	PHE	CA-CB-CG	5.20	119.00	113.80
1	J	101	SER	N-CA-CB	-5.19	103.35	111.56
1	B	268	LEU	CD1-CG-CD2	-5.19	99.38	110.80
1	C	80	LYS	CA-C-N	5.19	132.98	124.31
1	C	80	LYS	C-N-CA	5.19	132.98	124.31
1	D	42	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	D	66	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	D	271	LYS	CA-C-O	5.19	125.44	118.38
1	C	156	ILE	CB-CA-C	5.19	117.35	110.91
1	I	334	ILE	CA-CB-CG1	5.19	119.22	110.40
1	J	219	ILE	O-C-N	-5.19	117.08	123.00
1	G	169	SER	CA-C-O	-5.19	113.49	119.61
1	H	396	ARG	NH1-CZ-NH2	-5.19	112.56	119.30
1	I	342	THR	N-CA-C	5.19	118.63	112.72
1	J	107	ILE	CA-C-N	5.19	128.85	120.55
1	J	107	ILE	C-N-CA	5.19	128.85	120.55
1	G	281	VAL	CA-C-N	5.18	129.50	122.19
1	G	281	VAL	C-N-CA	5.18	129.50	122.19
1	J	332	SER	CA-C-N	5.18	124.50	118.85
1	J	332	SER	C-N-CA	5.18	124.50	118.85
1	B	263	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	255	ALA	N-CA-CB	-5.18	101.89	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	178	VAL	CA-C-N	5.18	131.13	122.73
1	I	178	VAL	C-N-CA	5.18	131.13	122.73
1	J	61	ILE	N-CA-C	5.18	114.66	106.32
1	F	404	ASN	CA-C-O	5.18	127.39	121.28
1	A	56	SER	CA-C-N	5.18	131.43	121.54
1	A	56	SER	C-N-CA	5.18	131.43	121.54
1	F	95	ASP	CA-CB-CG	5.18	117.78	112.60
1	K	40	SER	O-C-N	-5.18	117.15	123.16
1	H	38	VAL	CA-CB-CG1	5.18	119.20	110.40
1	B	73	PHE	O-C-N	-5.18	115.70	122.59
1	A	180	ALA	CB-CA-C	5.17	119.18	109.71
1	E	155	LYS	N-CA-C	5.17	116.74	108.41
1	H	361	GLN	OE1-CD-NE2	-5.17	117.42	122.60
1	J	196	ILE	O-C-N	-5.17	117.39	122.67
1	C	87	PHE	CA-C-N	5.17	126.31	119.84
1	C	87	PHE	C-N-CA	5.17	126.31	119.84
1	D	45	ILE	CA-C-N	5.17	127.46	120.38
1	D	45	ILE	C-N-CA	5.17	127.46	120.38
1	G	427	ILE	CA-CB-CG1	5.17	119.19	110.40
1	H	270	GLU	O-C-N	-5.17	115.37	122.46
1	I	52	VAL	N-CA-CB	5.17	117.45	112.28
1	A	283	ILE	CA-C-O	5.17	126.52	121.19
1	D	53	VAL	CA-CB-CG1	5.17	119.19	110.40
1	J	345	ILE	N-CA-C	5.17	116.68	109.80
1	D	347	GLN	CA-C-O	-5.17	115.93	121.56
1	D	402	ASP	CA-CB-CG	5.17	117.77	112.60
1	F	59	LYS	O-C-N	-5.17	117.14	123.19
1	H	397	LEU	N-CA-CB	-5.17	104.24	109.51
1	L	57	THR	CA-C-O	-5.17	115.51	122.44
1	E	161	LEU	O-C-N	-5.17	116.90	122.79
1	J	221	PRO	CB-CA-C	5.17	120.08	111.56
1	K	396	ARG	N-CA-C	5.17	121.81	110.80
1	F	63	ARG	CD-NE-CZ	5.17	131.63	124.40
1	D	58	SER	CA-C-O	5.16	127.89	120.51
1	H	118	ASN	N-CA-CB	5.16	117.56	110.07
1	J	355	ARG	NE-CZ-NH2	-5.16	114.55	119.20
1	B	208	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	C	344	GLU	CB-CG-CD	5.16	121.37	112.60
1	I	264	ILE	CA-C-N	5.16	127.96	120.79
1	I	264	ILE	C-N-CA	5.16	127.96	120.79
1	J	103	GLY	N-CA-C	5.16	119.89	111.27
1	J	305	VAL	CA-CB-CG2	-5.16	101.63	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ASN	N-CA-C	5.16	118.71	111.90
1	K	348	LYS	CA-C-N	5.16	130.23	123.11
1	K	348	LYS	C-N-CA	5.16	130.23	123.11
1	L	237	GLY	O-C-N	-5.16	117.98	123.45
1	B	326	ASN	O-C-N	-5.16	115.73	122.59
1	A	328	LYS	N-CA-C	5.15	117.75	108.48
1	B	140	ALA	CB-CA-C	5.15	118.32	109.51
1	E	147	PRO	CB-CA-C	-5.15	103.06	111.56
1	K	183	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	K	305	VAL	CA-C-O	-5.15	115.72	121.23
1	I	65	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	D	231	SER	CA-C-N	5.15	130.31	122.23
1	D	231	SER	C-N-CA	5.15	130.31	122.23
1	I	176	ASP	N-CA-C	5.15	117.70	110.23
1	C	140	ALA	CB-CA-C	5.15	118.20	109.50
1	C	380	LEU	CA-C-N	5.15	131.24	121.97
1	C	380	LEU	C-N-CA	5.15	131.24	121.97
1	H	197	SER	CA-C-O	-5.15	113.46	118.97
1	I	152	ALA	N-CA-C	5.15	117.07	108.99
1	I	433	GLN	CA-C-N	5.15	130.89	122.81
1	I	433	GLN	C-N-CA	5.15	130.89	122.81
1	I	444	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	G	424	GLU	CA-C-O	5.15	126.92	121.05
1	G	377	GLN	CG-CD-NE2	5.14	124.11	116.40
1	L	430	GLY	N-CA-C	5.14	120.65	110.83
1	F	240	SER	CA-C-N	5.14	130.64	122.10
1	F	240	SER	C-N-CA	5.14	130.64	122.10
1	B	202	ASP	CA-C-N	5.14	129.92	122.36
1	B	202	ASP	C-N-CA	5.14	129.92	122.36
1	F	399	ILE	O-C-N	-5.14	115.59	121.14
1	C	408	VAL	N-CA-C	5.14	114.69	106.88
1	F	455	THR	CB-CA-C	-5.14	101.76	110.19
1	I	392	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	L	445	ALA	N-CA-C	5.14	116.88	111.28
1	A	50	LYS	CA-C-N	5.14	131.52	122.79
1	A	50	LYS	C-N-CA	5.14	131.52	122.79
1	A	115	VAL	CA-C-N	5.14	130.28	122.11
1	A	115	VAL	C-N-CA	5.14	130.28	122.11
1	C	119	HIS	CA-C-O	5.14	125.91	120.10
1	D	158	ALA	N-CA-CB	-5.14	101.81	110.49
1	I	122	ASP	CB-CA-C	5.14	118.11	109.89
1	I	320	ASP	CA-CB-CG	5.14	117.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	250	ASN	CA-CB-CG	5.14	117.74	112.60
1	E	354	GLU	N-CA-C	5.13	117.61	109.50
1	G	258	SER	CA-C-O	-5.13	114.07	119.97
1	I	199	LEU	N-CA-C	5.13	117.77	109.40
1	I	428	ILE	O-C-N	5.13	128.58	122.83
1	J	376	VAL	CA-CB-CG1	5.13	119.12	110.40
1	K	372	ASN	CA-CB-CG	5.13	117.73	112.60
1	B	166	PHE	CA-CB-CG	5.13	118.93	113.80
1	F	121	VAL	O-C-N	-5.13	116.82	122.05
1	G	295	LYS	CB-CA-C	5.13	119.83	111.26
1	C	93	LYS	N-CA-C	5.13	116.56	111.07
1	F	42	HIS	N-CA-C	5.13	119.01	112.34
1	H	342	THR	CA-CB-CG2	5.13	119.22	110.50
1	J	210	GLU	CA-C-O	-5.13	115.11	121.11
1	F	319	GLY	CA-C-N	5.13	132.38	122.07
1	F	319	GLY	C-N-CA	5.13	132.38	122.07
1	J	176	ASP	N-CA-CB	5.13	117.61	109.51
1	K	252	ILE	CA-CB-CG1	5.13	119.11	110.40
1	G	291	LYS	CA-C-N	5.12	127.46	120.54
1	G	291	LYS	C-N-CA	5.12	127.46	120.54
1	I	227	ALA	N-CA-C	5.12	117.14	110.43
1	L	336	LEU	N-CA-C	5.12	116.87	111.28
1	G	122	ASP	CB-CA-C	5.12	117.94	110.26
1	G	141	LYS	CB-CA-C	5.12	118.20	109.80
1	J	108	ILE	N-CA-C	5.12	116.58	111.00
1	I	131	LEU	CB-CA-C	5.12	117.71	109.51
1	L	240	SER	CA-C-N	5.12	130.99	121.62
1	L	240	SER	C-N-CA	5.12	130.99	121.62
1	B	221	PRO	N-CA-CB	5.12	107.80	103.35
1	F	226	GLY	CA-C-O	-5.12	117.16	122.28
1	J	227	ALA	CA-C-O	-5.12	116.24	121.87
1	C	386	LEU	CB-CA-C	5.12	118.74	109.37
1	I	416	LYS	CA-C-N	5.12	131.44	121.41
1	I	416	LYS	C-N-CA	5.12	131.44	121.41
1	K	68	SER	CA-C-O	5.12	125.78	120.25
1	A	372	ASN	CA-C-N	5.12	124.78	119.56
1	A	372	ASN	C-N-CA	5.12	124.78	119.56
1	E	466	THR	CA-C-O	-5.12	114.83	120.30
1	F	167	THR	CA-C-O	-5.12	116.64	122.01
1	H	241	ALA	CA-C-O	-5.12	115.98	121.45
1	I	60	THR	CA-CB-OG1	-5.12	101.93	109.60
1	L	167	THR	N-CA-CB	5.12	117.68	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	374	LYS	N-CA-C	5.12	121.69	110.80
1	C	115	VAL	N-CA-C	5.11	115.27	108.11
1	C	277	GLY	N-CA-C	-5.11	103.87	112.77
1	I	320	ASP	N-CA-C	5.11	118.55	109.96
1	L	419	ASN	CA-CB-CG	5.11	117.71	112.60
1	E	409	ASP	O-C-N	-5.11	116.57	122.09
1	C	420	SER	N-CA-C	5.11	119.25	112.30
1	D	403	VAL	CA-CB-CG1	5.11	119.09	110.40
1	G	407	LEU	CB-CA-C	5.11	118.17	109.53
1	J	109	SER	CA-CB-OG	5.11	121.32	111.10
1	K	255	ALA	N-CA-C	5.11	117.82	109.59
1	A	441	ASP	CA-C-O	5.11	125.66	119.38
1	F	262	LYS	CA-C-N	5.11	127.12	120.28
1	F	262	LYS	C-N-CA	5.11	127.12	120.28
1	K	410	SER	N-CA-C	5.11	117.15	109.23
1	E	60	THR	CA-CB-CG2	5.10	119.18	110.50
1	E	372	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	117	ASN	CA-CB-CG	-5.10	107.50	112.60
1	A	382	ASP	CA-C-O	5.10	126.50	120.58
1	D	71	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	85	PHE	N-CA-CB	-5.10	101.87	110.49
1	G	279	LEU	CB-CA-C	5.10	119.34	110.72
1	B	160	ASN	CA-C-N	5.10	129.63	122.09
1	B	160	ASN	C-N-CA	5.10	129.63	122.09
1	H	393	LEU	CA-C-N	5.10	132.27	122.03
1	H	393	LEU	C-N-CA	5.10	132.27	122.03
1	B	121	VAL	N-CA-C	5.09	117.12	112.43
1	F	458	TRP	CG-CD2-CE3	5.09	138.99	133.90
1	H	123	ASP	CA-CB-CG	5.09	117.69	112.60
1	H	185	PHE	N-CA-CB	-5.09	104.44	112.13
1	H	352	SER	N-CA-C	5.09	118.42	110.32
1	K	85	PHE	CA-C-N	5.09	131.27	121.54
1	K	85	PHE	C-N-CA	5.09	131.27	121.54
1	G	410	SER	O-C-N	-5.09	117.44	123.25
1	G	107	ILE	CA-C-N	5.09	128.78	121.55
1	G	107	ILE	C-N-CA	5.09	128.78	121.55
1	I	230	ASP	N-CA-C	5.09	117.73	109.79
1	J	58	SER	O-C-N	-5.09	115.82	122.59
1	K	355	ARG	O-C-N	-5.09	117.15	123.36
1	G	95	ASP	CA-C-O	5.09	124.78	119.03
1	H	44	SER	CA-C-O	-5.09	115.45	120.90
