



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 07:23 AM UTC

PDB ID : 6WKK / pdb_00006wkk
EMDB ID : EMD-21695
Title : Phage G gp27 major capsid proteins and gp26 decoration proteins
Authors : Monroe, L.; Gonzalez, B.; Jiang, W.; Kihara, D.
Deposited on : 2020-04-16
Resolution : 6.10 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

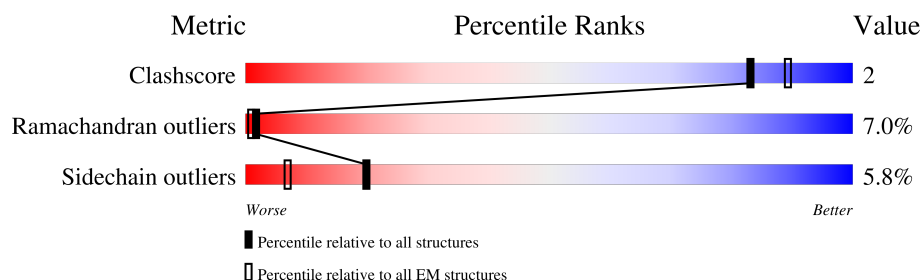
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.10 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.



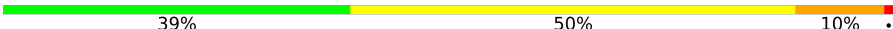
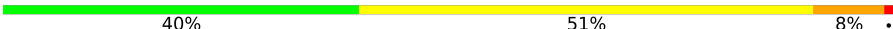
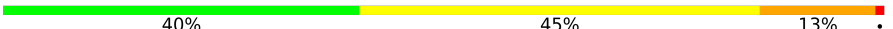
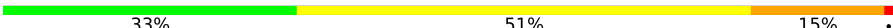
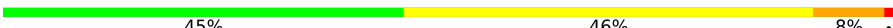
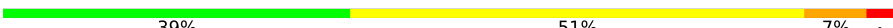
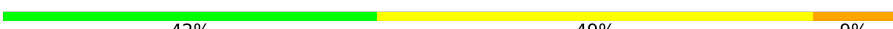
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	280	39% 51% 10% .
1	B	280	40% 52% 8%
1	C	280	40% 52% 6% .
1	D	280	37% 52% 9% .
1	E	280	42% 46% 10% .
1	F	280	44% 48% 7%
2	G	150	44% 47% 9% .
2	H	150	49% 39% 11% .
2	I	150	43% 45% 11% .

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Mol	Chain	Length	Quality of chain
2	J	150	 40% 51% 9%
2	K	150	 39% 50% 10%
2	L	150	 40% 51% 8%
2	M	150	 40% 45% 13%
2	N	150	 53% 40% 7%
2	O	150	 33% 51% 15%
2	P	150	 47% 45% 6%
2	Q	150	 47% 42% 11%
2	R	150	 45% 46% 8%
2	S	150	 48% 44% 7%
2	T	150	 39% 51% 7%
2	U	150	 42% 47% 11%
2	V	150	 39% 49% 11%
2	W	150	 56% 35% 9%
2	X	150	 42% 49% 9%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 33000 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 Gp27 major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	280	Total	C	N	O	S	0	0
			2182	1390	374	413	5		
1	B	280	Total	C	N	O	S	0	0
			2182	1390	374	413	5		
1	C	280	Total	C	N	O	S	0	0
			2182	1390	374	413	5		
1	D	280	Total	C	N	O	S	0	0
			2182	1390	374	413	5		
1	E	280	Total	C	N	O	S	0	0
			2182	1390	374	413	5		
1	F	280	Total	C	N	O	S	0	0
			2182	1390	374	413	5		

- Molecule 2 is a protein called Gp26 capsid decoration protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	H	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	I	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	J	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	K	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	L	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	M	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	N	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	O	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		

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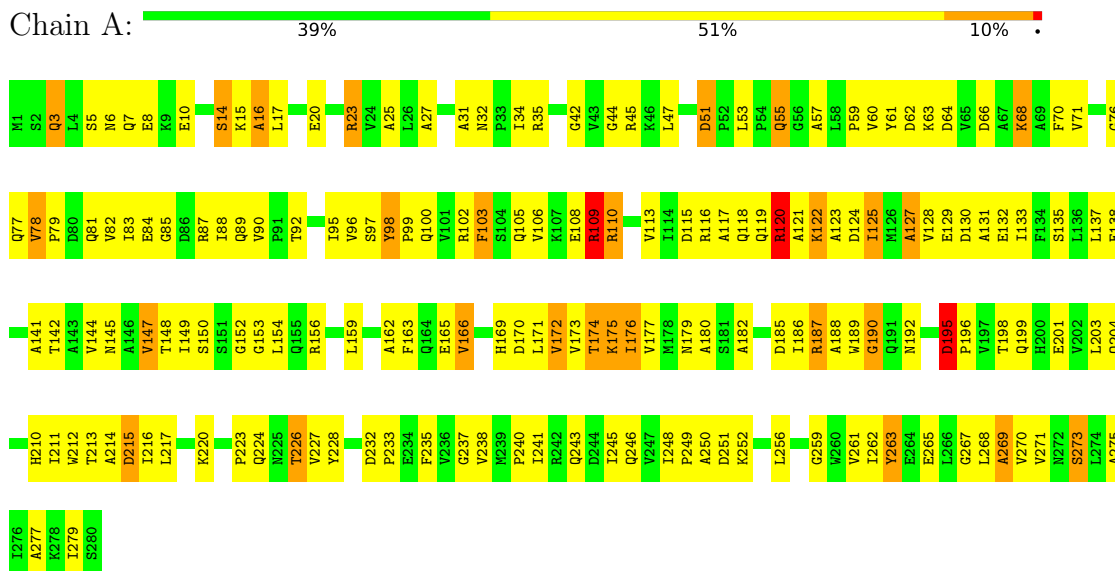
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	Q	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	R	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	S	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	T	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	U	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	V	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	W	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		
2	X	150	Total	C	N	O	S	0	0
			1106	696	186	219	5		

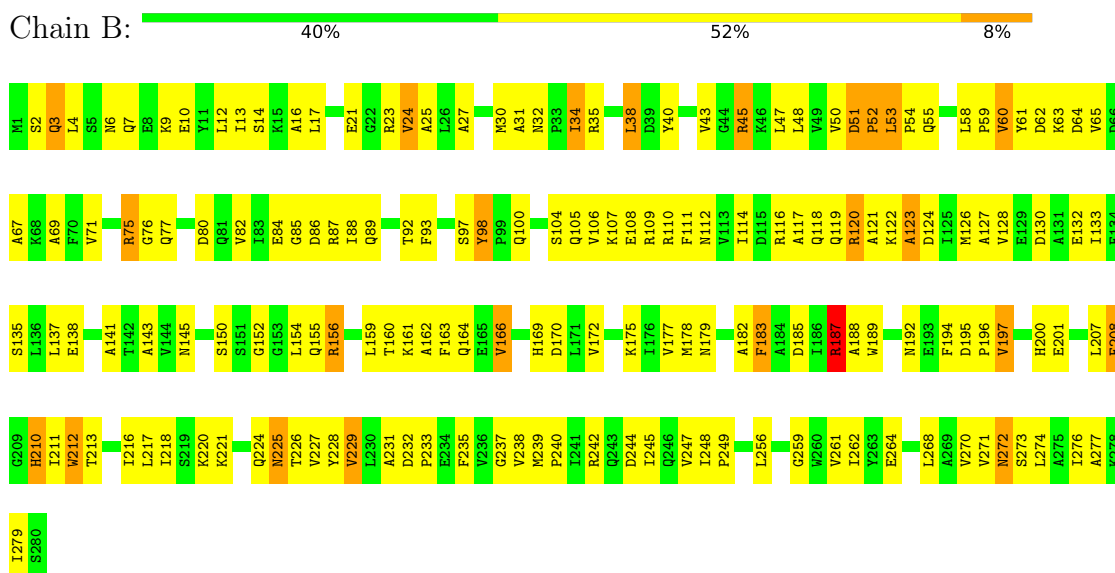
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Gp27 major capsid protein

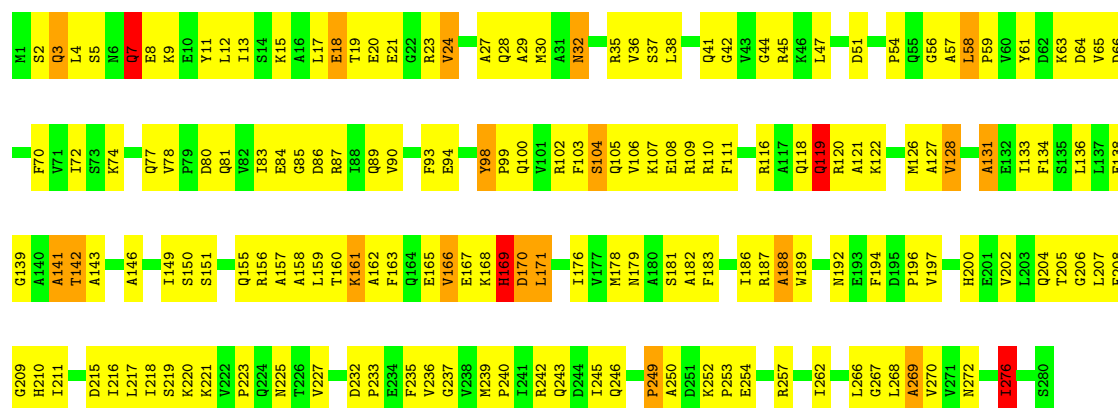


- Molecule 1: Gp27 major capsid protein



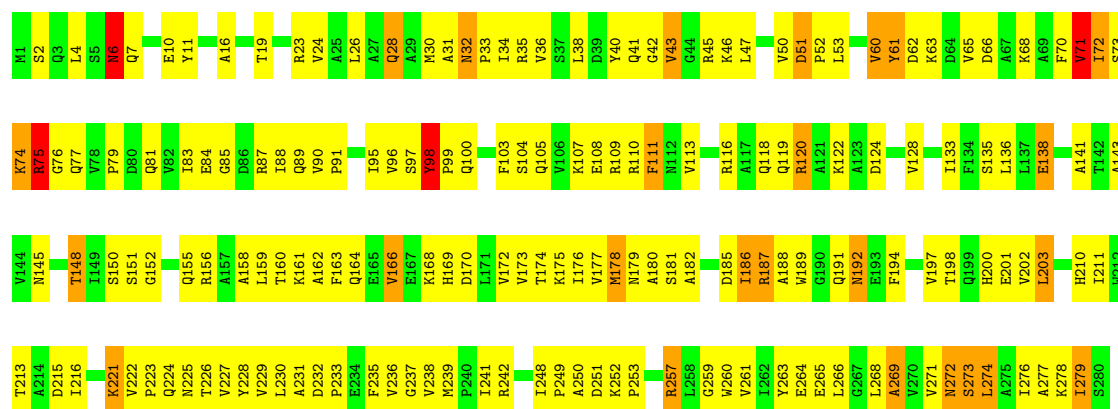
- Molecule 1: Gp27 major capsid protein

Chain C:  40% 52% 6% .



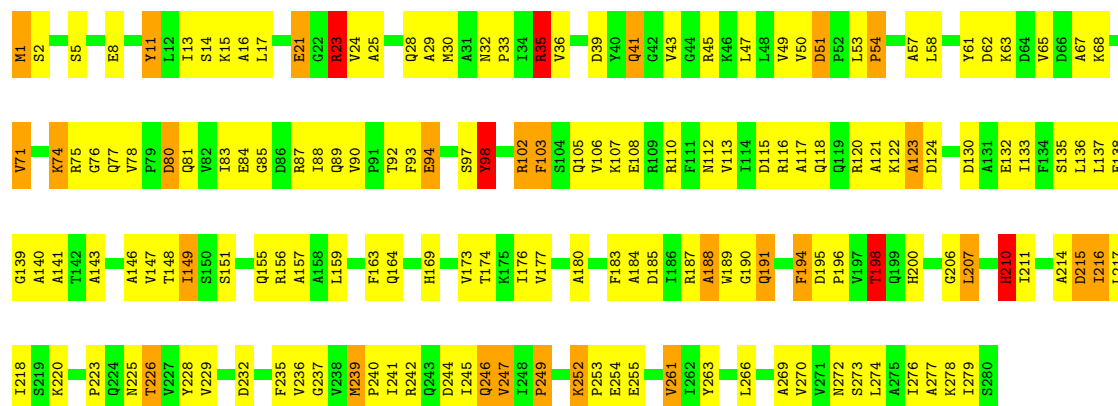
• Molecule 1: Gp27 major capsid protein

Chain D:  37% 52% 9% .

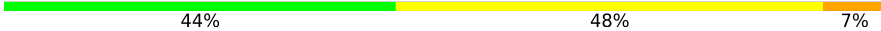


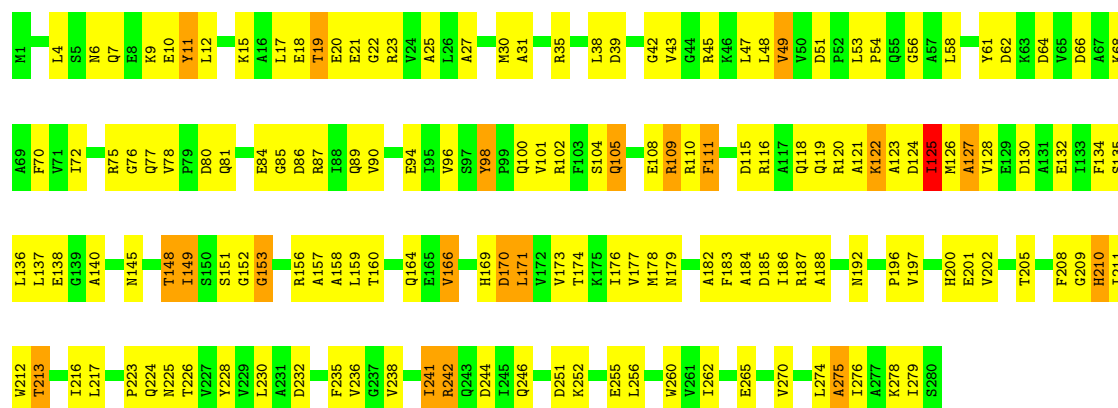
• Molecule 1: Gp27 major capsid protein

Chain E:  42% 46% 10% .

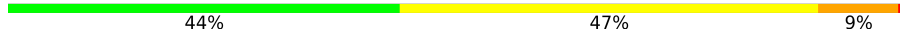


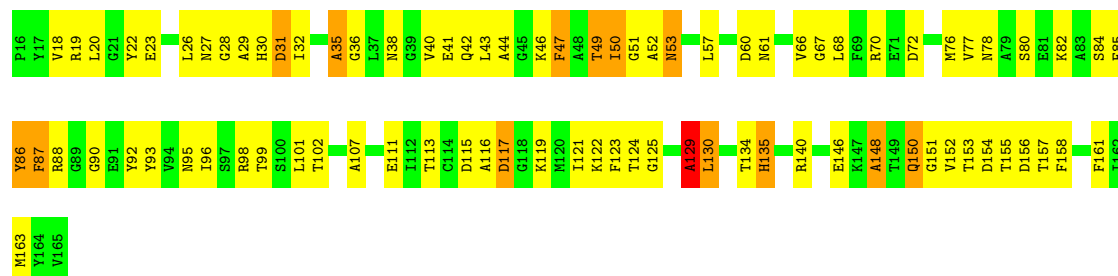
• Molecule 1: Gp27 major capsid protein

Chain F: 



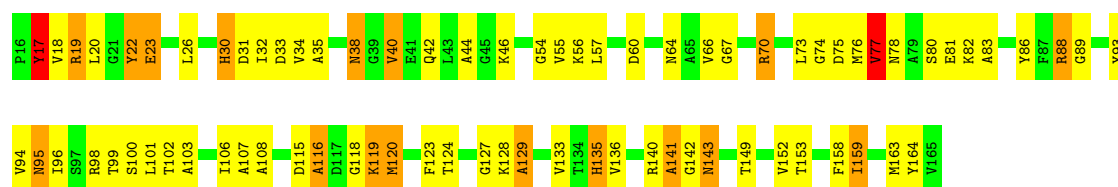
- Molecule 2: Gp26 capsid decoration protein

Chain G: 

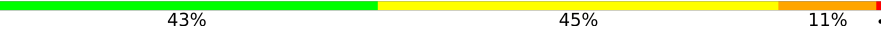


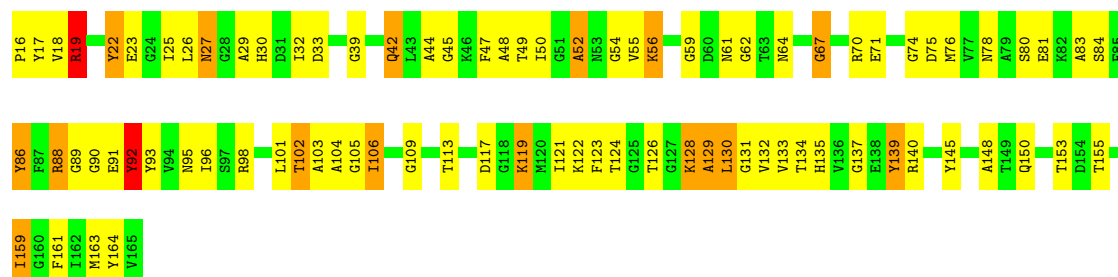
- Molecule 2: Gp26 capsid decoration protein

Chain H: 

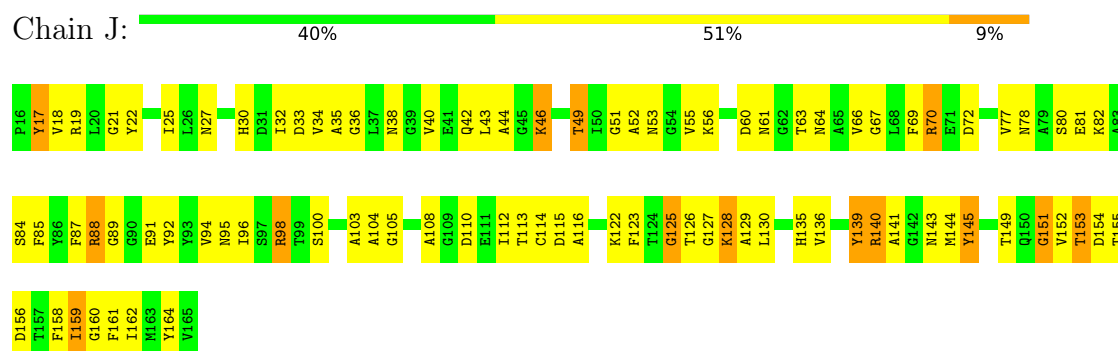


- Molecule 2: Gp26 capsid decoration protein

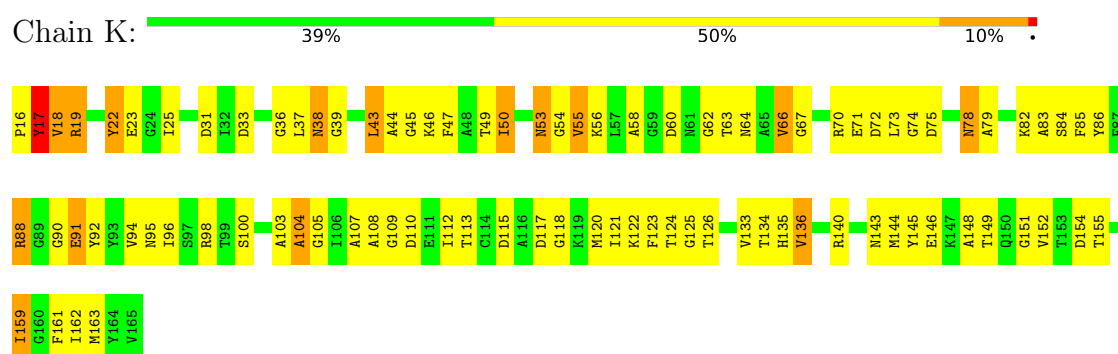
Chain I: 



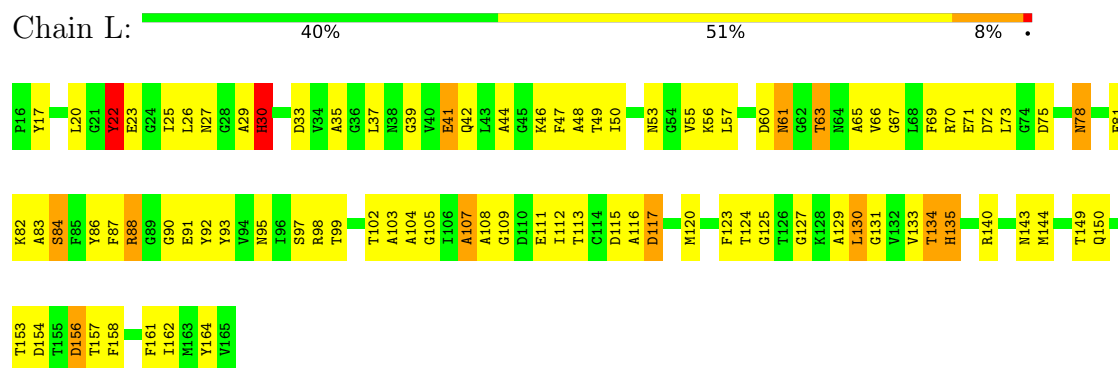
- Molecule 2: Gp26 capsid decoration protein



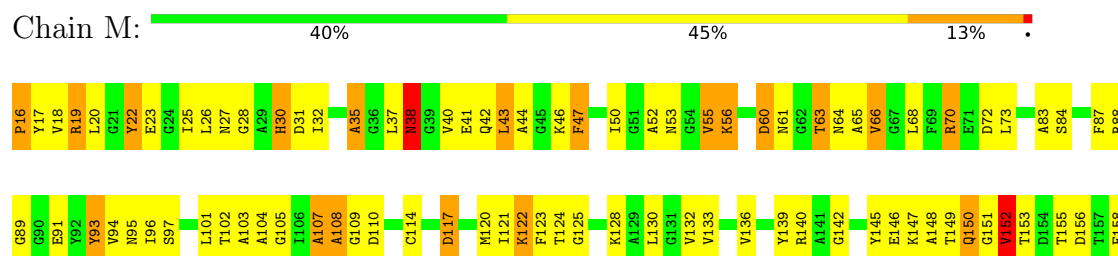
- Molecule 2: Gp26 capsid decoration protein

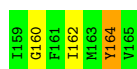


- Molecule 2: Gp26 capsid decoration protein



- Molecule 2: Gp26 capsid decoration protein





- Molecule 2: Gp26 capsid decoration protein

Chain N: 53% 40% 7%



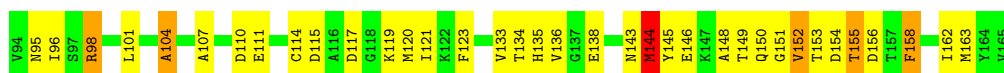
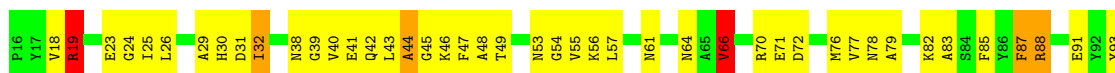
- Molecule 2: Gp26 capsid decoration protein

Chain O: 33% 51% 15%



- Molecule 2: Gp26 capsid decoration protein

Chain P: 47% 45% 6%

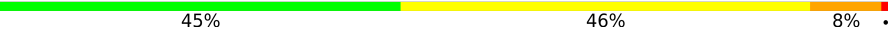


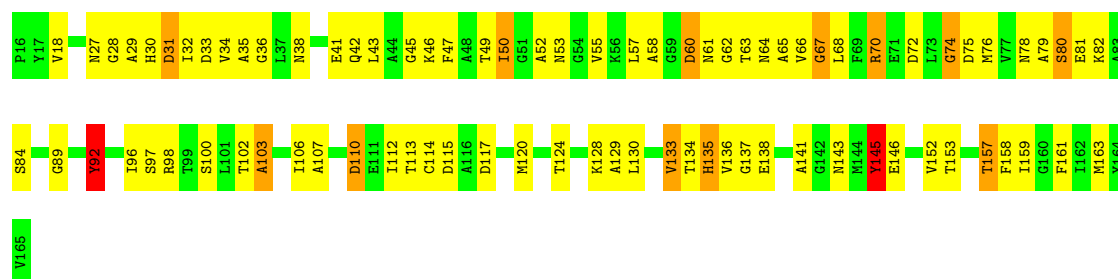
- Molecule 2: Gp26 capsid decoration protein

Chain Q: 47% 42% 11%

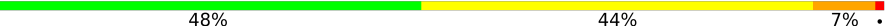


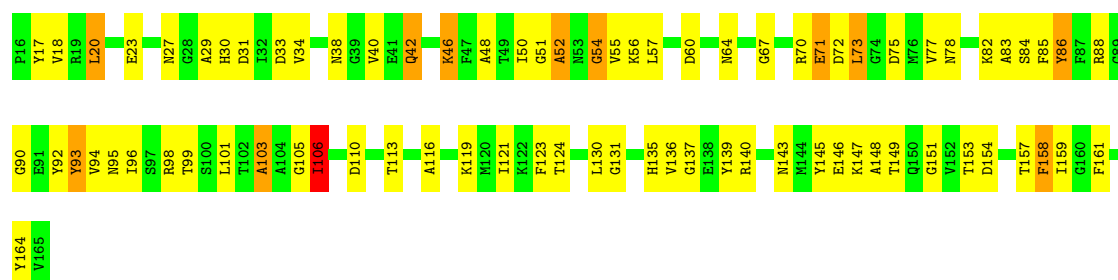
- Molecule 2: Gp26 capsid decoration protein

Chain R:  45% 46% 8%



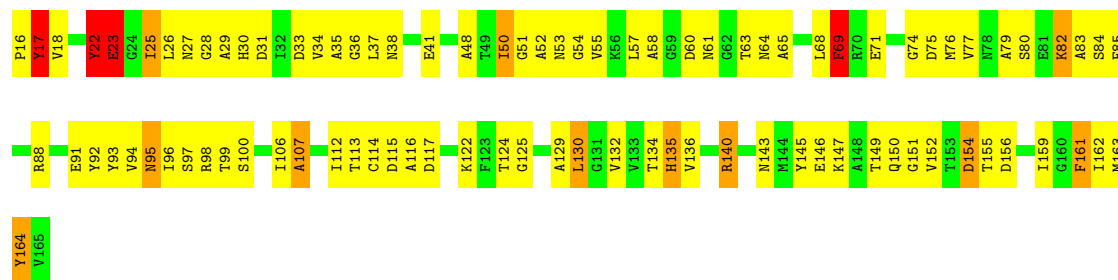
- Molecule 2: Gp26 capsid decoration protein

Chain S:  48% 44% 7%

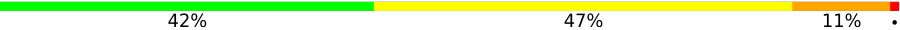


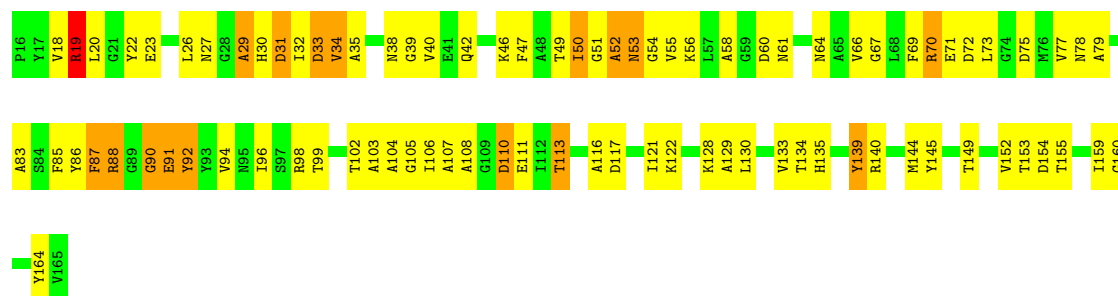
- Molecule 2: Gp26 capsid decoration protein

Chain T:  39% 51% 7%

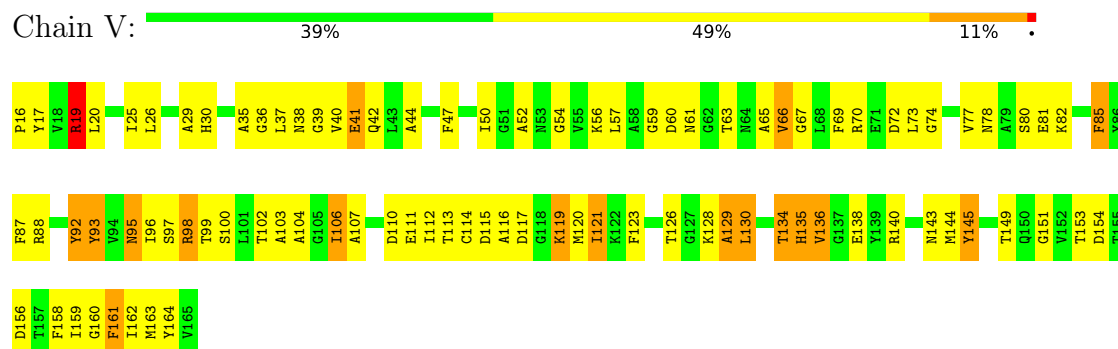


- Molecule 2: Gp26 capsid decoration protein

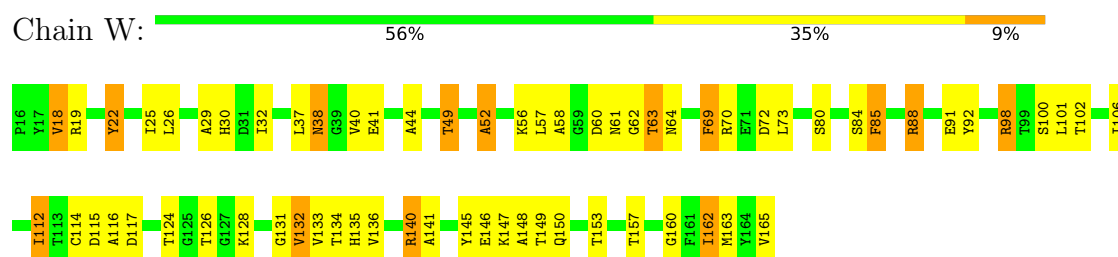
Chain U:  42% 47% 11%



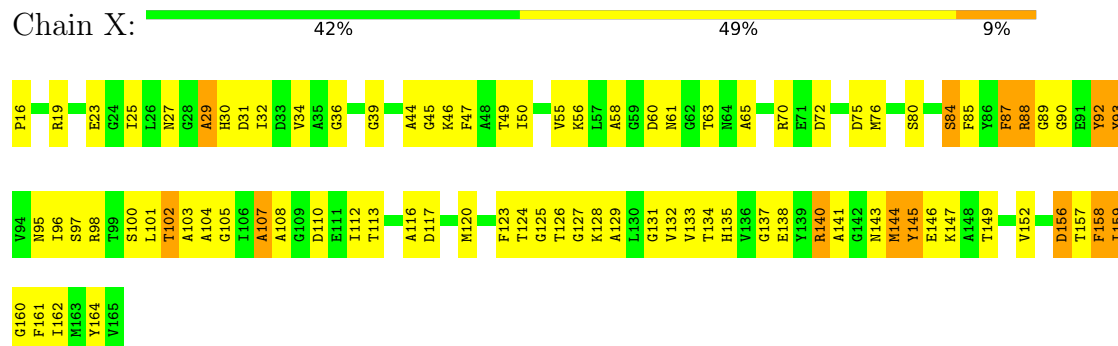
- Molecule 2: Gp26 capsid decoration protein



- Molecule 2: Gp26 capsid decoration protein



- Molecule 2: Gp26 capsid decoration protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	14.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	2.48	84/2219 (3.8%)	2.51	174/3012 (5.8%)
1	B	2.30	77/2219 (3.5%)	2.57	173/3012 (5.7%)
1	C	2.29	77/2219 (3.5%)	2.51	174/3012 (5.8%)
1	D	2.28	89/2219 (4.0%)	2.46	152/3012 (5.0%)
1	E	2.23	80/2219 (3.6%)	2.53	174/3012 (5.8%)
1	F	2.58	85/2219 (3.8%)	2.45	146/3012 (4.8%)
2	G	2.31	43/1123 (3.8%)	2.41	67/1515 (4.4%)
2	H	2.26	40/1123 (3.6%)	2.42	72/1515 (4.8%)
2	I	2.22	39/1123 (3.5%)	2.41	74/1515 (4.9%)
2	J	2.29	38/1123 (3.4%)	2.45	77/1515 (5.1%)
2	K	2.33	51/1123 (4.5%)	2.41	60/1515 (4.0%)
2	L	2.24	43/1123 (3.8%)	2.46	64/1515 (4.2%)
2	M	2.57	55/1123 (4.9%)	2.39	64/1515 (4.2%)
2	N	2.18	33/1123 (2.9%)	2.36	61/1515 (4.0%)
2	O	4.17	53/1123 (4.7%)	2.57	80/1515 (5.3%)
2	P	2.24	41/1123 (3.7%)	2.45	72/1515 (4.8%)
2	Q	2.31	45/1123 (4.0%)	2.36	67/1515 (4.4%)
2	R	2.27	48/1123 (4.3%)	2.40	69/1515 (4.6%)
2	S	2.29	41/1123 (3.7%)	2.43	69/1515 (4.6%)
2	T	2.31	47/1123 (4.2%)	2.39	69/1515 (4.6%)
2	U	2.36	47/1123 (4.2%)	2.41	70/1515 (4.6%)
2	V	2.27	44/1123 (3.9%)	2.28	59/1515 (3.9%)
2	W	2.26	39/1123 (3.5%)	2.37	51/1515 (3.4%)
2	X	2.25	42/1123 (3.7%)	2.35	66/1515 (4.4%)
All	All	2.41	1281/33528 (3.8%)	2.45	2204/45342 (4.9%)

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	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	9
1	C	0	2
1	D	0	11
1	E	0	6
1	F	0	6
2	G	1	6
2	H	3	5
2	I	0	8
2	J	1	7
2	K	3	3
2	L	0	4
2	M	1	3
2	N	3	3
2	O	0	4
2	P	1	4
2	Q	3	3
2	R	0	3
2	S	1	4
2	T	2	7
2	U	0	7
2	V	2	3
2	W	3	3
2	X	0	7
All	All	24	123

