



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:55 AM UTC

PDB ID : 6HE5 / pdb_00006he5
EMDB ID : EMD-0210
Title : 20S core particle of PAN-proteasomes
Authors : Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.
Deposited on : 2018-08-20
Resolution : 4.12 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

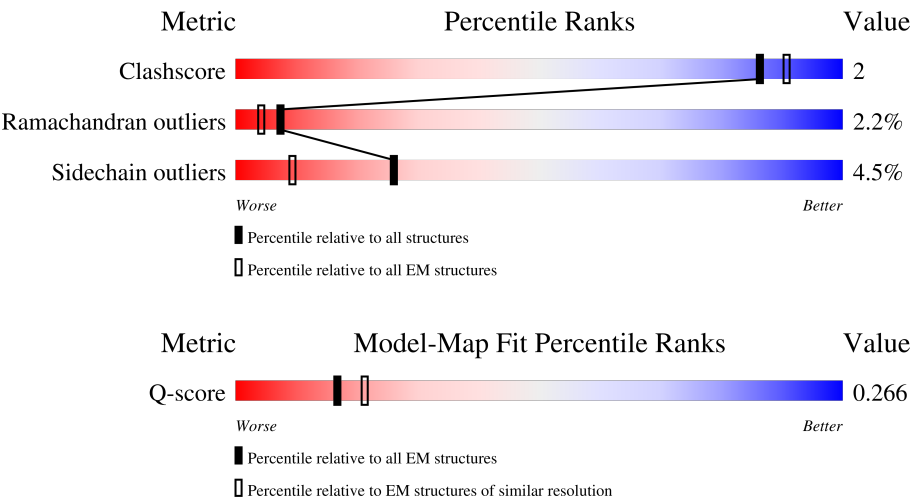
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.12 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5662 (3.62 - 4.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	247	23% 49% 44% 5% ..
1	B	247	21% 48% 45% ..
1	C	247	19% 44% 47% 5% ..
1	D	247	23% 48% 45% 5% .

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Mol	Chain	Length	Quality of chain
1	E	247	
1	F	247	
1	G	247	
2	1	210	
2	2	210	
2	3	210	
2	4	210	
2	5	210	
2	6	210	
2	7	210	
3	H	401	
3	I	401	
3	J	401	
3	K	401	
3	L	401	
3	M	401	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24633 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	B	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	C	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	D	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	E	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	F	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		
1	G	242	Total	C	N	O	S	0	0
			1907	1211	321	368	7		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O29760
A	1	GLY	-	expression tag	UNP O29760
B	0	MET	-	initiating methionine	UNP O29760
B	1	GLY	-	expression tag	UNP O29760
C	0	MET	-	initiating methionine	UNP O29760
C	1	GLY	-	expression tag	UNP O29760
D	0	MET	-	initiating methionine	UNP O29760
D	1	GLY	-	expression tag	UNP O29760
E	0	MET	-	initiating methionine	UNP O29760
E	1	GLY	-	expression tag	UNP O29760
F	0	MET	-	initiating methionine	UNP O29760
F	1	GLY	-	expression tag	UNP O29760
G	0	MET	-	initiating methionine	UNP O29760
G	1	GLY	-	expression tag	UNP O29760

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	202	Total	C	N	O	S	0	0
			1552	982	260	304	6		
2	2	202	Total	C	N	O	S	0	0
			1552	982	260	304	6		
2	3	202	Total	C	N	O	S	0	0
			1552	982	260	304	6		
2	4	202	Total	C	N	O	S	0	0
			1552	982	260	304	6		
2	5	202	Total	C	N	O	S	0	0
			1552	982	260	304	6		
2	6	202	Total	C	N	O	S	0	0
			1552	982	260	304	6		
2	7	202	Total	C	N	O	S	0	0
			1552	982	260	304	6		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	10	MET	-	initiating methionine	UNP Q9P996
1	214	HIS	-	expression tag	UNP Q9P996
1	215	HIS	-	expression tag	UNP Q9P996
1	216	HIS	-	expression tag	UNP Q9P996
1	217	HIS	-	expression tag	UNP Q9P996
1	218	HIS	-	expression tag	UNP Q9P996
1	219	HIS	-	expression tag	UNP Q9P996
2	10	MET	-	initiating methionine	UNP Q9P996
2	214	HIS	-	expression tag	UNP Q9P996
2	215	HIS	-	expression tag	UNP Q9P996
2	216	HIS	-	expression tag	UNP Q9P996
2	217	HIS	-	expression tag	UNP Q9P996
2	218	HIS	-	expression tag	UNP Q9P996
2	219	HIS	-	expression tag	UNP Q9P996
3	10	MET	-	initiating methionine	UNP Q9P996
3	214	HIS	-	expression tag	UNP Q9P996
3	215	HIS	-	expression tag	UNP Q9P996
3	216	HIS	-	expression tag	UNP Q9P996
3	217	HIS	-	expression tag	UNP Q9P996
3	218	HIS	-	expression tag	UNP Q9P996
3	219	HIS	-	expression tag	UNP Q9P996
4	10	MET	-	initiating methionine	UNP Q9P996
4	214	HIS	-	expression tag	UNP Q9P996
4	215	HIS	-	expression tag	UNP Q9P996
4	216	HIS	-	expression tag	UNP Q9P996
4	217	HIS	-	expression tag	UNP Q9P996