1	J	392	ARG	NE-CZ-NH1	5.09	126.59	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	446	LEU	CD1-CG-CD2	-5.09	99.60	110.80
1	E	130	ASN	CB-CG-ND2	5.09	124.03	116.40
1	I	461	ARG	CA-CB-CG	-5.09	103.93	114.10
1	K	408	VAL	CA-C-N	5.09	127.36	120.44
1	K	408	VAL	C-N-CA	5.09	127.36	120.44
1	J	238	ILE	CA-CB-CG1	5.08	119.04	110.40
1	A	387	ARG	CD-NE-CZ	5.08	131.52	124.40
1	C	260	MET	CA-C-O	-5.08	113.95	120.31
1	G	449	VAL	N-CA-C	5.08	119.21	111.89
1	L	356	ASP	N-CA-C	5.08	121.63	110.80
1	E	450	ASN	CB-CA-C	5.08	119.71	110.72
1	H	208	GLN	CA-C-N	5.08	129.91	122.39
1	H	208	GLN	C-N-CA	5.08	129.91	122.39
1	I	413	GLU	CA-CB-CG	5.08	124.26	114.10
1	J	350	SER	N-CA-C	5.08	121.62	110.80
1	K	73	PHE	CA-CB-CG	5.08	118.88	113.80
1	L	373	PRO	CB-CA-C	-5.08	103.17	111.56
1	C	344	GLU	CA-C-N	5.08	127.41	120.35
1	C	344	GLU	C-N-CA	5.08	127.41	120.35
1	H	293	ALA	CA-C-N	5.08	131.24	121.54
1	H	293	ALA	C-N-CA	5.08	131.24	121.54
1	K	114	ILE	N-CA-C	5.08	116.55	109.80
1	G	88	PRO	CA-N-CD	-5.08	104.89	112.00
1	A	296	ASN	CA-CB-CG	-5.08	107.52	112.60
1	K	151	LEU	CD1-CG-CD2	-5.08	99.64	110.80
1	C	200	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	G	86	ASP	CA-CB-CG	5.07	117.67	112.60
1	I	438	ASN	N-CA-C	5.07	115.03	107.88
1	A	321	LEU	CA-C-N	5.07	128.79	121.18
1	A	321	LEU	C-N-CA	5.07	128.79	121.18
1	I	220	ASN	O-C-N	-5.07	117.01	121.32
1	A	363	SER	N-CA-C	5.07	117.42	108.75
1	H	390	ASP	O-C-N	-5.07	115.59	121.47
1	K	138	TYR	CB-CG-CD2	-5.07	113.19	120.80
1	K	295	LYS	CA-C-N	5.07	129.53	122.08
1	K	295	LYS	C-N-CA	5.07	129.53	122.08
1	B	216	ASP	CA-C-O	5.07	125.41	119.28
1	J	347	GLN	CB-CA-C	5.07	119.23	110.77
1	L	291	LYS	O-C-N	5.07	127.29	122.07
1	I	257	PRO	N-CA-CB	5.07	108.00	103.19
1	J	67	PRO	O-C-N	5.07	128.50	122.98
1	J	242	ILE	CA-CB-CG1	5.07	119.01	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ILE	N-CA-CB	-5.06	107.15	112.06
1	F	254	PHE	N-CA-C	5.06	116.66	108.41
1	F	364	PHE	CA-CB-CG	5.06	118.86	113.80
1	F	366	LEU	N-CA-C	5.06	116.44	109.15
1	I	268	LEU	CA-C-N	5.06	127.40	120.46
1	I	268	LEU	C-N-CA	5.06	127.40	120.46
1	J	303	THR	N-CA-CB	5.06	118.04	110.19
1	J	377	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	360	LYS	CB-CG-CD	5.06	122.94	111.30
1	D	468	LEU	O-C-N	-5.06	116.01	122.94
1	E	405	GLY	N-CA-C	5.06	117.41	110.58
1	G	210	GLU	CA-C-O	-5.06	115.81	121.23
1	B	249	ASN	CA-CB-CG	-5.06	107.54	112.60
1	D	87	PHE	CA-C-O	-5.06	115.43	120.64
1	D	399	ILE	CA-C-N	5.06	124.55	119.19
1	D	399	ILE	C-N-CA	5.06	124.55	119.19
1	E	255	ALA	N-CA-CB	-5.06	102.05	110.80
1	K	441	ASP	CB-CA-C	5.06	120.38	110.67
1	L	209	TYR	CA-C-N	5.06	130.53	122.94
1	L	209	TYR	C-N-CA	5.06	130.53	122.94
1	A	159	ASN	CB-CA-C	5.06	121.95	110.67
1	C	426	ASP	CA-CB-CG	5.06	117.66	112.60
1	F	60	THR	CA-CB-CG2	5.06	119.10	110.50
1	F	318	ARG	O-C-N	5.06	128.72	123.06
1	H	208	GLN	CA-C-O	-5.06	112.88	118.69
1	I	76	ASP	O-C-N	5.06	125.87	121.17
1	A	130	ASN	N-CA-C	5.05	116.94	107.99
1	D	338	ASN	CB-CG-OD1	5.05	130.91	120.80
1	E	427	ILE	CA-C-O	-5.05	114.46	120.78
1	A	382	ASP	O-C-N	-5.05	116.59	122.96
1	E	356	ASP	CA-CB-CG	5.05	117.65	112.60
1	K	244	SER	N-CA-C	5.05	115.20	108.38
1	G	236	VAL	CA-CB-CG2	5.05	118.98	110.40
1	I	467	LEU	O-C-N	-5.05	117.46	123.22
1	B	282	THR	O-C-N	5.05	129.75	123.19
1	E	347	GLN	N-CA-C	5.05	117.55	110.23
1	E	368	GLY	O-C-N	-5.05	116.14	122.70
1	F	184	PRO	N-CD-CG	5.05	110.77	103.20
1	K	76	ASP	CB-CA-C	5.05	120.11	110.17
1	K	468	LEU	CA-C-N	5.05	131.06	121.97
1	K	468	LEU	C-N-CA	5.05	131.06	121.97
1	L	49	LYS	CA-CB-CG	5.05	124.19	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	LYS	O-C-N	-5.04	115.83	122.39
1	F	310	SER	CA-C-O	-5.04	113.59	119.14
1	L	66	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	A	422	PHE	O-C-N	-5.04	117.31	123.16
1	G	306	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	H	245	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	H	424	GLU	N-CA-C	5.04	116.79	110.24
1	J	248	GLY	CA-C-N	5.04	128.85	120.94
1	J	248	GLY	C-N-CA	5.04	128.85	120.94
1	L	281	VAL	CA-C-N	5.04	129.96	123.00
1	L	281	VAL	C-N-CA	5.04	129.96	123.00
1	E	90	ARG	CA-CB-CG	5.04	124.18	114.10
1	A	62	THR	OG1-CB-CG2	-5.04	99.22	109.30
1	C	225	GLY	CA-C-N	5.04	128.81	121.05
1	C	225	GLY	C-N-CA	5.04	128.81	121.05
1	F	390	ASP	CB-CA-C	5.04	116.88	110.13
1	G	372	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	I	396	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	D	60	THR	CA-CB-CG2	5.04	119.06	110.50
1	B	147	PRO	CA-C-N	5.04	129.04	120.88
1	B	147	PRO	C-N-CA	5.04	129.04	120.88
1	A	322	VAL	CA-C-O	-5.03	114.86	120.95
1	B	296	ASN	CB-CG-ND2	5.03	123.95	116.40
1	H	179	PHE	CA-CB-CG	5.03	118.83	113.80
1	H	334	ILE	CA-CB-CG2	-5.03	101.94	110.50
1	K	330	ILE	N-CA-C	5.03	115.22	107.77
1	D	190	SER	CA-C-N	5.03	129.96	122.71
1	D	190	SER	C-N-CA	5.03	129.96	122.71
1	D	249	ASN	N-CA-CB	-5.03	103.17	110.36
1	H	312	ASP	N-CA-C	5.03	117.54	111.40
1	K	55	ILE	O-C-N	-5.03	117.95	123.18
1	A	230	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	287	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	A	423	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	320	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	214	GLN	CA-C-N	5.03	130.49	122.59
1	D	214	GLN	C-N-CA	5.03	130.49	122.59
1	H	197	SER	CA-CB-OG	5.03	121.16	111.10
1	K	170	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	444	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	H	274	ILE	CA-C-O	5.03	126.55	120.67
1	J	166	PHE	CB-CA-C	5.03	119.51	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	309	SER	N-CA-CB	-5.03	102.80	110.39
1	F	196	ILE	O-C-N	5.03	127.80	122.67
1	A	153	VAL	CA-CB-CG2	5.03	118.94	110.40
1	C	444	GLN	N-CA-CB	5.03	117.30	110.01
1	G	225	GLY	CA-C-O	5.03	124.76	119.03
1	H	397	LEU	O-C-N	-5.03	119.34	123.11
1	J	67	PRO	CA-C-N	5.03	129.71	121.57
1	J	67	PRO	C-N-CA	5.03	129.71	121.57
1	J	235	LEU	N-CA-C	5.03	117.59	110.10
1	J	324	LYS	CA-C-N	5.03	128.09	120.75
1	J	324	LYS	C-N-CA	5.03	128.09	120.75
1	K	115	VAL	CB-CA-C	5.03	118.11	110.62
1	L	203	ASN	CA-CB-CG	5.03	117.62	112.60
1	C	101	SER	CB-CA-C	5.02	118.09	109.80
1	J	160	ASN	CA-CB-CG	5.02	117.62	112.60
1	L	97	GLU	CB-CA-C	5.02	120.02	110.27
1	E	204	ILE	CB-CA-C	5.02	115.48	111.06
1	H	364	PHE	O-C-N	-5.02	116.49	123.12
1	K	423	GLN	N-CA-C	5.02	117.31	109.52
1	L	45	ILE	CA-C-N	5.02	127.42	120.29
1	L	45	ILE	C-N-CA	5.02	127.42	120.29
1	E	51	SER	CA-C-N	5.02	131.01	121.97
1	E	51	SER	C-N-CA	5.02	131.01	121.97
1	A	468	LEU	N-CA-CB	-5.02	102.96	111.69
1	D	148	LYS	O-C-N	-5.02	115.52	122.30
1	C	345	ILE	CA-CB-CG2	5.02	119.03	110.50
1	D	154	ILE	CA-CB-CG1	5.02	118.93	110.40
1	J	297	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	K	151	LEU	CA-C-N	5.02	130.97	121.69
1	K	151	LEU	C-N-CA	5.02	130.97	121.69
1	L	43	ASP	CA-CB-CG	5.02	117.62	112.60
1	J	354	GLU	CB-CA-C	5.01	119.39	109.66
1	C	78	TYR	N-CA-CB	5.01	118.96	110.49
1	D	243	LEU	CD1-CG-CD2	-5.01	99.77	110.80
1	D	264	ILE	O-C-N	-5.01	117.00	121.91
1	B	286	LEU	O-C-N	-5.01	116.64	122.96
1	E	277	GLY	O-C-N	5.01	129.22	122.70
1	K	437	LYS	N-CA-C	5.01	120.77	114.31
1	D	305	VAL	CB-CA-C	-5.01	104.62	111.33
1	H	354	GLU	CA-C-O	-5.01	115.60	121.46
1	I	139	LYS	N-CA-C	-5.01	103.44	110.50
1	L	443	GLU	CA-C-O	-5.01	113.43	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	LYS	CA-C-N	5.01	130.30	120.99
1	A	96	LYS	C-N-CA	5.01	130.30	120.99
1	C	165	THR	CA-C-N	5.01	131.10	121.54
1	C	165	THR	C-N-CA	5.01	131.10	121.54
1	F	262	LYS	CA-C-O	-5.01	115.56	120.82
1	F	292	LYS	O-C-N	-5.01	116.68	122.09
1	I	44	SER	CA-C-N	5.01	128.58	120.82
1	I	44	SER	C-N-CA	5.01	128.58	120.82
1	C	86	ASP	CB-CA-C	5.00	115.96	109.80
1	L	195	ILE	CA-C-O	5.00	127.93	121.32
1	C	183	ASN	CB-CA-C	5.00	120.03	110.17
1	G	119	HIS	CB-CG-CD2	-5.00	124.69	131.20
1	D	282	THR	CA-C-O	-5.00	114.93	120.38
1	G	201	LYS	CB-CA-C	5.00	118.79	110.74
1	I	315	GLY	CA-C-O	-5.00	111.87	120.57
1	K	401	LYS	N-CA-CB	-5.00	102.24	110.14