All (1281) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	35	ALA	N-CA	115.48	2.95	1.46
1	A	55	GLN	CD-NE2	46.34	2.30	1.33
1	F	111	PHE	CG-CD1	31.37	2.04	1.38
1	F	111	PHE	CG-CD2	28.67	1.99	1.38
2	M	47	PHE	CG-CD2	22.00	1.85	1.38
1	F	111	PHE	CD2-CE2	21.63	2.03	1.38
1	F	111	PHE	CE1-CZ	20.39	1.99	1.38
2	M	47	PHE	CG-CD1	19.20	1.79	1.38
1	F	111	PHE	CD1-CE1	18.53	1.94	1.38
1	F	111	PHE	CE2-CZ	17.51	1.91	1.38
2	M	47	PHE	CE2-CZ	15.18	1.84	1.38
2	M	47	PHE	CE1-CZ	13.69	1.79	1.38
1	C	122	LYS	CA-C	-13.25	1.46	1.53
1	F	85	GLY	N-CA	-12.94	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	115	ASP	CA-C	-12.87	1.38	1.52
2	M	47	PHE	CD1-CE1	11.22	1.72	1.38
2	R	163	MET	CA-C	-10.85	1.39	1.52
2	M	47	PHE	CD2-CE2	10.84	1.71	1.38
2	J	30	HIS	CA-C	-10.83	1.39	1.52
1	B	277	ALA	CA-C	-10.51	1.40	1.52
1	F	90	VAL	N-CA	-10.50	1.38	1.46
2	G	36	GLY	CA-C	-10.22	1.42	1.52
2	S	164	TYR	C-N	10.06	1.47	1.33
1	C	151	SER	N-CA	10.05	1.58	1.46
1	A	78	VAL	N-CA	-9.70	1.38	1.45
1	D	248	ILE	N-CA	-9.67	1.34	1.46
2	S	29	ALA	N-CA	-9.61	1.34	1.46
2	V	78	ASN	CA-C	-9.57	1.41	1.52
2	S	51	GLY	N-CA	-9.33	1.36	1.45
2	O	35	ALA	CA-C	9.06	1.65	1.52
1	D	268	LEU	CA-C	-9.04	1.43	1.53
1	A	159	LEU	CA-C	-9.04	1.41	1.52
2	W	131	GLY	N-CA	-9.02	1.38	1.46
2	S	34	VAL	CA-C	-8.95	1.41	1.52
1	D	77	GLN	C-N	8.93	1.42	1.33
2	S	121	ILE	CA-C	-8.93	1.41	1.52
1	A	77	GLN	CA-C	-8.88	1.41	1.52
2	O	95	ASN	CA-C	-8.87	1.42	1.52
2	J	123	PHE	C-O	-8.81	1.17	1.23
2	X	141	ALA	CA-C	-8.76	1.41	1.52
2	W	147	LYS	C-N	8.73	1.44	1.33
2	R	30	HIS	ND1-CE1	8.71	1.41	1.32
2	K	31	ASP	CA-C	-8.70	1.42	1.52
1	C	38	LEU	CA-C	-8.67	1.41	1.52
2	U	61	ASN	CA-C	-8.65	1.41	1.53
1	E	90	VAL	CA-C	-8.58	1.45	1.52
1	B	114	ILE	CA-CB	-8.55	1.44	1.54
2	S	57	LEU	CA-CB	8.55	1.66	1.53
2	U	94	VAL	CA-C	-8.48	1.42	1.52
2	M	91	GLU	CA-C	-8.42	1.42	1.52
2	K	133	VAL	CA-C	-8.38	1.42	1.52
2	G	115	ASP	C-N	8.37	1.45	1.33
1	A	271	VAL	N-CA	-8.35	1.35	1.46
2	J	25	ILE	CA-C	-8.33	1.45	1.53
2	N	161	PHE	C-N	8.33	1.42	1.33
2	P	119	LYS	N-CA	-8.32	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	93	TYR	CA-C	-8.31	1.42	1.52
2	V	160	GLY	CA-C	8.31	1.60	1.51
1	D	118	GLN	CA-CB	8.30	1.66	1.53
2	S	38	ASN	N-CA	-8.28	1.35	1.46
2	H	135	HIS	ND1-CE1	8.28	1.40	1.32
1	F	255	GLU	CA-C	-8.27	1.42	1.52
1	F	242	ARG	NE-CZ	8.25	1.42	1.33
1	B	212	TRP	C-N	8.23	1.44	1.33
2	J	78	ASN	N-CA	-8.21	1.36	1.46
1	E	241	ILE	C-N	8.18	1.45	1.33
1	A	108	GLU	CA-C	-8.17	1.42	1.52
1	F	152	GLY	CA-C	-8.16	1.42	1.52
2	U	106	ILE	CA-CB	-8.15	1.46	1.54
1	B	164	GLN	C-N	8.13	1.45	1.33
1	B	238	VAL	CA-CB	-8.13	1.44	1.54
2	O	51	GLY	N-CA	8.10	1.50	1.44
2	G	150	GLN	CA-C	-8.10	1.42	1.52
2	P	48	ALA	CA-C	-8.10	1.42	1.52
2	G	119	LYS	C-N	8.09	1.44	1.33
1	C	28	GLN	CA-CB	8.09	1.63	1.53
1	A	100	GLN	N-CA	-8.08	1.36	1.46
2	V	159	ILE	CA-CB	-8.07	1.44	1.54
1	C	15	LYS	CA-CB	8.05	1.66	1.54
2	X	126	THR	C-N	8.05	1.40	1.33
2	L	22	TYR	N-CA	-8.05	1.35	1.46
2	N	111	GLU	CA-CB	8.04	1.63	1.53
2	N	46	LYS	N-CA	-8.04	1.36	1.46
2	R	143	ASN	CA-C	-8.04	1.42	1.52
1	A	212	TRP	CA-C	-8.04	1.43	1.52
2	N	135	HIS	ND1-CE1	8.03	1.40	1.32
2	L	25	ILE	CA-CB	8.02	1.63	1.54
2	R	70	ARG	NE-CZ	7.97	1.41	1.33
1	A	14	SER	CA-C	-7.96	1.42	1.52
2	R	100	SER	C-N	7.94	1.44	1.33
1	F	111	PHE	CA-C	-7.94	1.42	1.52
2	R	97	SER	N-CA	-7.92	1.36	1.46
1	E	76	GLY	CA-C	-7.90	1.45	1.51
2	N	57	LEU	N-CA	-7.89	1.36	1.46
2	Q	107	ALA	CA-C	-7.89	1.42	1.52
1	C	89	GLN	C-N	7.88	1.40	1.32
1	E	138	GLU	CA-C	-7.88	1.42	1.52
1	E	92	THR	C-N	7.87	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	200	HIS	N-CA	-7.86	1.36	1.46
1	E	90	VAL	CA-CB	-7.85	1.44	1.54
2	S	29	ALA	CA-C	-7.85	1.43	1.52
2	G	43	LEU	CA-C	-7.83	1.42	1.52
2	P	45	GLY	CA-C	7.83	1.61	1.51
2	H	136	VAL	CA-C	-7.83	1.43	1.52
2	T	115	ASP	CA-C	-7.82	1.44	1.53
2	J	44	ALA	C-O	-7.82	1.14	1.24
2	T	36	GLY	C-N	7.80	1.44	1.33
1	D	279	ILE	N-CA	-7.79	1.38	1.46
2	P	40	VAL	CA-C	7.75	1.63	1.52
1	B	21	GLU	C-N	7.74	1.40	1.33
2	M	130	LEU	N-CA	-7.70	1.36	1.46
2	U	50	ILE	CA-CB	-7.70	1.46	1.54
1	D	84	GLU	CA-C	7.70	1.61	1.52
1	F	137	LEU	N-CA	7.70	1.56	1.46
2	V	156	ASP	C-O	-7.70	1.18	1.24
2	P	70	ARG	NE-CZ	7.67	1.41	1.33
2	Q	150	GLN	N-CA	-7.65	1.37	1.46
2	R	18	VAL	CA-C	-7.61	1.43	1.52
2	U	30	HIS	CA-C	-7.60	1.43	1.52
1	E	75	ARG	NE-CZ	7.59	1.41	1.33
2	M	23	GLU	C-N	7.58	1.42	1.33
1	B	154	LEU	CA-C	-7.57	1.43	1.52
2	K	122	LYS	C-N	7.57	1.43	1.33
1	C	36	VAL	N-CA	-7.56	1.37	1.46
1	F	196	PRO	CA-CB	7.55	1.63	1.53
2	K	112	ILE	N-CA	-7.54	1.37	1.46
1	A	106	VAL	C-N	7.53	1.43	1.33
2	I	90	GLY	CA-C	-7.53	1.41	1.51
1	E	45	ARG	NE-CZ	7.51	1.41	1.33
1	C	126	MET	CA-CB	7.50	1.65	1.54
1	B	30	MET	CA-C	7.49	1.61	1.52
2	R	157	THR	CA-CB	7.48	1.64	1.53
2	Q	19	ARG	C-O	-7.48	1.15	1.24
2	X	131	GLY	N-CA	7.48	1.53	1.45
2	X	127	GLY	N-CA	-7.47	1.37	1.45
2	K	95	ASN	CA-C	-7.46	1.43	1.52
2	G	107	ALA	CA-C	-7.45	1.43	1.52
2	O	62	GLY	CA-C	-7.45	1.41	1.51
1	C	155	GLN	N-CA	-7.44	1.37	1.46
2	X	93	TYR	N-CA	-7.44	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	76	GLY	CA-C	-7.42	1.46	1.52
2	I	44	ALA	CA-CB	7.42	1.64	1.53
2	P	95	ASN	CA-C	-7.40	1.43	1.52
2	W	26	LEU	C-N	7.39	1.43	1.33
2	Q	150	GLN	C-N	7.39	1.43	1.33
2	Q	35	ALA	CA-C	-7.38	1.42	1.52
1	B	221	LYS	CA-C	-7.36	1.43	1.52
2	W	37	LEU	N-CA	-7.36	1.36	1.46
1	F	196	PRO	CA-C	-7.36	1.44	1.52
2	H	57	LEU	CA-CB	7.34	1.64	1.53
1	B	76	GLY	N-CA	-7.33	1.37	1.45
2	K	19	ARG	CA-C	-7.33	1.43	1.52
2	T	17	TYR	CA-CB	7.32	1.65	1.53
1	A	203	LEU	CA-CB	7.32	1.64	1.53
1	C	17	LEU	CA-C	-7.32	1.44	1.52
1	A	120	ARG	NE-CZ	7.32	1.41	1.33
2	X	117	ASP	N-CA	7.31	1.55	1.46
2	X	125	GLY	CA-C	-7.29	1.42	1.51
2	Q	98	ARG	CA-C	-7.27	1.43	1.52
2	X	44	ALA	CA-C	-7.27	1.43	1.52
2	T	77	VAL	CA-C	7.27	1.61	1.52
1	B	63	LYS	CA-CB	7.27	1.64	1.53
1	C	133	ILE	N-CA	-7.27	1.38	1.46
2	M	83	ALA	C-N	7.26	1.43	1.33
1	D	91	PRO	C-O	-7.26	1.15	1.24
1	E	75	ARG	CA-C	-7.26	1.44	1.52
2	N	70	ARG	NE-CZ	7.26	1.41	1.33
1	B	127	ALA	C-N	7.25	1.41	1.33
1	E	23	ARG	CZ-NH1	7.25	1.42	1.32
1	F	232	ASP	N-CA	7.25	1.54	1.46
2	M	122	LYS	CA-CB	7.24	1.64	1.53
2	Q	125	GLY	CA-C	-7.24	1.42	1.52
1	D	168	LYS	N-CA	-7.23	1.36	1.46
2	L	158	PHE	C-N	7.21	1.40	1.33
2	S	94	VAL	CA-CB	-7.20	1.43	1.54
1	D	136	LEU	CA-C	-7.20	1.43	1.52
2	L	87	PHE	N-CA	-7.18	1.36	1.45
1	B	270	VAL	CA-C	-7.17	1.43	1.52
2	Q	87	PHE	N-CA	-7.16	1.37	1.46
1	B	187	ARG	NE-CZ	7.15	1.41	1.33
2	M	22	TYR	N-CA	-7.15	1.36	1.45
2	T	79	ALA	CA-C	-7.14	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	167	GLU	CA-C	-7.14	1.43	1.52
2	N	159	ILE	CA-C	-7.13	1.44	1.52
1	A	268	LEU	C-N	7.13	1.43	1.33
2	L	29	ALA	CA-C	-7.12	1.44	1.52
2	I	88	ARG	CD-NE	7.12	1.56	1.46
2	M	19	ARG	CA-C	-7.12	1.43	1.52
2	M	43	LEU	N-CA	-7.12	1.38	1.46
1	B	47	LEU	CA-CB	7.11	1.68	1.54
1	C	237	GLY	N-CA	7.11	1.54	1.45
2	U	111	GLU	CA-C	-7.10	1.43	1.52
1	B	200	HIS	N-CA	-7.10	1.38	1.46
2	W	40	VAL	N-CA	-7.09	1.38	1.46
1	C	18	GLU	N-CA	-7.09	1.37	1.45
1	E	30	MET	CA-C	-7.09	1.44	1.52
2	W	136	VAL	CA-C	-7.09	1.44	1.52
2	K	82	LYS	N-CA	-7.07	1.37	1.46
2	R	98	ARG	CZ-NH1	7.07	1.42	1.32
2	G	52	ALA	C-N	7.07	1.43	1.33
1	F	125	ILE	CA-CB	-7.07	1.44	1.54
2	G	60	ASP	CA-C	7.07	1.61	1.52
2	R	141	ALA	N-CA	-7.06	1.37	1.46
1	A	35	ARG	NE-CZ	7.05	1.40	1.33
2	P	79	ALA	C-N	7.05	1.43	1.33
1	D	109	ARG	NE-CZ	7.04	1.40	1.33
1	E	191	GLN	CA-C	-7.04	1.43	1.52
1	A	62	ASP	CA-CB	7.04	1.64	1.53
1	F	17	LEU	N-CA	-7.03	1.37	1.46
2	H	123	PHE	CA-C	-7.03	1.44	1.52
2	I	164	TYR	C-N	7.03	1.43	1.33
2	J	70	ARG	CA-C	-7.03	1.44	1.52
2	P	111	GLU	C-N	7.02	1.44	1.33
1	B	268	LEU	CA-CB	7.02	1.62	1.53
2	I	122	LYS	N-CA	-7.01	1.37	1.46
2	L	30	HIS	CD2-NE2	7.00	1.45	1.37
1	E	116	ARG	NE-CZ	7.00	1.40	1.33
2	K	133	VAL	N-CA	-7.00	1.38	1.46
2	G	61	ASN	C-N	7.00	1.42	1.33
2	V	154	ASP	N-CA	-7.00	1.38	1.46
1	E	102	ARG	CD-NE	6.99	1.56	1.46
2	G	35	ALA	N-CA	-6.99	1.37	1.46
1	F	202	VAL	N-CA	-6.99	1.34	1.45
1	D	53	LEU	CA-CB	6.99	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	26	LEU	C-N	6.99	1.42	1.33
1	B	256	LEU	CA-CB	6.98	1.64	1.53
2	K	56	LYS	CA-CB	6.97	1.63	1.53
2	H	108	ALA	CA-C	-6.97	1.44	1.52
1	B	179	ASN	CA-CB	6.96	1.64	1.53
1	C	249	PRO	C-N	6.96	1.42	1.33
1	D	161	LYS	CA-CB	6.96	1.64	1.53
1	F	210	HIS	ND1-CE1	6.96	1.39	1.32
2	N	44	ALA	N-CA	-6.95	1.37	1.46
2	H	78	ASN	C-N	6.95	1.42	1.33
1	A	23	ARG	C-N	6.95	1.40	1.33
2	I	131	GLY	CA-C	-6.94	1.45	1.52
2	X	112	ILE	C-N	6.94	1.43	1.33
1	D	188	ALA	N-CA	-6.94	1.36	1.46
2	X	107	ALA	CA-C	-6.94	1.43	1.52
2	L	129	ALA	CA-C	-6.93	1.44	1.52
1	B	25	ALA	C-N	6.93	1.43	1.33
1	D	182	ALA	CA-C	-6.93	1.43	1.52
1	F	9	LYS	N-CA	-6.92	1.36	1.45
2	X	19	ARG	CD-NE	6.92	1.55	1.46
2	T	114	CYS	CA-C	-6.92	1.44	1.52
2	R	46	LYS	CA-C	-6.92	1.44	1.52
2	T	80	SER	CA-CB	6.92	1.65	1.53
2	U	77	VAL	CA-C	-6.91	1.44	1.52
1	A	170	ASP	CA-CB	6.91	1.63	1.54
1	B	225	ASN	CA-C	-6.90	1.46	1.53
1	E	180	ALA	N-CA	-6.90	1.38	1.46
1	D	7	GLN	CA-CB	6.89	1.64	1.53
2	L	111	GLU	C-N	6.89	1.43	1.33
2	S	18	VAL	CA-C	-6.88	1.44	1.52
1	F	12	LEU	CA-CB	6.88	1.62	1.53
2	W	106	ILE	N-CA	6.88	1.54	1.46
1	F	104	SER	CA-C	6.88	1.61	1.52
2	K	113	THR	CA-C	-6.87	1.44	1.52
1	E	261	VAL	N-CA	-6.87	1.37	1.46
2	K	91	GLU	N-CA	-6.86	1.37	1.46
2	T	37	LEU	CA-C	-6.86	1.43	1.52
1	C	257	ARG	C-N	6.85	1.42	1.33
1	E	235	PHE	CA-C	6.85	1.61	1.52
1	F	130	ASP	CA-C	-6.85	1.44	1.52
2	H	119	LYS	CA-C	-6.85	1.45	1.53
1	E	35	ARG	CA-CB	6.83	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	58	LEU	N-CA	-6.82	1.36	1.46
2	Q	82	LYS	CA-C	-6.80	1.44	1.52
2	R	28	GLY	CA-C	-6.80	1.42	1.51
2	J	152	VAL	CA-C	-6.80	1.44	1.52
1	B	216	ILE	CA-C	-6.79	1.44	1.52
2	W	58	ALA	CA-C	-6.79	1.43	1.52
2	M	41	GLU	C-O	-6.79	1.15	1.23
2	H	77	VAL	N-CA	-6.79	1.38	1.46
1	E	184	ALA	CA-C	-6.79	1.43	1.52
2	V	135	HIS	CB-CG	6.78	1.59	1.50
2	U	144	MET	CA-C	-6.77	1.44	1.52
2	H	54	GLY	N-CA	-6.77	1.37	1.45
2	M	28	GLY	C-N	6.77	1.39	1.33
1	E	62	ASP	CA-C	-6.76	1.43	1.52
2	G	151	GLY	CA-C	-6.74	1.44	1.52
2	O	115	ASP	CA-CB	6.74	1.63	1.54
2	L	60	ASP	CA-CB	6.73	1.61	1.53
1	E	77	GLN	CA-C	-6.73	1.44	1.52
1	B	35	ARG	NE-CZ	6.72	1.40	1.33
2	P	53	ASN	CA-C	-6.72	1.44	1.52
2	R	58	ALA	CA-C	-6.72	1.43	1.52
2	X	146	GLU	C-O	-6.72	1.18	1.23
2	G	26	LEU	N-CA	-6.72	1.37	1.46
2	U	52	ALA	C-N	6.72	1.43	1.33
1	B	71	VAL	N-CA	-6.71	1.38	1.46
1	D	179	ASN	N-CA	-6.71	1.38	1.46
2	M	88	ARG	CA-CB	6.71	1.64	1.53
1	C	2	SER	N-CA	-6.70	1.37	1.46
2	V	138	GLU	N-CA	-6.69	1.38	1.45
1	C	127	ALA	CA-C	-6.69	1.42	1.52
2	L	149	THR	CA-C	-6.68	1.43	1.52
2	U	104	ALA	CA-C	6.67	1.60	1.52
1	D	178	MET	C-N	6.67	1.42	1.33
1	D	46	LYS	C-N	6.67	1.43	1.33
1	D	278	LYS	CA-C	-6.66	1.44	1.52
2	X	135	HIS	CG-CD2	6.66	1.43	1.35
2	U	46	LYS	C-N	6.65	1.42	1.33
2	G	93	TYR	N-CA	-6.65	1.38	1.46
2	X	103	ALA	CA-C	-6.64	1.43	1.52
2	O	139	TYR	CA-C	-6.64	1.44	1.52
2	L	81	GLU	CA-C	-6.64	1.43	1.52
1	B	161	LYS	N-CA	-6.63	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	242	ARG	NE-CZ	6.63	1.40	1.33
2	I	96	ILE	CA-C	-6.63	1.44	1.52
2	U	60	ASP	CA-C	-6.63	1.47	1.53
2	J	35	ALA	C-N	6.63	1.42	1.33
2	I	133	VAL	CA-C	-6.62	1.44	1.52
1	B	52	PRO	CA-CB	6.62	1.62	1.53
1	E	194	PHE	C-N	6.62	1.41	1.32
2	H	119	LYS	C-O	6.61	1.29	1.24
1	D	42	GLY	C-N	6.61	1.42	1.34
2	M	27	ASN	CA-CB	6.60	1.63	1.53
2	O	132	VAL	CA-C	-6.60	1.44	1.52
1	B	135	SER	CA-CB	6.60	1.63	1.53
2	O	20	LEU	CA-C	-6.59	1.44	1.53
2	U	47	PHE	C-N	6.58	1.42	1.33
1	B	271	VAL	C-N	6.58	1.42	1.33
2	G	158	PHE	CA-C	-6.58	1.44	1.53
1	D	201	GLU	CA-C	-6.57	1.44	1.52
2	G	28	GLY	CA-C	-6.57	1.43	1.52
2	Q	120	MET	CA-C	-6.57	1.44	1.52
1	D	83	ILE	C-N	6.57	1.41	1.33
2	G	98	ARG	CD-NE	6.57	1.55	1.46
2	G	57	LEU	CA-CB	6.56	1.62	1.53
1	C	30	MET	N-CA	-6.56	1.37	1.46
1	E	110	ARG	NE-CZ	6.56	1.40	1.33
1	D	118	GLN	C-N	6.56	1.42	1.33
2	K	105	GLY	C-N	6.56	1.40	1.33
2	K	67	GLY	C-N	6.55	1.42	1.33
1	D	68	LYS	CA-C	-6.54	1.44	1.52
1	D	277	ALA	N-CA	-6.54	1.38	1.46
2	L	131	GLY	C-O	6.54	1.31	1.24
2	O	35	ALA	CA-CB	6.53	1.64	1.53
2	W	132	VAL	C-N	6.53	1.42	1.33
1	D	211	ILE	N-CA	-6.53	1.38	1.46
2	G	99	THR	CA-C	6.52	1.61	1.52
2	J	145	TYR	CA-C	-6.52	1.45	1.52
2	T	65	ALA	CA-C	-6.52	1.44	1.52
2	T	130	LEU	CA-C	-6.52	1.44	1.52
2	W	162	ILE	N-CA	-6.51	1.38	1.46
1	A	185	ASP	CA-C	-6.50	1.45	1.53
2	P	155	THR	N-CA	-6.50	1.38	1.46
1	F	35	ARG	NE-CZ	6.50	1.40	1.33
1	C	268	LEU	CA-CB	6.49	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	140	ARG	CD-NE	6.48	1.55	1.46
1	C	7	GLN	C-N	6.48	1.42	1.33
2	T	116	ALA	C-N	6.48	1.42	1.33
2	K	49	THR	CA-C	-6.48	1.45	1.52
2	U	116	ALA	C-N	6.47	1.42	1.33
2	X	96	ILE	CB-CG1	6.47	1.66	1.53
1	D	257	ARG	CA-C	-6.46	1.44	1.52
2	P	78	ASN	CA-C	-6.46	1.44	1.52
1	F	77	GLN	CA-C	-6.46	1.44	1.52
1	E	210	HIS	ND1-CE1	6.46	1.39	1.32
2	N	145	TYR	CA-C	-6.45	1.44	1.52
2	M	53	ASN	N-CA	-6.44	1.37	1.46
2	X	161	PHE	N-CA	-6.44	1.38	1.45
2	V	39	GLY	C-N	6.43	1.41	1.33
2	Q	145	TYR	CA-CB	6.43	1.64	1.53
1	A	238	VAL	CA-C	-6.43	1.44	1.52
1	A	90	VAL	N-CA	-6.42	1.41	1.46
1	B	6	ASN	C-N	6.42	1.42	1.33
2	H	30	HIS	ND1-CE1	6.42	1.39	1.32
2	O	101	LEU	N-CA	-6.42	1.37	1.45
2	O	44	ALA	CA-C	6.41	1.60	1.52
1	B	249	PRO	N-CA	6.41	1.55	1.47
2	R	134	THR	C-O	6.41	1.31	1.24
1	F	145	ASN	CA-C	-6.41	1.43	1.52
2	K	123	PHE	C-N	6.41	1.41	1.33
1	B	161	LYS	C-O	-6.41	1.16	1.24
1	F	124	ASP	CA-CB	6.41	1.62	1.53
1	C	240	PRO	C-N	6.40	1.42	1.33
2	U	153	THR	CA-C	-6.40	1.45	1.52
2	L	91	GLU	N-CA	-6.40	1.38	1.46
2	O	48	ALA	CA-C	-6.39	1.45	1.52
1	A	201	GLU	CA-C	-6.38	1.45	1.52
1	D	158	ALA	CA-C	-6.38	1.44	1.52
2	I	33	ASP	CA-C	-6.38	1.44	1.52
2	K	152	VAL	CA-C	-6.37	1.43	1.52
1	D	151	SER	CA-C	-6.37	1.44	1.52
2	R	41	GLU	C-N	6.37	1.41	1.33
1	E	110	ARG	CA-CB	6.37	1.63	1.53
1	E	229	VAL	C-N	6.36	1.42	1.33
2	I	22	TYR	CA-C	-6.36	1.44	1.52
2	S	60	ASP	CA-C	-6.36	1.44	1.52
1	B	231	ALA	N-CA	-6.36	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	153	THR	N-CA	-6.36	1.38	1.46
2	Q	152	VAL	CA-C	-6.36	1.43	1.52
1	A	210	HIS	ND1-CE1	6.35	1.39	1.32
2	W	88	ARG	NE-CZ	6.35	1.40	1.33
2	K	94	VAL	CA-C	-6.35	1.44	1.52
2	H	32	ILE	CA-CB	-6.34	1.47	1.54
1	C	104	SER	CA-C	-6.34	1.44	1.52
2	Q	52	ALA	C-N	6.34	1.42	1.33
2	R	76	MET	CA-C	6.34	1.60	1.52
2	N	49	THR	C-N	6.34	1.41	1.33
1	D	224	GLN	CA-C	-6.33	1.45	1.52
1	E	273	SER	CA-CB	6.33	1.64	1.52
2	I	119	LYS	CA-C	-6.33	1.44	1.52
2	U	83	ALA	C-N	6.33	1.41	1.33
1	B	120	ARG	CA-C	-6.33	1.44	1.52
1	B	98	TYR	CA-CB	6.33	1.63	1.53
1	D	216	ILE	C-O	-6.32	1.17	1.24
2	L	44	ALA	CA-CB	6.32	1.62	1.53
1	A	15	LYS	C-N	6.32	1.42	1.33
1	E	220	LYS	N-CA	-6.32	1.38	1.46
1	F	252	LYS	C-N	-6.32	1.28	1.33
1	E	211	ILE	CA-C	-6.32	1.45	1.52
1	F	173	VAL	C-N	6.32	1.42	1.33
2	O	73	LEU	CA-CB	6.32	1.64	1.53
2	Q	158	PHE	C-N	6.31	1.42	1.33
2	M	17	TYR	C-N	6.31	1.41	1.33
2	N	135	HIS	CD2-NE2	6.31	1.44	1.37
2	H	95	ASN	C-N	6.31	1.41	1.33
2	R	135	HIS	ND1-CE1	6.30	1.38	1.32
2	T	136	VAL	N-CA	-6.30	1.39	1.46
2	O	162	ILE	CA-C	-6.30	1.45	1.52
1	B	239	MET	C-N	-6.30	1.25	1.33
2	O	158	PHE	CA-C	-6.30	1.44	1.53
2	K	122	LYS	CA-C	-6.29	1.45	1.52
2	Q	111	GLU	C-N	6.29	1.43	1.33
2	Q	48	ALA	CA-C	-6.29	1.45	1.52
2	V	40	VAL	CA-CB	-6.29	1.47	1.54
1	A	120	ARG	CA-CB	6.29	1.63	1.53
1	E	87	ARG	NE-CZ	6.29	1.40	1.33
2	L	95	ASN	CA-CB	6.29	1.61	1.53
2	V	158	PHE	C-N	6.29	1.41	1.33
2	P	54	GLY	C-O	-6.28	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	88	ARG	CA-C	-6.28	1.44	1.52
2	J	91	GLU	N-CA	6.27	1.54	1.46
1	D	35	ARG	CA-CB	6.27	1.64	1.53
2	U	102	THR	C-N	6.26	1.41	1.33
1	D	120	ARG	CA-C	-6.26	1.44	1.52
2	U	92	TYR	C-N	6.25	1.42	1.33
1	D	124	ASP	CA-CB	6.25	1.62	1.53
2	J	18	VAL	CA-C	-6.25	1.45	1.52
2	K	18	VAL	N-CA	-6.25	1.39	1.46
2	O	145	TYR	C-N	6.25	1.42	1.33
2	V	87	PHE	C-N	6.24	1.43	1.33
1	A	199	GLN	C-N	6.24	1.42	1.33
1	C	110	ARG	NE-CZ	6.24	1.40	1.33
2	P	123	PHE	N-CA	-6.23	1.38	1.46
1	B	159	LEU	CA-CB	6.23	1.63	1.53
2	M	26	LEU	CA-C	-6.23	1.44	1.52
2	P	38	ASN	N-CA	-6.23	1.38	1.45
2	Q	91	GLU	C-N	6.22	1.42	1.33
1	D	141	ALA	N-CA	-6.21	1.38	1.46
2	K	94	VAL	C-O	-6.21	1.16	1.24
2	X	133	VAL	CA-CB	-6.21	1.46	1.54
1	D	192	ASN	CA-CB	6.21	1.63	1.53
2	U	47	PHE	N-CA	-6.21	1.38	1.45
2	S	17	TYR	CA-C	-6.20	1.45	1.52
2	X	140	ARG	NE-CZ	6.20	1.39	1.33
2	G	122	LYS	CA-C	-6.20	1.45	1.52
2	O	114	CYS	C-N	6.20	1.38	1.33
2	I	80	SER	CA-C	-6.19	1.45	1.52
1	E	207	LEU	CA-CB	6.19	1.64	1.53
2	I	135	HIS	N-CA	-6.19	1.39	1.46
1	D	198	THR	C-N	6.19	1.41	1.33
1	A	176	ILE	N-CA	-6.18	1.39	1.46
1	C	83	ILE	CA-C	-6.18	1.45	1.52
1	F	66	ASP	CA-C	-6.18	1.44	1.52
2	Q	35	ALA	CA-CB	6.18	1.64	1.53
1	F	127	ALA	CA-C	-6.18	1.44	1.52
2	Q	88	ARG	CD-NE	6.18	1.54	1.46
2	U	22	TYR	N-CA	-6.18	1.38	1.46
1	F	225	ASN	CA-CB	6.17	1.61	1.53
1	B	105	GLN	N-CA	6.17	1.53	1.46
2	V	47	PHE	CA-CB	6.17	1.63	1.53
2	T	41	GLU	CA-C	-6.15	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	22	TYR	C-N	6.14	1.42	1.33
2	H	116	ALA	CA-C	-6.14	1.44	1.52
2	X	88	ARG	CA-C	-6.14	1.45	1.53
1	B	183	PHE	CA-C	-6.13	1.44	1.52
2	W	69	PHE	CA-C	-6.13	1.45	1.52
1	D	252	LYS	CA-C	-6.13	1.46	1.52
2	X	19	ARG	NE-CZ	6.13	1.39	1.33
2	U	152	VAL	CA-CB	-6.13	1.46	1.53
1	B	164	GLN	CA-C	-6.13	1.44	1.52
1	B	238	VAL	C-O	-6.13	1.17	1.24
2	P	104	ALA	C-N	6.12	1.42	1.33
2	M	87	PHE	CA-C	-6.12	1.44	1.52
2	T	135	HIS	ND1-CE1	6.12	1.38	1.32
1	D	104	SER	C-N	6.12	1.41	1.33
1	F	118	GLN	CA-CB	6.12	1.62	1.53
2	P	114	CYS	N-CA	6.11	1.53	1.45
2	S	164	TYR	N-CA	-6.11	1.38	1.46
1	A	147	VAL	CA-C	-6.11	1.45	1.52
1	F	101	VAL	N-CA	-6.11	1.39	1.46
2	Q	23	GLU	C-N	6.10	1.41	1.33
2	Q	143	ASN	N-CA	-6.10	1.39	1.46
2	O	63	THR	N-CA	-6.10	1.38	1.46
1	E	105	GLN	C-N	6.10	1.41	1.33
2	V	104	ALA	CA-C	-6.10	1.45	1.52
1	D	163	PHE	CA-CB	6.09	1.63	1.53
2	O	55	VAL	C-N	6.09	1.41	1.33
2	U	139	TYR	CA-C	-6.09	1.45	1.52
2	U	34	VAL	N-CA	6.09	1.53	1.46
1	F	109	ARG	NE-CZ	6.09	1.39	1.33
2	S	71	GLU	N-CA	-6.08	1.38	1.46
2	S	110	ASP	CA-C	-6.08	1.45	1.52
2	W	38	ASN	CA-CB	6.08	1.63	1.53
1	D	202	VAL	C-N	6.07	1.42	1.33
1	F	42	GLY	N-CA	-6.07	1.39	1.45
2	J	156	ASP	CA-CB	6.07	1.63	1.53
1	E	67	ALA	C-N	6.07	1.41	1.33
1	F	278	LYS	C-N	6.07	1.40	1.34
2	M	103	ALA	CA-C	-6.07	1.45	1.52
2	S	105	GLY	C-N	6.07	1.39	1.33
1	A	228	TYR	CA-C	-6.07	1.45	1.52
2	K	135	HIS	ND1-CE1	6.06	1.38	1.32
2	H	34	VAL	N-CA	6.05	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	85	PHE	CA-CB	6.05	1.61	1.53
1	E	117	ALA	CA-CB	6.05	1.62	1.53
2	X	129	ALA	C-N	6.05	1.41	1.33
2	T	124	THR	C-N	6.04	1.41	1.32
2	M	160	GLY	C-O	-6.03	1.17	1.23
1	E	187	ARG	CZ-NH2	6.03	1.41	1.33
1	D	2	SER	C-O	-6.03	1.16	1.24
1	F	30	MET	CA-C	6.02	1.61	1.53
2	R	145	TYR	CA-C	-6.02	1.44	1.52
1	B	211	ILE	CA-CB	-6.02	1.46	1.54
1	E	151	SER	C-N	6.02	1.41	1.33
1	F	212	TRP	N-CA	-6.02	1.38	1.46
1	A	192	ASN	CA-C	-6.01	1.44	1.53
1	C	197	VAL	CA-CB	-6.01	1.47	1.54
1	F	209	GLY	CA-C	-6.01	1.46	1.52
2	R	112	ILE	CA-CB	-6.01	1.46	1.54
1	D	108	GLU	C-N	6.00	1.41	1.33
1	C	211	ILE	C-N	6.00	1.41	1.33
1	E	255	GLU	N-CA	-6.00	1.38	1.45
2	N	152	VAL	N-CA	-6.00	1.38	1.46
2	Q	46	LYS	C-N	6.00	1.42	1.33
2	S	77	VAL	CA-C	6.00	1.60	1.52
2	G	66	VAL	N-CA	-6.00	1.39	1.46
1	B	237	GLY	C-N	5.99	1.41	1.33
1	E	239	MET	C-O	5.99	1.31	1.24
1	C	119	GLN	C-N	5.99	1.41	1.33
1	C	233	PRO	CA-CB	-5.99	1.47	1.54
1	F	20	GLU	CA-CB	5.99	1.62	1.53
1	C	80	ASP	CA-C	-5.99	1.44	1.53
2	P	119	LYS	CA-C	-5.99	1.45	1.52
2	T	125	GLY	N-CA	-5.98	1.38	1.45
2	R	138	GLU	CA-C	5.98	1.60	1.52
2	T	64	ASN	CA-CB	5.98	1.63	1.53
1	E	173	VAL	N-CA	-5.98	1.38	1.46
2	R	80	SER	CA-C	-5.98	1.44	1.52
1	F	87	ARG	C-N	5.98	1.41	1.33
2	L	41	GLU	N-CA	-5.98	1.39	1.46
2	Q	70	ARG	CA-C	-5.98	1.45	1.52
2	Q	135	HIS	C-N	5.98	1.40	1.33
1	F	208	PHE	C-N	5.97	1.41	1.33
1	B	122	LYS	CA-C	-5.96	1.44	1.53
1	D	35	ARG	NE-CZ	5.96	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1	MET	C-N	5.96	1.41	1.33
2	P	87	PHE	N-CA	-5.96	1.38	1.46
2	X	100	SER	C-N	5.96	1.42	1.33
1	E	240	PRO	CA-C	-5.96	1.46	1.52
1	A	141	ALA	CA-C	-5.95	1.45	1.52
2	Q	114	CYS	CA-C	-5.95	1.45	1.52
2	V	114	CYS	C-N	5.95	1.40	1.33
2	L	50	ILE	C-N	5.95	1.43	1.33
2	O	70	ARG	CZ-NH1	5.95	1.41	1.32
1	D	257	ARG	CD-NE	5.94	1.54	1.46
1	C	128	VAL	CA-CB	-5.94	1.46	1.54
2	W	92	TYR	CA-C	-5.94	1.46	1.53
2	J	67	GLY	CA-C	-5.93	1.43	1.51
2	G	121	ILE	CA-C	-5.93	1.45	1.52
2	J	114	CYS	C-N	5.93	1.40	1.33
2	V	144	MET	C-N	5.93	1.42	1.33
2	K	118	GLY	CA-C	-5.93	1.43	1.51
2	O	50	ILE	C-N	5.93	1.40	1.33
2	T	140	ARG	NE-CZ	5.92	1.39	1.33
2	G	47	PHE	C-N	5.92	1.41	1.33
2	L	60	ASP	C-O	-5.92	1.17	1.24
1	A	275	ALA	CA-C	-5.92	1.45	1.52
2	G	53	ASN	CA-CB	5.92	1.63	1.53
2	P	96	ILE	CA-C	5.92	1.60	1.52
2	Q	122	LYS	CA-C	-5.92	1.45	1.52
2	V	17	TYR	CA-CB	5.92	1.63	1.53
1	E	223	PRO	CA-C	5.92	1.58	1.52
1	F	115	ASP	CA-C	-5.92	1.44	1.52
1	E	122	LYS	N-CA	5.91	1.53	1.46
2	G	44	ALA	CA-C	-5.91	1.45	1.52
1	C	217	LEU	C-N	5.90	1.40	1.33
2	T	33	ASP	C-N	5.90	1.41	1.33
2	S	54	GLY	C-N	5.90	1.38	1.33
2	W	32	ILE	C-N	5.90	1.41	1.33
2	I	92	TYR	CA-CB	5.90	1.63	1.53
2	X	100	SER	CA-CB	5.90	1.62	1.53
1	D	191	GLN	N-CA	-5.89	1.38	1.46
2	K	163	MET	CA-C	-5.89	1.45	1.52
2	M	148	ALA	CA-C	-5.89	1.45	1.52
2	H	33	ASP	C-N	5.89	1.39	1.33
2	Q	163	MET	N-CA	-5.89	1.38	1.46
2	O	121	ILE	CA-C	-5.89	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	122	LYS	N-CA	-5.88	1.38	1.45
2	O	114	CYS	CA-C	-5.88	1.45	1.53
2	S	78	ASN	N-CA	5.88	1.53	1.46
2	H	106	ILE	CA-CB	5.88	1.60	1.54
2	M	68	LEU	N-CA	-5.88	1.38	1.46
2	Q	77	VAL	N-CA	-5.88	1.39	1.46
2	W	73	LEU	C-N	5.88	1.41	1.33
2	N	151	GLY	C-N	5.88	1.40	1.33
2	T	146	GLU	CA-C	-5.88	1.44	1.53
2	U	108	ALA	CA-C	-5.88	1.45	1.52
1	C	28	GLN	CA-C	-5.88	1.45	1.53
1	D	116	ARG	CD-NE	5.88	1.54	1.46
2	G	96	ILE	N-CA	-5.88	1.39	1.46
2	S	51	GLY	C-N	5.88	1.42	1.33
2	V	35	ALA	N-CA	-5.88	1.38	1.46
2	J	159	ILE	C-N	5.88	1.42	1.33
2	T	115	ASP	C-N	5.88	1.42	1.33
1	F	102	ARG	C-O	-5.87	1.17	1.24
2	M	35	ALA	N-CA	-5.87	1.38	1.46
1	A	113	VAL	CA-C	5.87	1.60	1.52
2	K	161	PHE	C-N	5.87	1.41	1.33
1	C	108	GLU	CA-CB	5.87	1.62	1.53
1	A	88	ILE	CA-CB	-5.86	1.47	1.54
2	O	111	GLU	CA-CB	5.86	1.61	1.53
1	B	77	GLN	CA-C	-5.86	1.45	1.52
1	F	89	GLN	C-N	5.86	1.38	1.33
2	V	140	ARG	CD-NE	5.86	1.54	1.46
1	E	76	GLY	N-CA	-5.86	1.39	1.45
1	E	113	VAL	C-N	5.86	1.41	1.33
2	M	44	ALA	CA-C	-5.86	1.46	1.53
2	O	73	LEU	C-N	5.86	1.40	1.33
2	O	24	GLY	CA-C	5.86	1.59	1.52
1	A	27	ALA	N-CA	-5.85	1.38	1.46
1	A	96	VAL	N-CA	-5.85	1.39	1.46
1	D	124	ASP	CA-C	-5.85	1.45	1.53
1	A	35	ARG	CZ-NH2	5.85	1.41	1.33