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Chain	Residue	Modelled	Actual	Comment	Reference
4	218	HIS	-	expression tag	UNP Q9P996
4	219	HIS	-	expression tag	UNP Q9P996
5	10	MET	-	initiating methionine	UNP Q9P996
5	214	HIS	-	expression tag	UNP Q9P996
5	215	HIS	-	expression tag	UNP Q9P996
5	216	HIS	-	expression tag	UNP Q9P996
5	217	HIS	-	expression tag	UNP Q9P996
5	218	HIS	-	expression tag	UNP Q9P996
5	219	HIS	-	expression tag	UNP Q9P996
6	10	MET	-	initiating methionine	UNP Q9P996
6	214	HIS	-	expression tag	UNP Q9P996
6	215	HIS	-	expression tag	UNP Q9P996
6	216	HIS	-	expression tag	UNP Q9P996
6	217	HIS	-	expression tag	UNP Q9P996
6	218	HIS	-	expression tag	UNP Q9P996
6	219	HIS	-	expression tag	UNP Q9P996
7	10	MET	-	initiating methionine	UNP Q9P996
7	214	HIS	-	expression tag	UNP Q9P996
7	215	HIS	-	expression tag	UNP Q9P996
7	216	HIS	-	expression tag	UNP Q9P996
7	217	HIS	-	expression tag	UNP Q9P996
7	218	HIS	-	expression tag	UNP Q9P996
7	219	HIS	-	expression tag	UNP Q9P996

- Molecule 3 is a protein called Proteasome-activating nucleotidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	I	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	K	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	L	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	M	9	Total	C	N	O	S	0	0
			70	47	10	12	1		
3	J	9	Total	C	N	O	S	0	0
			70	47	10	12	1		

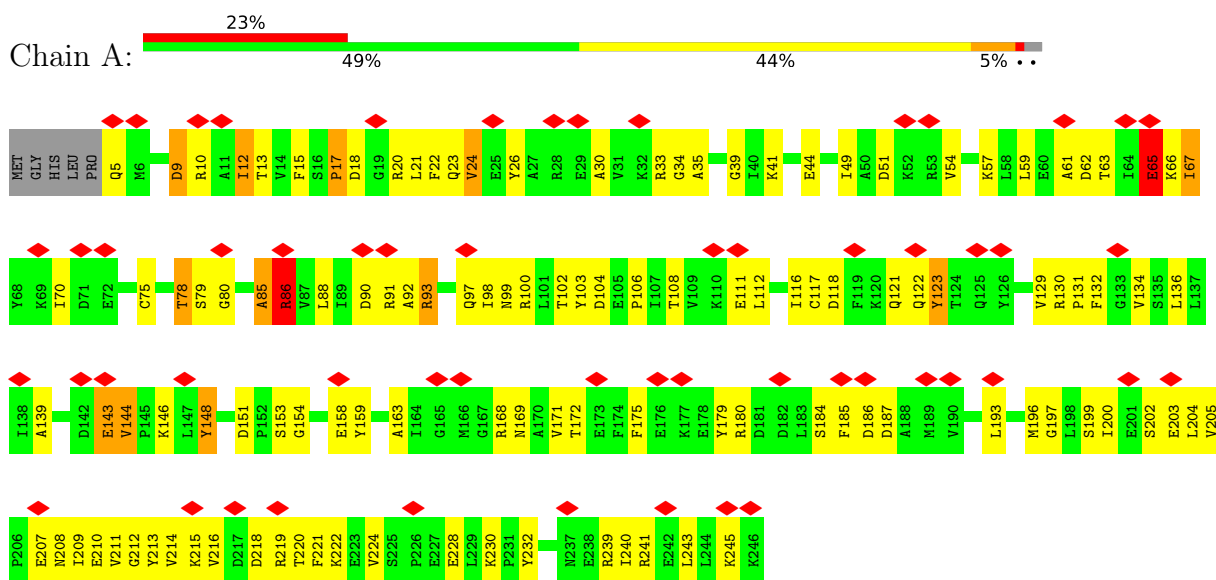
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLY	-	expression tag	UNP O28303
H	-1	HIS	-	expression tag	UNP O28303
H	0	MET	-	expression tag	UNP O28303
H	1	GLY	-	expression tag	UNP O28303
I	-2	GLY	-	expression tag	UNP O28303
I	-1	HIS	-	expression tag	UNP O28303
I	0	MET	-	expression tag	UNP O28303
I	1	GLY	-	expression tag	UNP O28303
K	-2	GLY	-	expression tag	UNP O28303
K	-1	HIS	-	expression tag	UNP O28303
K	0	MET	-	expression tag	UNP O28303
K	1	GLY	-	expression tag	UNP O28303
L	-2	GLY	-	expression tag	UNP O28303
L	-1	HIS	-	expression tag	UNP O28303
L	0	MET	-	expression tag	UNP O28303
L	1	GLY	-	expression tag	UNP O28303
M	-2	GLY	-	expression tag	UNP O28303
M	-1	HIS	-	expression tag	UNP O28303
M	0	MET	-	expression tag	UNP O28303
M	1	GLY	-	expression tag	UNP O28303
J	-2	GLY	-	expression tag	UNP O28303
J	-1	HIS	-	expression tag	UNP O28303
J	0	MET	-	expression tag	UNP O28303
J	1	GLY	-	expression tag	UNP O28303