There are no chirality outliers.

All (205) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	129	VAL	Peptide
1	A	185	PHE	Sidechain
1	A	230	ASP	Sidechain
1	A	234	TYR	Sidechain
1	A	294	TYR	Sidechain
1	A	371	GLU	Peptide
1	A	389	LEU	Peptide
1	A	396	ARG	Peptide
1	A	41	TYR	Sidechain
1	A	419	ASN	Peptide
1	A	460	TYR	Sidechain
1	A	461	ARG	Sidechain
1	A	83	PHE	Peptide
1	B	113	TYR	Sidechain
1	B	139	LYS	Mainchain
1	B	166	PHE	Sidechain
1	B	170	ASP	Mainchain
1	B	189	PHE	Sidechain
1	B	202	ASP	Peptide
1	B	209	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	245	ARG	Sidechain
1	B	318	ARG	Sidechain
1	B	374	LYS	Peptide
1	B	387	ARG	Sidechain
1	B	389	LEU	Peptide
1	B	396	ARG	Sidechain
1	B	41	TYR	Peptide
1	B	441	ASP	Mainchain
1	B	461	ARG	Sidechain
1	B	469	VAL	Mainchain
1	B	53	VAL	Mainchain,Peptide
1	C	138	TYR	Sidechain
1	C	159	ASN	Peptide
1	C	222	GLY	Peptide
1	C	245	ARG	Sidechain
1	C	289	ASP	Mainchain
1	C	318	ARG	Sidechain
1	C	353	TYR	Sidechain
1	C	364	PHE	Sidechain
1	C	368	GLY	Mainchain
1	C	387	ARG	Sidechain
1	C	389	LEU	Peptide
1	C	390	ASP	Peptide
1	C	404	ASN	Peptide
1	C	438	ASN	Mainchain
1	C	461	ARG	Sidechain
1	C	56	SER	Peptide
1	C	63	ARG	Sidechain
1	C	82	PHE	Sidechain
1	C	89	GLN	Mainchain
1	D	119	HIS	Sidechain
1	D	138	TYR	Sidechain
1	D	162	SER	Peptide
1	D	220	ASN	Peptide
1	D	245	ARG	Sidechain
1	D	247	GLY	Peptide
1	D	276	ARG	Sidechain
1	D	278	PHE	Peptide
1	D	282	THR	Peptide
1	D	364	PHE	Sidechain
1	D	375	GLY	Peptide
1	D	389	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	D	396	ARG	Peptide
1	D	460	TYR	Sidechain
1	D	53	VAL	Peptide
1	D	63	ARG	Sidechain
1	D	90	ARG	Sidechain
1	E	100	SER	Peptide
1	E	113	TYR	Sidechain
1	E	138	TYR	Sidechain
1	E	162	SER	Peptide
1	E	171	ASP	Peptide
1	E	185	PHE	Sidechain
1	E	202	ASP	Peptide
1	E	222	GLY	Peptide
1	E	389	LEU	Peptide
1	E	41	TYR	Sidechain
1	E	461	ARG	Sidechain
1	E	63	ARG	Sidechain
1	F	138	TYR	Sidechain
1	F	139	LYS	Mainchain
1	F	185	PHE	Sidechain
1	F	209	TYR	Sidechain
1	F	212	PHE	Sidechain
1	F	221	PRO	Peptide
1	F	232	ARG	Sidechain
1	F	318	ARG	Sidechain
1	F	340	ILE	Mainchain
1	F	344	GLU	Peptide
1	F	353	TYR	Sidechain
1	F	355	ARG	Sidechain
1	F	389	LEU	Peptide
1	F	415	SER	Mainchain
1	F	78	TYR	Sidechain
1	F	79	PHE	Sidechain
1	G	170	ASP	Peptide
1	G	185	PHE	Sidechain
1	G	199	LEU	Peptide
1	G	204	ILE	Peptide
1	G	232	ARG	Sidechain
1	G	249	ASN	Sidechain
1	G	318	ARG	Sidechain
1	G	339	TYR	Sidechain
1	G	344	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	G	345	ILE	Peptide
1	G	353	TYR	Sidechain
1	G	387	ARG	Sidechain
1	G	389	LEU	Peptide
1	G	460	TYR	Sidechain
1	G	461	ARG	Sidechain
1	G	51	SER	Mainchain
1	G	53	VAL	Peptide
1	G	74	PHE	Peptide
1	H	113	TYR	Sidechain
1	H	120	VAL	Mainchain
1	H	138	TYR	Sidechain
1	H	185	PHE	Sidechain
1	H	192	THR	Mainchain
1	H	220	ASN	Peptide
1	H	306	GLN	Peptide
1	H	345	ILE	Peptide
1	H	376	VAL	Peptide
1	H	389	LEU	Peptide
1	H	390	ASP	Peptide
1	H	395	ASP	Peptide
1	H	396	ARG	Sidechain
1	H	415	SER	Mainchain
1	H	461	ARG	Sidechain
1	H	78	TYR	Sidechain
1	I	185	PHE	Sidechain
1	I	201	LYS	Peptide
1	I	240	SER	Mainchain
1	I	256	ILE	Mainchain
1	I	318	ARG	Sidechain
1	I	337	LYS	Mainchain
1	I	339	TYR	Sidechain
1	I	353	TYR	Sidechain
1	I	355	ARG	Sidechain
1	I	373	PRO	Peptide
1	I	387	ARG	Sidechain
1	I	389	LEU	Peptide
1	I	395	ASP	Mainchain
1	I	40	SER	Mainchain
1	I	418	LYS	Peptide
1	I	43	ASP	Mainchain
1	I	84	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	J	121	VAL	Peptide
1	J	209	TYR	Sidechain
1	J	217	ALA	Mainchain
1	J	237	GLY	Mainchain
1	J	245	ARG	Sidechain
1	J	276	ARG	Sidechain
1	J	289	ASP	Peptide
1	J	306	GLN	Peptide
1	J	318	ARG	Sidechain,Peptide
1	J	326	ASN	Sidechain
1	J	353	TYR	Sidechain
1	J	355	ARG	Sidechain
1	J	373	PRO	Mainchain
1	J	375	GLY	Peptide
1	J	389	LEU	Peptide
1	J	392	ARG	Sidechain
1	J	446	LEU	Peptide
1	J	56	SER	Peptide
1	J	66	ARG	Sidechain
1	J	73	PHE	Sidechain
1	K	133	GLY	Peptide
1	K	185	PHE	Sidechain
1	K	276	ARG	Sidechain
1	K	289	ASP	Peptide
1	K	294	TYR	Sidechain
1	K	296	ASN	Peptide
1	K	298	GLU	Mainchain
1	K	312	ASP	Peptide
1	K	318	ARG	Sidechain
1	K	370	LYS	Peptide
1	K	371	GLU	Peptide
1	K	372	ASN	Mainchain
1	K	376	VAL	Peptide
1	K	389	LEU	Peptide
1	K	390	ASP	Peptide
1	K	396	ARG	Sidechain,Peptide
1	K	403	VAL	Peptide
1	K	460	TYR	Sidechain
1	K	63	ARG	Sidechain
1	K	83	PHE	Sidechain
1	L	220	ASN	Peptide
1	L	227	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	L	277	GLY	Peptide
1	L	278	PHE	Peptide
1	L	294	TYR	Sidechain
1	L	318	ARG	Sidechain
1	L	339	TYR	Sidechain
1	L	375	GLY	Peptide
1	L	389	LEU	Peptide
1	L	422	PHE	Mainchain,Sidechain
1	L	461	ARG	Sidechain
1	L	66	ARG	Sidechain
1	L	70	LEU	Mainchain
1	L	78	TYR	Sidechain

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	3323	0	3393	17	0
1	B	3323	0	3393	32	0
1	C	3323	0	3393	12	0
1	D	3323	0	3393	24	0
1	E	3323	0	3393	29	0
1	F	3323	0	3393	22	0
1	G	3323	0	3393	24	0
1	H	3323	0	3393	26	0
1	I	3323	0	3393	32	0
1	J	3323	0	3393	33	0
1	K	3323	0	3393	21	0
1	L	3322	0	3393	25	0
All	All	39875	0	40716	292	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 4.