1	A	232	ASP	CA-CB	5.85	1.60	1.53
1	C	220	LYS	N-CA	-5.85	1.38	1.46
2	L	108	ALA	N-CA	-5.85	1.39	1.46
2	U	164	TYR	CA-CB	5.85	1.61	1.53
1	A	71	VAL	C-N	5.84	1.41	1.33
2	U	30	HIS	ND1-CE1	5.84	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	215	ASP	CA-C	5.84	1.60	1.52
2	J	112	ILE	CA-C	-5.84	1.45	1.52
2	K	85	PHE	CA-CB	5.84	1.62	1.53
2	N	37	LEU	CA-C	-5.84	1.45	1.52
1	B	210	HIS	C-N	5.84	1.40	1.33
2	L	83	ALA	CA-CB	5.84	1.63	1.53
1	A	95	ILE	N-CA	-5.83	1.39	1.46
1	E	120	ARG	NE-CZ	5.83	1.39	1.33
2	W	60	ASP	CA-CB	5.83	1.63	1.53
1	F	187	ARG	CZ-NH2	5.83	1.41	1.33
2	W	64	ASN	N-CA	-5.83	1.38	1.46
1	E	43	VAL	CA-CB	-5.82	1.46	1.54
2	P	114	CYS	C-N	5.82	1.38	1.33
2	J	110	ASP	CA-CB	5.81	1.63	1.53
2	X	116	ALA	C-N	5.81	1.41	1.33
1	A	64	ASP	CA-C	5.81	1.60	1.53
1	C	83	ILE	N-CA	-5.81	1.39	1.46
2	J	122	LYS	CA-C	-5.81	1.45	1.52
2	M	89	GLY	CA-C	-5.81	1.43	1.52
2	X	56	LYS	CA-CB	5.81	1.62	1.53
2	K	25	ILE	C-N	5.80	1.40	1.33
2	P	66	VAL	CA-C	5.80	1.58	1.52
1	B	192	ASN	N-CA	-5.80	1.38	1.45
2	H	93	TYR	C-O	-5.80	1.17	1.23
1	A	223	PRO	N-CA	-5.79	1.40	1.46
1	F	105	GLN	CA-C	-5.79	1.45	1.52
2	K	25	ILE	N-CA	-5.79	1.38	1.46
2	U	152	VAL	N-CA	5.79	1.53	1.46
2	M	55	VAL	CA-CB	5.79	1.61	1.54
2	K	144	MET	CA-CB	5.78	1.60	1.53
2	J	135	HIS	ND1-CE1	5.78	1.38	1.32
2	X	156	ASP	CA-C	-5.78	1.45	1.52
2	V	59	GLY	C-N	5.78	1.41	1.33
2	N	152	VAL	CA-CB	-5.77	1.47	1.54
1	D	156	ARG	CD-NE	5.77	1.54	1.46
1	E	120	ARG	N-CA	-5.77	1.39	1.46
2	S	140	ARG	CD-NE	5.77	1.54	1.46
1	E	63	LYS	N-CA	-5.76	1.38	1.46
2	O	133	VAL	N-CA	-5.76	1.39	1.46
1	B	210	HIS	CA-C	-5.76	1.45	1.52
1	C	64	ASP	N-CA	-5.76	1.38	1.45
2	N	32	ILE	CA-C	5.76	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	107	ALA	N-CA	-5.76	1.39	1.46
1	E	35	ARG	CZ-NH2	5.75	1.41	1.33
1	F	4	LEU	CA-C	-5.75	1.45	1.52
2	X	103	ALA	C-N	5.75	1.41	1.33
2	K	74	GLY	CA-C	-5.75	1.43	1.51
2	U	135	HIS	ND1-CE1	5.75	1.38	1.32
2	O	159	ILE	C-N	5.75	1.41	1.33
2	P	24	GLY	C-N	5.75	1.41	1.33
2	J	115	ASP	CA-CB	5.74	1.61	1.53
1	C	80	ASP	C-N	5.74	1.41	1.33
2	I	32	ILE	N-CA	-5.74	1.40	1.46
2	L	57	LEU	CA-CB	5.74	1.63	1.53
2	U	107	ALA	CA-C	-5.74	1.45	1.52
1	A	78	VAL	C-N	5.74	1.40	1.33
1	D	269	ALA	CA-C	-5.74	1.45	1.52
2	Q	110	ASP	C-N	5.74	1.41	1.33
1	D	23	ARG	CA-C	-5.74	1.45	1.52
2	J	122	LYS	N-CA	-5.74	1.39	1.45
1	B	137	LEU	C-N	5.73	1.41	1.33
2	T	150	GLN	C-N	5.73	1.41	1.33
1	B	71	VAL	CA-CB	5.72	1.62	1.54
2	O	139	TYR	N-CA	-5.72	1.39	1.46
2	T	159	ILE	C-N	5.72	1.40	1.33
2	P	44	ALA	CA-C	-5.72	1.45	1.52
2	L	135	HIS	C-N	5.72	1.39	1.33
2	T	125	GLY	C-O	5.72	1.30	1.24
2	L	161	PHE	CA-CB	5.71	1.62	1.53
2	G	50	ILE	CA-CB	-5.71	1.46	1.54
2	K	86	TYR	CA-C	-5.71	1.45	1.52
2	J	116	ALA	CA-CB	5.71	1.61	1.53
2	H	82	LYS	CA-CB	5.71	1.62	1.53
2	W	114	CYS	CA-C	-5.71	1.45	1.52
2	H	38	ASN	CA-CB	5.71	1.63	1.53
1	B	220	LYS	CA-C	-5.71	1.45	1.52
2	M	104	ALA	CA-C	-5.71	1.46	1.52
2	M	114	CYS	CA-C	-5.71	1.45	1.52
2	S	33	ASP	CA-C	-5.71	1.45	1.52
1	F	10	GLU	CA-C	-5.70	1.45	1.52
1	C	12	LEU	C-N	5.70	1.41	1.33
2	U	54	GLY	N-CA	-5.70	1.37	1.45
2	H	80	SER	N-CA	-5.69	1.38	1.46
2	S	72	ASP	CA-C	-5.69	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	56	LYS	C-O	5.69	1.31	1.24
2	M	158	PHE	C-N	5.69	1.40	1.33
1	A	85	GLY	CA-C	-5.69	1.46	1.51
1	E	5	SER	CA-C	-5.69	1.45	1.52
2	R	34	VAL	C-N	5.69	1.41	1.33
1	F	236	VAL	CA-C	-5.69	1.45	1.52
2	G	129	ALA	N-CA	-5.68	1.38	1.46
2	M	27	ASN	CA-C	-5.68	1.45	1.52
2	N	132	VAL	N-CA	5.68	1.52	1.46
2	R	103	ALA	CA-C	-5.68	1.45	1.52
2	O	52	ALA	CA-CB	5.68	1.62	1.53
1	A	170	ASP	C-N	5.68	1.40	1.33
1	A	162	ALA	CA-C	-5.68	1.45	1.52
1	B	189	TRP	CD1-NE1	-5.68	1.25	1.37
2	K	25	ILE	CA-CB	5.67	1.61	1.54
1	E	216	ILE	C-N	5.67	1.41	1.33
1	A	176	ILE	CA-CB	-5.67	1.47	1.54
2	M	72	ASP	CA-CB	5.67	1.61	1.53
2	G	22	TYR	CZ-OH	5.67	1.50	1.38
2	T	92	TYR	C-N	5.66	1.41	1.33
2	L	65	ALA	N-CA	-5.66	1.38	1.45
1	B	179	ASN	C-N	5.66	1.41	1.33
1	F	210	HIS	CD2-NE2	5.66	1.44	1.37
2	G	67	GLY	CA-C	5.66	1.59	1.52
2	L	123	PHE	C-N	5.66	1.40	1.33
1	A	204	GLN	CA-C	-5.65	1.45	1.52
2	Q	70	ARG	NE-CZ	5.65	1.39	1.33
1	E	83	ILE	CA-C	-5.65	1.46	1.52
1	D	30	MET	C-N	5.65	1.41	1.33
2	H	42	GLN	N-CA	-5.65	1.39	1.46
2	W	30	HIS	ND1-CE1	5.65	1.38	1.32
1	A	195	ASP	CA-C	-5.64	1.45	1.52
2	V	82	LYS	CA-C	-5.64	1.45	1.52
1	C	131	ALA	CA-C	-5.64	1.45	1.52
2	W	38	ASN	CA-C	-5.64	1.45	1.52
2	H	118	GLY	C-N	5.64	1.38	1.33
2	U	20	LEU	CA-C	-5.63	1.45	1.52
2	V	50	ILE	C-N	5.63	1.40	1.33
1	F	96	VAL	C-N	5.63	1.41	1.33
2	V	114	CYS	CA-C	-5.63	1.45	1.52
2	V	163	MET	C-N	5.63	1.40	1.33
1	C	246	GLN	CA-CB	5.63	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	140	ARG	CZ-NH2	5.63	1.40	1.33
1	F	224	GLN	CA-CB	5.63	1.62	1.53
2	H	19	ARG	CD-NE	5.63	1.54	1.46
2	S	99	THR	C-N	5.63	1.40	1.33
2	O	94	VAL	C-N	5.62	1.41	1.33
2	U	42	GLN	CA-C	-5.62	1.45	1.52
1	C	250	ALA	CA-C	-5.62	1.45	1.52
2	R	52	ALA	C-N	5.62	1.40	1.33
1	A	25	ALA	CA-C	-5.62	1.45	1.52
1	A	45	ARG	CZ-NH2	5.62	1.40	1.33
2	T	71	GLU	CA-C	-5.61	1.45	1.52
1	B	120	ARG	CD-NE	5.61	1.54	1.46
2	I	98	ARG	CD-NE	5.61	1.54	1.46
1	A	3	GLN	CA-CB	5.60	1.63	1.53
2	T	100	SER	CA-C	-5.60	1.45	1.52
2	R	62	GLY	CA-C	-5.60	1.46	1.52
2	I	159	ILE	CA-CB	5.60	1.62	1.54
2	K	53	ASN	CA-C	-5.60	1.45	1.52
2	K	60	ASP	C-N	5.60	1.42	1.33
2	V	156	ASP	CA-C	-5.59	1.46	1.53
1	C	38	LEU	N-CA	-5.59	1.39	1.45
1	F	58	LEU	C-N	5.58	1.40	1.33
2	I	76	MET	N-CA	-5.58	1.38	1.45
2	S	56	LYS	C-N	5.58	1.42	1.33
2	U	67	GLY	N-CA	-5.58	1.37	1.45
2	K	143	ASN	N-CA	-5.58	1.38	1.45
2	O	51	GLY	C-N	5.58	1.40	1.33
2	U	135	HIS	CA-C	-5.58	1.45	1.53
2	O	29	ALA	C-N	5.58	1.41	1.33
2	T	129	ALA	CA-C	-5.58	1.45	1.52
1	A	176	ILE	C-N	5.57	1.41	1.33
1	E	279	ILE	CA-C	-5.57	1.45	1.52
2	M	123	PHE	N-CA	5.57	1.52	1.46
2	T	140	ARG	CD-NE	5.57	1.54	1.46
1	B	221	LYS	C-N	5.57	1.39	1.33
2	T	94	VAL	CA-CB	-5.57	1.45	1.54
2	X	98	ARG	CZ-NH2	5.57	1.40	1.33
2	S	135	HIS	C-N	5.57	1.40	1.33
1	F	78	VAL	CA-C	-5.57	1.48	1.52
2	R	129	ALA	C-N	5.57	1.40	1.33
1	A	57	ALA	CA-C	-5.57	1.45	1.52
1	A	256	LEU	N-CA	-5.57	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	87	PHE	CG-CD2	5.56	1.50	1.38
2	V	25	ILE	CA-C	-5.56	1.46	1.52
1	A	147	VAL	N-CA	5.56	1.53	1.46
1	D	43	VAL	C-O	-5.56	1.18	1.24
1	E	97	SER	C-O	-5.56	1.17	1.24
1	F	276	ILE	N-CA	-5.56	1.39	1.46
2	X	85	PHE	CA-C	-5.56	1.46	1.52
2	Q	17	TYR	CA-CB	5.56	1.62	1.53
1	B	141	ALA	C-N	5.56	1.41	1.34
2	T	25	ILE	C-N	5.55	1.40	1.33
2	W	57	LEU	CA-CB	5.55	1.62	1.53
2	P	18	VAL	CA-CB	5.55	1.60	1.54
2	L	71	GLU	CA-C	-5.55	1.45	1.52
2	J	112	ILE	CA-CB	5.55	1.61	1.54
2	K	107	ALA	N-CA	5.55	1.51	1.47
1	C	235	PHE	CA-C	5.54	1.59	1.52
1	F	200	HIS	CA-CB	5.54	1.62	1.53
2	I	16	PRO	C-N	5.54	1.40	1.33
2	Q	138	GLU	C-N	5.54	1.41	1.33
2	I	113	THR	C-N	5.54	1.41	1.33
1	F	15	LYS	N-CA	-5.54	1.38	1.46
2	Q	88	ARG	NE-CZ	5.54	1.39	1.33
1	D	32	ASN	C-O	-5.54	1.17	1.24
1	D	237	GLY	CA-C	-5.54	1.42	1.52
2	L	86	TYR	C-N	5.54	1.41	1.33
2	Q	133	VAL	C-N	-5.54	1.25	1.33
2	U	128	LYS	C-N	5.53	1.41	1.33
1	A	173	VAL	C-N	5.53	1.41	1.33
2	R	113	THR	CA-C	-5.53	1.46	1.52
1	A	212	TRP	CA-CB	5.53	1.60	1.53
2	Q	51	GLY	CA-C	-5.52	1.46	1.52
2	R	29	ALA	N-CA	-5.52	1.38	1.45
2	R	157	THR	N-CA	5.52	1.53	1.46
2	U	98	ARG	CZ-NH1	5.51	1.40	1.32
1	D	162	ALA	C-N	5.51	1.41	1.34
2	I	19	ARG	CZ-NH2	5.51	1.40	1.33
2	J	126	THR	C-N	5.51	1.40	1.33
2	J	70	ARG	CZ-NH2	5.51	1.40	1.33
1	C	35	ARG	NE-CZ	5.50	1.39	1.33
2	J	17	TYR	CA-C	-5.50	1.45	1.52
2	J	87	PHE	CA-C	-5.50	1.45	1.52
2	N	39	GLY	C-N	5.50	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	101	LEU	CA-CB	5.50	1.62	1.53
2	H	93	TYR	CA-CB	5.50	1.63	1.53
2	O	19	ARG	C-N	5.50	1.42	1.33
1	D	159	LEU	CA-C	5.50	1.59	1.52
2	H	107	ALA	CA-C	-5.50	1.45	1.52
2	L	104	ALA	C-N	5.50	1.41	1.33
1	A	211	ILE	N-CA	-5.50	1.39	1.46
1	C	44	GLY	C-N	5.50	1.41	1.33
2	L	61	ASN	N-CA	-5.50	1.39	1.46
1	E	84	GLU	C-N	5.49	1.40	1.33
1	F	78	VAL	C-N	-5.49	1.26	1.33
2	K	62	GLY	CA-C	-5.49	1.46	1.52
2	T	164	TYR	CA-CB	5.49	1.60	1.53
1	C	133	ILE	CA-CB	-5.48	1.48	1.54
1	E	2	SER	C-O	-5.48	1.17	1.23
2	V	106	ILE	N-CA	-5.48	1.40	1.46
2	V	88	ARG	CD-NE	5.48	1.53	1.46
2	W	70	ARG	CD-NE	5.48	1.53	1.46
2	R	79	ALA	N-CA	-5.48	1.39	1.46
2	V	164	TYR	N-CA	5.48	1.52	1.46
1	C	138	GLU	C-N	5.47	1.40	1.33
2	X	39	GLY	CA-C	-5.47	1.44	1.51
2	I	135	HIS	ND1-CE1	5.47	1.38	1.32
1	F	48	LEU	C-N	5.47	1.41	1.33
1	F	241	ILE	N-CA	-5.47	1.40	1.46
2	G	98	ARG	CA-CB	5.47	1.60	1.53
1	F	45	ARG	CZ-NH2	5.46	1.40	1.33
1	F	156	ARG	NE-CZ	5.46	1.39	1.33
2	K	86	TYR	N-CA	-5.46	1.39	1.46
2	S	136	VAL	CA-C	-5.46	1.46	1.53
2	H	100	SER	N-CA	-5.46	1.38	1.46
2	M	114	CYS	C-N	5.46	1.40	1.33
2	J	60	ASP	CA-CB	5.46	1.62	1.53
2	M	149	THR	CA-C	-5.45	1.46	1.52
2	I	19	ARG	CZ-NH1	5.45	1.40	1.32
1	E	246	GLN	N-CA	-5.45	1.39	1.46
1	E	49	VAL	CA-C	5.45	1.59	1.52
1	F	102	ARG	CZ-NH2	5.44	1.40	1.33
1	D	4	LEU	C-N	5.44	1.41	1.33
2	U	88	ARG	CD-NE	5.44	1.53	1.46
2	K	39	GLY	C-N	5.44	1.41	1.33
1	F	130	ASP	N-CA	5.43	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	145	TYR	N-CA	-5.43	1.39	1.46
1	E	274	LEU	N-CA	5.43	1.52	1.46
2	R	32	ILE	N-CA	-5.43	1.40	1.46
2	H	64	ASN	CA-C	-5.42	1.46	1.52
2	L	133	VAL	N-CA	-5.42	1.39	1.46
2	I	135	HIS	CA-C	-5.42	1.45	1.52
1	D	191	GLN	CA-C	-5.42	1.45	1.52
1	B	85	GLY	CA-C	-5.42	1.46	1.51
2	V	52	ALA	CA-C	-5.42	1.45	1.52
1	E	23	ARG	CA-C	-5.42	1.46	1.52
2	N	30	HIS	CB-CG	5.42	1.57	1.50
1	D	181	SER	CA-CB	5.41	1.62	1.53
1	E	198	THR	C-N	5.41	1.41	1.33
1	E	139	GLY	CA-C	-5.41	1.47	1.52
2	L	98	ARG	CZ-NH2	5.41	1.40	1.33
2	S	143	ASN	CA-CB	5.41	1.64	1.53
2	M	114	CYS	CA-CB	5.41	1.60	1.53
1	F	56	GLY	CA-C	-5.41	1.43	1.51
2	U	159	ILE	N-CA	5.41	1.52	1.46
1	B	145	ASN	CA-CB	5.40	1.62	1.53
1	F	116	ARG	N-CA	-5.40	1.40	1.46
2	W	49	THR	CA-C	5.40	1.59	1.52
1	B	161	LYS	C-N	5.40	1.41	1.34
2	L	48	ALA	CA-C	-5.40	1.46	1.52
2	W	128	LYS	CA-CB	5.40	1.63	1.53
1	D	84	GLU	C-N	5.39	1.40	1.32
1	E	17	LEU	N-CA	-5.39	1.39	1.45
1	E	118	GLN	CA-CB	5.39	1.61	1.53
2	G	152	VAL	C-N	5.39	1.40	1.33
2	S	67	GLY	C-N	5.38	1.40	1.33
1	D	166	VAL	CA-C	-5.38	1.46	1.52
1	B	50	VAL	CA-C	-5.38	1.46	1.52
2	S	34	VAL	N-CA	-5.38	1.39	1.46
2	V	44	ALA	N-CA	-5.38	1.41	1.46
1	B	6	ASN	N-CA	-5.38	1.39	1.46
2	N	66	VAL	CA-CB	-5.38	1.47	1.54
2	P	163	MET	CA-CB	5.38	1.61	1.53
2	T	30	HIS	ND1-CE1	5.38	1.38	1.32
1	B	175	LYS	N-CA	-5.37	1.39	1.46
2	K	58	ALA	CA-C	5.37	1.59	1.52
2	M	117	ASP	C-N	5.37	1.41	1.33
2	T	113	THR	CA-C	-5.37	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	ASP	C-N	5.37	1.40	1.33
1	A	267	GLY	C-N	5.37	1.41	1.33
1	D	176	ILE	CA-CB	5.37	1.61	1.54
2	K	84	SER	C-O	5.37	1.29	1.23
2	K	44	ALA	C-N	5.37	1.39	1.33
2	P	151	GLY	C-N	5.37	1.41	1.33
2	Q	22	TYR	N-CA	-5.37	1.39	1.46
2	O	136	VAL	C-O	-5.36	1.18	1.24
2	O	162	ILE	C-N	5.36	1.40	1.33
2	P	46	LYS	C-N	5.36	1.40	1.33
2	U	73	LEU	C-N	5.36	1.41	1.33
2	J	64	ASN	CA-CB	5.36	1.61	1.53
2	R	35	ALA	N-CA	-5.36	1.39	1.46
2	R	45	GLY	N-CA	5.36	1.52	1.45
1	A	127	ALA	N-CA	-5.36	1.39	1.46
2	G	156	ASP	C-N	5.36	1.41	1.33
2	V	92	TYR	CZ-OH	5.36	1.49	1.38
2	K	98	ARG	N-CA	-5.36	1.38	1.46
2	W	88	ARG	CA-CB	5.36	1.62	1.53
1	D	50	VAL	CA-C	-5.36	1.45	1.52
1	E	21	GLU	C-N	5.36	1.41	1.33
2	K	71	GLU	N-CA	-5.36	1.39	1.45
1	D	26	LEU	C-N	-5.36	1.26	1.33
2	O	125	GLY	CA-C	-5.36	1.43	1.51
2	T	16	PRO	N-CD	5.35	1.55	1.47
2	W	41	GLU	CA-C	-5.35	1.46	1.52
2	G	98	ARG	NE-CZ	5.35	1.39	1.33
1	B	201	GLU	CA-C	-5.35	1.45	1.52
1	A	117	ALA	N-CA	-5.34	1.39	1.46
2	I	84	SER	N-CA	-5.34	1.40	1.46
2	L	70	ARG	N-CA	-5.34	1.39	1.46
2	G	32	ILE	CA-C	5.34	1.59	1.52
2	H	103	ALA	CA-C	-5.34	1.46	1.52
2	N	133	VAL	CA-CB	5.34	1.59	1.54
2	O	145	TYR	N-CA	-5.34	1.39	1.46
2	R	67	GLY	CA-C	-5.33	1.44	1.51
1	D	90	VAL	CA-C	-5.33	1.48	1.53
2	K	96	ILE	CA-C	-5.33	1.45	1.52
2	K	121	ILE	N-CA	-5.33	1.39	1.46
2	K	143	ASN	C-N	-5.33	1.26	1.33
2	M	18	VAL	CA-C	-5.33	1.45	1.52
1	E	135	SER	CA-C	5.33	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	LYS	C-N	5.33	1.40	1.34
1	B	172	VAL	CA-C	5.32	1.58	1.52
2	G	23	GLU	N-CA	-5.32	1.39	1.46
1	D	95	ILE	C-N	5.32	1.40	1.33
1	D	170	ASP	C-N	5.32	1.40	1.33
2	T	51	GLY	C-O	-5.32	1.16	1.23
2	W	92	TYR	N-CA	5.32	1.52	1.46
2	T	112	ILE	CA-C	-5.32	1.46	1.52
2	T	162	ILE	N-CA	-5.32	1.39	1.46
1	B	116	ARG	CZ-NH2	5.31	1.40	1.33
1	C	85	GLY	N-CA	-5.31	1.40	1.45
1	D	2	SER	CA-C	5.31	1.60	1.52
1	F	98	TYR	CA-C	5.31	1.59	1.52
1	B	92	THR	C-N	5.31	1.40	1.33
2	G	77	VAL	N-CA	-5.31	1.40	1.46
2	H	98	ARG	CD-NE	5.31	1.53	1.46
2	J	113	THR	N-CA	-5.30	1.39	1.46
2	X	58	ALA	CA-C	-5.30	1.46	1.52
2	X	92	TYR	N-CA	-5.30	1.39	1.46
2	O	25	ILE	CA-CB	-5.30	1.47	1.54
1	B	185	ASP	CA-CB	5.30	1.61	1.53
1	D	180	ALA	C-N	5.30	1.41	1.34
2	O	84	SER	CA-C	-5.30	1.46	1.52
1	A	154	LEU	CA-C	-5.30	1.46	1.52
1	A	248	ILE	C-N	5.30	1.40	1.34
2	R	161	PHE	C-N	5.30	1.40	1.33
2	X	75	ASP	CA-C	-5.30	1.48	1.52
1	C	204	GLN	CA-C	-5.30	1.46	1.52
2	N	76	MET	C-N	5.30	1.41	1.33
1	F	244	ASP	C-N	5.29	1.40	1.33
1	D	173	VAL	C-N	5.29	1.40	1.33
2	R	114	CYS	C-N	5.29	1.39	1.33
2	K	148	ALA	CA-CB	5.29	1.60	1.53
2	V	30	HIS	CD2-NE2	-5.29	1.32	1.37
2	J	95	ASN	CA-CB	5.29	1.60	1.53
2	L	109	GLY	C-N	5.28	1.39	1.33
2	M	30	HIS	C-N	5.28	1.40	1.33
1	A	196	PRO	C-N	5.28	1.39	1.33
2	H	94	VAL	CA-C	-5.28	1.46	1.52
2	U	51	GLY	CA-C	-5.28	1.43	1.52
2	M	28	GLY	N-CA	-5.28	1.38	1.45
2	N	62	GLY	CA-C	-5.28	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	96	ILE	C-O	-5.27	1.18	1.24
1	D	155	GLN	CA-C	-5.27	1.45	1.52
2	L	125	GLY	C-N	5.27	1.40	1.33
2	O	152	VAL	N-CA	-5.27	1.39	1.46
2	R	136	VAL	CA-CB	-5.27	1.49	1.54
1	B	100	GLN	N-CA	5.27	1.52	1.46
2	O	119	LYS	CA-C	-5.27	1.45	1.53
1	A	261	VAL	CA-C	-5.27	1.46	1.52
1	B	128	VAL	C-N	5.26	1.40	1.33
1	C	116	ARG	CZ-NH2	5.26	1.40	1.33
2	L	92	TYR	CA-CB	5.26	1.59	1.52
2	L	134	THR	CA-C	-5.26	1.45	1.52
2	U	96	ILE	N-CA	-5.26	1.39	1.46
2	O	73	LEU	N-CA	-5.26	1.39	1.46
2	L	112	ILE	C-O	-5.26	1.18	1.24
1	E	156	ARG	CZ-NH1	5.26	1.40	1.32
2	R	57	LEU	C-O	-5.26	1.18	1.24
1	F	108	GLU	N-CA	-5.25	1.39	1.46
1	A	34	ILE	CA-C	-5.25	1.46	1.52
1	B	229	VAL	C-N	5.25	1.40	1.33
1	F	251	ASP	N-CA	5.25	1.52	1.46
2	I	19	ARG	CA-C	-5.25	1.46	1.52
2	I	56	LYS	CA-C	-5.25	1.46	1.53
2	I	90	GLY	C-N	5.25	1.40	1.33
1	A	109	ARG	NE-CZ	5.25	1.38	1.33
1	C	121	ALA	CA-C	-5.25	1.46	1.52
1	D	279	ILE	CA-C	-5.25	1.47	1.52
1	E	245	ILE	CA-C	-5.25	1.46	1.52
2	H	67	GLY	CA-C	-5.25	1.45	1.52
2	O	109	GLY	C-N	5.25	1.40	1.33
1	F	75	ARG	C-N	5.25	1.40	1.33
2	I	132	VAL	CA-CB	-5.25	1.47	1.54
2	P	23	GLU	CA-C	5.25	1.58	1.52
1	C	72	ILE	CA-C	-5.24	1.46	1.52
1	B	123	ALA	C-N	5.24	1.40	1.33
1	D	136	LEU	CA-CB	5.24	1.61	1.53
1	D	124	ASP	N-CA	-5.24	1.39	1.45
1	F	18	GLU	CA-CB	5.24	1.60	1.53
2	S	158	PHE	CA-C	5.24	1.59	1.52
1	C	136	LEU	C-N	5.23	1.40	1.33
2	I	25	ILE	CA-C	-5.23	1.45	1.53
2	R	113	THR	C-O	-5.23	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	63	THR	CA-C	-5.23	1.46	1.53
2	P	79	ALA	CA-CB	5.23	1.61	1.53
1	C	37	SER	N-CA	-5.23	1.39	1.46
2	I	84	SER	CA-CB	5.23	1.61	1.53
2	V	119	LYS	CA-CB	5.23	1.62	1.53
2	S	17	TYR	C-N	5.23	1.40	1.33
2	X	132	VAL	N-CA	-5.23	1.38	1.45
1	D	65	VAL	C-N	5.23	1.41	1.33
1	D	138	GLU	CA-C	-5.23	1.46	1.52
2	T	35	ALA	CA-CB	5.23	1.62	1.53
1	A	259	GLY	C-N	5.22	1.40	1.33
2	Q	26	LEU	CA-C	-5.22	1.46	1.52
2	W	70	ARG	NE-CZ	5.22	1.38	1.33
1	C	47	LEU	CA-C	-5.22	1.46	1.52
1	E	149	ILE	CA-C	-5.22	1.47	1.52
2	M	110	ASP	C-N	5.22	1.40	1.33
2	N	87	PHE	C-N	5.22	1.40	1.33
1	C	118	GLN	C-N	5.21	1.40	1.33
2	Q	24	GLY	N-CA	-5.21	1.39	1.45
2	S	103	ALA	C-N	5.21	1.40	1.33
2	U	55	VAL	CA-CB	-5.21	1.48	1.54
2	O	59	GLY	CA-C	-5.21	1.46	1.52
2	T	115	ASP	CA-CB	5.21	1.61	1.54
1	B	156	ARG	NE-CZ	5.21	1.38	1.33
2	R	152	VAL	CA-C	-5.21	1.46	1.52
2	O	98	ARG	N-CA	-5.20	1.39	1.45
1	B	132	GLU	CA-C	-5.20	1.46	1.52
2	P	78	ASN	C-N	5.20	1.40	1.33
2	S	137	GLY	CA-C	-5.20	1.44	1.51
2	O	92	TYR	CA-CB	5.19	1.58	1.53
2	P	158	PHE	N-CA	-5.19	1.39	1.46
2	R	47	PHE	CA-CB	5.19	1.61	1.53
2	V	70	ARG	CA-C	-5.19	1.46	1.52
2	H	26	LEU	CA-CB	5.19	1.62	1.53
2	R	124	THR	CA-C	5.19	1.58	1.52
1	D	261	VAL	C-N	5.19	1.40	1.33
1	E	189	TRP	C-N	5.19	1.40	1.33
2	P	39	GLY	CA-C	-5.19	1.45	1.51
2	G	152	VAL	CA-CB	5.18	1.61	1.54
1	C	107	LYS	CA-CB	5.18	1.61	1.53
2	M	70	ARG	NE-CZ	5.18	1.38	1.33
2	M	96	ILE	CA-CB	-5.18	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	91	GLU	CA-CB	5.18	1.61	1.53
2	X	145	TYR	CA-CB	5.18	1.62	1.53
1	B	218	ILE	CB-CG1	5.18	1.63	1.53
2	Q	23	GLU	CA-C	-5.18	1.45	1.52
1	E	138	GLU	N-CA	-5.18	1.39	1.45
2	I	74	GLY	C-N	5.18	1.41	1.33
1	D	76	GLY	CA-C	-5.18	1.47	1.51
1	A	34	ILE	CA-CB	5.18	1.61	1.54
1	D	45	ARG	N-CA	-5.18	1.39	1.45
2	Q	42	GLN	CA-CB	5.18	1.61	1.53
2	T	28	GLY	CA-C	-5.18	1.45	1.51
2	H	20	LEU	C-O	-5.17	1.17	1.24
2	M	40	VAL	CA-C	-5.17	1.46	1.52
2	P	25	ILE	C-O	-5.17	1.19	1.24
2	S	31	ASP	CA-CB	5.17	1.61	1.53
1	B	32	ASN	CA-CB	5.17	1.61	1.53
1	C	267	GLY	C-N	5.17	1.41	1.33
1	F	105	GLN	CA-CB	5.17	1.61	1.53
2	H	70	ARG	CD-NE	5.17	1.53	1.46
2	N	143	ASN	CA-CB	5.17	1.61	1.53
2	Q	107	ALA	C-N	5.17	1.40	1.33
2	J	87	PHE	CA-CB	5.17	1.61	1.53
1	D	260	TRP	CA-C	-5.16	1.46	1.52
2	M	156	ASP	N-CA	-5.16	1.39	1.46
2	K	159	ILE	C-N	5.15	1.41	1.33
2	T	159	ILE	CA-CB	-5.15	1.47	1.54
2	X	47	PHE	CA-CB	5.15	1.61	1.53
1	A	60	VAL	CA-CB	-5.15	1.47	1.54
1	F	275	ALA	C-N	5.15	1.40	1.33
2	N	80	SER	CA-C	-5.15	1.46	1.52
2	S	73	LEU	CA-CB	5.15	1.62	1.53
1	A	135	SER	CA-CB	5.15	1.61	1.53
1	E	232	ASP	C-N	5.15	1.40	1.33
2	V	36	GLY	CA-C	-5.15	1.44	1.51
2	W	126	THR	N-CA	-5.15	1.39	1.46
1	E	120	ARG	CZ-NH2	5.14	1.40	1.33
2	H	83	ALA	N-CA	-5.14	1.39	1.45
1	D	235	PHE	CA-CB	5.14	1.61	1.53
2	J	143	ASN	CA-C	-5.14	1.46	1.52
1	C	166	VAL	CA-C	-5.14	1.46	1.52
1	A	42	GLY	C-N	5.14	1.39	1.33
2	M	23	GLU	CA-C	-5.14	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	86	TYR	N-CA	5.14	1.52	1.46
2	S	130	LEU	CA-CB	5.14	1.62	1.53
2	S	106	ILE	CA-CB	-5.13	1.50	1.55
2	T	134	THR	N-CA	-5.13	1.39	1.46
2	V	116	ALA	CA-CB	-5.13	1.46	1.54
1	E	157	ALA	N-CA	-5.13	1.40	1.46
2	W	140	ARG	NE-CZ	5.13	1.38	1.33
2	T	52	ALA	CA-C	-5.13	1.46	1.52
1	B	47	LEU	CA-C	-5.13	1.46	1.52
2	I	70	ARG	CZ-NH1	5.12	1.40	1.32
2	K	110	ASP	CA-C	-5.12	1.46	1.52
2	I	104	ALA	N-CA	-5.12	1.39	1.45
1	C	225	ASN	N-CA	-5.12	1.40	1.46
1	F	242	ARG	N-CA	-5.12	1.40	1.46
2	J	151	GLY	C-N	5.12	1.40	1.33
2	V	57	LEU	C-N	5.12	1.41	1.33
2	I	23	GLU	CA-CB	5.12	1.61	1.53
2	L	113	THR	CA-CB	-5.12	1.46	1.53
2	X	23	GLU	CA-CB	-5.12	1.45	1.53
2	W	126	THR	C-N	5.12	1.41	1.33
2	X	159	ILE	CA-C	-5.12	1.46	1.52
1	A	175	LYS	CA-CB	5.12	1.61	1.53
1	F	108	GLU	CA-C	5.12	1.59	1.52
2	P	57	LEU	CA-CB	5.12	1.61	1.53
2	H	163	MET	CA-C	-5.11	1.46	1.52
2	O	120	MET	CA-C	-5.11	1.46	1.52
2	U	107	ALA	C-N	5.11	1.40	1.33
1	D	34	ILE	N-CA	-5.11	1.40	1.46
2	W	147	LYS	CA-CB	5.11	1.62	1.53
2	H	18	VAL	N-CA	-5.11	1.39	1.46
2	P	149	THR	CA-C	5.11	1.59	1.52
1	A	27	ALA	C-N	5.10	1.40	1.33
2	O	45	GLY	C-N	5.10	1.39	1.33
1	A	269	ALA	N-CA	-5.10	1.39	1.46
2	K	92	TYR	CZ-OH	5.10	1.48	1.38
2	M	70	ARG	CD-NE	5.10	1.53	1.46
1	B	110	ARG	NE-CZ	5.10	1.38	1.33
2	G	117	ASP	CA-CB	5.10	1.62	1.53
2	N	116	ALA	CA-C	5.10	1.59	1.53
1	A	105	GLN	CA-C	5.10	1.59	1.52
2	T	151	GLY	C-N	5.10	1.40	1.33
2	G	32	ILE	N-CA	-5.10	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	187	ARG	CD-NE	5.09	1.53	1.46
2	L	26	LEU	CA-CB	5.09	1.60	1.53
2	J	141	ALA	N-CA	5.09	1.52	1.46
2	G	124	THR	N-CA	-5.09	1.40	1.46
2	R	74	GLY	C-N	5.09	1.40	1.33
2	L	90	GLY	CA-C	-5.09	1.45	1.52
2	O	61	ASN	CA-CB	5.09	1.62	1.53
1	A	170	ASP	CA-C	-5.09	1.45	1.52
1	C	54	PRO	N-CA	-5.09	1.40	1.47
1	C	94	GLU	N-CA	-5.09	1.40	1.46
2	R	33	ASP	N-CA	-5.09	1.42	1.47
2	V	103	ALA	CA-C	-5.09	1.46	1.52
1	E	43	VAL	C-N	5.08	1.40	1.33
2	W	126	THR	CA-C	-5.08	1.46	1.52
1	F	7	GLN	N-CA	-5.08	1.39	1.46
1	F	51	ASP	CA-CB	5.08	1.61	1.53
2	U	85	PHE	N-CA	-5.08	1.39	1.46
2	V	72	ASP	N-CA	-5.08	1.39	1.45
2	S	48	ALA	CA-CB	5.07	1.60	1.53
1	C	93	PHE	CA-CB	5.07	1.61	1.53
2	N	115	ASP	CA-CB	5.07	1.61	1.54
2	T	23	GLU	C-N	5.07	1.41	1.33
2	G	158	PHE	CB-CG	5.07	1.62	1.50
2	J	51	GLY	N-CA	-5.07	1.38	1.45
2	W	60	ASP	CA-C	-5.07	1.46	1.52
1	D	229	VAL	C-N	5.07	1.40	1.33
2	M	148	ALA	CA-CB	5.07	1.62	1.53
2	N	68	LEU	CA-C	-5.07	1.46	1.52
2	W	56	LYS	CA-C	-5.07	1.46	1.53
1	D	113	VAL	C-N	5.07	1.40	1.33
2	L	82	LYS	C-N	5.07	1.40	1.33
1	C	8	GLU	N-CA	-5.06	1.39	1.46
1	C	110	ARG	CD-NE	5.06	1.53	1.46
2	P	49	THR	N-CA	-5.06	1.40	1.46
1	B	89	GLN	C-N	5.06	1.37	1.32
2	R	128	LYS	C-N	5.06	1.38	1.33
2	K	46	LYS	CA-CB	5.06	1.63	1.53
1	A	263	TYR	C-N	5.06	1.40	1.33
1	C	136	LEU	N-CA	-5.06	1.40	1.46
1	D	96	VAL	CA-C	-5.06	1.46	1.52
2	N	120	MET	C-N	5.05	1.40	1.33
2	S	70	ARG	NE-CZ	5.05	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	98	ARG	CZ-NH1	5.05	1.39	1.32
2	I	102	THR	C-N	5.05	1.40	1.33
2	W	38	ASN	C-O	-5.05	1.17	1.24
1	C	121	ALA	C-N	5.05	1.37	1.32
1	A	248	ILE	CA-C	5.05	1.58	1.52
2	I	45	GLY	N-CA	-5.05	1.39	1.45
2	M	25	ILE	CA-C	-5.05	1.46	1.52
2	R	146	GLU	C-N	5.05	1.40	1.33
2	Q	57	LEU	C-O	-5.04	1.17	1.24
1	A	76	GLY	CA-C	-5.04	1.47	1.51
1	C	119	GLN	C-O	-5.04	1.18	1.24
2	G	148	ALA	C-N	5.04	1.40	1.33
2	N	27	ASN	C-N	5.04	1.40	1.33
1	C	56	GLY	C-N	5.04	1.40	1.33
2	P	107	ALA	CA-C	-5.04	1.46	1.52
2	G	163	MET	C-N	5.04	1.40	1.33
2	M	136	VAL	N-CA	-5.04	1.39	1.46
2	V	74	GLY	CA-C	-5.04	1.46	1.52
1	D	187	ARG	CZ-NH2	5.04	1.40	1.33
1	F	116	ARG	C-N	5.04	1.40	1.33
2	U	39	GLY	CA-C	-5.04	1.44	1.52
1	C	192	ASN	CA-C	-5.04	1.46	1.52
1	A	172	VAL	CA-C	-5.03	1.46	1.52
2	O	104	ALA	N-CA	-5.03	1.39	1.46
1	C	87	ARG	CD-NE	5.03	1.53	1.46
1	C	194	PHE	CA-C	5.03	1.59	1.52
2	X	162	ILE	CA-C	-5.03	1.46	1.52
2	N	105	GLY	CA-C	-5.03	1.44	1.51
2	U	91	GLU	C-N	5.03	1.40	1.33
2	P	30	HIS	CD2-NE2	5.03	1.43	1.37
2	X	36	GLY	CA-C	-5.03	1.44	1.51
1	F	153	GLY	CA-C	-5.03	1.46	1.52
2	Q	56	LYS	CA-C	-5.03	1.46	1.52
2	M	145	TYR	CA-C	-5.02	1.48	1.52
2	W	100	SER	C-N	5.02	1.40	1.33
1	A	177	VAL	CA-CB	-5.02	1.48	1.54
2	J	98	ARG	NE-CZ	5.02	1.38	1.33
2	U	72	ASP	CA-C	-5.02	1.46	1.53
1	E	77	GLN	N-CA	-5.01	1.39	1.46
2	V	19	ARG	CA-CB	5.01	1.61	1.53
1	C	19	THR	N-CA	-5.01	1.39	1.46
2	H	142	GLY	CA-C	-5.01	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	155	THR	N-CA	-5.01	1.40	1.46
2	V	112	ILE	C-N	5.01	1.40	1.33
1	C	138	GLU	CA-CB	5.00	1.61	1.53
1	A	213	THR	C-O	5.00	1.30	1.23
2	N	65	ALA	C-N	5.00	1.40	1.33
1	D	200	HIS	CG-CD2	5.00	1.41	1.35
2	Q	135	HIS	ND1-CE1	5.00	1.37	1.32