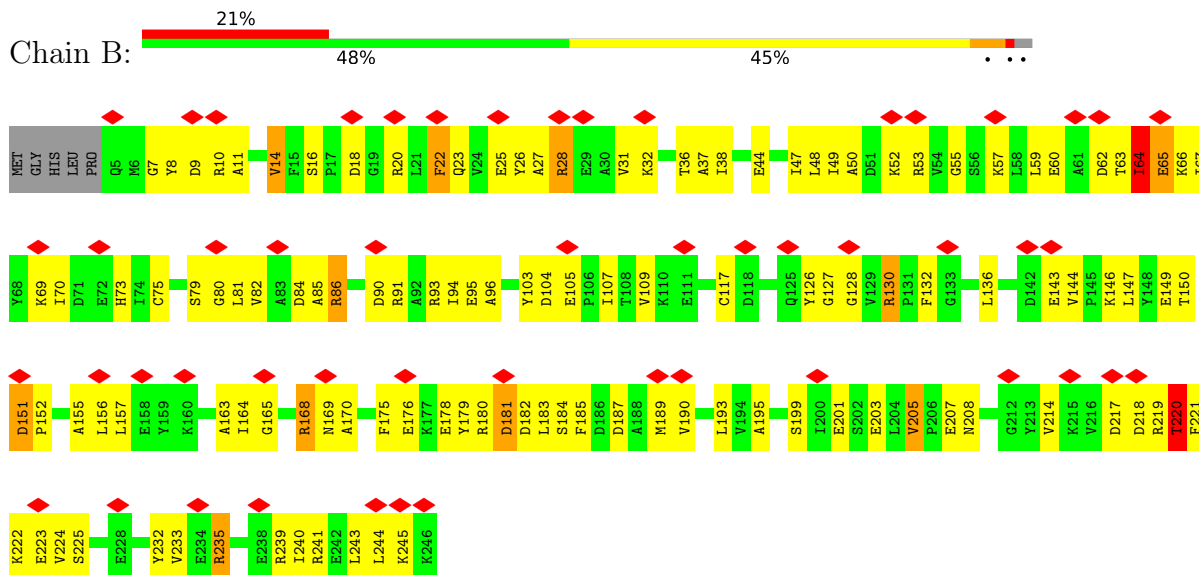
3 Residue-property plots [i](#)