All (292) 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:E:237:GLY:C	1:E:238:ILE:HD12	2.06	0.80
1:E:281:VAL:HG21	1:E:302:ILE:HD12	1.67	0.76
1:L:380:LEU:HB2	1:L:449:VAL:HG21	1.68	0.74
1:G:380:LEU:HB2	1:G:449:VAL:HG21	1.70	0.74
1:I:311:ALA:HB1	1:I:316:LEU:HD23	1.70	0.73
1:B:278:PHE:HA	1:B:340:ILE:HG21	1.76	0.67
1:I:380:LEU:HB2	1:I:449:VAL:HG21	1.76	0.67
1:J:294:TYR:CE2	1:J:416:LYS:HE3	2.31	0.65
1:I:294:TYR:CE2	1:I:416:LYS:HE3	2.31	0.64
1:E:139:LYS:HE3	1:E:141:LYS:HE3	1.78	0.64
1:I:302:ILE:HD11	1:I:316:LEU:HD21	1.78	0.64
1:L:365:ILE:HD12	1:L:367:LYS:HE3	1.79	0.64
1:G:302:ILE:HD11	1:G:322:VAL:HG23	1.81	0.62
1:L:384:LEU:HB3	1:L:386:LEU:HD13	1.82	0.61
1:G:446:LEU:O	1:G:449:VAL:HG22	2.00	0.61
1:J:457:VAL:HG22	1:J:470:LEU:HD13	1.83	0.60
1:D:267:LYS:HE2	1:D:267:LYS:HA	1.83	0.60
1:H:57:THR:HG23	1:H:127:ILE:HG22	1.82	0.60
1:D:281:VAL:HG21	1:D:302:ILE:HD12	1.84	0.60
1:E:340:ILE:HD12	1:E:366:LEU:HD11	1.84	0.59
1:K:282:THR:HG23	1:K:306:GLN:HE21	1.68	0.58
1:K:237:GLY:C	1:K:238:ILE:HD12	2.29	0.58
1:F:177:VAL:HG23	1:F:231:SER:HB3	1.86	0.58
1:B:318:ARG:HD2	1:B:377:GLN:HG3	1.86	0.57
1:C:278:PHE:CD1	1:C:340:ILE:HG21	2.39	0.57
1:L:264:ILE:HG23	1:L:274:ILE:HD11	1.85	0.57
1:H:384:LEU:HB3	1:H:386:LEU:HD13	1.85	0.57
1:K:380:LEU:HB2	1:K:449:VAL:HG21	1.87	0.57
1:I:312:ASP:CG	1:I:317:LYS:HZ1	2.13	0.57
1:L:302:ILE:HD11	1:L:322:VAL:CG2	2.34	0.57
1:L:218:SER:O	1:L:219:ILE:HD13	2.05	0.57
1:K:381:ILE:HB	1:K:446:LEU:HD13	1.87	0.56
1:D:198:ALA:HB3	1:D:214:GLN:HB3	1.88	0.56
1:I:317:LYS:HE3	1:I:376:VAL:CG1	2.35	0.56
1:J:241:ALA:C	1:J:242:ILE:HD12	2.30	0.56
1:H:131:LEU:HD12	1:H:132:PRO:HD2	1.86	0.56
1:J:385:SER:O	1:J:386:LEU:HD12	2.06	0.56
1:K:348:LYS:HE3	1:K:365:ILE:HG13	1.88	0.56
1:B:307:LYS:HE3	1:B:377:GLN:CD	2.30	0.56
1:J:325:VAL:HG23	1:J:330:ILE:HD11	1.88	0.56
1:I:340:ILE:HD12	1:I:366:LEU:HD11	1.88	0.55
1:B:380:LEU:HB2	1:B:449:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:297:GLN:HB2	1:K:321:LEU:HD12	1.87	0.55
1:L:294:TYR:CZ	1:L:416:LYS:HE3	2.41	0.55
1:B:446:LEU:O	1:B:449:VAL:HG22	2.07	0.55
1:F:267:LYS:HE2	1:F:267:LYS:HA	1.88	0.55
1:D:267:LYS:HA	1:D:267:LYS:CE	2.38	0.54
1:L:294:TYR:CE2	1:L:416:LYS:HE3	2.43	0.54
1:F:241:ALA:C	1:F:242:ILE:HD12	2.33	0.54
1:L:264:ILE:HG23	1:L:274:ILE:CD1	2.37	0.54
1:E:238:ILE:HD12	1:E:238:ILE:N	2.23	0.54
1:L:181:LEU:HD11	1:L:229:VAL:HG22	1.89	0.54
1:J:249:ASN:ND2	1:J:251:GLY:H	2.06	0.54
1:I:278:PHE:HA	1:I:340:ILE:HG21	1.90	0.53
1:I:385:SER:O	1:I:386:LEU:HD12	2.08	0.53
1:I:446:LEU:O	1:I:449:VAL:HG22	2.08	0.53
1:D:177:VAL:HG23	1:D:231:SER:HB3	1.91	0.53
1:L:328:LYS:HB3	1:L:339:TYR:CE2	2.44	0.53
1:B:328:LYS:HB3	1:B:339:TYR:CE2	2.44	0.52
1:H:81:GLN:HB3	1:H:185:PHE:CG	2.44	0.52
1:F:380:LEU:HB2	1:F:449:VAL:HG21	1.91	0.52
1:G:237:GLY:C	1:G:238:ILE:HD12	2.35	0.52
1:J:384:LEU:HB3	1:J:386:LEU:HD13	1.91	0.52
1:A:131:LEU:HD12	1:A:132:PRO:HD2	1.90	0.52
1:G:302:ILE:HD11	1:G:322:VAL:CG2	2.40	0.51
1:D:307:LYS:C	1:D:374:LYS:HA	2.36	0.51
1:C:117:ASN:HD22	1:C:119:HIS:CE1	2.29	0.51
1:D:81:GLN:HB3	1:D:185:PHE:CD2	2.47	0.51
1:I:317:LYS:HE3	1:I:376:VAL:HG13	1.92	0.50
1:E:307:LYS:C	1:E:374:LYS:HA	2.36	0.50
1:D:307:LYS:O	1:D:374:LYS:HA	2.11	0.50
1:I:177:VAL:HG23	1:I:231:SER:HB3	1.93	0.50
1:C:237:GLY:C	1:C:238:ILE:HD12	2.36	0.50
1:H:48:ALA:HB1	1:H:181:LEU:HD22	1.94	0.50
1:B:278:PHE:HB2	1:B:368:GLY:HA2	1.94	0.50
1:L:97:GLU:HG3	1:L:102:LEU:HD23	1.94	0.50
1:D:403:VAL:O	1:D:403:VAL:HG22	2.12	0.49
1:L:332:SER:HB2	1:L:333:PRO:HD2	1.94	0.49
1:F:365:ILE:HD12	1:F:367:LYS:HE3	1.94	0.49
1:H:246:GLY:HA3	1:I:245:ARG:HG3	1.93	0.49
1:L:318:ARG:HD3	1:L:377:GLN:HB2	1.93	0.49
1:I:208:GLN:O	1:I:337:LYS:HE2	2.13	0.49
1:A:307:LYS:C	1:A:374:LYS:HA	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:317:LYS:HE3	1:H:317:LYS:HA	1.93	0.49
1:C:107:ILE:HG12	1:C:114:ILE:HG22	1.95	0.49
1:E:454:PHE:C	1:E:454:PHE:CD2	2.90	0.49
1:B:449:VAL:C	1:B:451:LYS:H	2.20	0.49
1:C:81:GLN:HB3	1:C:185:PHE:CG	2.47	0.49
1:F:59:LYS:HE3	1:F:62:THR:HA	1.95	0.49
1:G:307:LYS:HB3	1:G:374:LYS:HA	1.94	0.49
1:L:153:VAL:HG23	1:L:268:LEU:HD12	1.93	0.49
1:B:433:GLN:HE21	1:B:456:LYS:HG3	1.78	0.49
1:I:81:GLN:HB3	1:I:185:PHE:CG	2.48	0.49
1:C:325:VAL:CG2	1:C:330:ILE:HD11	2.43	0.49
1:B:169:SER:HB3	1:B:258:SER:H	1.78	0.49
1:C:316:LEU:HD12	1:C:317:LYS:H	1.78	0.49
1:K:281:VAL:CG2	1:K:302:ILE:HG23	2.43	0.49
1:E:177:VAL:HG23	1:E:231:SER:HB3	1.95	0.48
1:H:380:LEU:HB2	1:H:449:VAL:HG21	1.95	0.48
1:I:307:LYS:C	1:I:309:SER:H	2.20	0.48
1:J:149:THR:HG23	1:J:276:ARG:HH22	1.78	0.48
1:J:307:LYS:HE3	1:J:377:GLN:OE1	2.12	0.48
1:J:325:VAL:CG2	1:J:330:ILE:HD11	2.43	0.48
1:E:279:LEU:HD12	1:E:336:LEU:HD11	1.95	0.48
1:J:264:ILE:HG23	1:J:274:ILE:HD11	1.95	0.48
1:L:184:PRO:O	1:L:187:VAL:HG22	2.14	0.48
1:H:81:GLN:HE22	1:H:102:LEU:HD11	1.78	0.48
1:J:380:LEU:HB2	1:J:449:VAL:HG21	1.96	0.48
1:A:311:ALA:HB1	1:A:316:LEU:HD23	1.96	0.47
1:A:294:TYR:CZ	1:A:416:LYS:HE3	2.48	0.47
1:D:79:PHE:CZ	1:D:93:LYS:HB3	2.49	0.47
1:H:54:ASN:HB3	1:H:183:ASN:HD22	1.80	0.47
1:J:386:LEU:HD11	1:J:408:VAL:HG13	1.96	0.47
1:B:371:GLU:CD	1:K:394:LYS:HE2	2.39	0.47
1:J:215:THR:HG23	1:J:217:ALA:HB3	1.97	0.47
1:J:249:ASN:HD21	1:J:251:GLY:HA2	1.79	0.47
1:E:275:ASP:HB3	1:E:345:ILE:HD12	1.96	0.47
1:F:113:TYR:CE1	1:F:143:ILE:HD11	2.50	0.47
1:I:345:ILE:HD12	1:I:345:ILE:H	1.80	0.47
1:L:307:LYS:HB3	1:L:375:GLY:H	1.78	0.47
1:B:177:VAL:HG23	1:B:231:SER:HB3	1.97	0.47
1:I:57:THR:CG2	1:I:101:SER:HB3	2.44	0.47
1:I:57:THR:HB	1:I:101:SER:HB3	1.95	0.47
1:J:237:GLY:C	1:J:238:ILE:HD12	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:VAL:CG2	1:A:302:ILE:HD12	2.45	0.47
1:G:129:VAL:HG22	1:G:156:ILE:HD13	1.96	0.47
1:D:302:ILE:HD11	1:D:322:VAL:HG23	1.97	0.46
1:D:380:LEU:HD13	1:D:449:VAL:HG23	1.96	0.46
1:J:57:THR:HA	1:J:127:ILE:HA	1.97	0.46
1:J:385:SER:C	1:J:386:LEU:HD12	2.40	0.46
1:H:237:GLY:C	1:H:238:ILE:HD12	2.39	0.46
1:K:380:LEU:CB	1:K:449:VAL:HG21	2.46	0.46
1:B:140:ALA:HB1	1:B:154:ILE:HG22	1.97	0.46
1:D:195:ILE:HD11	1:F:193:SER:H	1.79	0.46
1:D:284:LEU:HA	1:D:333:PRO:HG3	1.97	0.46
1:B:316:LEU:HD12	1:B:320:ASP:HB2	1.96	0.46
1:F:278:PHE:CD1	1:F:340:ILE:HG21	2.51	0.46
1:I:385:SER:C	1:I:386:LEU:HD12	2.40	0.46
1:L:143:ILE:HD11	1:L:155:LYS:HB2	1.97	0.46
1:D:467:LEU:HD23	1:D:467:LEU:H	1.80	0.46
1:G:406:VAL:HG11	1:G:442:LEU:HD22	1.97	0.46
1:J:307:LYS:C	1:J:374:LYS:HA	2.41	0.46
1:K:305:VAL:C	1:K:307:LYS:H	2.23	0.46
1:H:302:ILE:HG13	1:H:316:LEU:HD21	1.98	0.46
1:K:200:ASN:H	1:K:213:ILE:HG12	1.81	0.46
1:A:63:ARG:HH21	1:A:66:ARG:NH2	2.14	0.46
1:G:403:VAL:HG22	1:G:403:VAL:O	2.16	0.46
1:B:205:GLY:HA2	1:B:210:GLU:CD	2.41	0.45
1:H:219:ILE:HG23	1:H:223:ASN:CB	2.46	0.45
1:H:344:GLU:O	1:H:366:LEU:HD22	2.16	0.45
1:B:81:GLN:HB3	1:B:185:PHE:CG	2.52	0.45
1:F:63:ARG:HG2	1:F:63:ARG:HH21	1.82	0.45
1:J:394:LYS:HE3	1:J:395:ASP:CG	2.41	0.45
1:I:81:GLN:HB3	1:I:185:PHE:CD1	2.52	0.45
1:J:184:PRO:O	1:J:187:VAL:HG22	2.16	0.45
1:B:181:LEU:HD11	1:B:229:VAL:HG22	1.99	0.45
1:E:57:THR:HG23	1:E:127:ILE:HG22	1.99	0.45
1:E:237:GLY:CA	1:E:238:ILE:HD12	2.47	0.45
1:J:68:SER:HB3	1:J:70:LEU:HD13	1.97	0.45
1:D:318:ARG:HD3	1:D:377:GLN:HB2	1.98	0.45
1:F:185:PHE:CE1	1:F:221:PRO:HD2	2.51	0.45
1:B:182:GLY:CA	1:B:223:ASN:HD22	2.30	0.45
1:C:332:SER:HB2	1:C:333:PRO:HD2	1.98	0.45
1:G:208:GLN:O	1:G:337:LYS:HE2	2.17	0.45
1:H:351:LEU:C	1:H:351:LEU:HD23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:345:ILE:HD12	1:H:345:ILE:N	2.32	0.45
1:I:118:ASN:HB3	1:I:150:ASP:HA	1.98	0.45
1:I:406:VAL:HG12	1:I:428:ILE:HB	1.98	0.44
1:C:241:ALA:C	1:C:242:ILE:HD12	2.42	0.44
1:K:267:LYS:HE2	1:K:267:LYS:HA	1.99	0.44
1:A:52:VAL:HA	1:A:105:GLY:O	2.18	0.44
1:F:372:ASN:HA	1:F:373:PRO:HD3	1.89	0.44
1:I:181:LEU:HD11	1:I:229:VAL:HG22	2.00	0.44
1:I:237:GLY:C	1:I:238:ILE:HD12	2.43	0.44
1:E:49:LYS:HB3	1:E:189:PHE:CE2	2.53	0.44
1:E:267:LYS:HB3	1:E:274:ILE:HG23	2.00	0.44
1:G:307:LYS:C	1:G:309:SER:H	2.24	0.44
1:A:281:VAL:HG22	1:A:302:ILE:HD12	2.00	0.44
1:B:138:TYR:HB2	1:B:156:ILE:HD11	1.99	0.44
1:E:264:ILE:HG23	1:E:274:ILE:HD11	1.99	0.44
1:G:107:ILE:HG12	1:G:114:ILE:HG22	1.99	0.44
1:I:305:VAL:C	1:I:307:LYS:H	2.25	0.44
1:G:219:ILE:H	1:G:249:ASN:HB2	1.83	0.44
1:G:351:LEU:HD22	1:G:364:PHE:CZ	2.53	0.44
1:H:206:LEU:HD11	1:H:241:ALA:HB3	2.00	0.44
1:A:59:LYS:HD2	1:A:123:ASP:O	2.17	0.44
1:A:130:ASN:HD21	1:A:135:ASP:CG	2.26	0.44
1:B:149:THR:HG22	1:B:260:MET:HE3	1.99	0.44
1:E:213:ILE:HG22	1:E:214:GLN:N	2.33	0.43
1:E:117:ASN:HD22	1:E:224:SER:C	2.25	0.43
1:E:126:THR:HG23	1:E:139:LYS:HD2	1.99	0.43
1:E:328:LYS:HD3	1:E:339:TYR:CG	2.53	0.43
1:E:384:LEU:HB3	1:E:386:LEU:HD13	2.00	0.43
1:G:185:PHE:CE1	1:G:221:PRO:HD2	2.54	0.43
1:K:308:GLY:HA3	1:K:374:LYS:C	2.43	0.43
1:A:302:ILE:HD11	1:A:322:VAL:HG23	2.00	0.43
1:F:396:ARG:HD3	1:F:460:TYR:CE2	2.54	0.43
1:B:332:SER:HB2	1:B:333:PRO:HD2	1.99	0.43
1:C:380:LEU:HB2	1:C:449:VAL:HG21	2.00	0.43
1:E:281:VAL:CG2	1:E:302:ILE:HD12	2.45	0.43
1:G:245:ARG:HG3	1:I:246:GLY:HA3	2.00	0.43
1:L:394:LYS:HA	1:L:395:ASP:HA	1.82	0.43
1:H:206:LEU:CD1	1:H:241:ALA:HB3	2.48	0.43
1:C:446:LEU:O	1:C:449:VAL:HG22	2.18	0.43
1:E:241:ALA:C	1:E:242:ILE:HD12	2.44	0.43
1:G:146:ASP:CG	1:G:276:ARG:HH12	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:HB2	1:A:333:PRO:HD2	2.01	0.43
1:B:386:LEU:HD11	1:B:408:VAL:HG13	2.00	0.43
1:E:278:PHE:HA	1:E:340:ILE:HG21	2.00	0.43
1:G:469:VAL:HG13	1:G:469:VAL:O	2.19	0.43
1:C:281:VAL:HA	1:C:306:GLN:H	1.83	0.43
1:G:307:LYS:CB	1:G:374:LYS:HA	2.49	0.43
1:L:117:ASN:HD22	1:L:119:HIS:CE1	2.37	0.43
1:G:330:ILE:HD13	1:G:336:LEU:HB2	2.01	0.42
1:I:314:ALA:HB3	1:I:364:PHE:CE1	2.54	0.42
1:F:173:MET:HA	1:F:199:LEU:HD11	2.01	0.42
1:J:181:LEU:HD11	1:J:229:VAL:HG22	2.01	0.42
1:F:345:ILE:CD1	1:J:394:LYS:HE2	2.50	0.42
1:G:87:PHE:HA	1:G:88:PRO:HD3	1.92	0.42
1:J:446:LEU:O	1:J:449:VAL:HG22	2.19	0.42
1:K:400:PRO:HA	1:K:403:VAL:CG1	2.50	0.42
1:B:408:VAL:HG21	1:B:422:PHE:CZ	2.55	0.42
1:F:264:ILE:HG23	1:F:274:ILE:CD1	2.50	0.42
1:F:327:ASN:HD21	1:F:328:LYS:HE3	1.84	0.42
1:I:322:VAL:HG11	1:I:351:LEU:HD11	2.00	0.42
1:K:127:ILE:O	1:K:140:ALA:HB3	2.19	0.42
1:B:385:SER:O	1:B:386:LEU:HD12	2.18	0.42
1:E:422:PHE:CD1	1:E:459:VAL:HG11	2.54	0.42
1:H:320:ASP:CG	1:H:355:ARG:HG2	2.44	0.42
1:L:464:PHE:CG	1:L:465:ALA:N	2.87	0.42
1:K:281:VAL:HA	1:K:306:GLN:H	1.85	0.42
1:H:386:LEU:HD11	1:H:408:VAL:HG13	2.02	0.42
1:B:432:GLY:C	1:B:434:SER:H	2.28	0.42
1:F:335:ASP:HB3	1:F:339:TYR:CE2	2.55	0.42
1:G:294:TYR:CE2	1:G:416:LYS:HE3	2.54	0.42
1:B:219:ILE:HG23	1:B:223:ASN:CB	2.50	0.42
1:D:66:ARG:HG3	1:D:67:PRO:HD2	2.01	0.42
1:H:219:ILE:HG23	1:H:223:ASN:HB2	2.02	0.42
1:H:264:ILE:HG23	1:H:274:ILE:CD1	2.50	0.42
1:J:303:THR:HB	1:J:451:LYS:HG2	2.02	0.42
1:B:102:LEU:C	1:B:102:LEU:HD12	2.45	0.41
1:F:74:PHE:C	1:F:76:ASP:H	2.28	0.41
1:I:44:SER:O	1:I:48:ALA:HB2	2.20	0.41
1:D:42:HIS:ND1	1:D:46:LYS:HE3	2.35	0.41
1:K:180:ALA:CB	1:K:219:ILE:HD11	2.51	0.41
1:L:237:GLY:C	1:L:238:ILE:HD12	2.45	0.41
1:A:149:THR:HG23	1:A:276:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:276:ARG:NH1	1:J:341:GLY:O	2.53	0.41
1:A:206:LEU:HD12	1:A:212:PHE:CZ	2.56	0.41
1:A:218:SER:HA	1:A:249:ASN:ND2	2.35	0.41
1:E:283:ILE:HD12	1:E:302:ILE:HD13	2.02	0.41
1:L:76:ASP:N	1:L:77:PRO:CD	2.83	0.41
1:A:348:LYS:HE2	1:A:363:SER:OG	2.20	0.41
1:B:318:ARG:HD3	1:B:377:GLN:HB2	2.03	0.41
1:D:319:GLY:H	1:D:450:ASN:ND2	2.17	0.41
1:E:79:PHE:HB2	1:E:82:PHE:CD1	2.56	0.41
1:F:185:PHE:CD1	1:F:220:ASN:HB3	2.55	0.41
1:K:87:PHE:HA	1:K:88:PRO:HD3	1.87	0.41
1:D:218:SER:C	1:D:219:ILE:HG12	2.45	0.41
1:F:392:ARG:HA	1:F:392:ARG:NH1	2.36	0.41
1:J:303:THR:CG2	1:J:451:LYS:HG2	2.51	0.41
1:B:318:ARG:CD	1:B:377:GLN:HG3	2.50	0.41
1:B:399:ILE:HA	1:B:400:PRO:HD3	1.87	0.41
1:B:179:PHE:CE1	1:B:231:SER:HA	2.56	0.41
1:D:166:PHE:HB2	1:D:262:LYS:HE2	2.03	0.41
1:G:328:LYS:HB3	1:G:339:TYR:CE2	2.56	0.41
1:H:177:VAL:HG23	1:H:231:SER:HB3	2.03	0.41
1:I:393:LEU:HG	1:I:394:LYS:H	1.85	0.41
1:J:140:ALA:HB1	1:J:154:ILE:HG22	2.03	0.41
1:K:97:GLU:HG2	1:K:102:LEU:H	1.86	0.41
1:D:308:GLY:HA2	1:D:312:ASP:HB3	2.02	0.41
1:E:90:ARG:O	1:E:91:LYS:C	2.64	0.41
1:F:87:PHE:HA	1:F:88:PRO:HD3	1.88	0.41
1:H:417:GLY:C	1:H:422:PHE:HB3	2.46	0.41
1:H:457:VAL:HG22	1:H:470:LEU:HD13	2.02	0.41
1:J:156:ILE:HG23	1:J:161:LEU:HD13	2.03	0.41
1:L:324:LYS:HD2	1:L:329:VAL:HG22	2.02	0.41
1:D:117:ASN:HD22	1:D:119:HIS:CE1	2.39	0.40
1:D:185:PHE:CD1	1:D:220:ASN:HB3	2.56	0.40
1:E:180:ALA:HB1	1:E:219:ILE:CG1	2.52	0.40
1:G:307:LYS:HB3	1:G:375:GLY:H	1.86	0.40
1:J:142:LEU:HD21	1:J:145:LYS:HD3	2.02	0.40
1:K:317:LYS:H	1:K:320:ASP:CG	2.30	0.40
1:B:182:GLY:HA3	1:B:223:ASN:HD22	1.86	0.40
1:I:49:LYS:HB3	1:I:189:PHE:CE2	2.56	0.40
1:J:394:LYS:HE3	1:J:395:ASP:OD1	2.22	0.40
1:L:185:PHE:CE1	1:L:220:ASN:HB3	2.56	0.40
1:A:48:ALA:HB1	1:A:181:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:335:ASP:HB3	1:H:339:TYR:CE2	2.56	0.40
1:J:180:ALA:HB1	1:J:219:ILE:HD11	2.04	0.40
1:K:96:LYS:HE3	1:K:102:LEU:HB3	2.03	0.40
1:E:389:LEU:HD23	1:E:389:LEU:H	1.87	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 PDB entries followed by that with respect to all EM entries.