All (2204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	ASP	CA-CB-CG	16.94	129.54	112.60
1	A	55	GLN	CG-CD-OE1	-15.97	88.87	120.80
1	A	55	GLN	CG-CD-NE2	14.57	138.25	116.40
1	E	75	ARG	CA-C-N	13.81	132.25	121.61
1	E	75	ARG	C-N-CA	13.81	132.25	121.61
1	C	86	ASP	CA-CB-CG	12.97	125.58	112.60
2	H	32	ILE	N-CA-C	-12.97	100.81	113.53
2	O	34	VAL	CA-C-N	12.96	146.30	121.54
2	O	34	VAL	C-N-CA	12.96	146.30	121.54
2	O	35	ALA	CB-CA-C	-12.29	85.96	110.42
2	O	35	ALA	N-CA-CB	12.09	130.93	110.49
1	E	194	PHE	CA-CB-CG	12.05	125.85	113.80
2	J	69	PHE	CA-CB-CG	-11.87	101.93	113.80
2	P	136	VAL	N-CA-C	-11.70	101.67	112.43
2	T	60	ASP	CA-CB-CG	11.66	124.26	112.60
2	G	123	PHE	CA-CB-CG	-11.60	102.20	113.80
2	K	126	THR	O-C-N	11.32	135.76	122.85
2	O	35	ALA	N-CA-C	11.11	134.47	110.80
2	Q	136	VAL	N-CA-C	-11.01	101.94	112.29
2	S	161	PHE	CA-C-N	10.95	135.18	120.50
2	S	161	PHE	C-N-CA	10.95	135.18	120.50
1	B	75	ARG	CA-C-N	10.68	129.83	121.61
1	B	75	ARG	C-N-CA	10.68	129.83	121.61
2	O	55	VAL	N-CA-C	-10.65	102.05	112.17
2	O	110	ASP	CA-CB-CG	10.56	123.16	112.60
1	A	245	ILE	N-CA-C	-10.45	102.96	113.10
1	D	242	ARG	NE-CZ-NH2	10.24	128.42	119.20
2	V	161	PHE	N-CA-C	-10.24	93.50	109.07
1	A	55	GLN	OE1-CD-NE2	10.19	132.79	122.60
2	R	75	ASP	CA-CB-CG	-10.19	102.41	112.60
2	G	135	HIS	CA-CB-CG	-10.17	103.63	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	270	VAL	N-CA-C	-10.08	103.29	113.47
2	P	61	ASN	N-CA-C	-10.05	100.76	113.43
1	D	75	ARG	CA-C-N	10.00	129.31	121.61
1	D	75	ARG	C-N-CA	10.00	129.31	121.61
2	M	94	VAL	N-CA-CB	10.00	123.53	110.13
1	A	128	VAL	N-CA-C	-9.97	103.63	113.20
2	H	18	VAL	N-CA-C	-9.96	102.97	112.83
1	A	226	THR	CA-C-N	9.88	133.00	120.56
1	A	226	THR	C-N-CA	9.88	133.00	120.56
2	R	136	VAL	N-CA-C	-9.70	102.86	113.43
2	T	161	PHE	CA-CB-CG	9.67	123.47	113.80
2	S	64	ASN	CA-CB-CG	-9.63	102.97	112.60
1	A	96	VAL	N-CA-C	9.59	119.54	110.53
1	B	152	GLY	CA-C-N	9.55	130.58	119.98
1	B	152	GLY	C-N-CA	9.55	130.58	119.98
2	J	64	ASN	OD1-CG-ND2	9.52	132.12	122.60
1	F	94	GLU	CA-C-N	9.49	133.90	120.42
1	F	94	GLU	C-N-CA	9.49	133.90	120.42
2	X	132	VAL	O-C-N	9.45	132.84	122.92
1	F	108	GLU	CA-C-N	9.43	132.70	120.44
1	F	108	GLU	C-N-CA	9.43	132.70	120.44
2	V	38	ASN	CA-CB-CG	-9.41	103.19	112.60
2	L	92	TYR	CA-C-N	9.39	137.03	122.94
2	L	92	TYR	C-N-CA	9.39	137.03	122.94
1	B	93	PHE	CA-C-N	9.36	132.61	120.44
1	B	93	PHE	C-N-CA	9.36	132.61	120.44
1	A	16	ALA	N-CA-CB	9.28	126.17	110.49
1	D	133	ILE	N-CA-CB	9.27	120.80	110.51
1	A	142	THR	CA-C-N	9.27	133.63	120.28
1	A	142	THR	C-N-CA	9.27	133.63	120.28
1	A	176	ILE	CB-CA-C	9.24	123.79	111.97
2	W	61	ASN	CA-C-N	9.21	130.13	120.00
2	W	61	ASN	C-N-CA	9.21	130.13	120.00
2	G	20	LEU	CA-C-N	9.18	128.73	119.92
2	G	20	LEU	C-N-CA	9.18	128.73	119.92
2	R	158	PHE	CA-CB-CG	-9.15	104.65	113.80
2	W	72	ASP	N-CA-C	-9.13	99.46	113.89
2	Q	27	ASN	CA-C-O	9.12	130.18	119.32
1	B	261	VAL	N-CA-C	-9.05	95.47	108.42
2	N	50	ILE	N-CA-C	-9.01	92.95	107.28
1	D	150	SER	CA-C-N	8.97	132.30	120.28
1	D	150	SER	C-N-CA	8.97	132.30	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	HIS	CE1-NE2-CD2	-8.96	100.04	109.00
1	E	236	VAL	CA-C-N	8.90	134.76	121.05
1	E	236	VAL	C-N-CA	8.90	134.76	121.05
2	N	121	ILE	CA-CB-CG1	8.87	125.48	110.40
1	A	175	LYS	CA-C-N	8.87	131.73	120.56
1	A	175	LYS	C-N-CA	8.87	131.73	120.56
1	B	80	ASP	CA-C-O	-8.87	111.86	121.44
2	R	38	ASN	O-C-N	-8.81	113.02	122.00
1	B	120	ARG	N-CA-C	8.80	120.87	111.28
2	S	75	ASP	CA-CB-CG	8.79	121.39	112.60
2	O	86	TYR	N-CA-C	-8.77	100.46	113.61
2	I	117	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	233	PRO	CA-C-O	-8.71	111.03	121.48
1	E	169	HIS	ND1-CE1-NE2	8.71	117.11	108.40
2	G	95	ASN	N-CA-CB	8.70	124.60	110.43
1	B	200	HIS	CB-CG-CD2	-8.69	119.91	131.20
1	F	158	ALA	N-CA-C	8.68	120.74	111.28
1	E	246	GLN	N-CA-C	-8.65	96.71	108.38
1	D	71	VAL	N-CA-C	-8.62	94.66	107.51
2	X	140	ARG	CA-C-N	8.62	133.02	120.95
2	X	140	ARG	C-N-CA	8.62	133.02	120.95
1	C	45	ARG	N-CA-CB	8.61	125.81	110.83
2	H	57	LEU	N-CA-C	-8.61	95.50	109.96
1	E	164	GLN	CA-C-N	8.59	133.37	120.31
1	E	164	GLN	C-N-CA	8.59	133.37	120.31
2	W	153	THR	CA-C-O	-8.58	112.18	121.44
1	A	217	LEU	CA-C-N	8.57	132.82	120.91
1	A	217	LEU	C-N-CA	8.57	132.82	120.91
1	E	148	THR	CA-C-N	8.57	132.30	122.36
1	E	148	THR	C-N-CA	8.57	132.30	122.36
1	A	199	GLN	N-CA-C	-8.56	95.98	109.50
2	L	102	THR	N-CA-C	-8.55	95.56	108.46
2	W	72	ASP	CA-CB-CG	-8.54	104.06	112.60
1	E	184	ALA	N-CA-C	8.54	121.53	111.71
2	M	105	GLY	O-C-N	8.54	129.37	122.71
2	H	60	ASP	CA-C-O	-8.53	112.48	121.87
2	O	30	HIS	CA-CB-CG	-8.53	105.27	113.80
2	T	143	ASN	CA-CB-CG	-8.53	104.07	112.60
2	O	60	ASP	CA-CB-CG	8.50	121.10	112.60
2	T	75	ASP	N-CA-CB	8.50	120.12	110.35
2	U	29	ALA	N-CA-CB	8.50	124.85	110.49
1	F	211	ILE	N-CA-C	-8.47	96.31	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	90	VAL	O-C-N	-8.43	116.06	121.37
2	S	54	GLY	CA-C-N	8.41	131.27	122.27
2	S	54	GLY	C-N-CA	8.41	131.27	122.27
2	T	95	ASN	CA-CB-CG	-8.41	104.19	112.60
2	L	88	ARG	NE-CZ-NH2	8.40	126.76	119.20
2	M	142	GLY	O-C-N	8.39	130.56	122.92
1	C	156	ARG	CA-C-N	8.39	131.52	120.28
1	C	156	ARG	C-N-CA	8.39	131.52	120.28
2	K	161	PHE	CA-CB-CG	8.38	122.19	113.80
2	V	95	ASN	CA-CB-CG	8.37	120.97	112.60
2	O	123	PHE	CA-CB-CG	-8.35	105.45	113.80
2	T	147	LYS	N-CA-C	-8.35	97.47	110.42
1	E	90	VAL	O-C-N	-8.35	114.01	121.61
1	B	162	ALA	CA-C-N	8.33	131.44	120.28
1	B	162	ALA	C-N-CA	8.33	131.44	120.28
1	C	78	VAL	CA-C-O	-8.32	112.82	119.98
1	C	87	ARG	CA-C-N	8.32	133.51	123.19
1	C	87	ARG	C-N-CA	8.32	133.51	123.19
2	M	66	VAL	N-CA-C	-8.31	96.53	108.17
1	E	276	ILE	N-CA-C	-8.31	96.16	108.45
2	M	146	GLU	CA-C-O	-8.26	111.80	121.46
2	V	143	ASN	O-C-N	8.26	128.50	121.65
1	B	183	PHE	N-CA-C	8.24	120.26	111.28
2	U	46	LYS	N-CA-CB	8.23	124.39	110.49
1	F	128	VAL	N-CA-C	-8.21	104.87	112.43
1	A	174	THR	CA-C-N	8.21	133.16	121.42
1	A	174	THR	C-N-CA	8.21	133.16	121.42
2	K	108	ALA	N-CA-C	8.19	121.48	110.35
2	H	44	ALA	CA-C-N	8.18	129.78	120.53
2	H	44	ALA	C-N-CA	8.18	129.78	120.53
2	P	30	HIS	CE1-NE2-CD2	-8.18	100.82	109.00
1	B	156	ARG	NE-CZ-NH1	8.17	129.67	121.50
2	H	158	PHE	CB-CA-C	-8.17	97.79	110.37
1	D	89	GLN	CA-C-N	8.16	128.46	122.59
1	D	89	GLN	C-N-CA	8.16	128.46	122.59
2	H	141	ALA	CA-C-N	8.13	131.64	121.06
2	H	141	ALA	C-N-CA	8.13	131.64	121.06
2	X	84	SER	N-CA-C	-8.13	95.78	108.14
1	D	128	VAL	N-CA-C	-8.13	104.95	112.43
1	E	106	VAL	CA-C-N	8.13	131.01	120.44
1	E	106	VAL	C-N-CA	8.13	131.01	120.44
2	G	40	VAL	CA-C-O	-8.12	112.58	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	143	ASN	CA-CB-CG	-8.11	104.49	112.60
2	S	147	LYS	N-CA-C	-8.11	101.50	112.94
2	N	116	ALA	N-CA-C	-8.10	97.74	108.19
2	X	89	GLY	N-CA-C	-8.10	96.95	110.80
1	B	200	HIS	CB-CG-ND1	8.09	134.83	122.70
1	A	145	ASN	CA-CB-CG	-8.09	104.51	112.60
2	Q	130	LEU	CA-C-N	8.08	127.78	120.10
2	Q	130	LEU	C-N-CA	8.08	127.78	120.10
2	K	73	LEU	N-CA-C	-8.08	97.00	109.52
2	R	53	ASN	CA-CB-CG	-8.08	104.52	112.60
1	C	84	GLU	CA-C-N	8.07	131.93	121.27
1	C	84	GLU	C-N-CA	8.07	131.93	121.27
2	I	17	TYR	CA-C-N	8.06	131.30	120.50
2	I	17	TYR	C-N-CA	8.06	131.30	120.50
1	F	135	SER	N-CA-C	-8.05	102.45	111.14
2	M	120	MET	N-CA-CB	8.04	124.17	110.50
1	C	235	PHE	CA-CB-CG	8.04	121.84	113.80
2	R	34	VAL	N-CA-C	-8.04	96.01	107.75
1	C	227	VAL	N-CA-C	8.03	118.81	110.62
1	C	106	VAL	CB-CA-C	-8.03	101.30	112.14
2	R	31	ASP	CA-CB-CG	8.02	120.62	112.60
2	L	33	ASP	N-CA-C	-7.98	102.50	112.72
2	G	111	GLU	N-CA-CB	7.96	122.28	109.95
2	R	67	GLY	CA-C-N	7.96	132.01	120.71
2	R	67	GLY	C-N-CA	7.96	132.01	120.71
2	S	42	GLN	CA-C-N	7.94	130.92	120.28
2	S	42	GLN	C-N-CA	7.94	130.92	120.28
2	K	140	ARG	NE-CZ-NH2	7.93	126.34	119.20
1	A	273	SER	N-CA-C	-7.92	93.93	110.80
2	N	84	SER	N-CA-C	-7.92	103.76	113.50
2	Q	51	GLY	N-CA-C	-7.90	101.70	112.52
1	F	89	GLN	OE1-CD-NE2	-7.87	114.73	122.60
2	S	78	ASN	N-CA-C	-7.86	97.89	108.74
1	C	136	LEU	N-CA-C	7.85	119.91	111.36
2	S	123	PHE	CA-C-N	7.85	133.80	121.56
2	S	123	PHE	C-N-CA	7.85	133.80	121.56
2	X	144	MET	N-CA-CB	7.85	123.75	110.49
1	D	236	VAL	CA-C-N	7.85	130.53	120.64
1	D	236	VAL	C-N-CA	7.85	130.53	120.64
2	J	128	LYS	N-CA-C	7.84	121.12	109.59
2	O	41	GLU	N-CA-CB	7.83	123.72	110.49
1	B	276	ILE	CA-CB-CG1	7.82	123.70	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	78	ASN	CA-C-N	7.82	131.85	120.82
2	O	78	ASN	C-N-CA	7.82	131.85	120.82
1	D	250	ALA	CA-C-N	7.82	130.60	120.44
1	D	250	ALA	C-N-CA	7.82	130.60	120.44
2	O	30	HIS	CE1-NE2-CD2	-7.82	101.19	109.00
1	C	202	VAL	CA-C-O	-7.81	113.64	121.45
1	A	88	ILE	N-CA-C	-7.81	97.24	108.17
2	U	31	ASP	CA-CB-CG	7.80	120.40	112.60
1	E	261	VAL	CB-CA-C	-7.79	100.97	111.80
2	G	60	ASP	N-CA-C	-7.79	101.94	113.40
1	F	80	ASP	CA-C-O	-7.79	113.29	121.55
1	F	200	HIS	ND1-CE1-NE2	7.79	116.19	108.40
1	A	262	ILE	N-CA-C	-7.77	96.93	108.12
2	R	57	LEU	CA-C-N	7.77	136.38	121.54
2	R	57	LEU	C-N-CA	7.77	136.38	121.54
2	G	161	PHE	CA-CB-CG	-7.76	106.04	113.80
1	F	85	GLY	N-CA-C	-7.76	98.92	110.87
1	E	159	LEU	CB-CA-C	-7.75	97.92	110.79
2	Q	101	LEU	N-CA-C	-7.75	102.88	112.88
2	L	72	ASP	N-CA-C	-7.74	104.26	112.93
2	P	54	GLY	N-CA-C	-7.74	104.03	114.95
2	O	100	SER	N-CA-C	-7.74	101.77	112.30
1	F	151	SER	CA-C-N	7.73	128.50	120.00
1	F	151	SER	C-N-CA	7.73	128.50	120.00
2	G	78	ASN	CA-CB-CG	7.70	120.30	112.60
1	E	151	SER	CA-C-N	7.68	128.45	120.00
1	E	151	SER	C-N-CA	7.68	128.45	120.00
2	H	75	ASP	N-CA-C	-7.68	104.81	114.56
1	D	72	ILE	O-C-N	7.67	131.47	123.18
1	C	3	GLN	OE1-CD-NE2	7.67	130.27	122.60
2	T	147	LYS	CA-C-N	7.67	131.71	120.90
2	T	147	LYS	C-N-CA	7.67	131.71	120.90
2	U	54	GLY	N-CA-C	-7.66	95.02	113.18
1	A	186	ILE	CA-CB-CG2	7.65	123.51	110.50
2	N	41	GLU	CA-C-N	7.65	131.57	120.71
2	N	41	GLU	C-N-CA	7.65	131.57	120.71
1	B	200	HIS	CA-CB-CG	7.62	121.42	113.80
1	F	173	VAL	N-CA-CB	7.62	120.94	111.41
2	G	27	ASN	OD1-CG-ND2	7.60	130.20	122.60
1	A	87	ARG	NE-CZ-NH2	-7.60	112.36	119.20
1	B	212	TRP	CA-C-O	7.59	128.67	120.32
1	B	172	VAL	CA-C-N	7.59	132.36	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	VAL	C-N-CA	7.59	132.36	122.95
1	D	279	ILE	N-CA-C	-7.58	105.93	113.20
2	M	61	ASN	N-CA-C	-7.57	104.06	113.38
1	A	144	VAL	CA-C-N	7.55	132.67	121.72
1	A	144	VAL	C-N-CA	7.55	132.67	121.72
1	D	226	THR	CA-C-N	7.55	130.81	120.46
1	D	226	THR	C-N-CA	7.55	130.81	120.46
2	T	63	THR	CA-C-N	7.55	132.15	120.75
2	T	63	THR	C-N-CA	7.55	132.15	120.75
1	B	239	MET	CA-C-O	-7.54	112.52	120.28
1	F	31	ALA	CA-C-N	7.53	129.12	119.78
1	F	31	ALA	C-N-CA	7.53	129.12	119.78
1	D	111	PHE	CB-CA-C	-7.53	98.30	110.79
2	I	33	ASP	CA-CB-CG	7.52	120.12	112.60
2	V	110	ASP	N-CA-C	-7.52	97.98	109.41
1	D	120	ARG	N-CA-C	7.51	119.47	111.28
1	C	262	ILE	N-CA-C	-7.50	97.32	108.12
1	F	84	GLU	CA-C-N	7.49	131.16	121.27
1	F	84	GLU	C-N-CA	7.49	131.16	121.27
1	B	200	HIS	N-CA-C	-7.49	103.08	114.16
1	F	4	LEU	N-CA-C	-7.48	104.18	113.38
1	C	246	GLN	CA-C-N	7.47	130.56	120.77
1	C	246	GLN	C-N-CA	7.47	130.56	120.77
2	S	153	THR	N-CA-C	-7.47	94.88	107.80
1	E	218	ILE	CA-C-N	7.46	132.96	122.36
1	E	218	ILE	C-N-CA	7.46	132.96	122.36
1	A	270	VAL	O-C-N	-7.46	114.74	122.20
1	A	270	VAL	CA-C-N	7.45	132.25	121.52
1	A	270	VAL	C-N-CA	7.45	132.25	121.52
1	D	175	LYS	CA-C-N	7.45	130.66	120.46
1	D	175	LYS	C-N-CA	7.45	130.66	120.46
2	N	154	ASP	CA-CB-CG	-7.45	105.15	112.60
1	F	246	GLN	CA-C-N	7.44	130.00	120.70
1	F	246	GLN	C-N-CA	7.44	130.00	120.70
1	F	86	ASP	N-CA-C	-7.44	97.74	109.50
2	Q	35	ALA	N-CA-CB	7.43	123.06	110.49
2	M	164	TYR	N-CA-CB	7.43	123.05	110.49
2	K	36	GLY	CA-C-O	-7.41	113.13	122.61
1	C	61	TYR	N-CA-C	7.41	119.37	110.19
1	B	133	ILE	CA-C-N	7.40	130.20	120.28
1	B	133	ILE	C-N-CA	7.40	130.20	120.28
2	J	53	ASN	CA-CB-CG	-7.40	105.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	39	ASP	N-CA-C	-7.40	99.57	110.52
2	Q	49	THR	N-CA-C	-7.40	104.28	113.38
2	V	126	THR	N-CA-C	-7.40	97.89	109.72
2	P	72	ASP	CA-CB-CG	-7.39	105.21	112.60
2	Q	31	ASP	N-CA-C	-7.39	104.78	114.31
2	J	40	VAL	N-CA-C	-7.38	105.64	112.43
2	P	144	MET	N-CA-CB	7.38	122.97	110.49
1	B	137	LEU	N-CA-C	7.38	120.27	110.53
1	E	225	ASN	CA-C-N	7.38	130.49	120.38
1	E	225	ASN	C-N-CA	7.38	130.49	120.38
2	L	47	PHE	CA-CB-CG	7.37	121.17	113.80
1	F	210	HIS	CB-CG-CD2	-7.37	121.62	131.20
2	I	32	ILE	N-CA-C	-7.37	105.65	112.43
2	L	84	SER	CA-C-O	-7.36	110.76	119.15
1	B	264	GLU	CA-C-O	7.35	129.17	121.38
2	L	117	ASP	CA-CB-CG	7.35	119.95	112.60
2	Q	95	ASN	CA-C-N	7.35	130.63	120.49
2	Q	95	ASN	C-N-CA	7.35	130.63	120.49
2	V	63	THR	CA-C-O	-7.34	112.36	120.81
2	G	155	THR	N-CA-C	-7.34	104.18	113.72
2	S	95	ASN	N-CA-CB	7.33	122.26	110.16
2	H	70	ARG	CA-C-N	7.33	131.28	120.87
2	H	70	ARG	C-N-CA	7.33	131.28	120.87
1	C	242	ARG	NE-CZ-NH1	7.32	128.82	121.50
1	F	134	PHE	CA-C-N	7.32	130.40	120.44
1	F	134	PHE	C-N-CA	7.32	130.40	120.44
1	F	192	ASN	CA-C-O	7.32	128.41	120.43
2	P	53	ASN	N-CA-C	-7.32	97.94	109.50
2	H	74	GLY	CA-C-N	7.31	133.27	122.08
2	H	74	GLY	C-N-CA	7.31	133.27	122.08
2	M	26	LEU	N-CA-C	-7.31	103.97	114.12
1	A	279	ILE	CA-C-O	7.30	125.73	119.38
2	S	101	LEU	CA-C-N	7.30	133.27	123.05
2	S	101	LEU	C-N-CA	7.30	133.27	123.05
2	L	140	ARG	CA-C-N	7.30	131.17	120.95
2	L	140	ARG	C-N-CA	7.30	131.17	120.95
2	K	109	GLY	N-CA-C	-7.29	104.53	115.32
2	J	140	ARG	NE-CZ-NH2	-7.29	112.64	119.20
2	M	105	GLY	CA-C-O	-7.29	114.60	122.76
2	O	158	PHE	CA-CB-CG	-7.26	106.54	113.80
1	F	101	VAL	O-C-N	7.25	128.91	121.87
2	O	81	GLU	N-CA-C	-7.25	104.96	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	ASP	CA-C-O	-7.25	113.61	121.44
2	K	85	PHE	CA-CB-CG	-7.25	106.55	113.80
2	W	112	ILE	N-CA-C	-7.24	98.06	108.42
1	B	143	ALA	CA-C-O	-7.24	112.87	120.55
1	B	279	ILE	N-CA-C	-7.24	105.66	112.83
2	L	35	ALA	CA-C-O	-7.24	113.62	121.44
2	P	40	VAL	N-CA-C	-7.23	104.48	112.80
1	A	270	VAL	N-CA-C	-7.20	104.36	113.22
2	U	30	HIS	CA-C-N	7.19	132.85	122.35
2	U	30	HIS	C-N-CA	7.19	132.85	122.35
2	G	153	THR	N-CA-C	-7.19	103.60	112.88
2	L	117	ASP	N-CA-CB	7.19	122.64	110.49
1	E	211	ILE	CA-C-O	-7.18	112.86	120.48
2	R	133	VAL	CA-C-N	7.18	129.78	120.44
2	R	133	VAL	C-N-CA	7.18	129.78	120.44
1	D	169	HIS	CG-CD2-NE2	7.18	114.38	107.20
2	N	115	ASP	N-CA-C	-7.18	98.16	108.07
1	B	69	ALA	CA-C-N	7.18	132.76	121.56
1	B	69	ALA	C-N-CA	7.18	132.76	121.56
1	E	121	ALA	N-CA-C	7.18	119.00	111.03
1	E	276	ILE	CA-C-O	7.18	128.66	120.76
2	V	149	THR	N-CA-C	-7.17	103.09	112.41
2	P	98	ARG	NE-CZ-NH1	7.16	128.66	121.50
2	U	85	PHE	CA-CB-CG	-7.16	106.64	113.80
2	J	84	SER	CA-C-O	-7.16	113.57	121.23
2	P	48	ALA	CA-C-O	7.16	128.02	120.36
2	U	32	ILE	CA-C-N	7.15	135.20	121.54
2	U	32	ILE	C-N-CA	7.15	135.20	121.54
2	N	120	MET	N-CA-CB	7.15	121.16	110.29
1	D	169	HIS	ND1-CE1-NE2	7.14	115.55	108.40
2	J	161	PHE	CA-CB-CG	7.14	120.94	113.80
2	U	160	GLY	N-CA-C	-7.14	104.99	115.63
2	S	93	TYR	O-C-N	-7.14	113.97	122.96
2	M	162	ILE	O-C-N	-7.13	115.11	123.03
2	P	43	LEU	N-CA-C	-7.12	103.90	112.59
2	G	161	PHE	N-CA-C	-7.12	98.49	109.52
2	V	121	ILE	CA-C-O	7.12	128.99	120.67
2	J	53	ASN	N-CA-C	-7.11	98.20	109.23
2	Q	78	ASN	OD1-CG-ND2	7.11	129.71	122.60
2	H	98	ARG	N-CA-C	-7.11	103.17	112.41
1	E	261	VAL	CA-C-O	7.11	126.93	120.96
1	F	208	PHE	CA-C-N	7.11	127.09	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	208	PHE	C-N-CA	7.11	127.09	120.34
1	C	70	PHE	N-CA-C	-7.10	98.28	109.07
1	E	87	ARG	CA-C-O	-7.09	112.50	120.66
1	C	239	MET	O-C-N	-7.09	114.83	122.06
2	K	126	THR	CA-C-N	7.09	127.76	120.60
2	K	126	THR	C-N-CA	7.09	127.76	120.60
2	L	84	SER	O-C-N	7.09	131.70	122.42
2	W	52	ALA	CA-C-N	7.08	130.87	120.95
2	W	52	ALA	C-N-CA	7.08	130.87	120.95
2	J	33	ASP	N-CA-C	-7.08	105.17	114.31
2	Q	81	GLU	CA-C-N	7.08	132.49	122.72
2	Q	81	GLU	C-N-CA	7.08	132.49	122.72
2	K	88	ARG	NE-CZ-NH2	-7.07	112.83	119.20
2	X	44	ALA	N-CA-C	-7.07	98.27	109.23
2	T	63	THR	N-CA-C	-7.06	103.98	112.59
1	E	107	LYS	N-CA-CB	7.05	120.23	110.01
2	Q	77	VAL	N-CA-C	-7.05	98.00	108.85
1	B	163	PHE	CA-CB-CG	-7.04	106.76	113.80
1	A	227	VAL	N-CA-C	-7.04	103.66	110.42
2	R	64	ASN	N-CA-C	-7.04	104.96	113.97
2	P	48	ALA	CA-C-N	7.04	133.57	122.60
2	P	48	ALA	C-N-CA	7.04	133.57	122.60
1	F	100	GLN	CA-C-O	-7.03	113.09	120.55
2	L	124	THR	CA-C-O	-7.03	113.73	121.33
1	B	21	GLU	CA-C-N	7.03	126.66	119.92
1	B	21	GLU	C-N-CA	7.03	126.66	119.92
2	O	87	PHE	CA-C-N	7.03	134.96	121.54
2	O	87	PHE	C-N-CA	7.03	134.96	121.54
2	V	87	PHE	CA-CB-CG	-7.03	106.78	113.80
2	P	66	VAL	N-CA-C	-7.02	106.46	113.20
2	H	19	ARG	N-CA-C	-7.02	104.75	113.38
1	C	21	GLU	N-CA-C	-7.01	103.78	114.16
2	I	83	ALA	CA-C-O	7.01	127.93	120.36
1	A	210	HIS	CB-CG-CD2	-7.01	122.08	131.20
1	B	38	LEU	CA-C-O	-7.01	113.14	120.99
1	D	264	GLU	N-CA-C	-7.01	98.66	109.52
2	I	64	ASN	CA-C-N	7.01	130.24	120.29
2	I	64	ASN	C-N-CA	7.01	130.24	120.29
2	R	92	TYR	CA-C-O	7.00	127.92	120.36
1	C	162	ALA	CA-C-N	7.00	129.65	120.28
1	C	162	ALA	C-N-CA	7.00	129.65	120.28
2	K	124	THR	CA-CB-OG1	6.98	120.07	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	65	ALA	N-CA-C	-6.97	99.24	110.32
2	I	49	THR	CA-C-N	6.97	133.19	122.25
2	I	49	THR	C-N-CA	6.97	133.19	122.25
2	Q	96	ILE	O-C-N	-6.97	115.29	122.75
2	P	26	LEU	N-CA-C	-6.97	104.44	114.12
2	W	19	ARG	CA-C-N	6.97	134.24	121.70
2	W	19	ARG	C-N-CA	6.97	134.24	121.70
2	O	26	LEU	N-CA-C	-6.96	102.89	113.89
1	A	8	GLU	N-CA-C	-6.96	98.80	109.65
1	C	242	ARG	NE-CZ-NH2	-6.96	112.94	119.20
1	A	6	ASN	CA-C-N	6.96	130.17	120.29
1	A	6	ASN	C-N-CA	6.96	130.17	120.29
1	C	87	ARG	O-C-N	-6.95	114.79	123.27
1	A	241	ILE	N-CA-C	-6.95	97.56	108.81
1	F	21	GLU	N-CA-C	-6.95	102.67	113.02
1	B	23	ARG	NE-CZ-NH2	6.94	125.45	119.20
2	K	113	THR	N-CA-C	-6.94	97.89	109.07
2	P	64	ASN	CA-CB-CG	-6.94	105.66	112.60
1	B	123	ALA	CA-C-N	6.92	131.00	120.82
1	B	123	ALA	C-N-CA	6.92	131.00	120.82
1	F	9	LYS	N-CA-C	-6.92	98.79	109.52
1	A	87	ARG	NE-CZ-NH1	6.92	128.42	121.50
1	B	262	ILE	N-CA-C	-6.92	97.65	107.75
1	D	265	GLU	CA-C-N	6.91	132.94	122.93
1	D	265	GLU	C-N-CA	6.91	132.94	122.93
1	D	164	GLN	N-CA-CB	6.90	120.42	110.06
1	A	119	GLN	CA-C-N	6.90	129.53	120.28
1	A	119	GLN	C-N-CA	6.90	129.53	120.28
2	L	107	ALA	N-CA-CB	6.90	122.14	110.49
1	A	196	PRO	N-CA-C	6.90	121.19	111.33
2	V	162	ILE	CA-CB-CG2	-6.89	98.79	110.50
2	R	30	HIS	CE1-NE2-CD2	-6.89	102.11	109.00
2	P	30	HIS	CG-CD2-NE2	6.88	114.08	107.20
2	W	102	THR	N-CA-C	-6.88	104.77	113.72
1	B	58	LEU	CA-C-N	6.88	128.44	119.84
1	B	58	LEU	C-N-CA	6.88	128.44	119.84
2	Q	158	PHE	CA-C-O	6.88	128.06	119.95
2	J	80	SER	N-CA-C	6.88	120.34	110.10
1	E	102	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	A	232	ASP	CB-CA-C	-6.87	103.33	110.33
2	L	39	GLY	O-C-N	-6.86	113.79	122.70
1	E	159	LEU	N-CA-CB	6.85	120.20	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	67	GLY	CA-C-N	6.85	131.10	120.75
2	V	67	GLY	C-N-CA	6.85	131.10	120.75
2	G	32	ILE	N-CA-C	-6.85	97.65	108.95
2	H	56	LYS	CA-C-N	6.85	132.23	122.09
2	H	56	LYS	C-N-CA	6.85	132.23	122.09
1	A	273	SER	CA-C-N	6.84	132.22	122.09
1	A	273	SER	C-N-CA	6.84	132.22	122.09
2	T	122	LYS	N-CA-C	-6.84	98.25	109.40
2	X	63	THR	N-CA-C	-6.84	97.39	108.41
1	C	90	VAL	CA-C-N	6.84	126.64	119.05
1	C	90	VAL	C-N-CA	6.84	126.64	119.05
2	G	140	ARG	N-CA-C	-6.83	98.78	108.96
2	G	80	SER	N-CA-CB	6.82	120.13	110.24
2	J	36	GLY	CA-C-O	-6.82	115.66	121.66
2	O	138	GLU	N-CA-CB	6.81	120.84	109.94
2	V	136	VAL	N-CA-CB	6.81	122.47	111.23
1	A	7	GLN	N-CA-C	6.81	118.78	111.36
2	O	47	PHE	CA-CB-CG	-6.81	106.99	113.80
2	M	64	ASN	N-CA-CB	6.80	121.94	111.46
1	D	202	VAL	N-CA-C	-6.80	103.75	113.07
2	R	110	ASP	N-CA-CB	6.80	121.98	110.49
2	W	30	HIS	CE1-NE2-CD2	-6.80	102.20	109.00
1	F	201	GLU	CA-C-N	6.79	131.77	122.34
1	F	201	GLU	C-N-CA	6.79	131.77	122.34
1	E	210	HIS	N-CA-CB	6.79	122.08	110.68
2	J	70	ARG	CD-NE-CZ	-6.78	114.91	124.40
2	K	55	VAL	N-CA-C	-6.78	106.39	112.90
1	C	157	ALA	CA-C-N	6.78	129.92	120.29
1	C	157	ALA	C-N-CA	6.78	129.92	120.29
2	X	134	THR	N-CA-C	-6.77	98.80	109.50
1	B	226	THR	CA-C-N	6.77	130.07	120.53
1	B	226	THR	C-N-CA	6.77	130.07	120.53
1	D	52	PRO	CA-C-O	-6.77	113.41	121.67
2	U	103	ALA	N-CA-C	-6.76	97.18	108.75
1	A	251	ASP	O-C-N	6.76	129.29	122.12
1	D	119	GLN	CB-CG-CD	-6.75	101.12	112.60
1	B	82	VAL	CB-CA-C	6.75	120.67	110.62
1	E	261	VAL	O-C-N	-6.75	117.10	122.97
2	T	132	VAL	N-CA-CB	-6.75	104.89	112.45
2	X	85	PHE	CA-CB-CG	-6.75	107.05	113.80
2	T	17	TYR	CA-CB-CG	-6.74	101.76	113.90
1	D	133	ILE	CA-C-N	6.74	129.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	ILE	C-N-CA	6.74	129.31	120.28
1	A	270	VAL	CA-C-O	6.74	126.34	119.20
2	R	158	PHE	CA-C-O	6.74	129.40	121.58
1	F	226	THR	CA-C-N	6.74	129.05	120.56
1	F	226	THR	C-N-CA	6.74	129.05	120.56
2	V	66	VAL	CA-C-N	6.74	130.57	121.01
2	V	66	VAL	C-N-CA	6.74	130.57	121.01
1	E	28	GLN	O-C-N	-6.73	116.19	123.26
1	A	250	ALA	CA-C-N	6.73	129.30	120.28
1	A	250	ALA	C-N-CA	6.73	129.30	120.28
1	F	56	GLY	CA-C-N	6.73	130.71	120.82
1	F	56	GLY	C-N-CA	6.73	130.71	120.82
2	U	155	THR	CA-C-N	6.72	132.31	122.63
2	U	155	THR	C-N-CA	6.72	132.31	122.63
2	K	140	ARG	NE-CZ-NH1	-6.72	114.78	121.50
2	W	25	ILE	O-C-N	-6.72	115.24	123.10
1	A	103	PHE	CA-CB-CG	-6.71	107.08	113.80
2	J	77	VAL	CA-CB-CG1	6.71	121.81	110.40
1	F	256	LEU	N-CA-C	-6.71	98.27	109.07
2	M	27	ASN	OD1-CG-ND2	6.71	129.31	122.60
2	O	126	THR	CA-C-N	6.71	134.56	121.41
2	O	126	THR	C-N-CA	6.71	134.56	121.41
1	C	133	ILE	CA-C-N	6.71	129.26	120.28
1	C	133	ILE	C-N-CA	6.71	129.26	120.28
1	C	116	ARG	CA-C-N	6.70	129.26	120.28
1	C	116	ARG	C-N-CA	6.70	129.26	120.28
1	C	272	ASN	N-CA-C	-6.70	105.66	114.31
2	G	30	HIS	CB-CG-CD2	-6.70	122.49	131.20
1	A	277	ALA	CA-C-O	6.70	127.59	120.36
2	G	40	VAL	O-C-N	6.70	129.39	122.09
2	N	92	TYR	O-C-N	-6.69	114.30	122.20
2	Q	90	GLY	O-C-N	-6.69	117.49	122.71
2	L	41	GLU	N-CA-C	-6.69	96.32	108.02
2	L	55	VAL	N-CA-C	-6.68	105.82	112.17
1	A	81	GLN	CA-C-N	-6.68	114.39	123.14
1	A	81	GLN	C-N-CA	-6.68	114.39	123.14
1	F	23	ARG	CA-C-N	6.67	132.32	123.11
1	F	23	ARG	C-N-CA	6.67	132.32	123.11
2	P	41	GLU	N-CA-CB	6.67	119.79	109.85
2	S	84	SER	CA-C-N	6.67	133.03	122.62
2	S	84	SER	C-N-CA	6.67	133.03	122.62
1	C	146	ALA	O-C-N	-6.67	116.49	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	139	TYR	N-CA-C	-6.67	99.35	109.95
2	W	141	ALA	N-CA-C	-6.66	100.93	110.59
1	E	112	ASN	CA-CB-CG	6.66	119.26	112.60
2	U	121	ILE	CA-CB-CG1	6.66	121.72	110.40
2	K	38	ASN	CA-CB-CG	-6.66	105.94	112.60
2	G	96	ILE	N-CA-CB	6.66	120.59	111.41
1	E	225	ASN	CA-CB-CG	6.65	119.25	112.60
2	I	164	TYR	CA-CB-CG	-6.65	101.93	113.90
2	N	78	ASN	O-C-N	6.65	130.70	122.92
1	C	94	GLU	N-CA-C	6.65	118.61	111.36
1	C	236	VAL	N-CA-C	-6.65	98.61	108.45
2	H	19	ARG	NE-CZ-NH1	-6.65	114.85	121.50
1	B	107	LYS	N-CA-C	-6.65	104.11	111.36
1	C	2	SER	N-CA-C	6.65	119.42	109.25
1	C	58	LEU	CA-C-N	6.64	126.40	119.76
1	C	58	LEU	C-N-CA	6.64	126.40	119.76
2	S	73	LEU	N-CA-CB	6.64	119.80	110.04
2	R	134	THR	CA-C-N	6.64	134.22	121.54
2	R	134	THR	C-N-CA	6.64	134.22	121.54
1	B	40	TYR	O-C-N	-6.63	115.65	123.41
1	B	233	PRO	N-CA-CB	6.63	109.49	103.19
1	E	176	ILE	CA-C-N	6.63	128.92	120.56
1	E	176	ILE	C-N-CA	6.63	128.92	120.56
2	G	30	HIS	CE1-NE2-CD2	-6.63	102.37	109.00
2	K	72	ASP	N-CA-C	-6.63	106.14	114.56
1	F	64	ASP	N-CA-C	-6.62	104.94	113.16
2	G	30	HIS	CB-CG-ND1	6.62	132.63	122.70
2	J	89	GLY	N-CA-C	-6.62	102.85	111.52
2	O	126	THR	N-CA-C	-6.62	98.11	108.90
1	C	167	GLU	N-CA-C	-6.62	105.21	113.55
2	H	115	ASP	CA-C-N	6.62	134.18	121.54
2	H	115	ASP	C-N-CA	6.62	134.18	121.54
1	D	197	VAL	CA-CB-CG1	-6.61	99.16	110.40
1	D	201	GLU	N-CA-C	-6.61	99.28	109.52
1	A	156	ARG	CA-C-N	6.61	129.13	120.28
1	A	156	ARG	C-N-CA	6.61	129.13	120.28
2	R	115	ASP	CA-CB-CG	6.61	119.20	112.60
1	B	55	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	F	230	LEU	O-C-N	-6.60	113.89	122.94
1	B	247	VAL	N-CA-C	6.60	116.70	110.30
1	C	59	PRO	CA-C-O	-6.59	113.40	121.31
1	B	270	VAL	N-CA-C	-6.59	106.36	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	157	THR	CA-CB-OG1	6.59	119.49	109.60
1	B	259	GLY	N-CA-C	-6.59	97.56	113.18
1	F	217	LEU	CA-C-N	6.59	129.33	120.50
1	F	217	LEU	C-N-CA	6.59	129.33	120.50
2	T	53	ASN	N-CA-CB	6.59	121.29	111.01
2	J	38	ASN	CA-CB-CG	-6.59	106.01	112.60
2	X	157	THR	N-CA-C	-6.59	98.16	108.90
1	B	87	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	E	246	GLN	CA-C-N	6.58	128.93	120.70
1	E	246	GLN	C-N-CA	6.58	128.93	120.70
2	Q	135	HIS	N-CA-C	-6.58	101.89	111.30
1	F	53	LEU	N-CA-C	-6.57	100.65	110.24
1	A	277	ALA	N-CA-CB	6.57	121.71	110.68
1	A	176	ILE	CA-C-O	-6.56	114.21	121.17
1	C	202	VAL	O-C-N	6.56	129.97	122.82
2	O	141	ALA	N-CA-CB	6.56	119.62	109.97
2	S	99	THR	N-CA-C	-6.56	105.16	113.43
1	D	6	ASN	CA-CB-CG	6.56	119.16	112.60
2	K	78	ASN	CA-CB-CG	6.55	119.15	112.60
2	K	135	HIS	CA-C-N	6.55	129.06	120.60
2	K	135	HIS	C-N-CA	6.55	129.06	120.60
2	Q	159	ILE	N-CA-CB	6.55	122.04	111.23
1	E	155	GLN	CA-C-N	6.55	129.05	120.28
1	E	155	GLN	C-N-CA	6.55	129.05	120.28
2	I	39	GLY	CA-C-N	6.54	129.27	120.50
2	I	39	GLY	C-N-CA	6.54	129.27	120.50
2	N	158	PHE	CA-C-O	6.54	127.17	120.24
2	J	33	ASP	CA-CB-CG	-6.54	106.06	112.60
2	L	48	ALA	CB-CA-C	-6.54	98.49	109.48
1	A	153	GLY	CA-C-N	6.54	128.94	120.44
1	A	153	GLY	C-N-CA	6.54	128.94	120.44
2	R	50	ILE	N-CA-C	-6.53	105.18	113.22
1	A	199	GLN	O-C-N	-6.53	115.21	123.24
2	I	98	ARG	NE-CZ-NH2	6.53	125.08	119.20
2	V	104	ALA	N-CA-C	-6.53	99.28	109.72
1	A	82	VAL	N-CA-CB	6.52	120.41	111.41
2	V	123	PHE	CA-CB-CG	6.52	120.32	113.80
1	F	164	GLN	CA-C-N	6.52	129.67	120.28
1	F	164	GLN	C-N-CA	6.52	129.67	120.28
1	C	27	ALA	N-CA-C	-6.52	105.86	113.88
1	A	227	VAL	N-CA-CB	6.52	118.18	110.55
1	F	183	PHE	N-CA-CB	6.52	119.70	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	272	ASN	N-CA-CB	6.51	121.50	110.49
1	A	212	TRP	N-CA-CB	6.51	121.03	110.42
2	U	19	ARG	N-CA-CB	6.51	121.49	110.49
2	G	86	TYR	N-CA-CB	-6.50	100.81	110.24
1	E	183	PHE	O-C-N	6.50	129.01	122.12
2	M	31	ASP	CA-C-N	6.50	133.67	121.97
2	M	31	ASP	C-N-CA	6.50	133.67	121.97
2	M	65	ALA	N-CA-C	-6.49	103.52	112.03
1	B	14	SER	CA-C-N	6.49	131.34	122.19
1	B	14	SER	C-N-CA	6.49	131.34	122.19
1	E	140	ALA	CB-CA-C	6.49	120.49	109.72
1	E	151	SER	CA-C-O	6.49	127.42	120.55
2	L	75	ASP	N-CA-C	-6.48	102.55	112.99
2	J	135	HIS	N-CA-C	-6.48	105.53	113.50
2	R	36	GLY	O-C-N	-6.48	116.37	123.05
2	I	71	GLU	N-CA-C	-6.48	99.96	110.20
1	B	3	GLN	N-CA-C	-6.48	97.77	108.07
1	F	179	ASN	CA-C-N	6.48	128.96	120.28
1	F	179	ASN	C-N-CA	6.48	128.96	120.28
2	O	24	GLY	N-CA-C	-6.47	105.04	112.29
1	E	177	VAL	O-C-N	6.46	128.25	121.91
2	R	76	MET	N-CA-C	-6.46	99.29	109.50
1	E	80	ASP	N-CA-CB	6.45	119.53	110.04
1	D	145	ASN	CA-C-O	-6.45	113.70	121.05
2	P	95	ASN	OD1-CG-ND2	6.45	129.05	122.60
1	E	169	HIS	CE1-NE2-CD2	-6.45	102.55	109.00
1	D	19	THR	CA-C-N	6.45	130.30	120.82
1	D	19	THR	C-N-CA	6.45	130.30	120.82
1	D	2	SER	N-CA-CB	6.44	121.23	110.92
1	C	87	ARG	N-CA-C	-6.44	98.49	109.24
1	C	110	ARG	O-C-N	6.44	128.94	122.12
1	D	45	ARG	NE-CZ-NH2	6.44	124.99	119.20
2	N	106	ILE	CA-C-N	6.44	129.85	120.71
2	N	106	ILE	C-N-CA	6.44	129.85	120.71
2	R	50	ILE	CA-CB-CG1	6.44	121.34	110.40
2	N	150	GLN	N-CA-C	-6.43	98.95	108.79
2	K	79	ALA	CA-C-N	6.43	130.89	121.31
2	K	79	ALA	C-N-CA	6.43	130.89	121.31
2	P	77	VAL	CA-CB-CG1	-6.42	99.48	110.40
2	T	25	ILE	CA-CB-CG2	-6.42	99.58	110.50
2	I	25	ILE	N-CA-C	-6.42	99.85	108.96
2	Q	122	LYS	N-CA-C	-6.42	99.25	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	18	GLU	CA-C-N	6.42	132.04	122.99
1	F	18	GLU	C-N-CA	6.42	132.04	122.99
2	U	53	ASN	OD1-CG-ND2	6.42	129.02	122.60
2	I	61	ASN	OD1-CG-ND2	6.41	129.01	122.60
2	M	38	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	A	6	ASN	CA-CB-CG	6.40	119.00	112.60
2	M	53	ASN	OD1-CG-ND2	6.40	129.00	122.60
2	K	162	ILE	CB-CA-C	6.39	120.26	111.31
2	S	51	GLY	CA-C-N	6.39	133.75	121.54
2	S	51	GLY	C-N-CA	6.39	133.75	121.54
2	W	136	VAL	CA-CB-CG1	-6.39	99.53	110.40
1	B	84	GLU	CB-CG-CD	-6.39	101.73	112.60
1	C	163	PHE	CA-C-N	6.39	128.85	120.28
1	C	163	PHE	C-N-CA	6.39	128.85	120.28
1	D	155	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	A	121	ALA	N-CA-C	-6.39	103.94	111.03
1	E	102	ARG	NE-CZ-NH1	-6.38	115.11	121.50
1	E	195	ASP	CA-C-N	6.38	127.81	119.84
1	E	195	ASP	C-N-CA	6.38	127.81	119.84
2	U	83	ALA	CA-C-N	6.38	131.46	122.46
2	U	83	ALA	C-N-CA	6.38	131.46	122.46
1	C	133	ILE	N-CA-C	6.38	117.06	110.36
2	Q	62	GLY	CA-C-N	6.38	129.89	120.90
2	Q	62	GLY	C-N-CA	6.38	129.89	120.90
2	T	33	ASP	N-CA-C	-6.38	104.81	112.59
1	B	76	GLY	N-CA-C	-6.37	100.99	111.38
2	R	30	HIS	CG-CD2-NE2	6.37	113.57	107.20
1	B	183	PHE	CA-CB-CG	-6.37	107.43	113.80
2	P	154	ASP	N-CA-C	-6.37	98.52	108.90
2	N	121	ILE	N-CA-C	-6.37	101.05	108.82
2	H	35	ALA	CA-C-O	-6.37	113.86	120.99
2	M	108	ALA	N-CA-CB	6.37	121.25	110.49
1	B	64	ASP	N-CA-C	-6.36	97.25	110.80
2	M	97	SER	N-CA-C	-6.36	97.19	108.13
1	E	252	LYS	CA-C-N	6.36	127.79	119.84
1	E	252	LYS	C-N-CA	6.36	127.79	119.84
2	J	154	ASP	CA-CB-CG	6.36	118.96	112.60
2	L	130	LEU	N-CA-CB	6.35	121.22	110.49
1	D	79	PRO	N-CA-C	-6.35	101.17	111.77
1	C	99	PRO	CA-C-N	6.34	129.41	120.28
1	C	99	PRO	C-N-CA	6.34	129.41	120.28
1	E	124	ASP	N-CA-C	-6.34	99.96	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	102	THR	N-CA-C	-6.34	101.08	110.46
2	M	155	THR	CA-CB-OG1	6.34	119.11	109.60
2	I	132	VAL	N-CA-C	-6.34	101.09	108.82
2	O	34	VAL	N-CA-C	-6.34	99.98	108.35
2	J	46	LYS	O-C-N	-6.33	117.19	123.46
1	D	272	ASN	CA-CB-CG	-6.33	106.27	112.60
2	X	93	TYR	CA-C-O	-6.33	113.38	120.66
1	D	110	ARG	CB-CG-CD	6.33	125.86	111.30
1	D	151	SER	CA-C-O	6.33	127.26	120.55
2	N	113	THR	N-CA-C	-6.33	98.93	109.24
2	H	30	HIS	CA-CB-CG	6.32	120.12	113.80
2	N	48	ALA	CA-C-O	-6.32	113.59	120.36
1	D	251	ASP	CB-CA-C	-6.32	100.96	110.88
1	F	126	MET	CA-C-N	6.32	133.61	121.54
1	F	126	MET	C-N-CA	6.32	133.61	121.54
2	N	124	THR	CA-CB-OG1	6.32	119.07	109.60
2	M	30	HIS	CG-CD2-NE2	6.31	113.51	107.20
2	S	83	ALA	N-CA-CB	6.31	121.16	110.49
1	B	14	SER	N-CA-C	6.31	120.10	111.39
1	F	149	ILE	N-CA-C	-6.31	106.62	112.43
2	U	60	ASP	CA-C-N	6.31	132.45	120.97
2	U	60	ASP	C-N-CA	6.31	132.45	120.97
2	P	143	ASN	N-CA-C	-6.31	97.37	110.80
2	Q	153	THR	N-CA-C	-6.30	105.45	112.57
1	E	108	GLU	N-CA-C	-6.30	104.33	111.14
2	P	153	THR	O-C-N	6.30	129.88	123.26
1	D	169	HIS	N-CA-C	-6.30	97.99	108.32
1	B	55	GLN	N-CA-C	-6.30	105.60	113.28
1	E	81	GLN	OE1-CD-NE2	6.30	128.90	122.60
2	R	72	ASP	N-CA-C	-6.30	100.06	109.94
1	B	130	ASP	CA-C-N	6.29	133.56	121.54
1	B	130	ASP	C-N-CA	6.29	133.56	121.54
2	P	154	ASP	O-C-N	-6.29	115.81	123.30