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

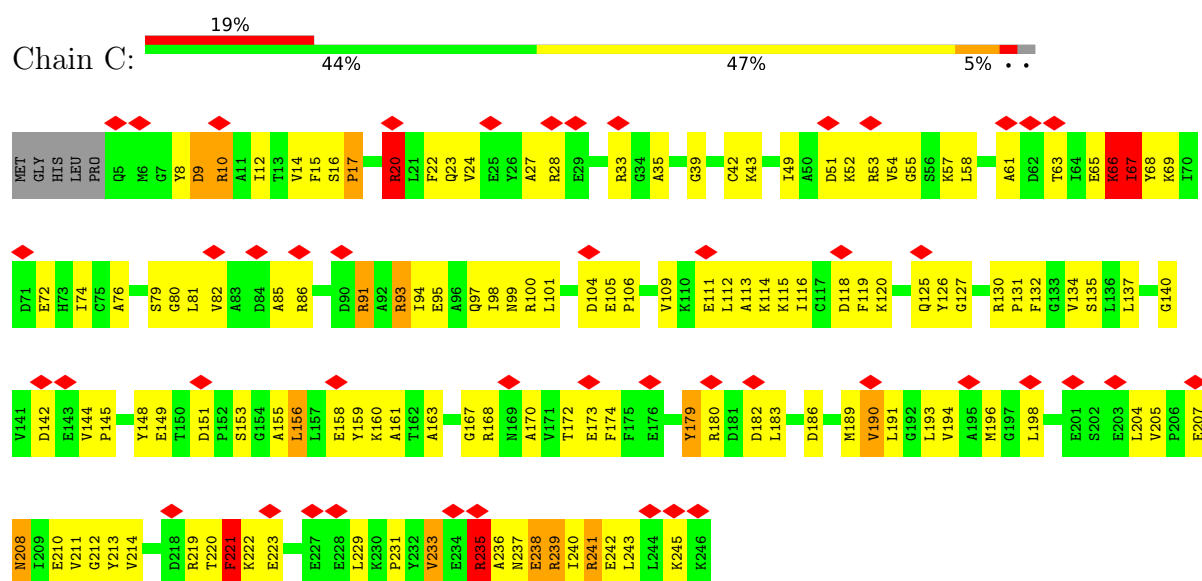
- Molecule 1: Proteasome subunit alpha



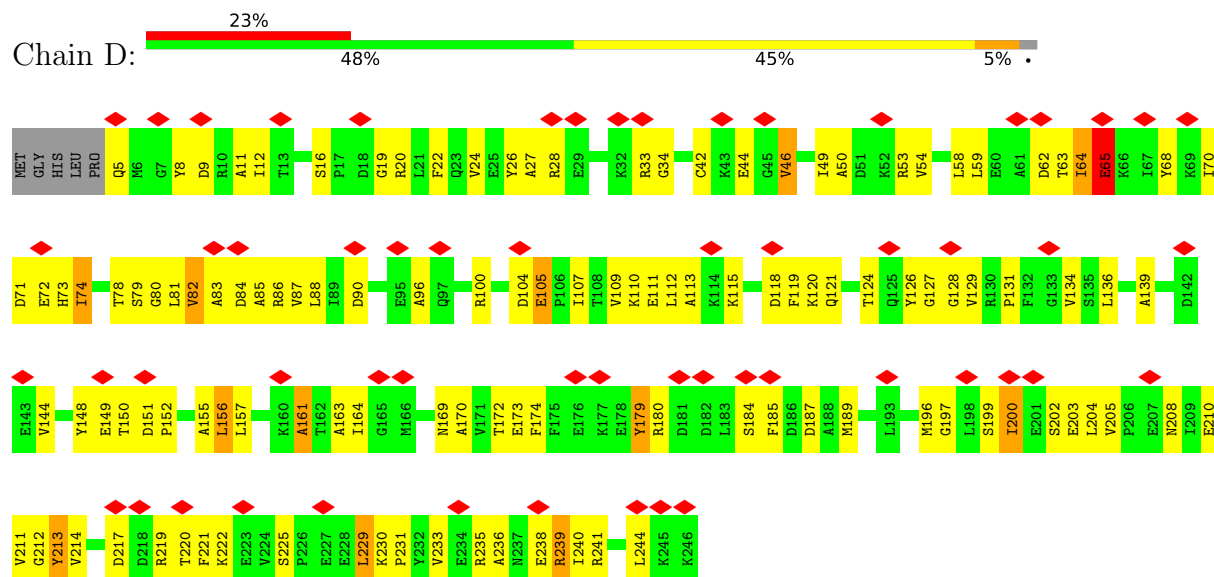
- Molecule 1: Proteasome subunit alpha



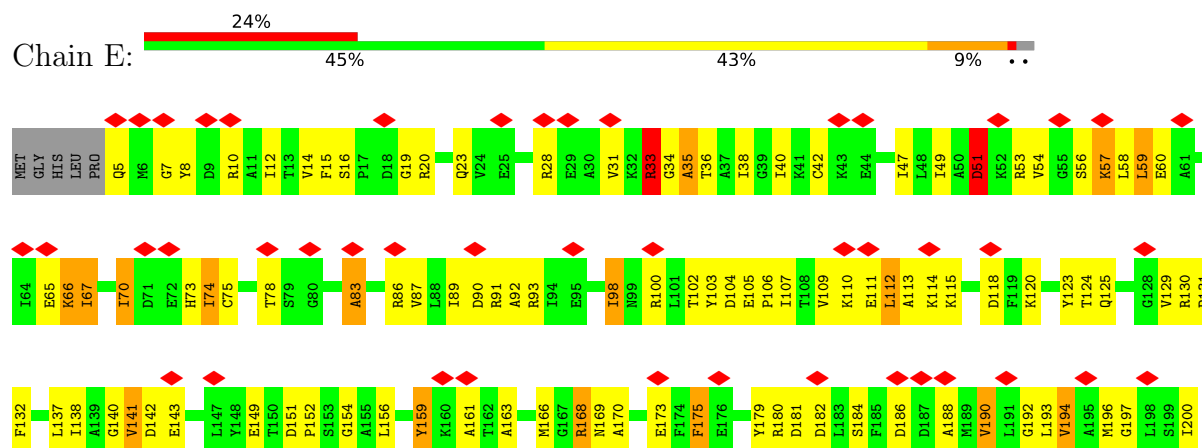
- Molecule 1: Proteasome subunit alpha

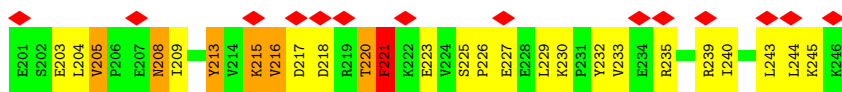


• Molecule 1: Proteasome subunit alpha

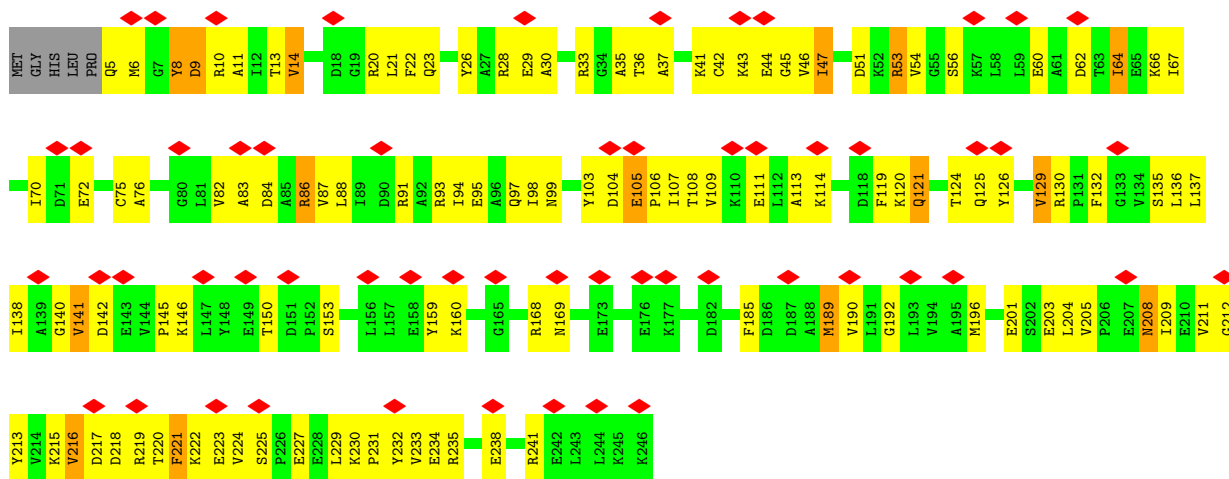


• Molecule 1: Proteasome subunit alpha

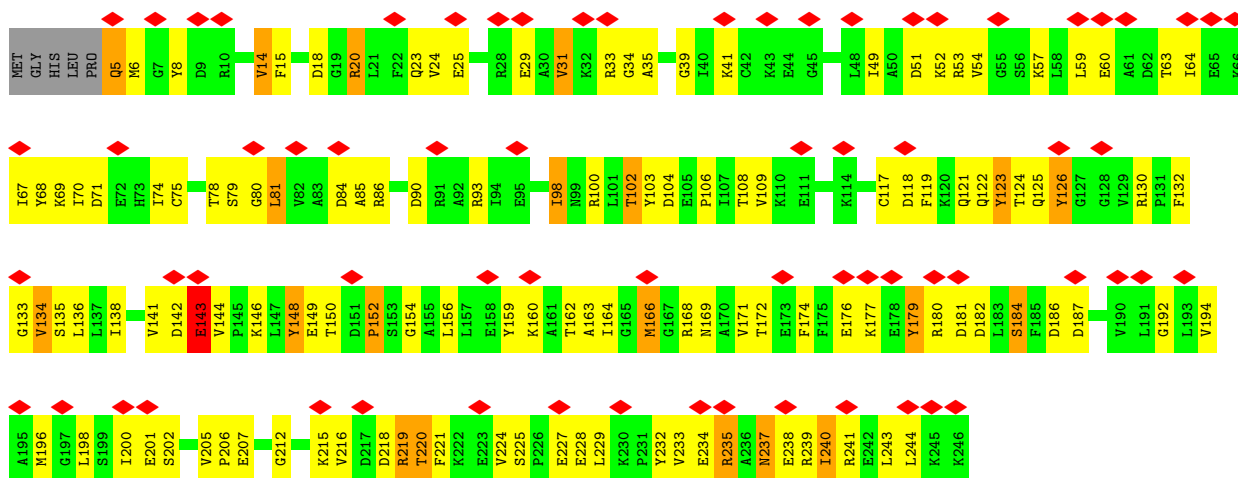




• Molecule 1: Proteasome subunit alpha

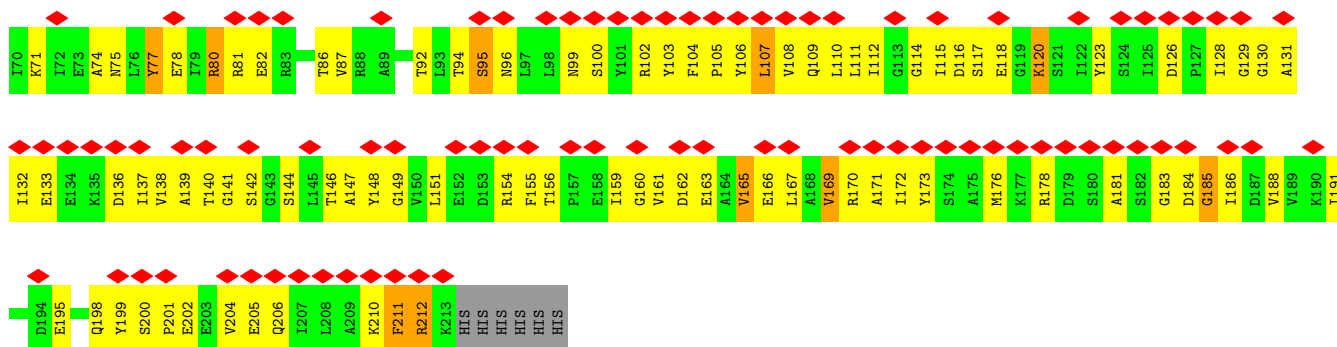