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	432/434 (100%)	356 (82%)	63 (15%)	13 (3%)	3	22
1	B	432/434 (100%)	364 (84%)	56 (13%)	12 (3%)	4	24
1	C	432/434 (100%)	353 (82%)	64 (15%)	15 (4%)	3	20
1	D	432/434 (100%)	351 (81%)	70 (16%)	11 (2%)	4	25
1	E	432/434 (100%)	351 (81%)	65 (15%)	16 (4%)	2	19
1	F	432/434 (100%)	366 (85%)	55 (13%)	11 (2%)	4	25
1	G	432/434 (100%)	367 (85%)	58 (13%)	7 (2%)	7	37
1	H	432/434 (100%)	348 (81%)	67 (16%)	17 (4%)	2	18
1	I	432/434 (100%)	361 (84%)	59 (14%)	12 (3%)	4	24
1	J	432/434 (100%)	350 (81%)	65 (15%)	17 (4%)	2	18
1	K	432/434 (100%)	356 (82%)	64 (15%)	12 (3%)	4	24
1	L	432/434 (100%)	356 (82%)	68 (16%)	8 (2%)	6	31
All	All	5184/5208 (100%)	4279 (82%)	754 (14%)	151 (3%)	5	23

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	LYS
1	B	373	PRO
1	B	396	ARG
1	C	200	ASN
1	C	307	LYS
1	C	356	ASP
1	C	433	GLN
1	D	200	ASN
1	D	309	SER
1	D	356	ASP
1	D	379	ASP
1	E	356	ASP
1	F	57	THR
1	F	307	LYS
1	F	356	ASP
1	H	356	ASP
1	I	57	THR
1	I	125	ASP
1	I	309	SER
1	J	374	LYS
1	K	224	SER
1	K	307	LYS
1	K	374	LYS
1	L	78	TYR
1	L	307	LYS
1	A	127	ILE
1	A	307	LYS
1	A	326	ASN
1	A	462	ASN
1	B	125	ASP
1	C	368	GLY
1	D	58	SER
1	E	127	ILE
1	E	231	SER
1	E	280	GLY
1	E	308	GLY
1	E	378	SER
1	E	382	ASP
1	G	309	SER
1	G	462	ASN
1	H	200	ASN
1	H	379	ASP
1	I	90	ARG

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Mol	Chain	Res	Type
1	I	307	LYS
1	I	308	GLY
1	I	356	ASP
1	I	380	LEU
1	I	396	ARG
1	J	58	SER
1	J	78	TYR
1	J	124	ALA
1	J	125	ASP
1	J	307	LYS
1	J	373	PRO
1	K	78	TYR
1	K	373	PRO
1	K	379	ASP
1	K	396	ARG
1	L	125	ASP
1	L	224	SER
1	L	231	SER
1	L	356	ASP
1	A	78	TYR
1	A	125	ASP
1	A	281	VAL
1	A	356	ASP
1	A	463	GLY
1	B	224	SER
1	B	296	ASN
1	B	463	GLY
1	C	125	ASP
1	C	463	GLY
1	D	71	ASP
1	D	396	ARG
1	E	86	ASP
1	E	171	ASP
1	E	309	SER
1	E	374	LYS
1	F	309	SER
1	F	326	ASN
1	F	371	GLU
1	G	75	ASN
1	G	78	TYR
1	G	307	LYS
1	G	379	ASP

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Mol	Chain	Res	Type
1	H	71	ASP
1	H	95	ASP
1	H	125	ASP
1	H	157	GLU
1	H	246	GLY
1	H	374	LYS
1	J	309	SER
1	J	396	ARG
1	A	57	THR
1	A	357	GLY
1	A	380	LEU
1	B	97	GLU
1	B	309	SER
1	B	356	ASP
1	C	69	PRO
1	C	335	ASP
1	C	374	LYS
1	E	110	LYS
1	E	368	GLY
1	F	91	LYS
1	F	396	ARG
1	H	75	ASN
1	H	307	LYS
1	I	92	GLY
1	J	86	ASP
1	J	208	GLN
1	J	357	GLY
1	K	86	ASP
1	K	356	ASP
1	K	433	GLN
1	A	374	LYS
1	B	218	SER
1	C	75	ASN
1	C	160	ASN
1	C	396	ARG
1	E	396	ARG
1	F	42	HIS
1	H	294	TYR
1	I	71	ASP
1	K	377	GLN
1	B	208	GLN
1	D	374	LYS

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Mol	Chain	Res	Type
1	H	337	LYS
1	I	463	GLY
1	J	95	ASP
1	J	96	LYS
1	J	134	SER
1	L	373	PRO
1	H	76	ASP
1	H	341	GLY
1	H	463	GLY
1	J	92	GLY
1	K	403	VAL
1	C	127	ILE
1	C	252	ILE
1	D	127	ILE
1	E	246	GLY
1	F	251	GLY
1	J	88	PRO
1	D	204	ILE
1	D	252	ILE
1	E	76	ASP
1	G	88	PRO
1	H	92	GLY
1	F	88	PRO
1	L	69	PRO

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 PDB entries followed by that with respect to all EM entries.