1	D	47	LEU	N-CA-C	-6.29	99.77	109.52
2	K	135	HIS	ND1-CE1-NE2	6.29	114.69	108.40
2	O	116	ALA	N-CA-C	-6.29	97.40	110.80
1	C	221	LYS	N-CA-C	-6.29	99.48	109.23
1	E	8	GLU	CA-C-O	6.29	127.87	120.58
2	J	33	ASP	CA-C-N	6.29	130.99	123.19
2	J	33	ASP	C-N-CA	6.29	130.99	123.19
2	R	67	GLY	N-CA-C	6.29	122.44	111.50
1	A	44	GLY	N-CA-C	-6.29	99.83	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	VAL	CA-C-N	6.29	126.47	120.31
1	C	78	VAL	C-N-CA	6.29	126.47	120.31
2	R	138	GLU	N-CA-CB	6.28	119.97	109.92
2	V	113	THR	N-CA-C	-6.28	99.46	109.76
1	E	11	TYR	N-CA-CB	6.28	121.10	110.49
2	X	113	THR	N-CA-CB	6.28	120.66	110.43
1	B	264	GLU	O-C-N	-6.28	116.67	123.26
1	C	104	SER	CA-C-O	-6.28	113.89	120.55
1	D	276	ILE	N-CA-C	-6.28	98.64	108.81
1	B	88	ILE	CB-CA-C	6.28	120.18	110.83
1	D	189	TRP	N-CA-C	-6.28	104.89	113.30
1	E	105	GLN	CA-C-N	6.28	129.06	120.46
1	E	105	GLN	C-N-CA	6.28	129.06	120.46
2	G	30	HIS	CG-CD2-NE2	6.27	113.47	107.20
1	D	2	SER	N-CA-C	-6.27	104.94	112.59
1	E	206	GLY	CA-C-N	6.27	133.51	121.54
1	E	206	GLY	C-N-CA	6.27	133.51	121.54
2	K	135	HIS	CE1-NE2-CD2	-6.26	102.73	109.00
2	O	150	GLN	N-CA-C	-6.26	103.69	113.02
2	I	155	THR	CA-CB-OG1	6.26	118.99	109.60
2	H	102	THR	CA-C-O	6.26	127.52	119.95
1	A	97	SER	O-C-N	6.25	129.28	122.15
1	D	152	GLY	CA-C-N	6.25	126.92	119.98
1	D	152	GLY	C-N-CA	6.25	126.92	119.98
2	M	93	TYR	CA-C-N	6.25	128.94	120.63
2	M	93	TYR	C-N-CA	6.25	128.94	120.63
1	A	237	GLY	CA-C-N	6.25	128.94	120.63
1	A	237	GLY	C-N-CA	6.25	128.94	120.63
2	I	27	ASN	CA-CB-CG	-6.25	106.35	112.60
2	J	84	SER	O-C-N	6.25	130.10	123.42
1	A	45	ARG	NE-CZ-NH1	6.25	127.75	121.50
1	A	88	ILE	N-CA-CB	6.24	119.74	111.25
1	E	39	ASP	CA-CB-CG	-6.24	106.36	112.60
1	E	76	GLY	N-CA-C	-6.24	101.22	111.38
2	O	145	TYR	N-CA-CB	6.24	121.03	110.49
2	S	86	TYR	N-CA-CB	6.24	119.90	109.92
1	C	66	ASP	O-C-N	6.23	130.57	122.97
2	T	31	ASP	CA-CB-CG	-6.23	106.37	112.60
2	U	87	PHE	CA-CB-CG	-6.23	107.57	113.80
2	U	113	THR	N-CA-C	-6.23	99.12	109.46
1	C	252	LYS	CA-C-N	6.23	127.62	119.84
1	C	252	LYS	C-N-CA	6.23	127.62	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	78	ASN	N-CA-C	-6.23	100.02	108.24
2	O	33	ASP	CA-CB-CG	6.23	118.83	112.60
2	W	30	HIS	CG-CD2-NE2	6.23	113.43	107.20
1	E	173	VAL	CA-C-O	-6.22	113.38	120.66
2	W	163	MET	N-CA-C	-6.22	99.57	109.59
2	K	134	THR	N-CA-C	-6.22	100.78	110.42
2	T	54	GLY	O-C-N	-6.22	116.36	122.77
2	J	63	THR	N-CA-C	-6.22	99.27	108.79
2	X	76	MET	CA-C-O	-6.22	113.83	121.11
1	D	76	GLY	N-CA-C	-6.22	101.25	111.38
1	D	2	SER	CB-CA-C	-6.21	101.02	111.02
1	B	25	ALA	O-C-N	-6.21	116.77	123.42
1	D	11	TYR	N-CA-C	-6.21	104.46	114.09
2	M	150	GLN	N-CA-CB	6.21	120.99	110.49
2	P	29	ALA	N-CA-C	-6.21	105.53	113.23
2	S	84	SER	N-CA-C	-6.21	104.87	112.88
2	V	54	GLY	O-C-N	-6.21	116.84	122.86
1	E	188	ALA	N-CA-CB	6.21	120.98	110.49
2	N	78	ASN	CA-C-O	-6.21	114.78	121.36
1	E	120	ARG	NE-CZ-NH2	6.21	124.78	119.20
1	C	196	PRO	CA-C-O	-6.20	114.59	121.23
1	C	216	ILE	N-CA-C	-6.20	98.71	108.95
2	J	49	THR	N-CA-C	-6.20	105.02	112.59
2	P	82	LYS	N-CA-C	-6.20	99.70	109.50
1	B	111	PHE	CA-C-O	6.20	127.33	120.82
2	X	140	ARG	NE-CZ-NH2	-6.20	113.62	119.20
2	S	116	ALA	CA-C-O	6.19	126.90	119.59
2	U	78	ASN	N-CA-C	-6.19	100.02	108.38
2	R	124	THR	CA-C-N	6.18	133.53	121.41
2	R	124	THR	C-N-CA	6.18	133.53	121.41
2	L	156	ASP	N-CA-CB	-6.18	100.05	110.49
2	O	49	THR	CA-C-N	6.18	130.19	121.66
2	O	49	THR	C-N-CA	6.18	130.19	121.66
2	V	111	GLU	N-CA-CB	6.18	119.53	109.95
1	A	125	ILE	CA-C-N	6.18	131.88	122.37
1	A	125	ILE	C-N-CA	6.18	131.88	122.37
2	Q	79	ALA	N-CA-CB	6.18	119.06	110.17
2	L	37	LEU	CA-C-O	6.17	126.07	119.34
1	A	153	GLY	N-CA-C	-6.17	105.33	112.73
1	B	272	ASN	N-CA-C	-6.16	99.67	109.59
1	D	200	HIS	ND1-CE1-NE2	6.16	114.56	108.40
2	U	27	ASN	CA-CB-CG	-6.16	106.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	159	ILE	CA-CB-CG1	6.16	120.88	110.40
2	X	133	VAL	CB-CA-C	6.16	120.18	110.81
1	F	200	HIS	CE1-NE2-CD2	-6.16	102.84	109.00
1	B	51	ASP	CA-CB-CG	-6.16	106.44	112.60
1	B	53	LEU	CA-C-O	-6.16	111.78	119.54
2	L	48	ALA	N-CA-C	-6.16	99.66	109.76
1	E	105	GLN	O-C-N	-6.16	115.13	122.15
2	P	133	VAL	CA-C-N	6.16	130.51	120.23
2	P	133	VAL	C-N-CA	6.16	130.51	120.23
1	E	39	ASP	CA-C-O	-6.15	114.46	121.72
2	O	124	THR	N-CA-C	-6.15	104.56	114.09
1	A	42	GLY	CA-C-O	6.15	126.68	121.88
2	U	130	LEU	N-CA-C	-6.15	104.27	112.94
2	J	143	ASN	N-CA-C	-6.14	100.09	108.38
1	C	109	ARG	CA-C-N	6.14	128.50	120.28
1	C	109	ARG	C-N-CA	6.14	128.50	120.28
2	L	115	ASP	N-CA-C	-6.14	100.72	108.45
1	B	108	GLU	CB-CG-CD	-6.13	102.17	112.60
2	Q	117	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	90	VAL	O-C-N	-6.13	115.28	120.92
2	O	53	ASN	N-CA-C	-6.13	99.41	109.40
2	T	113	THR	O-C-N	-6.13	116.23	123.22
2	O	95	ASN	CA-CB-CG	-6.12	106.47	112.60
1	A	133	ILE	CA-C-N	6.12	128.49	120.28
1	A	133	ILE	C-N-CA	6.12	128.49	120.28
2	M	20	LEU	N-CA-CB	6.12	122.49	112.63
2	R	96	ILE	N-CA-C	-6.12	98.81	107.75
2	S	124	THR	CA-CB-CG2	-6.12	100.09	110.50
2	X	55	VAL	CA-CB-CG1	6.12	120.81	110.40
1	A	182	ALA	CB-CA-C	-6.12	100.63	110.79
2	H	89	GLY	CA-C-N	6.12	133.41	121.41
2	H	89	GLY	C-N-CA	6.12	133.41	121.41
2	Q	120	MET	CG-SD-CE	-6.12	87.43	100.90
2	T	99	THR	N-CA-C	-6.12	99.42	109.40
2	S	27	ASN	OD1-CG-ND2	6.12	128.72	122.60
2	L	73	LEU	N-CA-CB	6.12	120.82	110.49
2	S	85	PHE	CA-C-N	6.11	129.81	120.82
2	S	85	PHE	C-N-CA	6.11	129.81	120.82
1	C	139	GLY	CA-C-O	-6.11	115.30	121.90
2	H	88	ARG	NE-CZ-NH2	-6.11	113.70	119.20
2	O	130	LEU	CA-C-O	6.11	129.24	120.51
2	P	49	THR	CA-C-N	6.11	130.76	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	49	THR	C-N-CA	6.11	130.76	123.19
1	D	222	VAL	CA-C-O	-6.11	111.77	119.95
1	E	130	ASP	CA-C-N	6.11	131.60	122.99
1	E	130	ASP	C-N-CA	6.11	131.60	122.99
2	U	117	ASP	CA-CB-CG	-6.10	106.50	112.60
1	E	54	PRO	CA-C-O	6.10	131.70	120.60
2	P	148	ALA	N-CA-C	6.10	118.64	110.35
2	O	145	TYR	CA-C-N	6.09	133.18	121.54
2	O	145	TYR	C-N-CA	6.09	133.18	121.54
1	F	11	TYR	CA-CB-CG	-6.09	102.94	113.90
1	F	182	ALA	N-CA-CB	6.09	118.90	110.07
1	E	141	ALA	CA-C-N	6.08	129.56	120.31
1	E	141	ALA	C-N-CA	6.08	129.56	120.31
2	V	80	SER	CA-C-N	6.08	132.65	121.70
2	V	80	SER	C-N-CA	6.08	132.65	121.70
2	L	93	TYR	CA-CB-CG	-6.08	102.95	113.90
2	P	154	ASP	CA-C-N	6.08	132.55	122.33
2	P	154	ASP	C-N-CA	6.08	132.55	122.33
2	W	101	LEU	N-CA-CB	6.08	120.76	110.49
1	F	178	MET	CG-SD-CE	-6.08	87.53	100.90
1	F	244	ASP	N-CA-C	-6.08	105.91	113.38
2	M	60	ASP	CA-CB-CG	6.08	118.67	112.60
2	U	23	GLU	N-CA-C	6.08	118.55	110.53
1	A	68	LYS	CG-CD-CE	6.07	125.27	111.30
2	V	73	LEU	N-CA-C	-6.07	101.29	110.28
2	G	135	HIS	CE1-NE2-CD2	-6.07	102.93	109.00
2	M	125	GLY	CA-C-N	6.07	129.45	120.95
2	M	125	GLY	C-N-CA	6.07	129.45	120.95
1	C	159	LEU	CA-C-N	6.07	128.42	120.28
1	C	159	LEU	C-N-CA	6.07	128.42	120.28
1	F	48	LEU	N-CA-C	-6.07	99.51	109.40
2	P	30	HIS	ND1-CE1-NE2	6.07	114.47	108.40
2	X	147	LYS	CA-C-N	6.07	133.13	121.54
2	X	147	LYS	C-N-CA	6.07	133.13	121.54
1	A	137	LEU	CA-C-N	6.06	131.02	121.56
1	A	137	LEU	C-N-CA	6.06	131.02	121.56
1	A	246	GLN	O-C-N	6.06	129.81	122.96
2	U	26	LEU	CA-C-N	6.06	131.27	122.36
2	U	26	LEU	C-N-CA	6.06	131.27	122.36
2	H	19	ARG	NE-CZ-NH2	6.06	124.65	119.20
2	K	151	GLY	CA-C-N	6.06	129.54	120.69
2	K	151	GLY	C-N-CA	6.06	129.54	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	128	LYS	N-CA-C	-6.06	105.93	113.38
2	G	40	VAL	N-CA-C	-6.05	106.86	112.43
2	W	56	LYS	CA-C-N	6.05	133.10	121.54
2	W	56	LYS	C-N-CA	6.05	133.10	121.54
1	B	118	GLN	CB-CA-C	-6.05	101.38	110.88
2	Q	110	ASP	N-CA-CB	6.05	119.61	110.42
2	S	30	HIS	CA-C-O	-6.05	114.27	121.11
1	D	176	ILE	CA-CB-CG2	6.04	120.78	110.50
1	F	223	PRO	N-CA-C	-6.04	101.68	111.77
1	A	216	ILE	N-CA-C	-6.04	105.79	113.22
1	A	66	ASP	N-CA-CB	6.03	118.94	109.83
2	V	115	ASP	N-CA-C	-6.03	100.44	108.34
2	W	62	GLY	N-CA-C	-6.03	105.05	112.77
1	A	70	PHE	CA-C-N	6.03	132.83	121.97
1	A	70	PHE	C-N-CA	6.03	132.83	121.97
2	M	40	VAL	CB-CA-C	6.03	118.39	110.91
1	E	149	ILE	N-CA-C	-6.03	107.41	113.20
2	V	16	PRO	CA-C-N	6.03	133.05	121.54
2	V	16	PRO	C-N-CA	6.03	133.05	121.54
2	X	87	PHE	CA-CB-CG	-6.03	107.78	113.80
1	E	83	ILE	N-CA-C	-6.02	99.81	108.48
2	L	49	THR	N-CA-C	-6.02	105.24	112.59
2	X	138	GLU	CA-C-O	-6.02	114.31	121.66
1	A	189	TRP	CA-C-N	6.02	126.66	119.98
1	A	189	TRP	C-N-CA	6.02	126.66	119.98
1	D	235	PHE	N-CA-C	-6.02	104.64	111.14
2	L	95	ASN	OD1-CG-ND2	6.02	128.62	122.60
2	T	136	VAL	N-CA-C	-6.02	106.87	113.43
1	F	115	ASP	CA-C-N	6.02	128.26	120.44
1	F	115	ASP	C-N-CA	6.02	128.26	120.44
2	W	61	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	B	17	LEU	N-CA-CB	6.01	120.66	110.49
1	A	17	LEU	N-CA-C	-6.01	104.59	113.61
1	E	163	PHE	O-C-N	6.01	129.25	122.22
1	F	166	VAL	N-CA-CB	6.01	121.15	111.23
2	I	159	ILE	N-CA-CB	6.01	121.15	111.23
1	C	160	THR	CA-C-N	6.01	128.33	120.28
1	C	160	THR	C-N-CA	6.01	128.33	120.28
1	E	189	TRP	CD2-CE3-CZ3	-6.00	110.79	118.60
2	T	85	PHE	CA-CB-CG	6.00	119.80	113.80
2	S	119	LYS	N-CA-C	6.00	119.04	110.10
2	I	124	THR	N-CA-C	-6.00	99.19	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	HIS	ND1-CE1-NE2	6.00	114.39	108.40
2	M	109	GLY	N-CA-C	-5.99	104.87	112.54
2	V	29	ALA	CA-C-N	5.99	131.10	122.35
2	V	29	ALA	C-N-CA	5.99	131.10	122.35
2	W	149	THR	CA-C-N	5.99	132.99	121.54
2	W	149	THR	C-N-CA	5.99	132.99	121.54
1	C	210	HIS	N-CA-CB	5.99	120.75	110.68
2	R	129	ALA	CA-C-N	5.99	129.38	120.87
2	R	129	ALA	C-N-CA	5.99	129.38	120.87
2	S	96	ILE	CA-C-O	-5.99	113.30	120.78
2	T	113	THR	CA-C-O	5.99	127.31	120.54
2	N	78	ASN	CA-CB-CG	5.99	118.59	112.60
2	O	102	THR	CA-C-N	5.99	132.97	121.54
2	O	102	THR	C-N-CA	5.99	132.97	121.54
2	Q	151	GLY	N-CA-C	-5.98	105.14	112.68
1	B	270	VAL	O-C-N	-5.98	115.57	122.09
2	L	39	GLY	CA-C-N	5.98	129.51	120.95
2	L	39	GLY	C-N-CA	5.98	129.51	120.95
2	T	107	ALA	CA-C-N	5.98	129.40	120.31
2	T	107	ALA	C-N-CA	5.98	129.40	120.31
1	E	78	VAL	O-C-N	5.98	126.45	120.59
2	M	35	ALA	N-CA-CB	5.98	120.60	110.49
1	F	230	LEU	CA-C-O	5.98	128.51	121.58
2	G	47	PHE	CA-CB-CG	5.98	119.78	113.80
1	C	42	GLY	CA-C-N	5.98	130.56	120.64
1	C	42	GLY	C-N-CA	5.98	130.56	120.64
2	K	47	PHE	CA-CB-CG	-5.97	107.83	113.80
2	P	71	GLU	CA-C-O	-5.97	114.47	121.16
1	C	156	ARG	CB-CA-C	-5.97	100.70	110.85
1	A	121	ALA	N-CA-CB	5.97	118.64	109.98
1	F	186	ILE	CA-CB-CG1	5.97	120.55	110.40
1	F	252	LYS	O-C-N	-5.97	115.32	120.99
1	F	255	GLU	CA-C-N	-5.97	114.77	123.00
1	F	255	GLU	C-N-CA	-5.97	114.77	123.00
2	O	159	ILE	CA-CB-CG1	5.97	120.54	110.40
2	J	155	THR	CA-CB-OG1	5.96	118.55	109.60
2	O	117	ASP	N-CA-CB	5.96	120.57	110.49
1	A	198	THR	CA-C-N	5.96	131.92	122.62
1	A	198	THR	C-N-CA	5.96	131.92	122.62
2	T	54	GLY	CA-C-O	5.96	128.11	121.67
1	D	250	ALA	CB-CA-C	-5.96	100.72	110.85
1	A	195	ASP	N-CA-CB	5.96	120.97	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ARG	NE-CZ-NH2	-5.95	113.84	119.20
2	V	61	ASN	CA-CB-CG	5.95	118.55	112.60
1	F	201	GLU	CA-C-O	-5.95	114.61	121.15
1	F	54	PRO	CA-C-O	-5.94	114.57	121.34
2	S	50	ILE	N-CA-CB	5.93	121.02	111.23
2	W	85	PHE	N-CA-CB	5.93	120.52	110.49
2	I	96	ILE	O-C-N	5.93	129.35	123.18
1	C	143	ALA	CA-C-N	5.93	128.58	120.46
1	C	143	ALA	C-N-CA	5.93	128.58	120.46
2	L	37	LEU	N-CA-C	-5.93	104.19	113.02
2	G	86	TYR	CA-C-N	5.92	132.86	121.54
2	G	86	TYR	C-N-CA	5.92	132.86	121.54
2	I	95	ASN	CA-CB-CG	5.92	118.52	112.60
1	F	184	ALA	CA-C-N	5.92	132.85	121.54
1	F	184	ALA	C-N-CA	5.92	132.85	121.54
2	K	43	LEU	CA-C-N	5.92	132.84	121.54
2	K	43	LEU	C-N-CA	5.92	132.84	121.54
2	Q	37	LEU	CA-C-N	5.92	131.15	122.63
2	Q	37	LEU	C-N-CA	5.92	131.15	122.63
1	B	210	HIS	CA-CB-CG	-5.91	107.89	113.80
1	E	51	ASP	CA-C-O	-5.91	112.06	120.16
2	W	148	ALA	N-CA-C	-5.91	100.08	109.07
2	K	17	TYR	CA-CB-CG	-5.91	103.26	113.90
1	A	45	ARG	CA-C-N	5.91	131.84	122.74
1	A	45	ARG	C-N-CA	5.91	131.84	122.74
1	D	51	ASP	O-C-N	-5.91	114.52	121.32
1	C	109	ARG	NH1-CZ-NH2	-5.91	111.62	119.30
1	D	176	ILE	CA-C-O	5.91	127.09	120.95
1	B	182	ALA	N-CA-CB	5.90	118.80	110.12
2	N	82	LYS	CA-C-N	5.90	132.82	121.54
2	N	82	LYS	C-N-CA	5.90	132.82	121.54
1	E	74	LYS	N-CA-C	-5.90	100.17	109.50
1	E	190	GLY	CA-C-O	-5.90	117.86	122.52
1	F	81	GLN	OE1-CD-NE2	5.90	128.50	122.60
1	F	19	THR	N-CA-CB	5.90	120.59	110.68
1	A	180	ALA	N-CA-C	-5.90	104.76	111.07
2	I	129	ALA	CA-C-O	-5.90	114.63	120.82
1	A	129	GLU	CA-C-N	5.89	129.08	120.71
1	A	129	GLU	C-N-CA	5.89	129.08	120.71
1	C	120	ARG	NE-CZ-NH1	-5.89	115.61	121.50
2	V	66	VAL	N-CA-CB	5.89	120.95	111.23
1	E	16	ALA	N-CA-C	-5.89	103.51	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	137	LEU	N-CA-C	5.89	117.89	110.24
2	T	154	ASP	N-CA-CB	5.89	120.44	110.49
2	G	31	ASP	CA-CB-CG	5.89	118.49	112.60
2	M	93	TYR	CA-C-O	-5.89	114.72	121.19
2	U	129	ALA	N-CA-CB	5.88	119.07	109.95
1	B	34	ILE	N-CA-CB	5.88	118.54	110.54
2	V	72	ASP	CA-C-N	5.88	129.22	120.87
2	V	72	ASP	C-N-CA	5.88	129.22	120.87
2	G	158	PHE	CA-C-N	5.88	128.45	120.63
2	G	158	PHE	C-N-CA	5.88	128.45	120.63
2	Q	93	TYR	N-CA-CB	5.88	118.71	109.83
2	V	88	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	D	143	ALA	O-C-N	5.88	128.35	122.12
1	F	213	THR	CA-C-N	5.88	130.67	120.68
1	F	213	THR	C-N-CA	5.88	130.67	120.68
2	J	130	LEU	N-CA-C	-5.88	100.95	109.59
2	N	159	ILE	CA-CB-CG2	5.88	120.49	110.50
1	D	28	GLN	N-CA-C	-5.87	100.03	108.60
2	O	139	TYR	N-CA-CB	5.87	119.44	109.87
2	G	152	VAL	CA-CB-CG2	-5.87	100.42	110.40
2	N	123	PHE	CB-CA-C	5.87	119.94	109.38
1	A	59	PRO	CA-C-N	5.87	131.72	122.33
1	A	59	PRO	C-N-CA	5.87	131.72	122.33
2	H	88	ARG	NE-CZ-NH1	5.87	127.36	121.50
2	W	165	VAL	CB-CA-C	-5.87	100.25	111.40
1	E	132	GLU	N-CA-CB	5.86	121.61	111.00
2	W	153	THR	O-C-N	5.86	130.32	122.82
1	F	6	ASN	CB-CG-ND2	5.86	125.19	116.40
2	H	140	ARG	CA-C-N	5.86	132.73	121.54
2	H	140	ARG	C-N-CA	5.86	132.73	121.54
1	C	100	GLN	CA-C-N	5.86	127.94	120.56
1	C	100	GLN	C-N-CA	5.86	127.94	120.56
1	C	178	MET	CA-C-N	5.86	128.13	120.28
1	C	178	MET	C-N-CA	5.86	128.13	120.28
2	P	88	ARG	N-CA-CB	5.86	118.67	109.83
2	S	55	VAL	N-CA-C	5.85	117.54	109.46
2	S	57	LEU	N-CA-C	-5.85	101.52	109.95
1	B	97	SER	N-CA-C	-5.85	104.98	111.36
2	M	84	SER	N-CA-CB	5.85	120.38	110.49
1	D	63	LYS	O-C-N	5.85	127.29	121.85
2	V	145	TYR	N-CA-CB	5.85	120.37	110.49
1	D	182	ALA	CA-C-N	5.85	128.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	182	ALA	C-N-CA	5.85	128.12	120.28
1	E	244	ASP	CA-CB-CG	-5.85	106.75	112.60
2	U	71	GLU	O-C-N	5.85	130.02	122.89
2	G	102	THR	O-C-N	-5.85	115.33	122.34
1	C	90	VAL	N-CA-C	-5.84	101.15	108.05
1	D	151	SER	CA-C-N	5.84	126.43	120.00
1	D	151	SER	C-N-CA	5.84	126.43	120.00
1	F	27	ALA	CA-C-N	5.84	129.01	120.71
1	F	27	ALA	C-N-CA	5.84	129.01	120.71
2	X	160	GLY	CA-C-O	5.84	126.32	119.19
2	J	56	LYS	CA-C-O	-5.84	114.81	121.65
1	A	150	SER	CA-C-N	5.84	128.59	120.29
1	A	150	SER	C-N-CA	5.84	128.59	120.29
2	T	117	ASP	N-CA-C	-5.84	102.12	110.59
2	U	38	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	99	PRO	O-C-N	5.84	130.52	122.35
1	F	90	VAL	N-CA-C	-5.84	101.77	107.55
2	L	90	GLY	CA-C-O	-5.84	116.44	122.28
2	P	31	ASP	CA-CB-CG	5.84	118.44	112.60
1	D	60	VAL	N-CA-C	-5.84	97.20	109.34
2	V	128	LYS	N-CA-CB	5.84	119.79	110.16
2	O	99	THR	CA-CB-OG1	5.83	118.35	109.60
2	U	64	ASN	N-CA-CB	5.83	120.34	110.49
2	U	159	ILE	CA-C-N	5.83	130.57	122.29
2	U	159	ILE	C-N-CA	5.83	130.57	122.29
2	R	46	LYS	CG-CD-CE	5.83	124.71	111.30
2	P	138	GLU	N-CA-CB	5.83	119.96	110.17
1	E	71	VAL	O-C-N	-5.83	116.62	122.62
1	C	243	GLN	CA-C-N	5.83	131.69	122.60
1	C	243	GLN	C-N-CA	5.83	131.69	122.60
2	O	82	LYS	N-CA-CB	5.83	120.43	111.46
2	J	27	ASN	N-CA-CB	5.82	121.97	111.37
1	E	173	VAL	N-CA-C	-5.82	98.76	107.37
2	W	165	VAL	CA-CB-CG2	-5.82	100.50	110.40
2	X	25	ILE	CA-C-O	-5.82	113.99	120.74
1	B	169	HIS	ND1-CE1-NE2	5.82	114.22	108.40
1	B	271	VAL	CB-CA-C	-5.82	104.39	112.36
1	C	218	ILE	CB-CA-C	5.82	117.89	111.08
2	N	18	VAL	O-C-N	-5.82	116.77	123.00
2	N	114	CYS	N-CA-C	-5.82	100.91	109.81
1	D	233	PRO	N-CD-CG	5.82	111.92	103.20
2	M	121	ILE	CA-CB-CG2	-5.82	100.61	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	PRO	N-CD-CG	5.81	111.92	103.20
2	N	48	ALA	CA-C-N	5.81	132.65	121.54
2	N	48	ALA	C-N-CA	5.81	132.65	121.54
1	E	226	THR	CA-C-N	5.81	128.42	120.46
1	E	226	THR	C-N-CA	5.81	128.42	120.46
2	I	42	GLN	CA-C-N	5.81	128.34	120.38
2	I	42	GLN	C-N-CA	5.81	128.34	120.38
1	E	149	ILE	CA-CB-CG1	5.81	120.27	110.40
2	L	42	GLN	OE1-CD-NE2	5.81	128.41	122.60
2	S	27	ASN	CA-C-N	5.81	130.18	122.75
2	S	27	ASN	C-N-CA	5.81	130.18	122.75
2	S	135	HIS	CA-C-N	5.81	128.40	121.84
2	S	135	HIS	C-N-CA	5.81	128.40	121.84
2	W	88	ARG	N-CA-CB	5.81	121.01	111.31
2	O	91	GLU	N-CA-C	-5.80	101.77	110.06
2	H	55	VAL	N-CA-CB	5.80	118.44	111.31
2	U	23	GLU	CA-C-N	5.80	127.59	122.43
2	U	23	GLU	C-N-CA	5.80	127.59	122.43
2	H	34	VAL	N-CA-C	-5.80	107.61	113.47
1	B	141	ALA	CA-C-N	5.79	128.62	120.28
1	B	141	ALA	C-N-CA	5.79	128.62	120.28
2	T	145	TYR	CA-CB-CG	-5.79	103.47	113.90
2	V	69	PHE	CA-C-N	5.79	132.06	122.33
2	V	69	PHE	C-N-CA	5.79	132.06	122.33
1	C	204	GLN	N-CA-C	-5.79	98.06	108.48
2	J	94	VAL	CA-C-N	5.79	130.35	122.19
2	J	94	VAL	C-N-CA	5.79	130.35	122.19
1	D	277	ALA	CA-C-N	5.79	129.06	120.90
1	D	277	ALA	C-N-CA	5.79	129.06	120.90
1	F	90	VAL	N-CA-CB	5.79	118.14	111.31
1	F	197	VAL	CA-CB-CG2	5.79	120.23	110.40
2	I	44	ALA	CA-C-N	5.78	129.63	121.30
2	I	44	ALA	C-N-CA	5.78	129.63	121.30
2	U	33	ASP	CA-C-N	5.78	132.38	121.97
2	U	33	ASP	C-N-CA	5.78	132.38	121.97
2	G	88	ARG	CA-C-N	5.78	129.82	121.44
2	G	88	ARG	C-N-CA	5.78	129.82	121.44
1	D	41	GLN	N-CA-C	-5.78	100.28	109.59
2	Q	29	ALA	CB-CA-C	-5.78	100.21	109.75
1	C	41	GLN	O-C-N	5.78	130.07	123.31
1	C	239	MET	CA-C-O	5.78	125.62	119.50
2	J	42	GLN	OE1-CD-NE2	-5.78	116.82	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	146	GLU	CB-CG-CD	-5.78	102.78	112.60
2	U	46	LYS	N-CA-C	-5.78	98.50	110.80
1	A	132	GLU	CA-C-N	5.78	128.37	120.46
1	A	132	GLU	C-N-CA	5.78	128.37	120.46
1	E	90	VAL	CA-CB-CG1	5.78	120.22	110.40
1	F	124	ASP	CA-C-N	5.78	132.36	121.97
1	F	124	ASP	C-N-CA	5.78	132.36	121.97
2	L	144	MET	N-CA-CB	5.78	118.55	109.83
2	T	69	PHE	CA-CB-CG	5.78	119.58	113.80
1	B	122	LYS	CA-C-N	5.77	132.57	121.54
1	B	122	LYS	C-N-CA	5.77	132.57	121.54
2	I	153	THR	CA-CB-OG1	5.77	118.26	109.60
1	C	9	LYS	N-CA-C	-5.77	105.50	112.54
2	K	144	MET	N-CA-C	5.77	117.61	108.67
2	G	125	GLY	N-CA-C	-5.77	99.50	113.18
2	P	64	ASN	N-CA-C	-5.77	106.28	113.38
2	R	50	ILE	CA-C-O	-5.77	113.08	119.20
2	G	154	ASP	N-CA-C	-5.77	104.91	112.41
2	N	52	ALA	CA-C-N	5.77	129.46	120.75
2	N	52	ALA	C-N-CA	5.77	129.46	120.75
1	D	38	LEU	N-CA-C	-5.77	100.53	109.24
1	C	272	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	F	137	LEU	N-CA-C	5.76	118.71	110.24
2	Q	31	ASP	CA-CB-CG	5.76	118.36	112.60
2	P	70	ARG	CA-C-N	5.76	129.05	120.87
2	P	70	ARG	C-N-CA	5.76	129.05	120.87
2	R	158	PHE	CA-C-N	5.76	129.61	121.66
2	R	158	PHE	C-N-CA	5.76	129.61	121.66
2	I	101	LEU	N-CA-C	-5.76	98.90	108.34
2	M	60	ASP	N-CA-C	-5.76	98.54	110.80
1	F	228	TYR	O-C-N	-5.75	115.88	122.09
1	B	61	TYR	CA-C-O	-5.75	115.30	121.45
1	D	231	ALA	O-C-N	-5.75	116.68	123.41
2	S	123	PHE	N-CA-C	-5.75	99.78	108.52
2	I	137	GLY	N-CA-C	-5.75	106.81	115.32
2	Q	88	ARG	CA-C-O	-5.75	114.72	121.16
1	D	74	LYS	CA-C-N	5.75	132.12	122.87
1	D	74	LYS	C-N-CA	5.75	132.12	122.87
2	I	81	GLU	N-CA-C	-5.75	104.94	112.41
2	I	134	THR	CA-C-O	-5.75	114.90	121.68
2	N	29	ALA	CB-CA-C	-5.75	99.44	110.24
2	X	137	GLY	N-CA-C	-5.75	104.99	114.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	92	TYR	CA-CB-CG	-5.75	103.56	113.90
1	C	189	TRP	N-CA-C	-5.74	106.31	113.55
2	H	60	ASP	CA-C-N	5.74	132.51	121.54
2	H	60	ASP	C-N-CA	5.74	132.51	121.54
2	H	30	HIS	CG-CD2-NE2	5.74	112.94	107.20
2	W	149	THR	N-CA-C	-5.74	100.62	109.52
1	D	99	PRO	CA-C-N	5.74	127.97	120.28
1	D	99	PRO	C-N-CA	5.74	127.97	120.28
2	T	38	ASN	CA-CB-CG	5.74	118.34	112.60
2	W	135	HIS	N-CA-C	5.74	118.31	111.71
1	D	259	GLY	N-CA-C	-5.74	99.58	113.18
2	I	30	HIS	CA-CB-CG	5.74	119.54	113.80
1	B	228	TYR	CA-CB-CG	5.73	124.22	113.90
1	D	85	GLY	N-CA-C	-5.73	101.00	110.80
1	D	238	VAL	CG1-CB-CG2	5.73	123.41	110.80
1	A	20	GLU	N-CA-CB	5.73	119.13	110.42
2	M	23	GLU	CA-C-O	-5.73	115.14	121.33
2	T	27	ASN	N-CA-C	-5.73	104.86	112.94
1	A	235	PHE	O-C-N	5.73	128.28	122.09
2	S	157	THR	O-C-N	5.73	129.98	122.93
1	C	23	ARG	CA-C-N	5.73	131.06	122.58
1	C	23	ARG	C-N-CA	5.73	131.06	122.58
2	Q	23	GLU	CA-C-N	5.72	127.49	120.22
2	Q	23	GLU	C-N-CA	5.72	127.49	120.22
1	C	151	SER	CA-C-N	5.72	126.33	119.98
1	C	151	SER	C-N-CA	5.72	126.33	119.98
2	X	34	VAL	CA-C-N	5.72	130.26	122.19
2	X	34	VAL	C-N-CA	5.72	130.26	122.19
2	U	58	ALA	N-CA-C	-5.72	98.97	108.75
2	H	102	THR	N-CA-C	-5.72	104.98	112.41
1	F	87	ARG	NE-CZ-NH2	-5.71	114.06	119.20
2	J	81	GLU	O-C-N	-5.71	117.10	123.04
1	B	88	ILE	CA-C-O	-5.71	114.43	120.48
1	C	236	VAL	CA-C-O	5.71	127.04	120.76
1	E	189	TRP	CE2-CD2-CE3	5.71	124.51	118.80
2	P	134	THR	N-CA-C	-5.71	103.80	112.99
2	T	79	ALA	O-C-N	5.70	129.85	122.89
2	U	88	ARG	CA-C-N	5.70	126.66	120.44
2	U	88	ARG	C-N-CA	5.70	126.66	120.44
2	I	27	ASN	O-C-N	-5.70	115.01	122.59
2	N	30	HIS	CE1-NE2-CD2	-5.70	103.30	109.00
2	O	139	TYR	CB-CA-C	-5.70	100.94	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	19	ARG	CA-C-N	5.70	129.36	120.75
2	P	19	ARG	C-N-CA	5.70	129.36	120.75
1	D	122	LYS	N-CA-CB	5.70	118.38	110.17
2	Q	135	HIS	CG-CD2-NE2	5.70	112.90	107.20
1	C	215	ASP	CA-CB-CG	5.70	118.30	112.60
2	I	22	TYR	N-CA-C	-5.70	98.67	110.80
1	F	100	GLN	N-CA-C	5.69	117.49	111.28
1	F	17	LEU	N-CA-C	-5.69	98.23	108.48
2	Q	34	VAL	CB-CA-C	5.69	120.62	111.29
1	E	239	MET	O-C-N	-5.69	116.26	122.06
2	I	78	ASN	CA-CB-CG	5.69	118.29	112.60
1	A	248	ILE	CA-C-N	5.69	125.22	119.19
1	A	248	ILE	C-N-CA	5.69	125.22	119.19
1	E	93	PHE	CA-C-N	5.69	128.37	120.29
1	E	93	PHE	C-N-CA	5.69	128.37	120.29
1	E	247	VAL	CB-CA-C	-5.69	104.70	111.81
1	C	13	ILE	CA-C-N	5.68	128.84	120.82
1	C	13	ILE	C-N-CA	5.68	128.84	120.82
2	G	67	GLY	CA-C-O	-5.68	116.59	122.28
2	S	20	LEU	N-CA-CB	5.68	120.10	110.49
1	E	90	VAL	CA-C-N	5.68	125.36	119.05
1	E	90	VAL	C-N-CA	5.68	125.36	119.05
2	J	140	ARG	N-CA-C	-5.68	100.68	109.14
1	D	185	ASP	CA-C-N	5.68	130.43	123.10
1	D	185	ASP	C-N-CA	5.68	130.43	123.10
2	P	115	ASP	N-CA-C	-5.68	100.23	108.07
1	B	195	ASP	N-CA-C	-5.68	99.22	108.82
1	A	145	ASN	CA-C-O	5.68	127.08	120.49
1	B	10	GLU	CB-CG-CD	-5.68	102.95	112.60
2	M	110	ASP	CA-C-O	-5.68	114.55	121.36
2	N	47	PHE	CA-C-O	-5.68	115.02	121.72
1	B	240	PRO	N-CD-CG	5.67	111.71	103.20
1	C	182	ALA	O-C-N	5.67	128.62	122.15
2	M	37	LEU	N-CA-C	-5.67	102.89	110.55
1	C	4	LEU	N-CA-C	-5.67	106.17	114.39
2	S	88	ARG	O-C-N	5.67	129.85	123.27
1	B	62	ASP	CA-CB-CG	5.67	118.27	112.60
1	C	205	THR	N-CA-CB	5.67	121.26	111.00
1	A	113	VAL	CA-C-N	5.67	127.81	120.56
1	A	113	VAL	C-N-CA	5.67	127.81	120.56
2	I	135	HIS	CG-CD2-NE2	5.67	112.87	107.20
2	I	159	ILE	CA-C-N	5.67	129.65	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	159	ILE	C-N-CA	5.67	129.65	122.00
2	O	30	HIS	CB-CG-CD2	-5.66	123.84	131.20
2	R	143	ASN	CA-C-N	5.66	128.75	120.71
2	R	143	ASN	C-N-CA	5.66	128.75	120.71
1	E	94	GLU	N-CA-C	-5.66	105.19	111.36
1	B	31	ALA	CB-CA-C	-5.66	101.15	110.72
1	F	169	HIS	CE1-NE2-CD2	-5.66	103.34	109.00
1	F	174	THR	CA-C-N	5.66	129.51	121.42
1	F	174	THR	C-N-CA	5.66	129.51	121.42
2	Q	156	ASP	CB-CA-C	-5.66	100.91	110.64
1	D	74	LYS	N-CA-C	-5.65	100.57	109.50
1	E	169	HIS	CA-CB-CG	5.65	119.45	113.80
1	F	228	TYR	CB-CA-C	-5.65	101.97	110.90
2	I	126	THR	CA-CB-OG1	5.65	118.08	109.60
2	G	156	ASP	N-CA-C	-5.65	106.28	112.72
2	X	133	VAL	N-CA-C	-5.65	100.34	108.53
2	U	70	ARG	NE-CZ-NH2	-5.65	114.12	119.20
1	F	160	THR	N-CA-C	5.65	118.37	111.82
2	G	146	GLU	N-CA-C	-5.65	101.17	109.81
2	O	66	VAL	N-CA-C	-5.65	99.41	107.77
2	S	113	THR	N-CA-C	-5.65	100.50	109.76
1	B	196	PRO	CA-C-N	5.64	127.88	120.60
1	B	196	PRO	C-N-CA	5.64	127.88	120.60
1	F	279	ILE	CA-CB-CG2	-5.64	100.90	110.50
2	H	120	MET	N-CA-CB	5.64	118.58	110.06
2	T	149	THR	N-CA-C	-5.64	101.83	109.95
2	X	97	SER	O-C-N	5.64	128.86	122.20
2	G	42	GLN	CB-CG-CD	-5.64	103.02	112.60
2	X	72	ASP	N-CA-C	-5.64	100.21	109.40
1	D	33	PRO	CA-C-N	5.63	128.42	120.42
1	D	33	PRO	C-N-CA	5.63	128.42	120.42
2	H	60	ASP	O-C-N	5.63	129.34	122.75
1	D	228	TYR	CA-C-N	5.63	127.77	120.56
1	D	228	TYR	C-N-CA	5.63	127.77	120.56
2	Q	161	PHE	CA-C-O	-5.63	114.60	121.36
1	E	147	VAL	N-CA-CB	5.63	116.97	110.49
1	C	209	GLY	N-CA-C	5.63	119.74	112.54
1	D	105	GLN	CG-CD-NE2	5.63	124.84	116.40
2	K	159	ILE	CA-CB-CG2	-5.63	100.94	110.50
1	A	98	TYR	CA-C-N	5.62	125.72	119.87
1	A	98	TYR	C-N-CA	5.62	125.72	119.87
2	O	144	MET	O-C-N	5.62	129.39	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	17	TYR	O-C-N	5.62	130.22	123.36
2	K	134	THR	N-CA-CB	5.62	119.33	110.56
2	R	137	GLY	CA-C-N	5.62	129.09	120.82
2	R	137	GLY	C-N-CA	5.62	129.09	120.82
2	T	26	LEU	O-C-N	-5.62	116.66	123.29
2	W	30	HIS	CB-CG-ND1	5.62	131.13	122.70
1	B	235	PHE	CA-C-O	-5.62	114.91	120.70
1	B	109	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	F	98	TYR	CA-C-O	-5.62	112.46	120.16
1	A	163	PHE	CA-CB-CG	-5.62	108.18	113.80
1	B	227	VAL	CA-C-O	-5.62	115.21	121.05
1	B	242	ARG	N-CA-C	-5.62	99.51	109.06
1	F	22	GLY	N-CA-C	-5.61	105.07	112.82
2	J	61	ASN	O-C-N	-5.61	115.13	122.20
2	X	90	GLY	N-CA-C	-5.61	102.66	112.53
1	D	135	SER	CA-C-N	5.61	128.83	120.31
1	D	135	SER	C-N-CA	5.61	128.83	120.31
2	Q	113	THR	CA-C-N	5.61	130.69	121.39
2	Q	113	THR	C-N-CA	5.61	130.69	121.39
1	F	119	GLN	OE1-CD-NE2	5.60	128.20	122.60
2	U	90	GLY	CA-C-N	5.60	132.24	121.54
2	U	90	GLY	C-N-CA	5.60	132.24	121.54
1	B	166	VAL	N-CA-CB	5.60	120.47	111.23
1	F	102	ARG	NE-CZ-NH2	-5.60	114.16	119.20
2	P	48	ALA	CB-CA-C	-5.60	101.12	110.19
2	Q	83	ALA	CA-C-N	5.60	129.30	121.02
2	Q	83	ALA	C-N-CA	5.60	129.30	121.02
1	D	10	GLU	N-CA-C	-5.59	105.77	112.59
2	J	112	ILE	N-CA-C	5.59	116.64	108.53
2	R	67	GLY	O-C-N	5.59	128.93	122.61
2	N	38	ASN	N-CA-CB	5.59	118.27	109.83
1	C	208	PHE	CA-C-N	5.59	126.84	120.53
1	C	208	PHE	C-N-CA	5.59	126.84	120.53
1	D	118	GLN	N-CA-C	5.58	117.05	111.07
2	W	61	ASN	O-C-N	5.58	129.70	122.89
1	B	85	GLY	N-CA-C	-5.58	102.27	110.87
2	U	122	LYS	N-CA-C	-5.58	100.30	109.40
1	C	266	LEU	CA-C-N	5.58	132.35	121.41
1	C	266	LEU	C-N-CA	5.58	132.35	121.41
1	A	51	ASP	N-CA-CB	-5.58	100.44	110.37
2	L	124	THR	N-CA-C	-5.58	100.59	109.07
1	B	43	VAL	CA-CB-CG1	5.58	119.89	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	LYS	CA-C-O	5.58	128.42	121.89
2	N	148	ALA	CB-CA-C	-5.58	101.47	109.84
2	R	84	SER	N-CA-C	5.58	117.94	110.35
2	X	98	ARG	CA-C-O	5.58	126.37	119.79
2	V	69	PHE	CA-CB-CG	-5.57	108.23	113.80
1	E	65	VAL	CA-C-O	5.57	126.53	120.57
2	I	84	SER	CB-CA-C	-5.57	102.14	110.88
1	C	77	GLN	N-CA-C	-5.57	99.94	109.24
1	E	116	ARG	CB-CA-C	5.57	119.62	110.88
1	E	214	ALA	N-CA-C	-5.57	100.17	109.24
1	C	134	PHE	CA-CB-CG	5.57	119.36	113.80
1	E	146	ALA	CA-C-N	5.57	128.90	120.77
1	E	146	ALA	C-N-CA	5.57	128.90	120.77
2	X	72	ASP	CA-C-N	5.57	129.26	121.02
2	X	72	ASP	C-N-CA	5.57	129.26	121.02
1	C	51	ASP	O-C-N	-5.56	114.92	121.32
1	E	122	LYS	CA-C-N	5.56	132.17	121.54
1	E	122	LYS	C-N-CA	5.56	132.17	121.54
2	K	78	ASN	N-CA-C	-5.56	101.44	108.45
1	A	79	PRO	N-CA-C	-5.56	103.12	111.57
2	U	52	ALA	CA-C-O	-5.56	115.32	121.33
1	B	9	LYS	N-CA-C	-5.56	104.74	112.30
1	D	230	LEU	CB-CA-C	-5.56	99.79	110.24
1	F	90	VAL	CA-C-N	5.56	125.22	119.05
1	F	90	VAL	C-N-CA	5.56	125.22	119.05
2	J	155	THR	N-CA-C	-5.56	105.10	112.94
2	L	88	ARG	NH1-CZ-NH2	-5.56	112.07	119.30
2	M	60	ASP	N-CA-CB	5.56	119.89	110.49
1	B	30	MET	CA-C-N	5.56	131.27	122.60
1	B	30	MET	C-N-CA	5.56	131.27	122.60
1	D	203	LEU	N-CA-C	-5.56	98.97	110.80
2	H	60	ASP	CA-CB-CG	5.56	118.16	112.60
2	X	45	GLY	N-CA-C	-5.56	104.18	113.02
1	C	42	GLY	N-CA-C	-5.55	98.55	110.66
1	C	267	GLY	O-C-N	-5.55	115.48	122.70
2	H	129	ALA	N-CA-C	-5.55	98.97	110.80
2	S	146	GLU	N-CA-C	-5.55	105.86	113.30
2	G	27	ASN	CB-CG-ND2	-5.55	108.07	116.40
1	B	67	ALA	N-CA-C	-5.55	102.30	110.52
1	A	190	GLY	O-C-N	5.55	127.52	122.19
2	X	120	MET	CG-SD-CE	-5.55	88.69	100.90
2	V	140	ARG	CB-CA-C	-5.55	99.31	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	HIS	O-C-N	-5.55	116.14	121.85
2	M	44	ALA	N-CA-C	-5.55	104.06	112.99
1	A	250	ALA	N-CA-C	5.54	117.00	111.07
1	D	177	VAL	N-CA-C	5.54	115.74	110.53
2	O	136	VAL	CA-C-N	5.54	126.26	119.99
2	O	136	VAL	C-N-CA	5.54	126.26	119.99
1	A	53	LEU	CB-CA-C	5.54	116.84	108.86
1	C	257	ARG	N-CA-CB	5.54	119.27	110.57
2	J	127	GLY	N-CA-C	-5.54	105.62	112.33
2	P	47	PHE	CA-C-O	5.54	128.42	121.66
2	P	53	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	131	ALA	N-CA-C	5.54	117.69	110.43
1	C	233	PRO	N-CA-CB	5.54	108.71	102.67
1	D	143	ALA	CA-C-N	5.54	128.05	120.46
1	D	143	ALA	C-N-CA	5.54	128.05	120.46
1	E	196	PRO	CA-C-N	5.54	129.13	122.26
1	E	196	PRO	C-N-CA	5.54	129.13	122.26
1	A	210	HIS	CA-C-N	5.54	130.47	123.10
1	A	210	HIS	C-N-CA	5.54	130.47	123.10
1	B	238	VAL	N-CA-C	5.54	116.22	109.30
2	K	133	VAL	N-CA-CB	5.54	121.03	111.39
2	H	78	ASN	N-CA-CB	5.54	119.99	111.24
2	P	47	PHE	O-C-N	-5.54	116.77	123.03
1	F	49	VAL	CA-C-O	-5.54	114.86	121.28
2	L	44	ALA	CA-C-N	-5.54	113.33	121.30
2	L	44	ALA	C-N-CA	-5.54	113.33	121.30
2	N	53	ASN	N-CA-C	-5.54	102.82	110.35
2	T	135	HIS	ND1-CE1-NE2	5.54	113.94	108.40
1	C	183	PHE	CA-C-N	5.53	128.25	120.28
1	C	183	PHE	C-N-CA	5.53	128.25	120.28
2	H	124	THR	N-CA-CB	5.53	121.18	111.55
1	A	130	ASP	N-CA-CB	5.53	118.18	109.83
1	A	47	LEU	CA-C-O	-5.53	114.64	121.11
1	A	78	VAL	CB-CA-C	5.53	115.74	110.16
1	C	246	GLN	N-CA-C	-5.53	101.12	108.74
2	I	25	ILE	N-CA-CB	5.53	119.73	112.60
2	J	22	TYR	CA-C-N	5.53	128.95	121.05
2	J	22	TYR	C-N-CA	5.53	128.95	121.05
1	C	41	GLN	CA-C-O	-5.52	114.19	120.32
2	J	89	GLY	CA-C-N	5.52	129.95	121.45
2	J	89	GLY	C-N-CA	5.52	129.95	121.45
1	C	98	TYR	N-CA-CB	5.52	120.20	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ILE	CA-C-O	-5.52	115.33	121.23
1	D	202	VAL	CA-C-N	5.52	132.08	121.54
1	D	202	VAL	C-N-CA	5.52	132.08	121.54
2	U	18	VAL	CA-C-O	-5.52	113.88	120.78
2	X	55	VAL	N-CA-C	-5.52	98.49	106.88
2	H	143	ASN	N-CA-CB	5.52	119.81	110.49
2	J	136	VAL	CA-C-N	5.52	126.11	119.98
2	J	136	VAL	C-N-CA	5.52	126.11	119.98
1	E	15	LYS	N-CA-CB	5.51	118.08	109.97
2	O	158	PHE	N-CA-CB	5.51	118.83	110.45
1	C	161	LYS	CA-C-N	5.51	128.22	120.28
1	C	161	LYS	C-N-CA	5.51	128.22	120.28
2	V	81	GLU	N-CA-C	-5.51	95.57	111.00