• Molecule 1: Proteasome subunit alpha

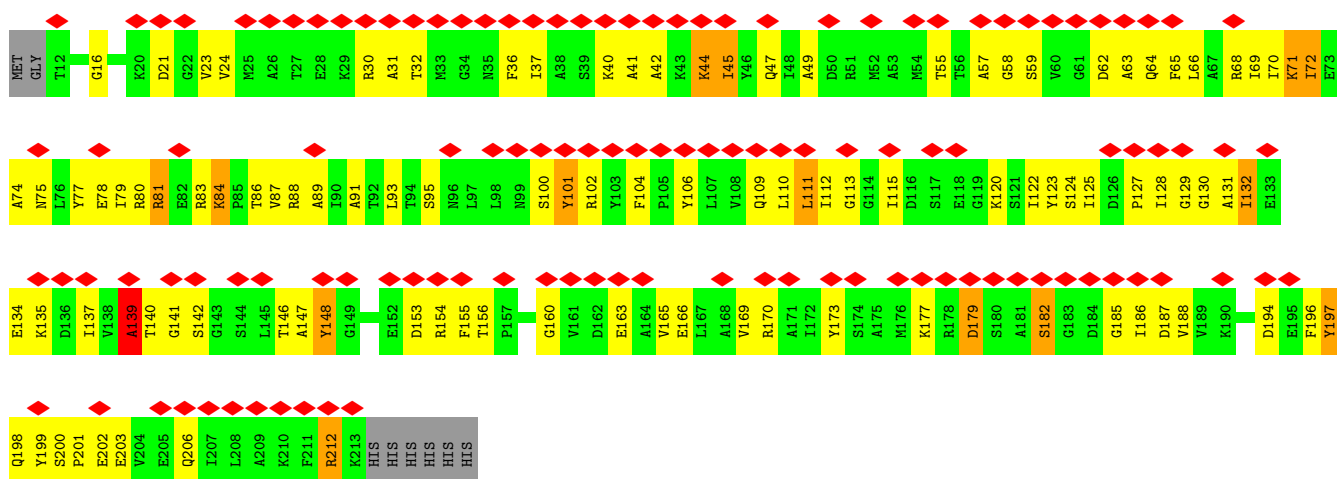


• Molecule 2: Proteasome subunit beta





- Molecule 2: Proteasome subunit beta

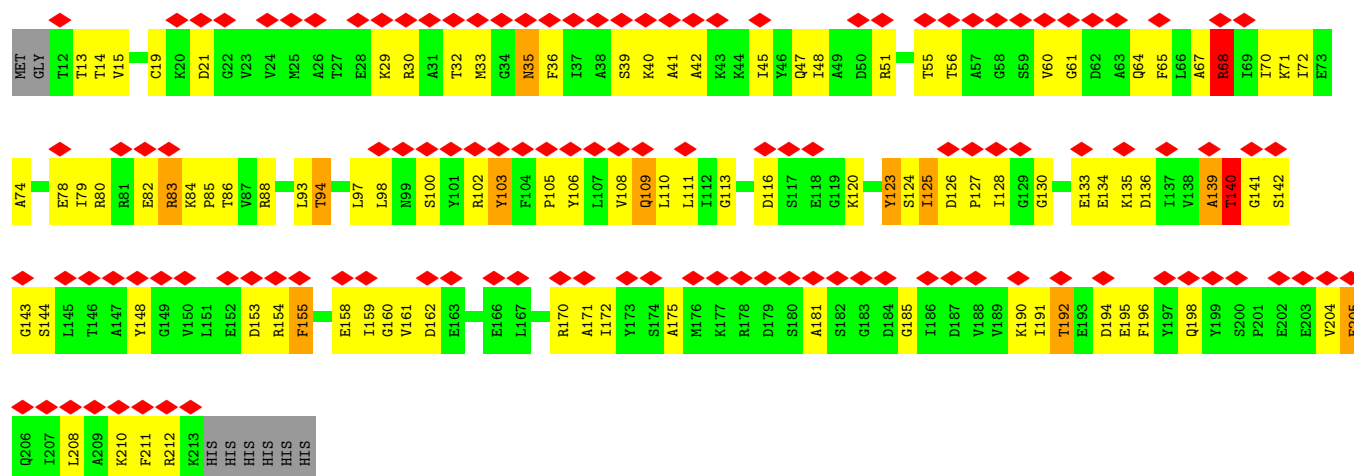


- Molecule 2: Proteasome subunit beta

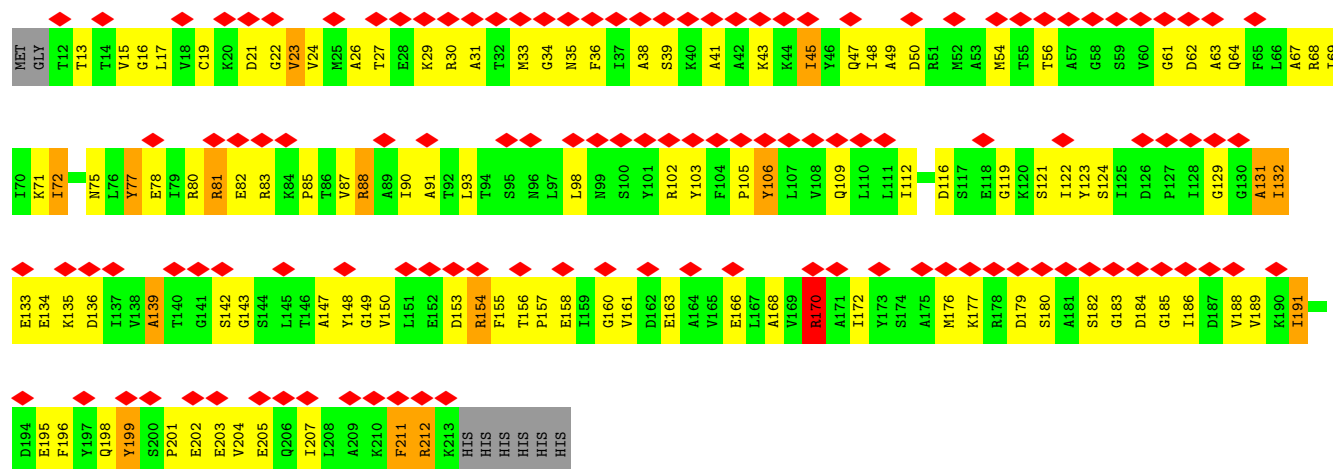


- Molecule 2: Proteasome subunit beta

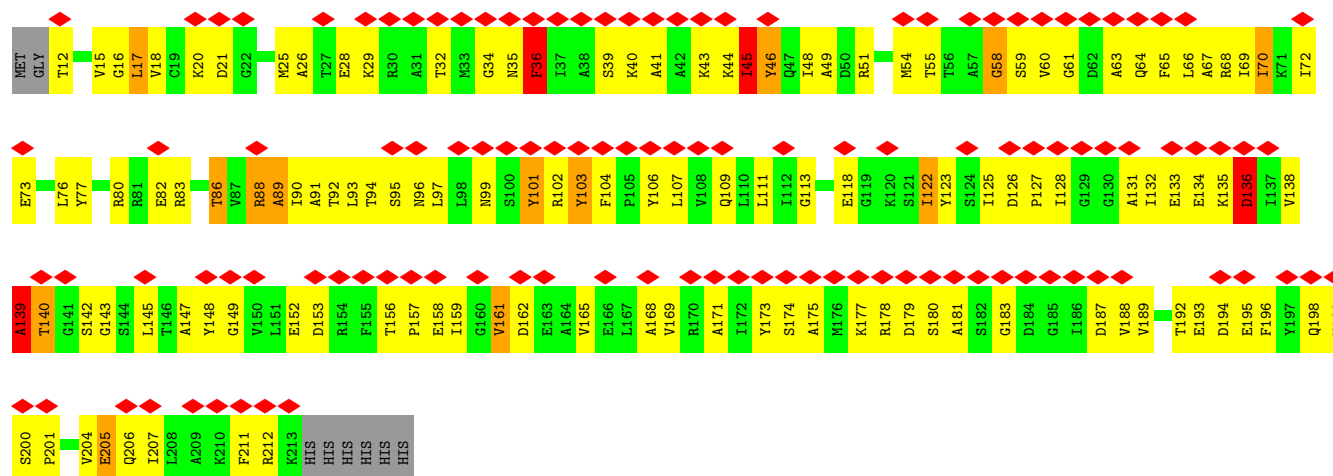




• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



Chain 7: 60% 38% 50% 7%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182989	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0372	Depositor