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	369/369 (100%)	330 (89%)	39 (11%)	6	21
1	B	369/369 (100%)	351 (95%)	18 (5%)	22	43
1	C	369/369 (100%)	339 (92%)	30 (8%)	11	30
1	D	369/369 (100%)	342 (93%)	27 (7%)	13	33
1	E	369/369 (100%)	345 (94%)	24 (6%)	15	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	369/369 (100%)	346 (94%)	23 (6%)	16	37
1	G	369/369 (100%)	342 (93%)	27 (7%)	13	33
1	H	369/369 (100%)	343 (93%)	26 (7%)	14	35
1	I	369/369 (100%)	347 (94%)	22 (6%)	17	38
1	J	369/369 (100%)	335 (91%)	34 (9%)	8	26
1	K	369/369 (100%)	341 (92%)	28 (8%)	12	32
1	L	369/369 (100%)	339 (92%)	30 (8%)	11	30
All	All	4428/4428 (100%)	4100 (93%)	328 (7%)	15	33

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	56	SER
1	A	57	THR
1	A	60	THR
1	A	74	PHE
1	A	83	PHE
1	A	96	LYS
1	A	97	GLU
1	A	114	ILE
1	A	117	ASN
1	A	126	THR
1	A	135	ASP
1	A	137	GLU
1	A	177	VAL
1	A	197	SER
1	A	204	ILE
1	A	214	GLN
1	A	224	SER
1	A	242	ILE
1	A	245	ARG
1	A	252	ILE
1	A	261	VAL
1	A	264	ILE
1	A	276	ARG
1	A	290	THR
1	A	295	LYS
1	A	317	LYS
1	A	335	ASP

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Mol	Chain	Res	Type
1	A	340	ILE
1	A	364	PHE
1	A	366	LEU
1	A	376	VAL
1	A	392	ARG
1	A	397	LEU
1	A	431	VAL
1	A	442	LEU
1	A	444	GLN
1	A	467	LEU
1	A	469	VAL
1	B	47	ASP
1	B	56	SER
1	B	57	THR
1	B	60	THR
1	B	83	PHE
1	B	97	GLU
1	B	102	LEU
1	B	149	THR
1	B	178	VAL
1	B	187	VAL
1	B	230	ASP
1	B	252	ILE
1	B	287	GLN
1	B	317	LYS
1	B	320	ASP
1	B	380	LEU
1	B	392	ARG
1	B	395	ASP
1	C	53	VAL
1	C	57	THR
1	C	83	PHE
1	C	84	ASP
1	C	85	PHE
1	C	98	VAL
1	C	99	VAL
1	C	101	SER
1	C	102	LEU
1	C	111	ASP
1	C	135	ASP
1	C	170	ASP
1	C	218	SER

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Mol	Chain	Res	Type
1	C	219	ILE
1	C	238	ILE
1	C	245	ARG
1	C	252	ILE
1	C	261	VAL
1	C	276	ARG
1	C	281	VAL
1	C	289	ASP
1	C	313	GLU
1	C	317	LYS
1	C	325	VAL
1	C	340	ILE
1	C	363	SER
1	C	373	PRO
1	C	377	GLN
1	C	392	ARG
1	C	397	LEU
1	D	53	VAL
1	D	57	THR
1	D	68	SER
1	D	81	GLN
1	D	83	PHE
1	D	97	GLU
1	D	114	ILE
1	D	121	VAL
1	D	122	ASP
1	D	123	ASP
1	D	157	GLU
1	D	174	GLU
1	D	214	GLN
1	D	229	VAL
1	D	243	LEU
1	D	274	ILE
1	D	276	ARG
1	D	295	LYS
1	D	317	LYS
1	D	340	ILE
1	D	351	LEU
1	D	358	GLU
1	D	373	PRO
1	D	377	GLN
1	D	453	GLU

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Mol	Chain	Res	Type
1	D	467	LEU
1	D	471	LYS
1	E	90	ARG
1	E	106	VAL
1	E	107	ILE
1	E	110	LYS
1	E	137	GLU
1	E	156	ILE
1	E	167	THR
1	E	197	SER
1	E	203	ASN
1	E	219	ILE
1	E	238	ILE
1	E	252	ILE
1	E	256	ILE
1	E	261	VAL
1	E	276	ARG
1	E	305	VAL
1	E	317	LYS
1	E	325	VAL
1	E	331	LYS
1	E	340	ILE
1	E	353	TYR
1	E	364	PHE
1	E	466	THR
1	E	467	LEU
1	F	60	THR
1	F	80	LYS
1	F	85	PHE
1	F	99	VAL
1	F	107	ILE
1	F	111	ASP
1	F	122	ASP
1	F	137	GLU
1	F	167	THR
1	F	197	SER
1	F	252	ILE
1	F	261	VAL
1	F	267	LYS
1	F	303	THR
1	F	313	GLU
1	F	317	LYS

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Mol	Chain	Res	Type
1	F	332	SER
1	F	340	ILE
1	F	358	GLU
1	F	364	PHE
1	F	371	GLU
1	F	377	GLN
1	F	392	ARG
1	G	55	ILE
1	G	57	THR
1	G	97	GLU
1	G	99	VAL
1	G	107	ILE
1	G	118	ASN
1	G	119	HIS
1	G	156	ILE
1	G	177	VAL
1	G	197	SER
1	G	204	ILE
1	G	229	VAL
1	G	238	ILE
1	G	245	ARG
1	G	252	ILE
1	G	313	GLU
1	G	317	LYS
1	G	320	ASP
1	G	332	SER
1	G	334	ILE
1	G	340	ILE
1	G	358	GLU
1	G	373	PRO
1	G	374	LYS
1	G	384	LEU
1	G	392	ARG
1	G	427	ILE
1	H	55	ILE
1	H	60	THR
1	H	96	LYS
1	H	99	VAL
1	H	118	ASN
1	H	135	ASP
1	H	165	THR
1	H	192	THR

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Mol	Chain	Res	Type
1	H	197	SER
1	H	214	GLN
1	H	215	THR
1	H	261	VAL
1	H	287	GLN
1	H	295	LYS
1	H	313	GLU
1	H	317	LYS
1	H	320	ASP
1	H	332	SER
1	H	351	LEU
1	H	377	GLN
1	H	382	ASP
1	H	392	ARG
1	H	397	LEU
1	H	459	VAL
1	H	461	ARG
1	H	469	VAL
1	I	53	VAL
1	I	58	SER
1	I	66	ARG
1	I	70	LEU
1	I	83	PHE
1	I	90	ARG
1	I	114	ILE
1	I	117	ASN
1	I	127	ILE
1	I	224	SER
1	I	242	ILE
1	I	303	THR
1	I	313	GLU
1	I	317	LYS
1	I	320	ASP
1	I	335	ASP
1	I	351	LEU
1	I	358	GLU
1	I	377	GLN
1	I	413	GLU
1	I	428	ILE
1	I	444	GLN
1	J	38	VAL
1	J	43	ASP

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Mol	Chain	Res	Type
1	J	55	ILE
1	J	71	ASP
1	J	83	PHE
1	J	96	LYS
1	J	97	GLU
1	J	102	LEU
1	J	111	ASP
1	J	118	ASN
1	J	119	HIS
1	J	131	LEU
1	J	135	ASP
1	J	177	VAL
1	J	193	SER
1	J	214	GLN
1	J	224	SER
1	J	238	ILE
1	J	242	ILE
1	J	252	ILE
1	J	261	VAL
1	J	276	ARG
1	J	281	VAL
1	J	295	LYS
1	J	313	GLU
1	J	317	LYS
1	J	332	SER
1	J	340	ILE
1	J	360	LYS
1	J	377	GLN
1	J	397	LEU
1	J	444	GLN
1	J	467	LEU
1	J	469	VAL
1	K	39	LEU
1	K	57	THR
1	K	84	ASP
1	K	97	GLU
1	K	99	VAL
1	K	101	SER
1	K	102	LEU
1	K	149	THR
1	K	157	GLU
1	K	177	VAL

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Mol	Chain	Res	Type
1	K	197	SER
1	K	203	ASN
1	K	214	GLN
1	K	252	ILE
1	K	281	VAL
1	K	290	THR
1	K	313	GLU
1	K	317	LYS
1	K	332	SER
1	K	335	ASP
1	K	340	ILE
1	K	351	LEU
1	K	364	PHE
1	K	366	LEU
1	K	380	LEU
1	K	392	ARG
1	K	397	LEU
1	K	434	SER
1	L	49	LYS
1	L	57	THR
1	L	58	SER
1	L	66	ARG
1	L	83	PHE
1	L	97	GLU
1	L	101	SER
1	L	102	LEU
1	L	167	THR
1	L	177	VAL
1	L	203	ASN
1	L	238	ILE
1	L	252	ILE
1	L	261	VAL
1	L	282	THR
1	L	317	LYS
1	L	320	ASP
1	L	322	VAL
1	L	325	VAL
1	L	340	ILE
1	L	351	LEU
1	L	358	GLU
1	L	366	LEU
1	L	389	LEU

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Mol	Chain	Res	Type
1	L	395	ASP
1	L	403	VAL
1	L	409	ASP
1	L	414	LYS
1	L	459	VAL
1	L	464	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	117	ASN
1	A	119	HIS
1	A	130	ASN
1	A	208	GLN
1	A	211	ASN
1	A	249	ASN
1	A	419	ASN
1	A	448	GLN
1	B	118	ASN
1	B	183	ASN
1	B	450	ASN
1	C	81	GLN
1	C	117	ASN
1	C	119	HIS
1	C	200	ASN
1	C	203	ASN
1	C	296	ASN
1	C	419	ASN
1	C	423	GLN
1	C	450	ASN
1	D	117	ASN
1	D	119	HIS
1	D	404	ASN
1	D	419	ASN
1	D	450	ASN
1	E	117	ASN
1	E	119	HIS
1	E	159	ASN
1	E	208	GLN
1	E	287	GLN
1	E	296	ASN

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Mol	Chain	Res	Type
1	F	200	ASN
1	F	208	GLN
1	F	239	ASN
1	F	448	GLN
1	G	54	ASN
1	G	65	ASN
1	G	81	GLN
1	H	117	ASN
1	H	118	ASN
1	H	119	HIS
1	H	200	ASN
1	H	207	ASN
1	H	296	ASN
1	H	297	GLN
1	H	404	ASN
1	I	214	GLN
1	I	296	ASN
1	I	372	ASN
1	I	450	ASN
1	J	54	ASN
1	J	75	ASN
1	J	81	GLN
1	J	94	ASN
1	J	130	ASN
1	J	159	ASN
1	J	183	ASN
1	J	200	ASN
1	J	207	ASN
1	J	249	ASN
1	J	404	ASN
1	J	448	GLN
1	J	450	ASN
1	J	462	ASN
1	K	75	ASN
1	K	117	ASN
1	K	160	ASN
1	K	208	GLN
1	K	327	ASN
1	K	448	GLN
1	L	81	GLN
1	L	119	HIS
1	L	214	GLN

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Mol	Chain	Res	Type
1	L	220	ASN
1	L	419	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11003. These allow visual inspection of the internal detail of the map and identification of artifacts.

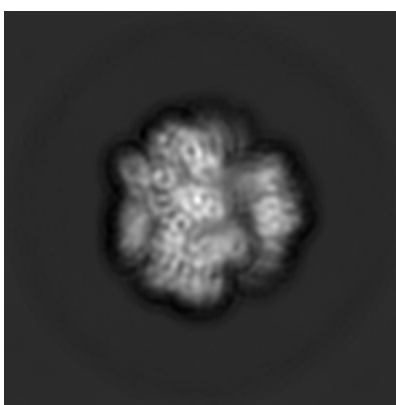
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

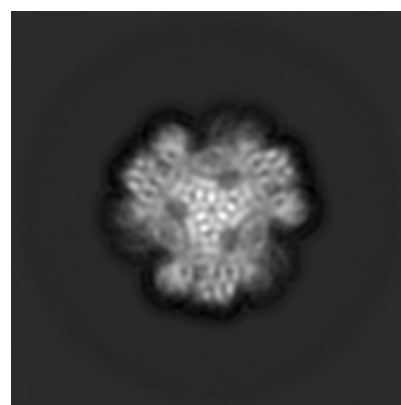
6.1.1 Primary map



X



Y

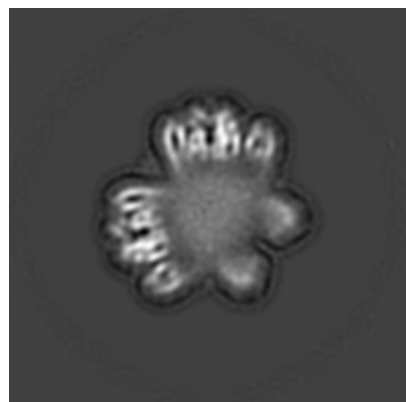


Z

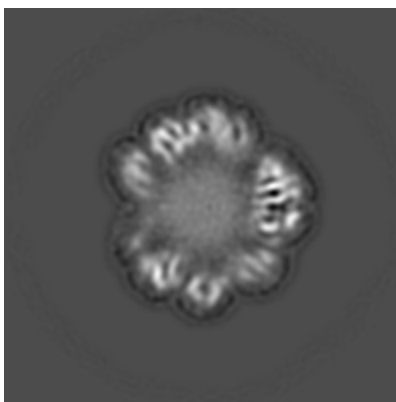
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