1	B	53	LEU	CA-C-N	5.51	127.95	120.79
1	B	53	LEU	C-N-CA	5.51	127.95	120.79
2	N	97	SER	CB-CA-C	-5.51	102.09	111.02
2	X	143	ASN	O-C-N	5.51	129.92	122.59
1	E	249	PRO	CA-C-N	5.51	127.60	120.44
1	E	249	PRO	C-N-CA	5.51	127.60	120.44
1	C	2	SER	CA-C-O	5.51	126.88	120.49
2	K	70	ARG	N-CA-C	-5.51	101.39	109.81
2	K	143	ASN	CA-CB-CG	-5.51	107.09	112.60
1	A	179	ASN	CA-C-N	5.50	127.60	120.44
1	A	179	ASN	C-N-CA	5.50	127.60	120.44
1	A	192	ASN	CA-C-N	5.50	128.68	120.31
1	A	192	ASN	C-N-CA	5.50	128.68	120.31
1	B	121	ALA	N-CA-C	5.50	117.14	111.03
1	E	136	LEU	CA-C-O	-5.50	114.72	120.55
1	E	118	GLN	CA-C-N	5.50	127.92	120.44
1	E	118	GLN	C-N-CA	5.50	127.92	120.44
2	N	41	GLU	O-C-N	-5.50	115.58	122.35
2	T	94	VAL	CA-C-N	5.50	129.95	122.19
2	T	94	VAL	C-N-CA	5.50	129.95	122.19
1	C	109	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	C	111	PHE	N-CA-CB	5.50	118.30	110.16
1	E	245	ILE	N-CA-C	-5.50	97.90	109.34
2	J	21	GLY	CA-C-N	5.50	131.12	122.21
2	J	21	GLY	C-N-CA	5.50	131.12	122.21
2	W	134	THR	CA-C-O	-5.50	115.23	121.72
2	Q	30	HIS	CE1-NE2-CD2	-5.50	103.50	109.00
2	S	23	GLU	CB-CG-CD	-5.50	103.25	112.60
2	W	98	ARG	CA-C-N	-5.50	115.36	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	98	ARG	C-N-CA	-5.50	115.36	123.05
2	M	56	LYS	N-CA-CB	5.49	119.78	110.49
2	S	123	PHE	CA-CB-CG	-5.49	108.31	113.80
2	J	153	THR	N-CA-C	-5.49	100.94	109.72
2	H	99	THR	N-CA-CB	5.49	118.16	109.71
2	S	106	ILE	CA-CB-CG1	5.49	119.72	110.40
2	U	149	THR	N-CA-C	-5.49	106.36	113.16
1	D	221	LYS	N-CA-CB	5.48	120.92	111.00
1	E	270	VAL	CB-CA-C	5.48	116.54	110.62
2	L	95	ASN	CA-C-N	5.48	131.84	121.97
2	L	95	ASN	C-N-CA	5.48	131.84	121.97
2	R	61	ASN	CA-CB-CG	-5.48	107.12	112.60
2	H	78	ASN	CA-CB-CG	5.48	118.08	112.60
2	Q	163	MET	CA-C-N	5.48	129.92	122.19
2	Q	163	MET	C-N-CA	5.48	129.92	122.19
1	C	8	GLU	CB-CA-C	-5.48	98.83	109.68
2	I	76	MET	N-CA-C	-5.48	101.03	109.52
1	B	76	GLY	CA-C-O	5.48	126.34	121.57
1	B	211	ILE	N-CA-C	-5.48	99.75	107.75
1	C	223	PRO	CA-C-N	5.48	132.00	121.54
1	C	223	PRO	C-N-CA	5.48	132.00	121.54
2	X	46	LYS	O-C-N	-5.48	118.48	123.41
1	B	116	ARG	CA-C-N	5.48	127.62	120.28
1	B	116	ARG	C-N-CA	5.48	127.62	120.28
2	O	39	GLY	CA-C-N	5.47	127.83	120.50
2	O	39	GLY	C-N-CA	5.47	127.83	120.50
2	S	149	THR	CA-CB-CG2	-5.47	101.19	110.50
1	F	238	VAL	N-CA-CB	5.47	118.67	110.13
2	Q	30	HIS	CA-CB-CG	-5.47	108.33	113.80
1	E	75	ARG	NH1-CZ-NH2	5.47	126.41	119.30
1	E	155	GLN	CA-C-O	-5.47	114.75	120.55
2	P	150	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	B	119	GLN	CA-C-N	5.47	127.61	120.28
1	B	119	GLN	C-N-CA	5.47	127.61	120.28
1	D	32	ASN	CA-CB-CG	5.47	118.07	112.60
2	P	40	VAL	CA-C-N	5.47	128.61	120.95
2	P	40	VAL	C-N-CA	5.47	128.61	120.95
2	T	71	GLU	N-CA-CB	5.47	118.01	109.97
1	D	45	ARG	CD-NE-CZ	-5.47	116.75	124.40
1	D	226	THR	N-CA-C	5.47	117.24	111.28
1	D	274	LEU	O-C-N	-5.47	117.57	123.42
2	L	93	TYR	CG-CD1-CE1	5.47	129.40	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	135	HIS	CE1-NE2-CD2	-5.46	103.53	109.00
1	F	98	TYR	CA-CB-CG	5.46	123.73	113.90
2	J	85	PHE	CA-CB-CG	-5.46	108.34	113.80
2	M	47	PHE	CB-CA-C	-5.46	102.30	110.16
2	M	52	ALA	N-CA-C	-5.46	105.24	112.94
2	H	18	VAL	CA-C-N	5.46	131.71	122.26
2	H	18	VAL	C-N-CA	5.46	131.71	122.26
2	J	88	ARG	CA-C-O	-5.46	114.16	120.49
2	O	156	ASP	N-CA-C	-5.46	101.01	109.14
1	C	276	ILE	N-CA-C	-5.45	99.97	108.86
1	C	103	PHE	CA-C-N	5.45	127.59	120.28
1	C	103	PHE	C-N-CA	5.45	127.59	120.28
1	B	208	PHE	CA-C-N	5.45	126.69	120.53
1	B	208	PHE	C-N-CA	5.45	126.69	120.53
1	B	54	PRO	N-CD-CG	5.45	111.37	103.20
2	T	60	ASP	N-CA-CB	5.45	118.23	110.44
1	B	224	GLN	CA-C-N	5.45	129.63	122.06
1	B	224	GLN	C-N-CA	5.45	129.63	122.06
2	R	98	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	B	177	VAL	O-C-N	5.44	127.56	121.90
1	C	232	ASP	N-CA-CB	5.44	119.30	110.05
1	F	262	ILE	N-CA-CB	5.44	119.22	111.82
2	H	127	GLY	O-C-N	5.44	129.78	122.70
2	P	119	LYS	CA-C-O	-5.44	115.45	121.33
2	Q	107	ALA	N-CA-CB	5.44	119.68	110.49
2	X	31	ASP	CA-C-N	5.44	127.91	120.35
2	X	31	ASP	C-N-CA	5.44	127.91	120.35
2	L	153	THR	N-CA-C	-5.44	101.03	109.24
2	O	76	MET	CA-C-O	-5.44	114.91	120.89
1	D	81	GLN	CA-C-N	5.43	130.26	123.14
1	D	81	GLN	C-N-CA	5.43	130.26	123.14
2	I	105	GLY	O-C-N	-5.43	115.63	122.70
2	R	46	LYS	CA-CB-CG	5.43	124.97	114.10
1	A	214	ALA	CA-C-N	5.43	131.92	121.54
1	A	214	ALA	C-N-CA	5.43	131.92	121.54
2	J	154	ASP	N-CA-C	-5.43	101.12	109.76
2	U	145	TYR	N-CA-C	-5.43	106.65	113.28
1	D	73	SER	N-CA-C	-5.43	100.92	109.50
2	L	105	GLY	CA-C-O	-5.43	115.55	122.01
2	M	97	SER	N-CA-CB	5.42	119.54	110.59
2	M	32	ILE	CB-CA-C	5.42	120.18	111.29
2	V	149	THR	CA-C-N	5.42	129.25	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	149	THR	C-N-CA	5.42	129.25	121.50
2	G	96	ILE	N-CA-C	-5.42	100.52	108.11
1	E	25	ALA	CA-C-N	5.42	128.46	120.82
1	E	25	ALA	C-N-CA	5.42	128.46	120.82
1	B	12	LEU	N-CA-CB	5.42	119.97	110.27
2	L	143	ASN	OD1-CG-ND2	5.42	128.02	122.60
2	N	30	HIS	CB-CG-CD2	-5.42	124.16	131.20
2	S	17	TYR	CB-CG-CD1	-5.42	112.67	120.80
2	H	40	VAL	N-CA-CB	5.42	120.17	111.23
1	A	188	ALA	N-CA-C	-5.41	104.57	113.50
1	C	74	LYS	N-CA-C	-5.41	101.06	109.72
2	G	76	MET	N-CA-C	-5.41	100.95	109.50
2	J	158	PHE	CA-C-O	-5.41	115.20	121.15
2	I	153	THR	CB-CA-C	5.41	120.00	110.37
2	J	70	ARG	NE-CZ-NH1	5.41	126.91	121.50
2	T	57	LEU	CA-C-O	5.41	128.24	120.51
2	L	154	ASP	CA-CB-CG	5.41	118.00	112.60
2	Q	64	ASN	N-CA-CB	5.41	119.63	110.49
2	X	124	THR	CA-C-N	5.40	128.78	122.19
2	X	124	THR	C-N-CA	5.40	128.78	122.19
2	Q	158	PHE	CA-C-N	5.40	131.69	121.97
2	Q	158	PHE	C-N-CA	5.40	131.69	121.97
2	T	22	TYR	CA-CB-CG	-5.40	104.17	113.90
2	T	34	VAL	N-CA-CB	5.40	118.59	111.25
2	T	159	ILE	O-C-N	-5.40	115.82	122.57
2	X	27	ASN	N-CA-CB	5.40	120.28	112.13
1	E	58	LEU	CA-C-N	5.40	126.58	119.84
1	E	58	LEU	C-N-CA	5.40	126.58	119.84
1	B	248	ILE	CA-C-O	-5.39	112.72	119.95
1	B	261	VAL	CA-CB-CG1	-5.39	101.23	110.40
2	J	122	LYS	N-CA-C	-5.39	101.49	110.17
1	F	177	VAL	CA-C-N	5.39	127.50	120.28
1	F	177	VAL	C-N-CA	5.39	127.50	120.28
1	D	172	VAL	N-CA-CB	5.39	118.58	111.25
1	D	77	GLN	O-C-N	-5.39	117.01	123.31
1	F	251	ASP	CA-CB-CG	-5.39	107.21	112.60
2	K	82	LYS	CA-C-N	5.39	131.83	121.54
2	K	82	LYS	C-N-CA	5.39	131.83	121.54
2	P	44	ALA	N-CA-CB	5.39	119.59	110.49
2	J	105	GLY	CA-C-N	5.38	128.63	120.77
2	J	105	GLY	C-N-CA	5.38	128.63	120.77
2	M	101	LEU	N-CA-C	-5.38	106.02	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	88	ARG	CD-NE-CZ	-5.38	116.86	124.40
2	V	77	VAL	N-CA-C	-5.38	100.56	108.85
2	V	130	LEU	N-CA-CB	5.38	119.65	110.50
1	A	45	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	C	206	GLY	CA-C-N	5.38	131.82	121.54
1	C	206	GLY	C-N-CA	5.38	131.82	121.54
1	B	232	ASP	N-CA-CB	5.38	119.20	110.05
2	H	23	GLU	N-CA-CB	5.38	119.58	110.49
1	B	86	ASP	N-CA-C	-5.38	101.00	109.50
2	R	38	ASN	N-CA-C	-5.38	102.01	113.20
2	U	152	VAL	CB-CA-C	-5.38	103.78	111.31
2	S	154	ASP	N-CA-C	-5.38	99.76	108.52
1	A	118	GLN	CA-C-O	-5.37	115.18	120.82
2	V	85	PHE	CA-C-O	-5.37	112.83	120.51
2	X	123	PHE	N-CA-CB	5.37	118.98	110.87
2	G	135	HIS	CB-CG-CD2	-5.37	124.22	131.20
2	J	34	VAL	N-CA-C	-5.37	100.65	108.17
1	A	223	PRO	CA-C-O	-5.37	115.42	122.19
1	B	112	ASN	N-CA-CB	5.37	117.86	110.07
1	E	123	ALA	N-CA-CB	5.37	119.56	110.49
2	G	113	THR	CB-CA-C	5.37	118.50	109.48
1	C	176	ILE	CA-C-N	5.37	127.81	120.46
1	C	176	ILE	C-N-CA	5.37	127.81	120.46
1	E	39	ASP	N-CA-CB	5.37	119.05	110.46
1	F	265	GLU	N-CA-CB	5.37	119.83	110.81
2	G	35	ALA	N-CA-C	-5.37	99.37	110.80
1	B	104	SER	N-CA-C	5.37	117.13	111.28
1	E	155	GLN	CB-CA-C	-5.37	101.88	110.79
2	G	90	GLY	CA-C-O	-5.36	115.29	121.46
2	N	64	ASN	N-CA-C	-5.36	100.92	109.07
1	C	104	SER	CA-C-N	5.36	127.73	120.44
1	C	104	SER	C-N-CA	5.36	127.73	120.44
2	X	126	THR	CA-C-N	5.36	125.07	119.92
2	X	126	THR	C-N-CA	5.36	125.07	119.92
2	X	162	ILE	O-C-N	-5.36	115.89	122.97
2	N	135	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
2	U	99	THR	CA-CB-OG1	5.36	117.64	109.60
1	D	223	PRO	N-CA-C	-5.36	102.15	112.01
1	E	62	ASP	N-CA-C	-5.36	105.97	112.88
2	H	54	GLY	CA-C-N	5.36	129.18	122.43
2	H	54	GLY	C-N-CA	5.36	129.18	122.43
2	V	128	LYS	O-C-N	5.36	129.32	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	132	GLU	CA-C-N	5.35	127.51	120.60
1	E	132	GLU	C-N-CA	5.35	127.51	120.60
1	A	8	GLU	CA-C-N	5.35	130.39	123.00
1	A	8	GLU	C-N-CA	5.35	130.39	123.00
1	E	36	VAL	N-CA-C	5.35	116.94	109.55
2	R	107	ALA	CA-C-N	5.35	131.76	121.54
2	R	107	ALA	C-N-CA	5.35	131.76	121.54
2	T	82	LYS	N-CA-C	-5.35	99.40	110.80
2	U	29	ALA	CB-CA-C	-5.35	99.77	110.42
2	U	50	ILE	CB-CA-C	-5.35	103.89	111.28
1	E	266	LEU	CA-C-O	-5.35	115.04	120.71
1	C	245	ILE	O-C-N	5.35	129.26	122.57
2	H	54	GLY	CA-C-O	5.35	126.05	121.88
1	A	122	LYS	N-CA-CB	5.35	119.53	110.49
1	B	51	ASP	CA-C-N	5.35	125.61	119.83
1	B	51	ASP	C-N-CA	5.35	125.61	119.83
1	F	70	PHE	CA-CB-CG	-5.35	108.45	113.80
2	L	82	LYS	N-CA-C	-5.35	100.99	109.76
2	W	160	GLY	N-CA-C	-5.34	107.41	115.32
1	C	87	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
2	I	106	ILE	N-CA-C	5.34	115.98	109.30
2	L	78	ASN	N-CA-CB	5.34	119.68	111.24
1	B	98	TYR	O-C-N	-5.34	115.18	121.32
2	Q	134	THR	N-CA-C	-5.34	101.42	109.85
1	A	78	VAL	CA-C-N	5.34	125.54	120.31
1	A	78	VAL	C-N-CA	5.34	125.54	120.31
1	D	232	ASP	CA-C-N	5.34	125.75	119.99
1	D	232	ASP	C-N-CA	5.34	125.75	119.99
1	D	266	LEU	N-CA-C	-5.34	101.00	109.59
2	Q	27	ASN	O-C-N	-5.34	115.78	122.24
2	R	65	ALA	O-C-N	5.34	129.46	123.06
1	D	225	ASN	OD1-CG-ND2	5.33	127.94	122.60
2	J	125	GLY	N-CA-C	-5.33	105.26	112.57
1	D	40	TYR	N-CA-C	-5.33	100.41	108.52
1	C	200	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
1	D	158	ALA	CA-C-N	5.33	127.42	120.28
1	D	158	ALA	C-N-CA	5.33	127.42	120.28
1	F	158	ALA	CB-CA-C	-5.33	101.94	110.79
1	C	179	ASN	N-CA-C	-5.33	105.47	111.28
1	E	24	VAL	N-CA-CB	5.33	120.23	111.38
1	B	27	ALA	N-CA-C	-5.33	99.76	108.76
1	D	186	ILE	N-CA-C	-5.32	100.81	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	261	VAL	N-CA-CB	5.32	118.88	111.05
2	S	72	ASP	CA-C-N	5.32	128.79	120.75
2	S	72	ASP	C-N-CA	5.32	128.79	120.75
2	U	134	THR	CA-CB-OG1	5.32	117.58	109.60
2	G	30	HIS	N-CA-C	-5.32	101.20	109.24
2	J	96	ILE	N-CA-C	-5.32	100.09	108.23
1	C	200	HIS	CA-CB-CG	-5.32	108.48	113.80
2	H	78	ASN	N-CA-C	-5.32	101.20	108.38
2	J	95	ASN	CA-C-N	5.32	129.02	122.37
2	J	95	ASN	C-N-CA	5.32	129.02	122.37
2	X	61	ASN	CA-CB-CG	5.32	117.92	112.60
1	C	65	VAL	N-CA-CB	5.32	116.85	110.31
2	L	30	HIS	CB-CG-CD2	-5.32	124.29	131.20
2	N	69	PHE	CA-CB-CG	-5.32	108.48	113.80
2	L	124	THR	O-C-N	5.31	129.31	123.25
1	D	160	THR	N-CA-CB	-5.31	102.31	110.12
1	D	181	SER	N-CA-CB	5.31	118.51	110.28
1	E	277	ALA	CA-C-N	5.31	131.69	121.54
1	E	277	ALA	C-N-CA	5.31	131.69	121.54
2	G	53	ASN	N-CA-CB	5.31	119.47	110.49
2	O	155	THR	N-CA-CB	5.31	121.41	111.53
2	P	121	ILE	CA-C-O	5.31	126.32	120.48
1	F	225	ASN	N-CA-C	-5.31	98.59	107.99
1	E	58	LEU	N-CA-C	5.31	121.54	109.81
1	C	11	TYR	CA-C-N	5.31	127.39	120.28
1	C	11	TYR	C-N-CA	5.31	127.39	120.28
2	T	84	SER	CA-C-O	5.31	125.64	119.32
1	A	210	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	186	ILE	CA-C-N	5.30	131.67	121.54
1	A	186	ILE	C-N-CA	5.30	131.67	121.54
1	D	61	TYR	N-CA-C	-5.30	100.04	109.06
2	I	164	TYR	CB-CA-C	5.30	118.50	109.75
2	M	16	PRO	CA-N-CD	-5.30	104.57	112.00
1	E	97	SER	CA-C-O	-5.30	114.80	120.42
1	F	38	LEU	O-C-N	-5.30	117.20	123.25
1	B	48	LEU	N-CA-CB	5.30	119.22	110.69
1	B	160	THR	CA-C-N	5.30	127.39	120.28
1	B	160	THR	C-N-CA	5.30	127.39	120.28
2	N	106	ILE	CB-CA-C	5.30	119.96	111.80
2	O	129	ALA	CA-C-N	5.30	131.67	121.54
2	O	129	ALA	C-N-CA	5.30	131.67	121.54
2	U	110	ASP	CA-CB-CG	5.30	117.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	52	ALA	N-CA-CB	5.30	119.45	110.49
2	K	120	MET	CG-SD-CE	-5.30	89.24	100.90
2	I	130	LEU	N-CA-C	-5.30	101.70	109.81
2	M	140	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	N	135	HIS	N-CA-CB	5.30	119.44	110.49
2	U	104	ALA	CB-CA-C	-5.30	98.42	110.07
1	C	63	LYS	N-CA-C	-5.29	106.05	112.88
1	C	168	LYS	N-CA-C	-5.29	104.83	111.92
2	O	30	HIS	ND1-CE1-NE2	5.29	113.69	108.40
2	T	50	ILE	N-CA-C	-5.29	100.79	108.36
1	A	153	GLY	CA-C-O	-5.29	115.30	120.75
2	X	95	ASN	OD1-CG-ND2	5.29	127.89	122.60
1	E	103	PHE	CA-C-N	5.29	127.36	120.28
1	E	103	PHE	C-N-CA	5.29	127.36	120.28
2	J	100	SER	CB-CA-C	5.29	120.94	110.42
1	E	157	ALA	O-C-N	-5.28	116.52	122.12
2	X	152	VAL	CB-CA-C	-5.28	104.65	111.20
2	L	57	LEU	O-C-N	5.28	129.51	122.43
1	B	124	ASP	O-C-N	5.28	129.58	122.82
2	L	150	GLN	N-CA-C	-5.28	105.49	112.94
2	U	71	GLU	CA-C-O	-5.28	115.25	121.16
1	C	204	GLN	N-CA-CB	5.28	119.47	110.71
2	I	67	GLY	CA-C-N	5.28	131.62	121.54
2	I	67	GLY	C-N-CA	5.28	131.62	121.54
2	R	89	GLY	CA-C-N	5.28	129.06	121.56
2	R	89	GLY	C-N-CA	5.28	129.06	121.56
2	O	68	LEU	CA-C-N	5.28	130.88	122.59
2	O	68	LEU	C-N-CA	5.28	130.88	122.59
2	O	72	ASP	N-CA-C	-5.28	106.70	112.72
2	X	89	GLY	CA-C-O	5.28	125.99	121.19
2	N	67	GLY	O-C-N	5.28	129.56	122.70
2	U	88	ARG	N-CA-C	-5.28	101.28	109.14
1	D	4	LEU	CA-C-O	5.27	125.70	119.48
2	K	33	ASP	CA-CB-CG	-5.27	107.33	112.60
2	X	30	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
2	W	63	THR	N-CA-CB	5.27	118.02	110.06
2	W	102	THR	CA-C-O	-5.27	113.25	119.05
2	K	103	ALA	CA-C-N	5.27	131.61	121.54
2	K	103	ALA	C-N-CA	5.27	131.61	121.54
1	B	106	VAL	CA-C-N	5.27	127.77	120.29
1	B	106	VAL	C-N-CA	5.27	127.77	120.29
1	E	28	GLN	N-CA-C	-5.27	100.91	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	157	ALA	CA-C-N	5.27	127.34	120.28
1	F	157	ALA	C-N-CA	5.27	127.34	120.28
2	J	135	HIS	CA-CB-CG	-5.27	108.53	113.80
1	D	216	ILE	CA-C-N	5.27	131.60	121.54
1	D	216	ILE	C-N-CA	5.27	131.60	121.54
1	A	89	GLN	CA-C-O	5.26	127.17	121.06
1	B	228	TYR	O-C-N	5.26	127.78	122.09
1	E	92	THR	CA-C-N	5.26	127.33	120.28
1	E	92	THR	C-N-CA	5.26	127.33	120.28
2	I	30	HIS	CB-CG-CD2	-5.26	124.36	131.20
2	I	161	PHE	CA-C-N	5.26	129.64	122.90
2	I	161	PHE	C-N-CA	5.26	129.64	122.90
2	K	45	GLY	CA-C-O	-5.26	115.95	121.53
2	Q	22	TYR	N-CA-C	-5.26	99.59	110.80
2	R	124	THR	O-C-N	-5.26	117.79	123.42
2	W	124	THR	N-CA-C	-5.26	101.18	109.50
2	H	76	MET	N-CA-C	-5.26	100.45	109.24
2	N	81	GLU	CB-CA-C	-5.26	101.17	109.80
2	X	29	ALA	CA-C-N	5.26	131.59	121.54
2	X	29	ALA	C-N-CA	5.26	131.59	121.54
1	B	155	GLN	CA-C-N	5.26	127.28	120.44
1	B	155	GLN	C-N-CA	5.26	127.28	120.44
2	N	48	ALA	O-C-N	5.26	129.22	123.22
2	R	61	ASN	CA-C-O	-5.26	114.96	121.06
1	E	92	THR	CA-CB-OG1	5.26	117.49	109.60
1	D	107	LYS	N-CA-CB	5.26	117.85	110.12
2	O	154	ASP	N-CA-C	-5.26	105.15	112.30
2	U	42	GLN	CA-C-N	5.26	130.87	122.93
2	U	42	GLN	C-N-CA	5.26	130.87	122.93
2	M	150	GLN	N-CA-C	-5.25	99.61	110.80
1	C	87	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	E	139	GLY	CA-C-N	5.25	128.17	120.71
1	E	139	GLY	C-N-CA	5.25	128.17	120.71
1	E	215	ASP	O-C-N	5.25	129.57	122.59
1	F	244	ASP	CA-C-O	5.25	125.14	119.15
2	I	64	ASN	N-CA-CB	5.25	117.76	109.83
2	R	43	LEU	N-CA-CB	5.25	118.21	109.60
2	U	105	GLY	CA-C-N	5.25	127.65	120.35
2	U	105	GLY	C-N-CA	5.25	127.65	120.35
1	B	177	VAL	CA-C-O	-5.25	115.22	121.05
2	J	82	LYS	CA-C-N	5.25	128.25	120.17
2	J	82	LYS	C-N-CA	5.25	128.25	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	GLN	N-CA-CB	5.25	119.36	110.49
2	P	56	LYS	CA-C-N	5.25	129.74	120.87
2	P	56	LYS	C-N-CA	5.25	129.74	120.87
2	T	92	TYR	N-CA-C	-5.25	106.11	112.88
2	U	69	PHE	CA-CB-CG	-5.25	108.55	113.80
2	G	72	ASP	CA-CB-CG	5.24	117.84	112.60
2	J	159	ILE	CA-CB-CG2	5.24	119.41	110.50
2	S	158	PHE	CB-CA-C	-5.24	99.99	110.42
1	D	273	SER	N-CA-C	-5.24	99.64	110.80
2	H	101	LEU	N-CA-C	-5.24	106.75	112.72
2	X	108	ALA	N-CA-CB	5.24	119.35	110.49
1	B	117	ALA	CA-C-N	5.24	127.25	120.44
1	B	117	ALA	C-N-CA	5.24	127.25	120.44
2	I	30	HIS	CA-C-N	5.24	128.66	120.75
2	I	30	HIS	C-N-CA	5.24	128.66	120.75
2	N	123	PHE	CA-C-N	5.24	130.39	123.00
2	N	123	PHE	C-N-CA	5.24	130.39	123.00
2	J	145	TYR	N-CA-C	-5.24	106.41	114.16
2	G	95	ASN	CA-CB-CG	-5.24	107.36	112.60
2	Q	37	LEU	N-CA-CB	5.23	119.33	110.49
2	V	162	ILE	N-CA-C	5.23	115.44	110.42
2	I	75	ASP	CB-CA-C	5.23	120.83	110.42
2	M	132	VAL	N-CA-C	-5.23	102.44	108.82
2	T	55	VAL	N-CA-CB	5.23	122.72	112.00
2	W	32	ILE	CB-CA-C	-5.23	104.42	110.91
2	T	149	THR	N-CA-CB	5.23	118.54	110.60
1	D	108	GLU	N-CA-C	-5.22	105.67	111.36
1	E	98	TYR	CA-C-O	-5.22	113.01	120.16
2	H	86	TYR	CA-C-N	5.22	128.64	120.75
2	H	86	TYR	C-N-CA	5.22	128.64	120.75
2	L	164	TYR	N-CA-CB	5.22	118.78	110.16
2	G	18	VAL	O-C-N	5.22	128.90	122.11
2	P	42	GLN	N-CA-C	-5.22	99.27	108.20
1	C	170	ASP	N-CA-C	-5.22	99.68	110.80
1	D	241	ILE	N-CA-C	-5.22	100.35	108.81
1	F	101	VAL	CB-CA-C	-5.22	105.09	112.14
2	G	130	LEU	N-CA-CB	5.22	119.99	111.74
2	R	106	ILE	O-C-N	5.22	128.88	122.83
2	V	100	SER	CA-CB-OG	5.22	121.53	111.10
2	M	153	THR	CA-CB-OG1	5.21	117.42	109.60
1	B	87	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	C	210	HIS	ND1-CE1-NE2	5.21	113.61	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	55	VAL	CA-C-N	5.21	129.58	122.34
2	J	55	VAL	C-N-CA	5.21	129.58	122.34
2	N	106	ILE	N-CA-C	-5.21	101.39	108.06
2	X	102	THR	N-CA-C	-5.21	106.43	112.89
2	O	70	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	Q	159	ILE	CA-C-N	5.21	128.65	121.26
2	Q	159	ILE	C-N-CA	5.21	128.65	121.26
1	A	145	ASN	N-CA-C	-5.20	101.29	109.25
1	C	141	ALA	CA-C-N	5.20	128.22	120.31
1	C	141	ALA	C-N-CA	5.20	128.22	120.31
1	E	108	GLU	O-C-N	-5.20	116.47	122.09
1	F	121	ALA	CA-C-O	-5.20	115.34	120.80
2	M	42	GLN	OE1-CD-NE2	5.20	127.80	122.60
1	C	158	ALA	CA-C-N	5.20	127.25	120.28
1	C	158	ALA	C-N-CA	5.20	127.25	120.28
2	S	135	HIS	CE1-NE2-CD2	-5.20	103.80	109.00
1	F	262	ILE	N-CA-C	-5.20	100.08	107.77
2	K	64	ASN	OD1-CG-ND2	5.20	127.80	122.60
2	O	157	THR	N-CA-C	-5.20	101.17	109.07
2	X	49	THR	CA-C-N	5.20	128.05	120.98
2	X	49	THR	C-N-CA	5.20	128.05	120.98
2	K	115	ASP	N-CA-C	-5.20	101.51	109.41
2	W	133	VAL	N-CA-C	5.19	115.96	108.48
2	T	35	ALA	N-CA-CB	5.19	119.26	110.49
1	A	90	VAL	CA-C-N	5.19	124.81	119.05
1	A	90	VAL	C-N-CA	5.19	124.81	119.05
2	H	127	GLY	N-CA-C	-5.19	100.89	113.18
2	N	19	ARG	NE-CZ-NH2	-5.19	114.53	119.20
2	Q	156	ASP	CA-C-O	5.19	125.60	119.48
2	T	96	ILE	CA-C-O	-5.19	113.96	120.86
1	D	113	VAL	CA-CB-CG1	5.19	119.22	110.40
2	G	68	LEU	N-CA-CB	5.19	117.89	110.06
1	A	243	GLN	CB-CG-CD	-5.18	103.78	112.60
1	C	9	LYS	CA-C-N	5.18	128.19	120.31
1	C	9	LYS	C-N-CA	5.18	128.19	120.31
2	H	153	THR	CA-CB-OG1	5.18	117.38	109.60
1	F	136	LEU	CA-C-N	5.18	128.46	121.05
1	F	136	LEU	C-N-CA	5.18	128.46	121.05
2	L	42	GLN	CA-C-N	5.18	129.95	122.44
2	L	42	GLN	C-N-CA	5.18	129.95	122.44
1	B	21	GLU	N-CA-CB	-5.18	103.53	111.56
1	D	32	ASN	O-C-N	-5.18	115.36	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	152	VAL	N-CA-CB	5.18	119.78	111.23
2	Q	143	ASN	N-CA-CB	5.18	119.32	110.57
1	C	169	HIS	CA-CB-CG	5.18	118.98	113.80
2	R	130	LEU	N-CA-CB	5.18	117.58	109.97
1	D	97	SER	N-CA-C	5.18	117.00	111.36
1	F	7	GLN	N-CA-CB	5.18	120.45	111.39
2	I	59	GLY	N-CA-C	-5.17	100.92	113.18
2	L	81	GLU	N-CA-C	-5.17	106.55	112.92
2	I	139	TYR	CA-CB-CG	-5.17	104.59	113.90
1	F	132	GLU	CA-C-N	5.17	127.27	120.60
1	F	132	GLU	C-N-CA	5.17	127.27	120.60
1	A	92	THR	N-CA-C	-5.17	105.73	111.36
1	B	217	LEU	CD1-CG-CD2	5.17	122.17	110.80
1	F	138	GLU	O-C-N	5.17	129.58	123.33
2	G	49	THR	CA-C-N	5.17	131.27	121.97
2	G	49	THR	C-N-CA	5.17	131.27	121.97
2	J	88	ARG	N-CA-CB	5.17	118.29	109.87
1	B	12	LEU	CA-C-N	5.17	131.27	121.97
1	B	12	LEU	C-N-CA	5.17	131.27	121.97
1	F	80	ASP	O-C-N	5.17	129.16	122.81
2	K	91	GLU	N-CA-CB	5.17	119.22	110.49
1	E	237	GLY	CA-C-N	5.16	128.09	120.91
1	E	237	GLY	C-N-CA	5.16	128.09	120.91
2	L	56	LYS	N-CA-C	-5.16	106.66	113.17
2	S	124	THR	CB-CA-C	-5.16	102.53	109.71
2	X	105	GLY	N-CA-C	-5.16	100.94	113.18
2	R	78	ASN	O-C-N	-5.16	116.78	122.72
2	K	88	ARG	NE-CZ-NH1	5.16	126.66	121.50
2	M	73	LEU	N-CA-CB	5.16	119.21	110.49
2	K	135	HIS	CG-CD2-NE2	5.16	112.36	107.20
2	J	103	ALA	O-C-N	5.16	128.50	122.67
1	C	168	LYS	CA-C-N	5.16	131.39	121.54
1	C	168	LYS	C-N-CA	5.16	131.39	121.54
1	C	254	GLU	CA-C-O	-5.16	115.76	121.33
2	H	152	VAL	CA-C-N	5.16	131.39	121.54
2	H	152	VAL	C-N-CA	5.16	131.39	121.54
2	V	37	LEU	CA-C-O	-5.16	113.10	119.18
1	C	165	GLU	N-CA-C	5.15	118.83	112.54
1	E	13	ILE	N-CA-C	-5.15	101.21	108.27
1	E	32	ASN	CA-C-O	-5.15	113.10	120.16
1	A	102	ARG	N-CA-C	-5.15	105.75	111.36
2	I	91	GLU	CB-CG-CD	-5.15	103.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	97	SER	CA-C-O	-5.15	115.48	121.15
2	M	133	VAL	CA-C-N	5.15	130.60	122.36
2	M	133	VAL	C-N-CA	5.15	130.60	122.36
1	A	169	HIS	CA-C-O	5.15	126.48	120.20
1	B	45	ARG	NE-CZ-NH2	-5.15	114.57	119.20
2	X	50	ILE	CA-C-O	-5.15	115.17	121.04
1	B	138	GLU	CA-C-O	-5.14	115.19	121.78
2	H	96	ILE	CA-CB-CG2	-5.14	101.75	110.50
2	U	53	ASN	CA-CB-CG	-5.14	107.46	112.60
1	A	76	GLY	O-C-N	-5.14	118.84	123.37
2	I	106	ILE	CA-CB-CG1	5.14	119.14	110.40
2	O	44	ALA	N-CA-C	-5.14	101.48	109.24
2	W	30	HIS	ND1-CE1-NE2	5.14	113.54	108.40
1	B	65	VAL	N-CA-C	-5.14	100.91	108.11
2	R	61	ASN	OD1-CG-ND2	5.14	127.74	122.60
1	F	62	ASP	N-CA-C	-5.14	100.03	108.41
1	A	118	GLN	OE1-CD-NE2	5.14	127.74	122.60
2	I	92	TYR	CA-C-N	5.14	131.35	121.54
2	I	92	TYR	C-N-CA	5.14	131.35	121.54
2	S	52	ALA	N-CA-CB	5.14	119.17	110.49
2	T	156	ASP	CA-C-N	5.14	128.76	121.42
2	T	156	ASP	C-N-CA	5.14	128.76	121.42
2	V	99	THR	CB-CA-C	5.14	120.47	110.30
2	H	33	ASP	N-CA-CB	5.13	118.95	110.69
1	B	238	VAL	CA-C-O	5.13	126.89	121.04
2	T	30	HIS	ND1-CE1-NE2	5.13	113.53	108.40
2	V	41	GLU	O-C-N	5.13	128.22	122.27
1	B	59	PRO	CA-C-N	5.13	131.21	121.97
1	B	59	PRO	C-N-CA	5.13	131.21	121.97
1	B	225	ASN	CA-C-N	5.13	127.41	120.38
1	B	225	ASN	C-N-CA	5.13	127.41	120.38
1	E	50	VAL	N-CA-CB	5.13	117.29	110.26
1	A	152	GLY	CA-C-N	5.13	125.67	119.98
1	A	152	GLY	C-N-CA	5.13	125.67	119.98
1	D	98	TYR	CA-C-N	5.13	125.58	120.04
1	D	98	TYR	C-N-CA	5.13	125.58	120.04
2	L	157	THR	CA-C-N	5.13	130.62	122.62
2	L	157	THR	C-N-CA	5.13	130.62	122.62
2	M	88	ARG	NE-CZ-NH2	-5.13	114.58	119.20
2	V	80	SER	N-CA-C	5.13	116.87	111.28
2	W	44	ALA	N-CA-CB	5.13	118.77	110.41
1	E	115	ASP	CA-C-N	5.13	127.11	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	115	ASP	C-N-CA	5.13	127.11	120.44
2	G	92	TYR	CA-C-N	5.13	130.23	123.05
2	G	92	TYR	C-N-CA	5.13	130.23	123.05
2	P	121	ILE	O-C-N	-5.12	117.51	122.99
2	S	17	TYR	CB-CG-CD2	5.12	128.49	120.80
2	H	31	ASP	N-CA-C	-5.12	102.43	110.17
2	I	54	GLY	CA-C-N	5.12	127.02	120.56
2	I	54	GLY	C-N-CA	5.12	127.02	120.56
2	I	55	VAL	CA-CB-CG2	-5.12	101.69	110.40
2	J	72	ASP	CA-C-N	5.12	129.41	121.26
2	J	72	ASP	C-N-CA	5.12	129.41	121.26
2	T	48	ALA	N-CA-CB	5.12	118.59	110.55
1	F	39	ASP	CA-CB-CG	5.12	117.72	112.60
2	U	30	HIS	N-CA-CB	5.12	119.66	110.80
2	V	99	THR	N-CA-C	-5.12	101.62	109.41
1	A	172	VAL	N-CA-CB	5.12	118.21	111.25
2	V	19	ARG	N-CA-C	-5.12	99.90	110.80
1	D	178	MET	N-CA-CB	-5.12	102.59	110.16
2	I	140	ARG	NE-CZ-NH2	-5.12	114.59	119.20
2	K	152	VAL	CA-C-N	5.12	128.97	120.94
2	K	152	VAL	C-N-CA	5.12	128.97	120.94
1	E	29	ALA	N-CA-CB	5.12	118.23	110.45
2	R	30	HIS	ND1-CE1-NE2	5.12	113.52	108.40
2	R	159	ILE	N-CA-CB	5.11	116.10	110.53
2	T	84	SER	CA-C-N	5.11	127.13	120.28
2	T	84	SER	C-N-CA	5.11	127.13	120.28
2	O	88	ARG	NH1-CZ-NH2	5.11	125.95	119.30
1	B	178	MET	CA-C-N	5.11	127.13	120.28
1	B	178	MET	C-N-CA	5.11	127.13	120.28
1	B	197	VAL	N-CA-C	5.11	115.73	110.36
1	C	272	ASN	CA-C-O	5.11	124.44	118.77
2	P	95	ASN	CA-CB-CG	5.11	117.71	112.60
2	R	55	VAL	N-CA-CB	5.11	118.71	110.13
2	W	92	TYR	CA-C-N	5.11	129.81	122.40
2	W	92	TYR	C-N-CA	5.11	129.81	122.40
2	G	41	GLU	CA-C-N	5.11	131.30	121.54
2	G	41	GLU	C-N-CA	5.11	131.30	121.54
2	I	74	GLY	N-CA-C	-5.11	108.40	114.48
2	O	154	ASP	CA-C-O	-5.11	113.86	119.78
2	P	110	ASP	N-CA-CB	5.11	118.38	110.46
2	Q	43	LEU	N-CA-C	-5.11	106.90	112.72
1	B	64	ASP	N-CA-CB	5.11	119.12	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	LYS	O-C-N	-5.11	115.45	121.32
2	W	100	SER	CA-C-N	5.11	131.29	121.54
2	W	100	SER	C-N-CA	5.11	131.29	121.54
2	S	30	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
1	B	240	PRO	N-CA-C	-5.10	102.62	112.01
1	F	43	VAL	N-CA-C	-5.10	108.15	113.10
2	J	161	PHE	N-CA-CB	5.10	119.11	110.49
1	A	78	VAL	CA-C-O	-5.10	117.29	119.94
2	T	54	GLY	CA-C-N	5.10	129.19	122.51
2	T	54	GLY	C-N-CA	5.10	129.19	122.51
2	K	104	ALA	N-CA-CB	5.10	119.10	110.49
1	A	121	ALA	CA-C-N	5.09	131.27	121.54
1	A	121	ALA	C-N-CA	5.09	131.27	121.54
2	P	83	ALA	CA-C-N	5.09	130.80	122.65
2	P	83	ALA	C-N-CA	5.09	130.80	122.65
1	D	148	THR	CB-CA-C	5.09	118.34	111.82
1	F	152	GLY	CA-C-O	-5.09	115.26	120.66
1	F	235	PHE	CA-CB-CG	5.09	118.89	113.80
2	H	141	ALA	O-C-N	5.09	129.36	122.59
2	L	44	ALA	CB-CA-C	-5.09	102.54	110.74
2	N	81	GLU	N-CA-CB	5.09	118.56	110.16
1	D	97	SER	CA-C-N	5.09	134.22	121.80
1	D	97	SER	C-N-CA	5.09	134.22	121.80
1	E	236	VAL	O-C-N	-5.09	117.40	123.05
1	D	100	GLN	CA-C-O	-5.09	115.16	120.55
1	E	151	SER	O-C-N	-5.09	116.73	122.12
1	F	176	ILE	CB-CA-C	-5.09	105.27	112.14
2	O	99	THR	N-CA-C	-5.09	106.32	112.88
1	D	84	GLU	N-CA-C	-5.08	101.18	108.60
1	D	90	VAL	CA-C-O	-5.08	116.15	119.15
2	X	80	SER	N-CA-C	5.08	117.48	111.33
1	D	98	TYR	CA-C-O	-5.08	113.20	120.16
2	P	162	ILE	CA-C-N	-5.08	115.99	123.00
2	P	162	ILE	C-N-CA	-5.08	115.99	123.00
1	A	47	LEU	CA-C-N	5.08	130.16	122.99
1	A	47	LEU	C-N-CA	5.08	130.16	122.99
2	K	109	GLY	CA-C-N	-5.08	113.93	123.03
2	K	109	GLY	C-N-CA	-5.08	113.93	123.03
2	R	60	ASP	CA-CB-CG	5.08	117.68	112.60
2	R	81	GLU	CA-C-N	5.08	127.98	120.82
2	R	81	GLU	C-N-CA	5.08	127.98	120.82
1	A	10	GLU	N-CA-CB	5.08	118.15	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	ILE	CA-C-N	5.08	129.57	122.36
1	B	13	ILE	C-N-CA	5.08	129.57	122.36
2	G	49	THR	N-CA-C	-5.08	104.38	110.88
2	K	66	VAL	CA-C-O	5.08	127.13	120.78
2	M	23	GLU	O-C-N	5.08	129.04	123.25
2	P	156	ASP	O-C-N	-5.08	116.45	122.65
2	O	105	GLY	CA-C-N	5.08	127.38	120.63
2	O	105	GLY	C-N-CA	5.08	127.38	120.63
2	M	87	PHE	N-CA-CB	5.08	117.46	109.69
1	F	225	ASN	N-CA-CB	5.07	118.89	110.47
1	B	98	TYR	N-CA-CB	5.07	119.40	110.37
2	H	128	LYS	CG-CD-CE	5.07	122.97	111.30
1	F	170	ASP	CA-C-O	5.07	125.74	119.81
2	Q	30	HIS	CG-CD2-NE2	5.07	112.27	107.20
2	R	42	GLN	O-C-N	5.07	129.27	123.29
2	T	98	ARG	CA-C-N	-5.07	115.33	122.94
2	T	98	ARG	C-N-CA	-5.07	115.33	122.94
1	E	143	ALA	O-C-N	5.07	127.49	122.12
2	N	126	THR	CA-CB-OG1	-5.07	102.00	109.60
2	P	163	MET	CA-C-O	5.07	125.91	120.38
1	C	240	PRO	CB-CA-C	5.07	118.17	110.21
2	H	135	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
2	P	120	MET	CA-C-N	5.07	129.92	123.13
2	P	120	MET	C-N-CA	5.07	129.92	123.13
1	E	33	PRO	N-CA-C	5.06	120.26	114.03
2	I	47	PHE	CA-C-O	5.06	127.70	121.72
2	O	30	HIS	N-CA-C	-5.06	100.01	110.80
2	O	56	LYS	CA-C-O	-5.06	116.30	121.87
2	S	99	THR	CA-C-N	5.06	128.89	120.94
2	S	99	THR	C-N-CA	5.06	128.89	120.94
2	I	49	THR	CA-C-O	5.06	126.31	120.84
2	K	115	ASP	CA-CB-CG	5.06	117.66	112.60
2	R	34	VAL	N-CA-CB	5.06	118.22	111.64
2	T	83	ALA	CB-CA-C	-5.06	101.00	109.65
2	H	99	THR	CA-C-O	5.06	126.45	120.58
2	S	159	ILE	N-CA-C	5.06	119.86	109.34
2	V	135	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
1	D	34	ILE	CA-C-N	5.06	127.89	120.71
1	D	34	ILE	C-N-CA	5.06	127.89	120.71
2	G	22	TYR	N-CA-C	-5.06	101.16	109.40
2	M	68	LEU	O-C-N	5.06	129.11	123.19
2	N	70	ARG	CA-C-O	-5.05	114.33	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	GLN	CA-C-N	-5.05	116.09	123.06
1	C	81	GLN	C-N-CA	-5.05	116.09	123.06
1	C	171	LEU	N-CA-CB	5.05	119.39	111.56
1	E	107	LYS	CB-CA-C	-5.04	102.96	110.88
1	F	178	MET	CA-C-N	5.04	127.04	120.28
1	F	178	MET	C-N-CA	5.04	127.04	120.28
2	N	158	PHE	N-CA-C	-5.04	100.06	108.34
1	A	138	GLU	N-CA-C	5.04	117.78	110.42
1	E	143	ALA	N-CA-C	5.04	116.78	111.28
1	E	207	LEU	CA-C-N	5.04	130.73	122.81
1	E	207	LEU	C-N-CA	5.04	130.73	122.81
2	G	122	LYS	N-CA-C	-5.04	101.65	109.72
2	O	21	GLY	N-CA-C	-5.04	105.66	112.57
2	S	18	VAL	N-CA-C	5.04	119.83	109.34
1	F	72	ILE	N-CA-C	-5.04	101.22	108.48
2	O	72	ASP	O-C-N	5.04	128.55	122.35
2	Q	59	GLY	CA-C-N	5.04	130.63	121.92
2	Q	59	GLY	C-N-CA	5.04	130.63	121.92
2	S	131	GLY	N-CA-C	-5.04	103.45	110.96
2	J	32	ILE	N-CA-CB	5.04	117.64	111.60
2	Q	139	TYR	N-CA-C	-5.04	101.66	109.72
1	A	110	ARG	NH1-CZ-NH2	-5.03	112.76	119.30
2	G	51	GLY	CA-C-O	-5.03	114.08	119.82
2	N	30	HIS	CG-CD2-NE2	5.03	112.23	107.20
1	A	32	ASN	CA-CB-CG	-5.03	107.57	112.60
1	A	251	ASP	CA-CB-CG	-5.03	107.57	112.60
2	X	126	THR	N-CA-C	-5.03	105.87	112.41
2	X	132	VAL	CA-C-N	5.03	129.59	123.10
2	X	132	VAL	C-N-CA	5.03	129.59	123.10
2	N	92	TYR	CA-C-O	5.03	125.12	119.18
1	A	82	VAL	CA-CB-CG2	-5.03	101.86	110.40
1	B	164	GLN	O-C-N	-5.03	116.79	122.12
1	E	116	ARG	CA-C-N	5.03	127.02	120.28
1	E	116	ARG	C-N-CA	5.03	127.02	120.28
2	S	124	THR	CA-CB-OG1	5.03	117.14	109.60
2	U	92	TYR	CA-CB-CG	-5.03	104.85	113.90
2	X	110	ASP	N-CA-CB	5.03	118.99	110.49
2	M	63	THR	O-C-N	-5.03	116.33	123.01
2	N	54	GLY	O-C-N	5.03	127.68	122.91
2	X	84	SER	N-CA-CB	5.03	120.01	111.57
1	D	87	ARG	CG-CD-NE	-5.02	100.95	112.00
1	F	274	LEU	CA-C-O	5.02	126.89	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	136	VAL	CB-CA-C	-5.02	104.33	111.21
1	C	169	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	C	219	SER	N-CA-CB	5.02	118.98	110.49
1	D	70	PHE	CD1-CG-CD2	-5.02	111.07	118.60
2	H	33	ASP	CA-CB-CG	5.02	117.62	112.60
2	S	64	ASN	N-CA-C	-5.02	101.56	109.50
1	E	85	GLY	O-C-N	-5.02	119.45	123.27
1	F	118	GLN	CA-C-N	5.02	127.27	120.44
1	F	118	GLN	C-N-CA	5.02	127.27	120.44
2	W	157	THR	CA-CB-OG1	5.02	117.13	109.60
1	B	182	ALA	CB-CA-C	-5.02	102.46	110.79
2	N	113	THR	CA-CB-OG1	5.02	117.13	109.60
2	U	133	VAL	O-C-N	5.02	128.84	122.57
2	V	82	LYS	CG-CD-CE	5.02	122.84	111.30
2	K	120	MET	O-C-N	-5.02	117.09	123.01
2	K	50	ILE	O-C-N	-5.01	116.30	122.57
2	V	151	GLY	CA-C-O	-5.01	115.09	122.06
2	T	53	ASN	N-CA-C	-5.01	106.32	114.09
1	B	166	VAL	CA-CB-CG2	5.01	118.92	110.40
2	M	40	VAL	O-C-N	-5.01	117.24	122.95
2	S	158	PHE	N-CA-CB	5.01	118.96	110.49
2	T	29	ALA	N-CA-C	-5.01	101.12	108.99
2	T	50	ILE	CB-CA-C	-5.01	104.03	110.84
2	V	42	GLN	N-CA-CB	5.01	118.56	110.85
1	E	263	TYR	CB-CG-CD1	-5.01	113.29	120.80
2	L	161	PHE	CA-CB-CG	-5.01	108.79	113.80
1	B	201	GLU	O-C-N	5.01	129.32	122.46
2	L	30	HIS	CE1-NE2-CD2	-5.00	104.00	109.00
1	A	224	GLN	CB-CA-C	5.00	119.97	110.56
2	R	102	THR	CA-CB-OG1	5.00	117.10	109.60
2	U	31	ASP	O-C-N	5.00	129.07	122.47