Map size ($\text{\AA}$)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	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	2.24	81/1934 (4.2%)	2.31	107/2605 (4.1%)
1	B	2.19	62/1934 (3.2%)	2.42	135/2605 (5.2%)
1	C	2.20	58/1934 (3.0%)	2.39	119/2605 (4.6%)
1	D	2.17	58/1934 (3.0%)	2.34	106/2605 (4.1%)
1	E	2.37	62/1934 (3.2%)	2.49	123/2605 (4.7%)
1	F	2.16	61/1934 (3.2%)	2.35	107/2605 (4.1%)
1	G	2.19	75/1934 (3.9%)	2.39	115/2605 (4.4%)
2	1	2.29	70/1572 (4.5%)	2.44	100/2121 (4.7%)
2	2	2.26	53/1572 (3.4%)	2.44	91/2121 (4.3%)
2	3	2.24	50/1572 (3.2%)	2.49	113/2121 (5.3%)
2	4	2.27	66/1572 (4.2%)	2.41	93/2121 (4.4%)
2	5	3.19	73/1572 (4.6%)	2.54	101/2121 (4.8%)
2	6	2.19	48/1572 (3.1%)	2.52	121/2121 (5.7%)
2	7	2.33	69/1572 (4.4%)	2.51	99/2121 (4.7%)
3	H	2.14	3/71 (4.2%)	2.32	5/92 (5.4%)
3	I	1.79	2/71 (2.8%)	2.40	4/92 (4.3%)
3	J	1.92	3/71 (4.2%)	2.53	5/92 (5.4%)
3	K	1.47	0/71	2.38	6/92 (6.5%)
3	L	2.10	1/71 (1.4%)	2.48	4/92 (4.3%)
3	M	2.04	2/71 (2.8%)	2.38	4/92 (4.3%)
All	All	2.30	897/24968 (3.6%)	2.43	1558/33634 (4.6%)

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	8
1	B	0	7
1	C	0	13
1	D	0	6
1	E	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	8
1	G	0	10
2	1	0	4
2	2	0	8
2	3	0	4
2	4	0	6
2	5	0	8
2	6	0	9
2	7	0	7
3	H	0	1
3	I	0	2
3	J	0	1
3	L	0	1
All	All	0	114