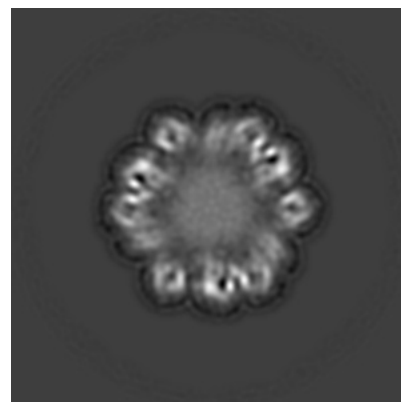
6.2.1 Primary map



X Index: 136



Y Index: 136

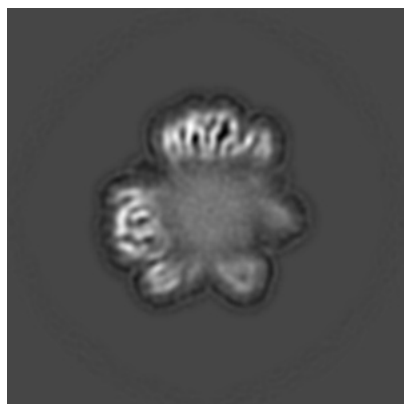


Z Index: 136

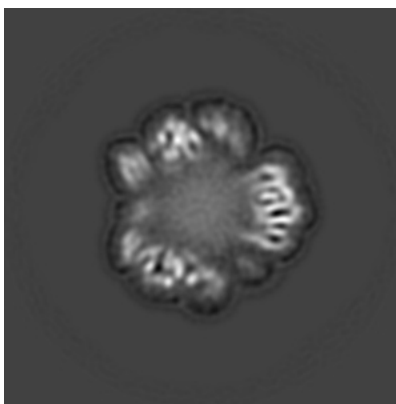
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

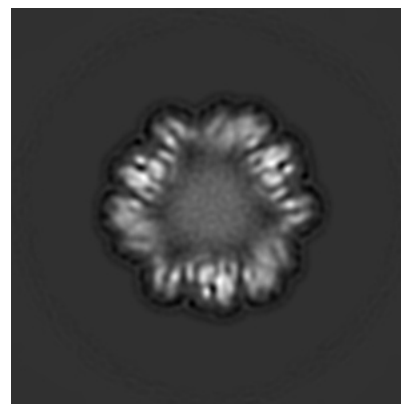
6.3.1 Primary map



X Index: 132



Y Index: 146

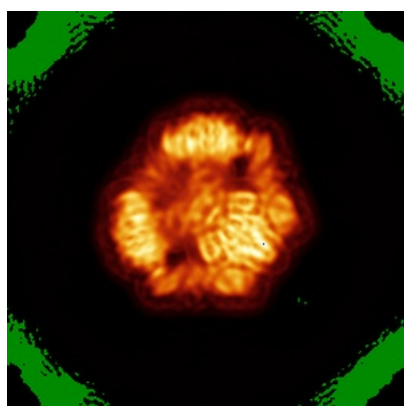


Z Index: 131

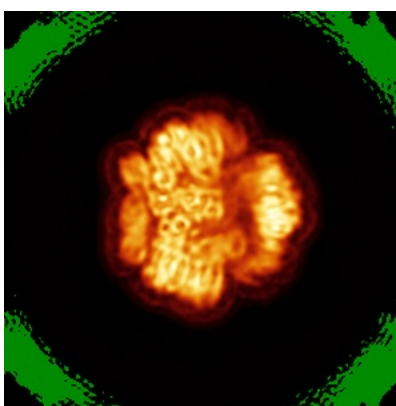
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

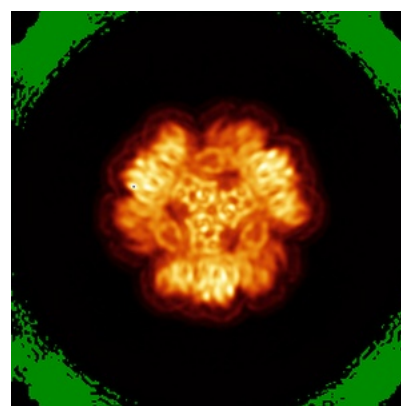
6.4.1 Primary map



X



Y

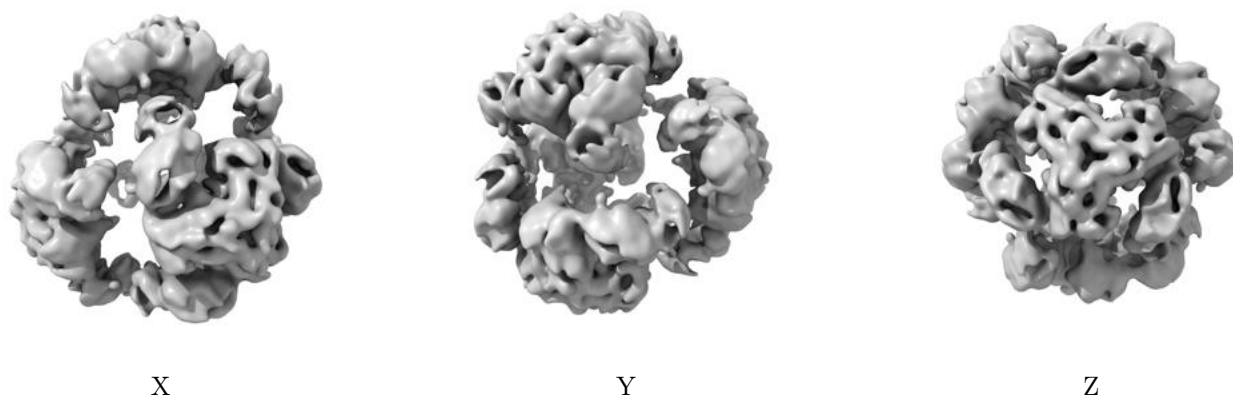


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

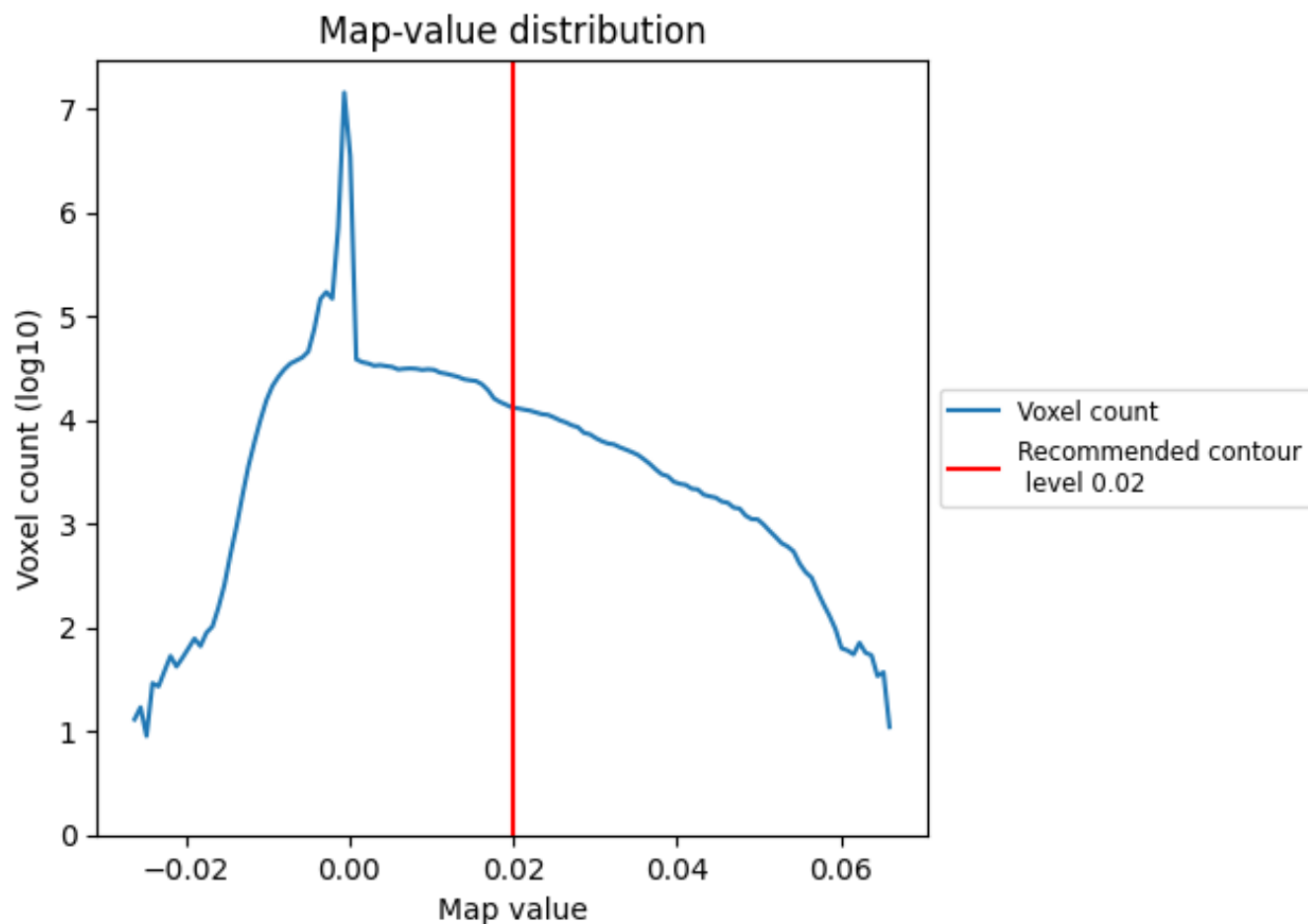
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

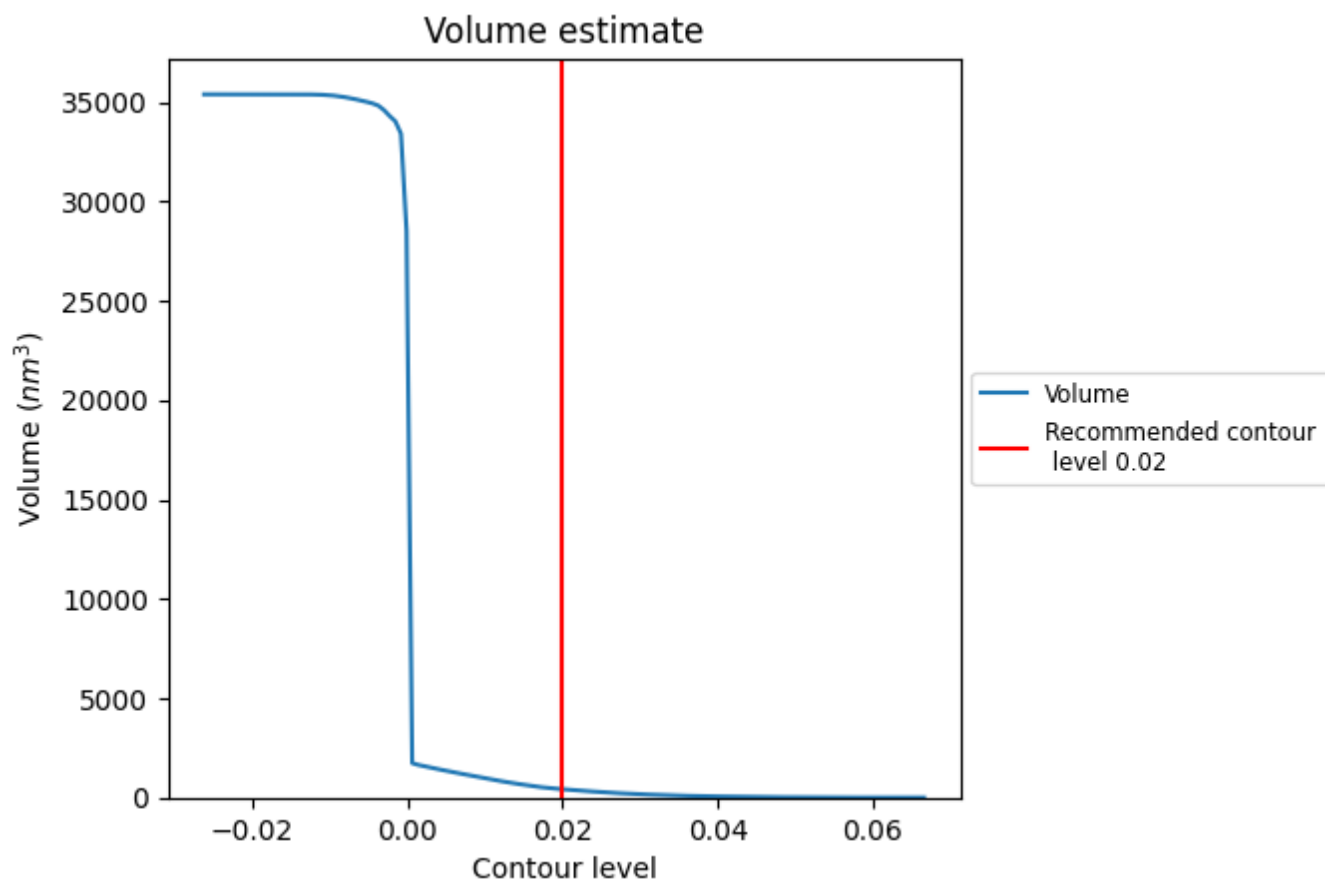
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