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	19	ARG	CA
2	H	17	TYR	CA
2	H	22	TYR	CA
2	H	23	GLU	CA
2	J	19	ARG	CA
2	K	17	TYR	CA
2	K	22	TYR	CA

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Mol	Chain	Res	Type	Atom
2	K	23	GLU	CA
2	M	19	ARG	CA
2	N	17	TYR	CA
2	N	22	TYR	CA
2	N	23	GLU	CA
2	P	19	ARG	CA
2	Q	17	TYR	CA
2	Q	22	TYR	CA
2	Q	23	GLU	CA
2	S	19	ARG	CA
2	T	17	TYR	CA
2	T	23	GLU	CA
2	V	19	ARG	CA
2	V	85	PHE	CA
2	W	18	VAL	CA
2	W	22	TYR	CA
2	W	23	GLU	CA

All (123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	110	ARG	Sidechain
1	A	116	ARG	Sidechain
1	A	120	ARG	Sidechain
1	A	187	ARG	Sidechain
1	B	120	ARG	Sidechain
1	B	156	ARG	Sidechain
1	B	183	PHE	Sidechain
1	B	187	ARG	Sidechain
1	B	188	ALA	Peptide
1	B	208	PHE	Sidechain
1	B	210	HIS	Sidechain
1	B	45	ARG	Sidechain
1	B	75	ARG	Sidechain
1	C	102	ARG	Sidechain
1	C	188	ALA	Peptide
1	D	103	PHE	Sidechain
1	D	111	PHE	Sidechain
1	D	120	ARG	Sidechain
1	D	187	ARG	Sidechain
1	D	194	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	D	210	HIS	Sidechain
1	D	257	ARG	Sidechain
1	D	263	TYR	Sidechain
1	D	61	TYR	Sidechain
1	D	75	ARG	Sidechain
1	D	98	TYR	Sidechain
1	E	102	ARG	Sidechain
1	E	210	HIS	Sidechain
1	E	228	TYR	Sidechain
1	E	35	ARG	Sidechain
1	E	61	TYR	Sidechain
1	E	98	TYR	Sidechain
1	F	109	ARG	Sidechain
1	F	11	TYR	Sidechain
1	F	110	ARG	Sidechain
1	F	120	ARG	Sidechain
1	F	210	HIS	Sidechain
1	F	61	TYR	Sidechain
2	G	129	ALA	Peptide
2	G	135	HIS	Sidechain
2	G	47	PHE	Sidechain
2	G	70	ARG	Sidechain
2	G	86	TYR	Sidechain
2	G	87	PHE	Sidechain
2	H	135	HIS	Sidechain
2	H	164	TYR	Sidechain
2	H	17	TYR	Sidechain
2	H	19	ARG	Sidechain
2	H	88	ARG	Sidechain
2	I	139	TYR	Sidechain
2	I	145	TYR	Sidechain
2	I	19	ARG	Sidechain
2	I	22	TYR	Sidechain
2	I	86	TYR	Sidechain
2	I	88	ARG	Sidechain
2	I	92	TYR	Sidechain
2	I	93	TYR	Sidechain
2	J	139	TYR	Sidechain
2	J	140	ARG	Peptide
2	J	145	TYR	Sidechain
2	J	164	TYR	Sidechain
2	J	17	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	J	43	LEU	Peptide
2	J	92	TYR	Sidechain
2	K	145	TYR	Sidechain
2	K	17	TYR	Sidechain
2	K	19	ARG	Sidechain
2	L	17	TYR	Sidechain
2	L	22	TYR	Sidechain
2	L	30	HIS	Sidechain
2	L	88	ARG	Sidechain
2	M	22	TYR	Sidechain
2	M	70	ARG	Sidechain
2	M	93	TYR	Sidechain
2	N	145	TYR	Sidechain
2	N	154	ASP	Peptide
2	N	22	TYR	Sidechain
2	O	123	PHE	Sidechain
2	O	145	TYR	Sidechain
2	O	86	TYR	Sidechain
2	O	88	ARG	Sidechain
2	P	145	TYR	Sidechain
2	P	87	PHE	Sidechain
2	P	88	ARG	Sidechain
2	P	98	ARG	Peptide
2	Q	17	TYR	Sidechain
2	Q	19	ARG	Sidechain
2	Q	86	TYR	Sidechain
2	R	103	ALA	Peptide
2	R	145	TYR	Sidechain
2	R	92	TYR	Peptide
2	S	139	TYR	Sidechain
2	S	46	LYS	Peptide
2	S	86	TYR	Sidechain
2	S	93	TYR	Sidechain
2	T	135	HIS	Sidechain
2	T	140	ARG	Sidechain
2	T	161	PHE	Sidechain
2	T	164	TYR	Sidechain
2	T	17	TYR	Sidechain
2	T	22	TYR	Sidechain
2	T	69	PHE	Sidechain
2	U	139	TYR	Sidechain
2	U	19	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	U	70	ARG	Sidechain
2	U	86	TYR	Sidechain
2	U	87	PHE	Sidechain
2	U	88	ARG	Sidechain
2	U	92	TYR	Sidechain
2	V	19	ARG	Sidechain
2	V	93	TYR	Sidechain
2	V	98	ARG	Sidechain
2	W	18	VAL	Mainchain
2	W	69	PHE	Sidechain
2	W	88	ARG	Sidechain
2	X	140	ARG	Sidechain
2	X	164	TYR	Sidechain
2	X	70	ARG	Sidechain
2	X	87	PHE	Peptide
2	X	88	ARG	Sidechain
2	X	92	TYR	Sidechain
2	X	93	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2182	0	2222	28	0
1	B	2182	0	2222	6	0
1	C	2182	0	2222	13	0
1	D	2182	0	2222	10	0
1	E	2182	0	2222	9	0
1	F	2182	0	2222	32	0
2	G	1106	0	1072	3	0
2	H	1106	0	1072	4	0
2	I	1106	0	1072	5	0
2	J	1106	0	1072	5	0
2	K	1106	0	1072	5	0
2	L	1106	0	1072	3	0
2	M	1106	0	1072	34	0
2	N	1106	0	1072	2	0
2	O	1106	0	1072	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1106	0	1072	1	0
2	Q	1106	0	1072	3	0
2	R	1106	0	1072	4	0
2	S	1106	0	1072	5	0
2	T	1106	0	1072	4	0
2	U	1106	0	1072	1	0
2	V	1106	0	1072	5	0
2	W	1106	0	1072	2	0
2	X	1106	0	1072	2	0
All	All	33000	0	32628	155	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 2.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:47:PHE:CG	2:M:47:PHE:CD1	1.79	1.70
2:M:47:PHE:CE1	2:M:47:PHE:CZ	1.79	1.65
2:M:47:PHE:CZ	2:M:47:PHE:CE2	1.84	1.63
2:M:47:PHE:CG	2:M:47:PHE:CD2	1.85	1.63
1:F:111:PHE:CE2	1:F:111:PHE:CZ	1.91	1.57
1:F:111:PHE:CE1	1:F:111:PHE:CD1	1.94	1.52
1:F:111:PHE:CD2	1:F:111:PHE:CG	1.99	1.51
1:F:111:PHE:CZ	1:F:111:PHE:CE1	1.99	1.50
2:M:47:PHE:CD1	2:O:35:ALA:HA	1.45	1.49
2:M:47:PHE:CE1	2:O:35:ALA:HA	1.48	1.49
1:F:111:PHE:CD1	1:F:111:PHE:CG	2.04	1.46
1:F:111:PHE:CE2	1:F:111:PHE:CD2	2.03	1.44
2:M:47:PHE:CD2	2:O:35:ALA:CA	2.28	1.16
1:A:55:GLN:CD	1:F:111:PHE:CD1	2.25	1.15
2:M:47:PHE:CZ	2:O:35:ALA:CA	2.30	1.15
2:M:47:PHE:CG	2:O:35:ALA:CA	2.30	1.14
2:M:47:PHE:CD1	2:O:35:ALA:CA	2.28	1.14
2:M:47:PHE:CE1	2:O:35:ALA:CA	2.31	1.14
2:M:47:PHE:CE2	2:O:35:ALA:CA	2.30	1.13
1:A:55:GLN:CD	1:F:111:PHE:CE2	2.27	1.13
1:A:55:GLN:CD	1:F:111:PHE:CE1	2.32	1.07
1:A:55:GLN:CD	1:F:111:PHE:CD2	2.33	1.06
1:A:55:GLN:CD	1:F:111:PHE:CZ	2.33	1.06
1:A:55:GLN:CD	1:F:111:PHE:CG	2.34	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLN:NE2	1:F:111:PHE:CG	2.27	1.03
1:A:55:GLN:NE2	1:F:111:PHE:CD1	2.27	1.03
1:A:55:GLN:NE2	1:F:111:PHE:CD2	2.27	1.02
1:A:55:GLN:NE2	1:F:111:PHE:CE1	2.28	1.01
1:A:55:GLN:NE2	1:F:111:PHE:CE2	2.29	1.00
1:A:55:GLN:NE2	1:F:111:PHE:CZ	2.30	0.99
2:M:47:PHE:CE1	2:O:35:ALA:N	2.30	0.99
2:M:47:PHE:CD2	2:O:35:ALA:N	2.33	0.97
2:M:47:PHE:CZ	2:O:35:ALA:N	2.33	0.97
2:M:47:PHE:CG	2:O:35:ALA:N	2.32	0.96
2:M:47:PHE:CD1	2:O:35:ALA:N	2.35	0.95
2:M:47:PHE:CE2	2:O:35:ALA:N	2.35	0.95
1:A:55:GLN:CD	1:A:55:GLN:NE2	2.30	0.90
1:A:55:GLN:CG	1:F:111:PHE:CE1	2.60	0.84
2:M:47:PHE:CG	2:O:35:ALA:HA	2.16	0.81
2:M:47:PHE:CZ	2:O:35:ALA:HA	2.16	0.80
1:A:55:GLN:HG2	1:F:111:PHE:CZ	2.18	0.79
1:A:55:GLN:CG	1:F:111:PHE:CZ	2.66	0.78
2:M:47:PHE:CZ	2:O:35:ALA:CB	2.67	0.77
1:A:55:GLN:HG2	1:F:111:PHE:CE1	2.22	0.75
1:A:55:GLN:OE1	1:F:111:PHE:CG	2.42	0.73
2:S:92:TYR:H	2:S:151:GLY:HA3	1.52	0.72
2:M:47:PHE:CE2	2:O:35:ALA:CB	2.73	0.72
1:A:55:GLN:OE1	1:F:111:PHE:CD2	2.43	0.71
2:M:47:PHE:CG	2:O:35:ALA:C	2.72	0.67
2:J:149:THR:HG22	2:J:151:GLY:H	1.68	0.58
2:I:123:PHE:CD1	2:I:163:MET:HE2	2.39	0.57
1:E:35:ARG:HH22	1:E:133:ILE:HD11	1.68	0.57
2:J:125:GLY:HA2	2:J:139:TYR:HB2	1.87	0.57
2:M:47:PHE:CZ	2:O:35:ALA:HB2	2.39	0.57
2:I:89:GLY:HA3	2:I:148:ALA:HB3	1.87	0.56
2:M:107:ALA:H	2:O:37:LEU:HD13	1.71	0.55
2:U:52:ALA:H	2:U:79:ALA:HB3	1.71	0.55
2:M:47:PHE:CE2	2:O:35:ALA:HB3	2.41	0.55
1:A:125:ILE:HG22	1:A:127:ALA:H	1.71	0.54
2:M:47:PHE:CG	2:O:34:VAL:C	2.85	0.54
2:M:47:PHE:CD2	2:O:35:ALA:C	2.86	0.53
2:H:119:LYS:HG3	2:H:120:MET:H	1.74	0.53
1:C:32:ASN:HD22	1:C:32:ASN:H	1.58	0.52
1:D:75:ARG:HD3	1:D:75:ARG:H	1.74	0.52
1:C:24:VAL:CG1	1:D:272:ASN:HD21	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:GLU:HG2	1:C:20:GLU:H	1.75	0.50
2:M:30:HIS:CD2	2:M:30:HIS:H	2.29	0.50
1:C:119:GLN:HE21	1:C:119:GLN:HA	1.76	0.50
1:C:270:VAL:O	1:C:270:VAL:HG12	2.12	0.50
2:O:71:GLU:HG3	2:O:93:TYR:CE2	2.46	0.50
2:H:70:ARG:HE	2:H:81:GLU:H	1.60	0.49
1:A:109:ARG:HA	1:A:109:ARG:HE	1.77	0.49
2:V:98:ARG:HB3	2:V:106:ILE:HD13	1.94	0.49
1:C:149:ILE:HD12	1:C:150:SER:H	1.78	0.49
2:J:125:GLY:HA2	2:J:139:TYR:CB	2.42	0.49
1:C:3:GLN:HG3	1:C:5:SER:H	1.79	0.48
2:M:55:VAL:HG22	2:O:147:LYS:HB2	1.96	0.47
2:L:66:VAL:HB	2:L:69:PHE:CE2	2.49	0.47
2:N:85:PHE:HB2	2:O:75:ASP:H	1.79	0.47
2:V:20:LEU:HD13	2:X:149:THR:HG21	1.97	0.47
1:A:83:ILE:HG23	1:A:115:ASP:HB2	1.97	0.46
2:M:151:GLY:O	2:M:152:VAL:HG13	2.15	0.46
2:Q:85:PHE:HB3	2:R:74:GLY:H	1.80	0.46
1:C:104:SER:HA	1:D:71:VAL:HG11	1.97	0.46
2:I:129:ALA:C	2:I:130:LEU:HD23	2.41	0.46
2:R:67:GLY:H	2:R:120:MET:HE2	1.81	0.46
1:B:229:VAL:HG22	1:B:272:ASN:HB3	1.98	0.46
2:K:18:VAL:HG23	2:L:41:GLU:H	1.81	0.46
2:V:119:LYS:HB3	2:V:120:MET:HA	1.98	0.46
2:M:43:LEU:HD22	2:O:97:SER:O	2.16	0.45
2:O:146:GLU:H	2:O:146:GLU:CD	2.23	0.45
2:T:22:TYR:H	2:T:61:ASN:HB3	1.81	0.45
2:J:70:ARG:HH22	2:K:38:ASN:HD22	1.64	0.45
2:J:88:ARG:NH1	2:K:90:GLY:H	2.15	0.45
1:F:241:ILE:HG13	1:F:260:TRP:HE1	1.81	0.45
2:K:125:GLY:H	2:K:159:ILE:HG22	1.80	0.45
1:F:170:ASP:HB3	1:F:171:LEU:HD23	1.97	0.45
1:C:169:HIS:CG	1:C:170:ASP:H	2.35	0.45
1:B:126:MET:HE2	2:G:130:LEU:HD11	1.98	0.45
2:G:129:ALA:HA	2:G:150:GLN:HG3	1.99	0.45
2:R:82:LYS:HG2	2:R:133:VAL:HG21	1.99	0.45
1:F:125:ILE:CG2	2:Q:53:ASN:HD21	2.30	0.44
2:H:77:VAL:HG11	2:H:95:ASN:HD21	1.82	0.44
2:S:148:ALA:HB2	2:T:76:MET:HE3	1.99	0.44
2:V:134:THR:HG22	2:V:135:HIS:H	1.83	0.44
2:I:48:ALA:HB1	2:I:106:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:47:PHE:CD2	2:O:34:VAL:C	2.96	0.44
1:D:239:MET:HB3	1:D:239:MET:HE2	1.86	0.44
1:D:178:MET:HE1	1:D:221:LYS:HD2	1.99	0.44
2:W:132:VAL:HG23	2:W:140:ARG:HE	1.81	0.44
1:A:109:ARG:HA	1:A:109:ARG:NE	2.33	0.43
1:E:246:GLN:HG3	1:E:247:VAL:H	1.82	0.43
1:E:89:GLN:HE21	1:E:94:GLU:HG2	1.83	0.43
2:S:42:GLN:HA	2:S:46:LYS:HE2	2.00	0.43
1:E:23:ARG:HD3	1:E:103:PHE:CE2	2.54	0.43
1:D:138:GLU:H	1:D:274:LEU:HA	1.84	0.43
2:P:32:ILE:HA	2:P:66:VAL:HG11	2.01	0.43
2:T:95:ASN:HD21	2:T:106:ILE:HD12	1.83	0.43
2:H:30:HIS:HB2	2:H:66:VAL:HG11	2.00	0.43
1:A:120:ARG:HH12	1:A:265:GLU:HA	1.83	0.42
1:D:36:VAL:CG1	1:D:227:VAL:HG13	2.50	0.42
2:G:101:LEU:N	2:G:101:LEU:HD23	2.34	0.42
1:E:252:LYS:HD3	1:E:254:GLU:HG3	2.01	0.42
1:A:190:GLY:H	1:B:187:ARG:HG2	1.84	0.42
1:A:23:ARG:HB3	1:A:103:PHE:CE2	2.55	0.42
1:C:142:THR:HG23	1:C:276:ILE:HG21	2.02	0.42
1:D:88:ILE:HG22	1:E:68:LYS:HB3	2.00	0.42
1:E:41:GLN:H	1:E:41:GLN:CD	2.27	0.42
1:B:207:LEU:HD23	1:B:207:LEU:HA	2.01	0.42
2:S:92:TYR:H	2:S:151:GLY:CA	2.26	0.42
2:T:152:VAL:HG23	2:T:163:MET:HB3	2.02	0.42
1:F:125:ILE:HG22	2:Q:53:ASN:HD21	1.82	0.41
2:I:26:LEU:HD23	2:I:26:LEU:H	1.85	0.41
1:D:186:ILE:HD13	1:D:192:ASN:HD22	1.85	0.41
2:R:68:LEU:HA	2:R:92:TYR:CE1	2.55	0.41
2:X:156:ASP:HB3	2:X:158:PHE:CE1	2.55	0.41
1:B:170:ASP:H	1:B:225:ASN:HA	1.86	0.41
1:F:213:THR:HG23	1:F:216:ILE:HG22	2.02	0.41
2:L:84:SER:HA	2:L:135:HIS:HB2	2.03	0.41
1:C:141:ALA:C	1:C:161:LYS:HZ1	2.28	0.41
1:B:24:VAL:HA	1:C:269:ALA:HA	2.02	0.41
1:C:7:GLN:HE21	2:K:136:VAL:HG13	1.86	0.41
2:W:112:ILE:HD12	2:W:112:ILE:HA	1.98	0.41
1:D:213:THR:HG22	1:D:215:ASP:H	1.86	0.41
1:F:148:THR:HG21	1:F:153:GLY:HA3	2.02	0.41
2:M:47:PHE:CD2	2:M:47:PHE:CB	2.88	0.41
2:O:61:ASN:HA	2:O:110:ASP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:LEU:HD22	1:E:71:VAL:HB	2.03	0.40
2:S:106:ILE:HD12	2:S:106:ILE:HA	2.00	0.40
1:A:166:VAL:O	1:F:25:ALA:HB1	2.22	0.40
2:V:129:ALA:HA	2:V:130:LEU:C	2.45	0.40
2:N:148:ALA:HA	2:O:47:PHE:CD2	2.57	0.40
2:O:61:ASN:HD22	2:O:110:ASP:CB	2.34	0.40
1:A:175:LYS:HZ3	1:A:215:ASP:H	1.69	0.40
1:E:200:HIS:HE1	1:F:159:LEU:HD12	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	278/280 (99%)	240 (86%)	20 (7%)	18 (6%)	1	12
1	B	278/280 (99%)	242 (87%)	25 (9%)	11 (4%)	2	18
1	C	278/280 (99%)	244 (88%)	23 (8%)	11 (4%)	2	18
1	D	278/280 (99%)	245 (88%)	19 (7%)	14 (5%)	1	15
1	E	278/280 (99%)	233 (84%)	25 (9%)	20 (7%)	1	10
1	F	278/280 (99%)	248 (89%)	20 (7%)	10 (4%)	2	20
2	G	148/150 (99%)	115 (78%)	20 (14%)	13 (9%)	0	8
2	H	148/150 (99%)	114 (77%)	24 (16%)	10 (7%)	1	11
2	I	148/150 (99%)	118 (80%)	18 (12%)	12 (8%)	1	9
2	J	148/150 (99%)	118 (80%)	21 (14%)	9 (6%)	1	12
2	K	148/150 (99%)	115 (78%)	15 (10%)	18 (12%)	0	4
2	L	148/150 (99%)	119 (80%)	14 (10%)	15 (10%)	0	7
2	M	148/150 (99%)	113 (76%)	22 (15%)	13 (9%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	148/150 (99%)	119 (80%)	19 (13%)	10 (7%)	1	11
2	O	148/150 (99%)	114 (77%)	20 (14%)	14 (10%)	0	8
2	P	148/150 (99%)	115 (78%)	23 (16%)	10 (7%)	1	11
2	Q	148/150 (99%)	118 (80%)	15 (10%)	15 (10%)	0	7
2	R	148/150 (99%)	123 (83%)	16 (11%)	9 (6%)	1	12
2	S	148/150 (99%)	120 (81%)	20 (14%)	8 (5%)	1	14
2	T	148/150 (99%)	121 (82%)	14 (10%)	13 (9%)	0	8
2	U	148/150 (99%)	116 (78%)	19 (13%)	13 (9%)	0	8
2	V	148/150 (99%)	117 (79%)	16 (11%)	15 (10%)	0	7
2	W	148/150 (99%)	116 (78%)	19 (13%)	13 (9%)	0	8
2	X	148/150 (99%)	114 (77%)	25 (17%)	9 (6%)	1	12
All	All	4332/4380 (99%)	3557 (82%)	472 (11%)	303 (7%)	2	11

All (303) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	16	ALA
1	A	98	TYR
1	A	122	LYS
1	A	123	ALA
1	A	187	ARG
1	A	273	SER
1	B	98	TYR
1	B	123	ALA
1	B	150	SER
1	B	194	PHE
1	C	29	ALA
1	C	98	TYR
1	D	16	ALA
1	D	66	ASP
1	D	98	TYR
1	D	271	VAL
1	D	273	SER
1	E	11	TYR
1	E	14	SER
1	E	57	ALA
1	E	98	TYR

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Mol	Chain	Res	Type
1	E	123	ALA
1	E	185	ASP
1	E	188	ALA
1	E	216	ILE
1	E	278	LYS
1	F	98	TYR
1	F	123	ALA
1	F	127	ALA
1	F	185	ASP
2	G	19	ARG
2	H	17	TYR
2	H	38	ASN
2	H	116	ALA
2	H	141	ALA
2	H	159	ILE
2	I	102	THR
2	I	103	ALA
2	J	19	ARG
2	J	52	ALA
2	J	108	ALA
2	K	17	TYR
2	K	50	ILE
2	K	154	ASP
2	L	20	LEU
2	L	23	GLU
2	L	53	ASN
2	L	117	ASP
2	M	56	LYS
2	M	60	ASP
2	M	108	ALA
2	M	152	VAL
2	M	164	TYR
2	N	17	TYR
2	N	22	TYR
2	N	23	GLU
2	N	87	PHE
2	O	41	GLU
2	P	19	ARG
2	P	144	MET
2	Q	17	TYR
2	Q	22	TYR
2	Q	23	GLU

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Mol	Chain	Res	Type
2	Q	117	ASP
2	R	31	ASP
2	R	66	VAL
2	R	135	HIS
2	R	145	TYR
2	S	20	LEU
2	S	52	ALA
2	T	17	TYR
2	T	23	GLU
2	U	29	ALA
2	U	35	ALA
2	U	91	GLU
2	V	19	ARG
2	V	65	ALA
2	V	85	PHE
2	V	97	SER
2	V	117	ASP
2	V	145	TYR
2	W	18	VAL
2	W	22	TYR
2	W	29	ALA
2	W	80	SER
2	X	107	ALA
2	X	145	TYR
1	A	31	ALA
1	A	269	ALA
1	B	166	VAL
1	C	57	ALA
1	C	131	ALA
1	D	203	LEU
1	D	269	ALA
1	F	140	ALA
1	F	166	VAL
1	F	275	ALA
2	G	35	ALA
2	G	38	ASN
2	G	84	SER
2	G	87	PHE
2	G	116	ALA
2	G	117	ASP
2	H	22	TYR
2	H	129	ALA

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Mol	Chain	Res	Type
2	I	27	ASN
2	I	52	ALA
2	I	159	ILE
2	J	104	ALA
2	J	129	ALA
2	K	23	GLU
2	K	37	LEU
2	K	53	ASN
2	K	54	GLY
2	K	66	VAL
2	K	75	ASP
2	K	100	SER
2	K	104	ALA
2	K	146	GLU
2	L	22	TYR
2	L	156	ASP
2	M	117	ASP
2	N	153	THR
2	O	35	ALA
2	O	129	ALA
2	O	148	ALA
2	P	101	LEU
2	Q	20	LEU
2	Q	35	ALA
2	Q	68	LEU
2	Q	85	PHE
2	Q	107	ALA
2	Q	146	GLU
2	R	110	ASP
2	S	103	ALA
2	S	158	PHE
2	T	58	ALA
2	T	74	GLY
2	T	82	LYS
2	T	91	GLU
2	T	107	ALA
2	U	34	VAL
2	U	56	LYS
2	U	66	VAL
2	V	60	ASP
2	V	66	VAL
2	W	38	ASN

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Mol	Chain	Res	Type
2	W	52	ALA
2	W	84	SER
2	W	91	GLU
2	W	116	ALA
2	W	150	GLN
2	X	65	ALA
1	A	215	ASP
1	B	4	LEU
1	C	128	VAL
1	C	169	HIS
1	C	269	ALA
1	D	6	ASN
1	D	62	ASP
1	F	188	ALA
1	F	270	VAL
2	H	23	GLU
2	I	62	GLY
2	I	67	GLY
2	I	92	TYR
2	I	128	LYS
2	K	22	TYR
2	K	63	THR
2	L	27	ASN
2	L	30	HIS
2	L	67	GLY
2	L	107	ALA
2	L	130	LEU
2	N	74	GLY
2	N	135	HIS
2	O	103	ALA
2	O	116	ALA
2	O	117	ASP
2	O	142	GLY
2	P	44	ALA
2	P	117	ASP
2	P	135	HIS
2	P	152	VAL
2	P	158	PHE
2	Q	37	LEU
2	Q	64	ASN
2	Q	145	TYR
2	R	80	SER

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Mol	Chain	Res	Type
2	S	82	LYS
2	T	130	LEU
2	U	19	ARG
2	U	75	ASP
2	U	110	ASP
2	V	92	TYR
2	V	129	ALA
1	A	51	ASP
1	A	63	LYS
1	A	124	ASP
1	A	195	ASP
1	B	2	SER
1	B	60	VAL
1	B	273	SER
1	C	188	ALA
1	C	207	LEU
1	D	60	VAL
1	E	194	PHE
1	E	207	LEU
1	E	253	PRO
1	E	269	ALA
2	G	148	ALA
2	I	29	ALA
2	J	98	ARG
2	K	83	ALA
2	K	88	ARG
2	K	91	GLU
2	L	116	ALA
2	L	127	GLY
2	M	38	ASN
2	M	147	LYS
2	M	150	GLN
2	N	49	THR
2	N	66	VAL
2	O	22	TYR
2	O	107	ALA
2	O	130	LEU
2	Q	44	ALA
2	R	60	ASP
2	S	54	GLY
2	S	90	GLY
2	T	68	LEU

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Mol	Chain	Res	Type
2	T	69	PHE
2	V	93	TYR
2	V	107	ALA
2	X	29	ALA
2	X	104	ALA
2	X	144	MET
2	X	158	PHE
2	X	159	ILE
1	A	14	SER
1	A	61	TYR
1	A	147	VAL
1	C	166	VAL
1	D	51	ASP
1	E	21	GLU
1	E	54	PRO
1	E	191	GLN
1	E	198	THR
1	E	215	ASP
1	E	217	LEU
1	F	125	ILE
2	G	29	ALA
2	G	82	LYS
2	G	129	ALA
2	H	40	VAL
2	I	109	GLY
2	I	150	GLN
2	J	66	VAL
2	L	99	THR
2	L	103	ALA
2	M	35	ALA
2	O	73	LEU
2	Q	159	ILE
2	R	117	ASP
2	T	93	TYR
2	T	97	SER
2	T	154	ASP
2	U	33	ASP
2	U	53	ASN
2	V	96	ILE
2	V	102	THR
2	V	136	VAL
2	W	85	PHE

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Mol	Chain	Res	Type
2	W	117	ASP
2	W	146	GLU
2	X	60	ASP
1	A	166	VAL
1	B	16	ALA
1	D	31	ALA
1	D	166	VAL
1	D	253	PRO
2	G	53	ASN
2	H	143	ASN
2	J	159	ILE
2	K	149	THR
2	M	19	ARG
2	M	107	ALA
2	N	127	GLY
2	O	147	LYS
2	P	104	ALA
2	R	27	ASN
2	S	98	ARG
2	U	154	ASP
1	B	51	ASP
1	E	51	ASP
2	P	55	VAL
1	C	253	PRO
2	G	50	ILE
2	M	50	ILE
2	O	54	GLY
2	U	90	GLY
2	J	160	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	235/235 (100%)	219 (93%)	16 (7%)	14	36
1	B	235/235 (100%)	223 (95%)	12 (5%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	235/235 (100%)	224 (95%)	11 (5%)	23	44
1	D	235/235 (100%)	222 (94%)	13 (6%)	19	41
1	E	235/235 (100%)	220 (94%)	15 (6%)	16	37
1	F	235/235 (100%)	224 (95%)	11 (5%)	23	44
2	G	109/109 (100%)	104 (95%)	5 (5%)	24	45
2	H	109/109 (100%)	102 (94%)	7 (6%)	16	37
2	I	109/109 (100%)	101 (93%)	8 (7%)	13	34
2	J	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	K	109/109 (100%)	101 (93%)	8 (7%)	13	34
2	L	109/109 (100%)	101 (93%)	8 (7%)	13	34
2	M	109/109 (100%)	99 (91%)	10 (9%)	8	27
2	N	109/109 (100%)	106 (97%)	3 (3%)	38	59
2	O	109/109 (100%)	100 (92%)	9 (8%)	10	30
2	P	109/109 (100%)	102 (94%)	7 (6%)	16	37
2	Q	109/109 (100%)	99 (91%)	10 (9%)	8	27
2	R	109/109 (100%)	104 (95%)	5 (5%)	24	45
2	S	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	T	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	U	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	V	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	W	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	X	109/109 (100%)	104 (95%)	5 (5%)	24	45
All	All	3372/3372 (100%)	3177 (94%)	195 (6%)	20	40

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	68	LYS
1	A	78	VAL
1	A	84	GLU
1	A	148	THR
1	A	149	ILE
1	A	165	GLU

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Mol	Chain	Res	Type
1	A	171	LEU
1	A	172	VAL
1	A	174	THR
1	A	176	ILE
1	A	195	ASP
1	A	220	LYS
1	A	226	THR
1	A	249	PRO
1	A	263	TYR
1	B	3	GLN
1	B	24	VAL
1	B	34	ILE
1	B	38	LEU
1	B	52	PRO
1	B	53	LEU
1	B	60	VAL
1	B	197	VAL
1	B	212	TRP
1	B	213	THR
1	B	245	ILE
1	B	274	LEU
1	C	7	GLN
1	C	24	VAL
1	C	32	ASN
1	C	58	LEU
1	C	105	GLN
1	C	119	GLN
1	C	142	THR
1	C	171	LEU
1	C	181	SER
1	C	249	PRO
1	C	276	ILE
1	D	6	ASN
1	D	24	VAL
1	D	28	GLN
1	D	32	ASN
1	D	43	VAL
1	D	71	VAL
1	D	72	ILE
1	D	74	LYS
1	D	75	ARG
1	D	148	THR

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Mol	Chain	Res	Type
1	D	174	THR
1	D	249	PRO
1	D	279	ILE
1	E	1	MET
1	E	23	ARG
1	E	41	GLN
1	E	47	LEU
1	E	74	LYS
1	E	80	ASP
1	E	88	ILE
1	E	149	ILE
1	E	174	THR
1	E	198	THR
1	E	210	HIS
1	E	226	THR
1	E	239	MET
1	E	249	PRO
1	E	261	VAL
1	F	19	THR
1	F	47	LEU
1	F	49	VAL
1	F	68	LYS
1	F	105	GLN
1	F	122	LYS
1	F	148	THR
1	F	149	ILE
1	F	171	LEU
1	F	205	THR
1	F	242	ARG
2	G	31	ASP
2	G	46	LYS
2	G	49	THR
2	G	85	PHE
2	G	134	THR
2	H	17	TYR
2	H	22	TYR
2	H	46	LYS
2	H	73	LEU
2	H	77	VAL
2	H	133	VAL
2	H	149	THR
2	I	18	VAL

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Mol	Chain	Res	Type
2	I	19	ARG
2	I	42	GLN
2	I	50	ILE
2	I	56	LYS
2	I	119	LYS
2	I	121	ILE
2	I	128	LYS
2	J	46	LYS
2	J	49	THR
2	J	128	LYS
2	J	144	MET
2	J	153	THR
2	J	162	ILE
2	K	16	PRO
2	K	22	TYR
2	K	43	LEU
2	K	55	VAL
2	K	78	ASN
2	K	117	ASP
2	K	136	VAL
2	K	155	THR
2	L	30	HIS
2	L	46	LYS
2	L	61	ASN
2	L	63	THR
2	L	78	ASN
2	L	120	MET
2	L	134	THR
2	L	162	ILE
2	M	16	PRO
2	M	38	ASN
2	M	46	LYS
2	M	63	THR
2	M	66	VAL
2	M	95	ASN
2	M	122	LYS
2	M	124	THR
2	M	128	LYS
2	M	152	VAL
2	N	143	ASN
2	N	150	GLN
2	N	162	ILE

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Mol	Chain	Res	Type
2	O	25	ILE
2	O	49	THR
2	O	76	MET
2	O	94	VAL
2	O	97	SER
2	O	120	MET
2	O	132	VAL
2	O	153	THR
2	O	157	THR
2	P	19	ARG
2	P	32	ILE
2	P	66	VAL
2	P	76	MET
2	P	85	PHE
2	P	144	MET
2	P	155	THR
2	Q	18	VAL
2	Q	20	LEU
2	Q	32	ILE
2	Q	82	LYS
2	Q	120	MET
2	Q	128	LYS
2	Q	130	LEU
2	Q	134	THR
2	Q	157	THR
2	Q	162	ILE
2	R	49	THR
2	R	50	ILE
2	R	63	THR
2	R	70	ARG
2	R	157	THR
2	S	40	VAL
2	S	71	GLU
2	S	73	LEU
2	S	106	ILE
2	T	18	VAL
2	T	23	GLU
2	T	25	ILE
2	T	50	ILE
2	U	31	ASP
2	U	40	VAL
2	U	49	THR

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Mol	Chain	Res	Type
2	U	50	ILE
2	U	113	THR
2	U	140	ARG
2	V	41	GLU
2	V	95	ASN
2	V	121	ILE
2	V	134	THR
2	V	153	THR
2	V	161	PHE
2	W	22	TYR
2	W	49	THR
2	W	63	THR
2	W	98	ARG
2	W	145	TYR
2	W	162	ILE
2	X	16	PRO
2	X	32	ILE
2	X	84	SER
2	X	102	THR
2	X	128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	55	GLN
1	A	81	GLN
1	A	105	GLN
1	A	118	GLN
1	A	145	ASN
1	A	169	HIS
1	A	191	GLN
1	A	246	GLN
1	B	105	GLN
1	B	199	GLN
1	B	210	HIS
1	B	272	ASN
1	C	7	GLN
1	C	32	ASN
1	C	81	GLN
1	C	105	GLN
1	C	118	GLN

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Mol	Chain	Res	Type
1	C	119	GLN
1	C	145	ASN
1	C	191	GLN
1	C	199	GLN
1	C	225	ASN
1	D	6	ASN
1	D	28	GLN
1	D	55	GLN
1	D	77	GLN
1	D	100	GLN
1	D	118	GLN
1	D	155	GLN
1	D	192	ASN
1	D	199	GLN
1	D	200	HIS
1	D	204	GLN
1	D	210	HIS
1	D	225	ASN
1	D	246	GLN
1	D	272	ASN
1	E	32	ASN
1	E	81	GLN
1	E	118	GLN
1	E	169	HIS
1	E	179	ASN
1	E	199	GLN
1	F	3	GLN
1	F	28	GLN
1	F	105	GLN
1	F	192	ASN
1	F	200	HIS
2	G	27	ASN
2	G	150	GLN
2	H	42	GLN
2	H	61	ASN
2	H	135	HIS
2	I	30	HIS
2	I	78	ASN
2	I	95	ASN
2	I	150	GLN
2	J	27	ASN
2	J	30	HIS

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Mol	Chain	Res	Type
2	J	42	GLN
2	K	42	GLN
2	K	53	ASN
2	K	95	ASN
2	K	135	HIS
2	L	30	HIS
2	M	30	HIS
2	M	61	ASN
2	M	78	ASN
2	N	27	ASN
2	N	30	HIS
2	N	78	ASN
2	N	135	HIS
2	O	27	ASN
2	O	61	ASN
2	O	150	GLN
2	P	30	HIS
2	P	42	GLN
2	P	95	ASN
2	Q	53	ASN
2	Q	78	ASN
2	Q	135	HIS
2	Q	143	ASN
2	Q	150	GLN
2	R	42	GLN
2	R	53	ASN
2	R	135	HIS
2	R	143	ASN
2	S	30	HIS
2	S	95	ASN
2	S	135	HIS
2	S	150	GLN
2	T	27	ASN
2	T	30	HIS
2	T	53	ASN
2	T	95	ASN
2	T	135	HIS
2	U	30	HIS
2	U	38	ASN
2	U	53	ASN
2	U	135	HIS
2	V	27	ASN

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Mol	Chain	Res	Type
2	V	30	HIS
2	W	27	ASN
2	W	78	ASN
2	W	150	GLN
2	X	53	ASN
2	X	64	ASN
2	X	135	HIS

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

This section contains visualisations of the EMDB entry EMD-21695. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.