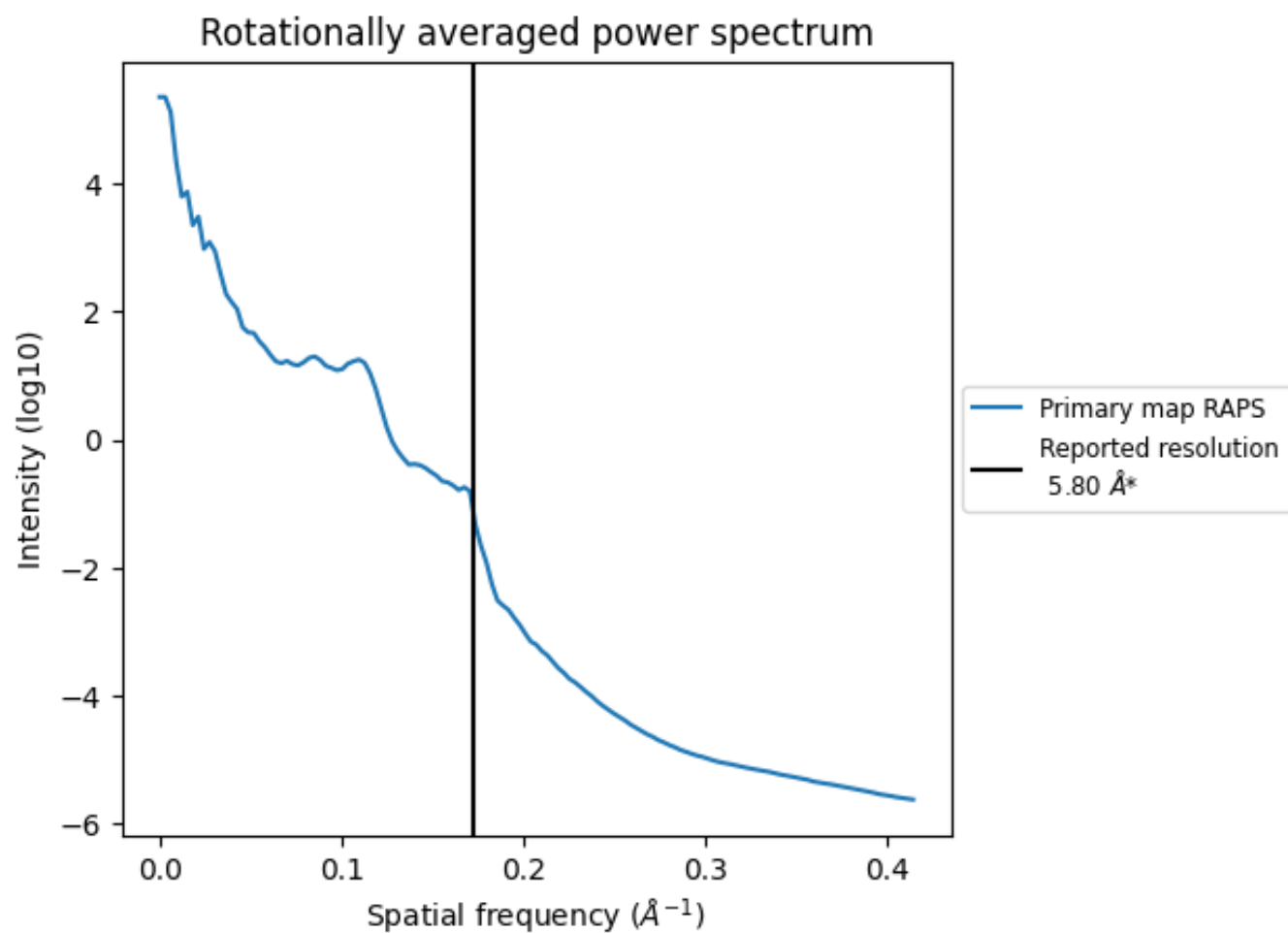
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 420 nm³; this corresponds to an approximate mass of 380 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.172 Å⁻¹

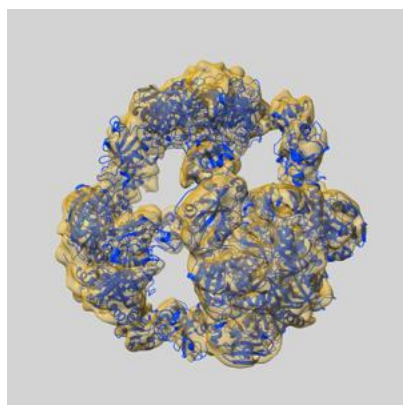
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

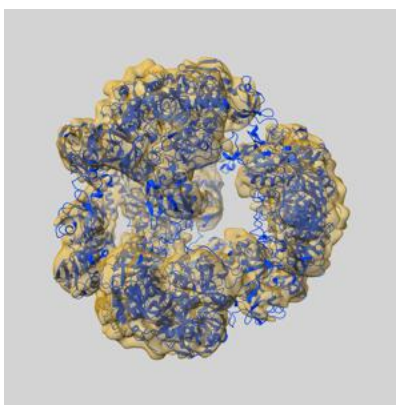
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11003 and PDB model 6Z05. Per-residue inclusion information can be found in section 3 on page 5.

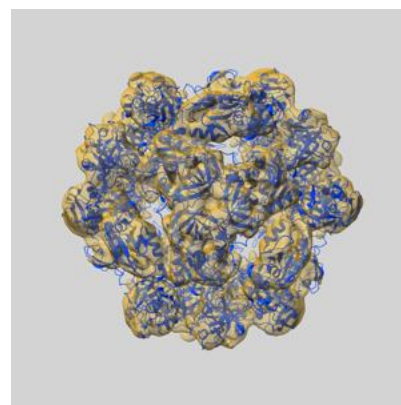
9.1 Map-model overlay [i](#)



X



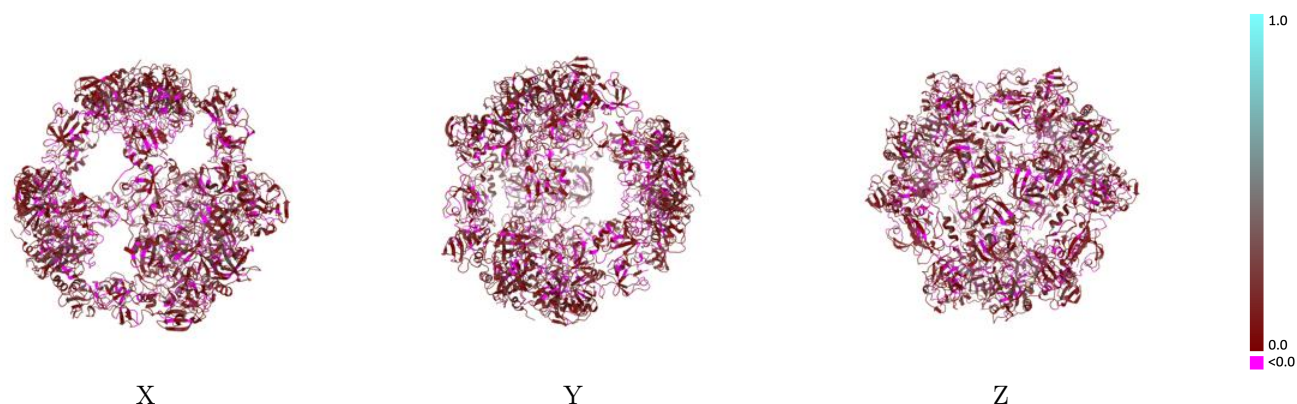
Y



Z

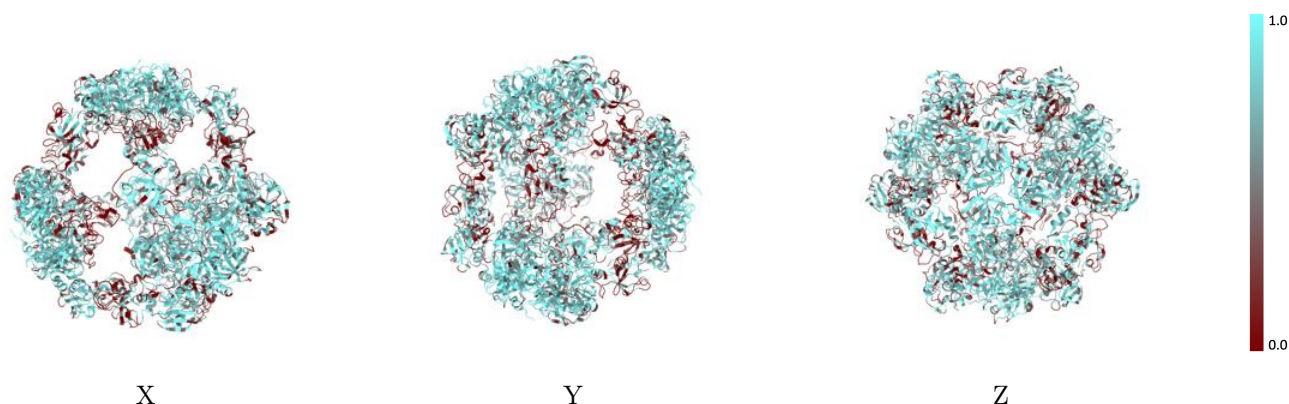
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



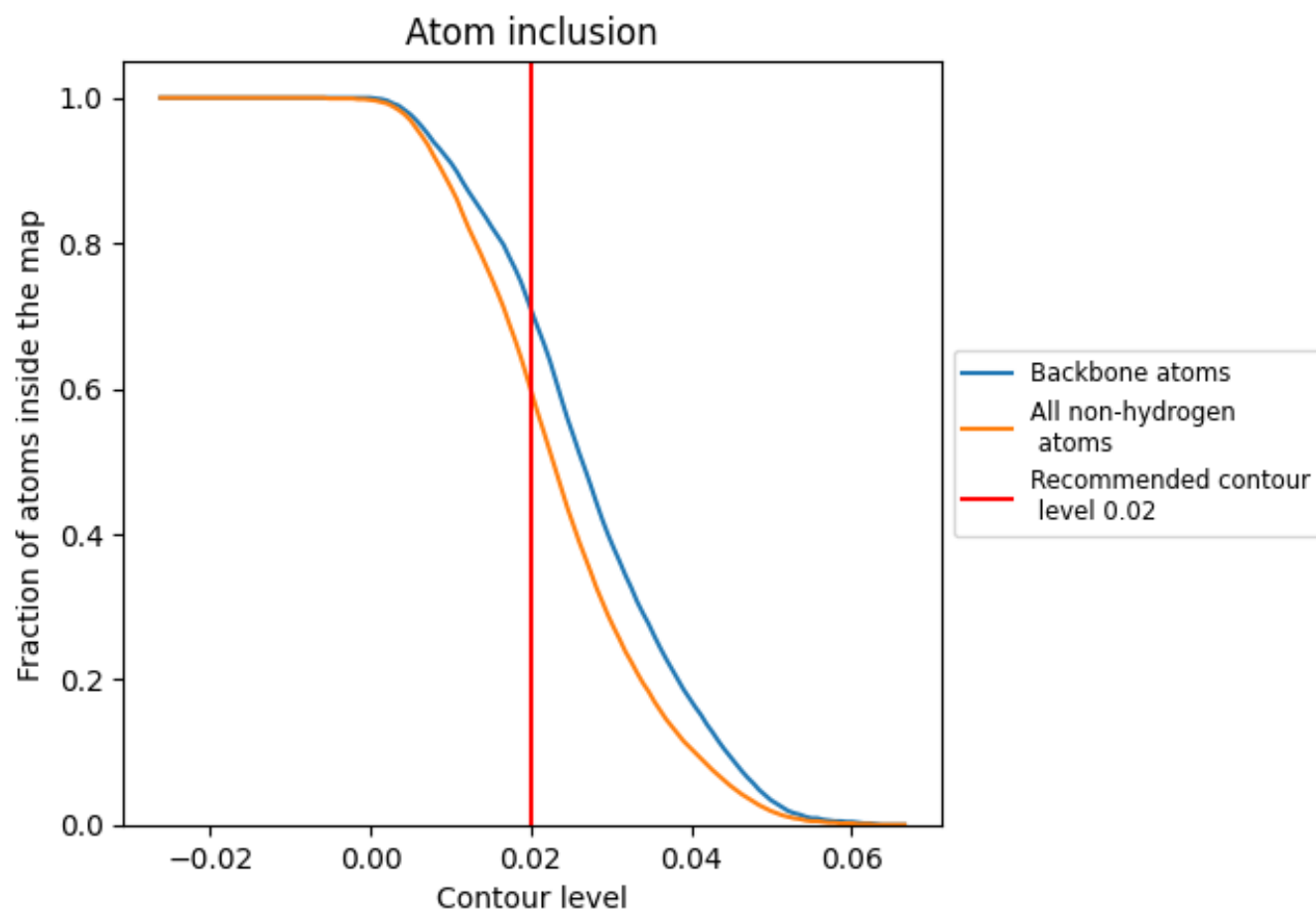
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.1100
A	0.5920	0.1090
B	0.6100	0.1130
C	0.5920	0.1100
D	0.6050	0.1090
E	0.6110	0.1120
F	0.5860	0.1030
G	0.6080	0.1110
H	0.5980	0.1090
I	0.5920	0.1130
J	0.6000	0.1100
K	0.5910	0.1080
L	0.5920	0.1080