All (897) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	170	ARG	CZ-NH1	58.83	2.15	1.32
2	5	211	PHE	CG-CD2	34.27	2.10	1.38
2	5	211	PHE	CG-CD1	31.30	2.04	1.38
1	E	66	LYS	C-N	30.86	1.71	1.33
1	E	5	GLN	N-CA	-24.09	1.00	1.46
2	5	211	PHE	CD2-CE2	23.12	2.08	1.38
2	5	211	PHE	CD1-CE1	21.97	2.04	1.38
2	5	211	PHE	CE2-CZ	21.56	2.03	1.38
2	5	211	PHE	CE1-CZ	21.42	2.02	1.38
2	7	212	ARG	NE-CZ	11.36	1.45	1.33
2	6	67	ALA	CA-C	-11.20	1.38	1.52
2	3	89	ALA	CA-C	-10.33	1.39	1.52
2	7	111	LEU	CA-C	-10.26	1.40	1.52
2	4	135	LYS	CA-C	-10.20	1.39	1.52
2	7	13	THR	CA-C	-10.10	1.39	1.52
2	7	110	LEU	CA-C	-9.81	1.40	1.52
1	A	134	VAL	CA-C	-9.65	1.41	1.52
1	E	65	GLU	C-N	9.42	1.46	1.33
1	A	93	ARG	CA-C	-9.15	1.40	1.52
2	1	201	PRO	C-N	9.13	1.44	1.33
1	D	149	GLU	CA-C	-9.01	1.41	1.52
1	A	214	VAL	CA-C	-8.99	1.40	1.52
2	5	69	ILE	CA-C	-8.97	1.41	1.52
2	7	58	GLY	C-N	8.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	219	ARG	CD-NE	8.90	1.58	1.46
1	G	180	ARG	NE-CZ	8.88	1.42	1.33
2	3	198	GLN	CA-C	-8.87	1.42	1.52
1	C	23	GLN	N-CA	-8.83	1.35	1.46
2	2	109	GLN	CA-C	-8.76	1.42	1.52
1	B	47	ILE	CA-C	-8.73	1.42	1.52
1	D	11	ALA	CA-C	-8.71	1.41	1.52
2	7	125	ILE	CA-C	-8.65	1.42	1.52
1	B	219	ARG	NE-CZ	8.59	1.42	1.33
2	7	169	VAL	CA-CB	-8.56	1.44	1.54
2	1	100	SER	C-N	8.49	1.43	1.33
2	3	53	ALA	CA-C	-8.45	1.42	1.52
2	7	28	GLU	N-CA	-8.33	1.36	1.46
1	G	239	ARG	NE-CZ	8.32	1.42	1.33
1	B	155	ALA	CA-C	-8.29	1.42	1.52
1	A	146	LYS	N-CA	-8.29	1.35	1.45
1	C	241	ARG	CA-C	-8.20	1.42	1.52
2	3	60	VAL	CA-C	-8.19	1.42	1.52
1	C	137	LEU	CA-C	-8.15	1.42	1.52
1	D	9	ASP	N-CA	-8.15	1.40	1.47
1	D	44	GLU	N-CA	-8.12	1.36	1.46
2	6	25	MET	CA-C	-8.10	1.42	1.52
1	D	241	ARG	CD-NE	8.04	1.57	1.46
1	E	137	LEU	CA-C	-8.03	1.43	1.52
2	5	31	ALA	C-N	8.03	1.44	1.33
2	4	190	LYS	N-CA	-7.94	1.36	1.46
1	G	75	CYS	CA-C	-7.92	1.42	1.52
1	G	98	ILE	CA-C	-7.88	1.42	1.52
1	D	150	THR	N-CA	-7.80	1.36	1.46
2	2	21	ASP	N-CA	-7.79	1.37	1.46
2	2	84	LYS	CA-CB	7.78	1.65	1.53
2	1	24	VAL	CA-CB	-7.78	1.43	1.54
2	4	106	TYR	N-CA	7.76	1.55	1.46
1	C	196	MET	CA-C	-7.74	1.42	1.52
2	2	58	GLY	C-N	7.74	1.44	1.33
2	6	177	LYS	N-CA	-7.74	1.36	1.46
1	B	132	PHE	CA-C	-7.73	1.42	1.52
1	A	180	ARG	CD-NE	7.71	1.57	1.46
1	G	241	ARG	CA-C	-7.69	1.42	1.52
1	B	50	ALA	C-N	7.69	1.43	1.33
2	3	206	GLN	C-N	7.69	1.43	1.33
1	D	96	ALA	CA-C	-7.68	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	41	ALA	CA-C	-7.67	1.42	1.52
2	6	109	GLN	CA-C	-7.67	1.43	1.52
2	5	212	ARG	NE-CZ	7.66	1.41	1.33
2	6	46	TYR	CA-C	-7.65	1.43	1.52
1	G	133	GLY	C-N	7.65	1.42	1.33
2	5	68	ARG	C-N	7.61	1.43	1.33
2	1	173	TYR	N-CA	-7.60	1.37	1.46
1	E	10	ARG	CD-NE	7.60	1.56	1.46
2	6	152	GLU	C-O	-7.59	1.15	1.24
1	D	157	LEU	CA-C	-7.59	1.43	1.52
1	E	86	ARG	NE-CZ	7.57	1.41	1.33
2	4	159	ILE	CA-C	-7.57	1.43	1.52
1	F	221	PHE	CA-CB	7.54	1.66	1.53
1	B	241	ARG	CZ-NH1	7.52	1.43	1.32
1	G	205	VAL	CA-CB	-7.52	1.48	1.54
1	A	130	ARG	CA-C	-7.49	1.44	1.53
2	7	96	ASN	CA-C	-7.48	1.43	1.52
1	B	144	VAL	CA-C	-7.45	1.44	1.52
1	E	180	ARG	C-N	7.43	1.43	1.33
2	5	81	ARG	NE-CZ	7.42	1.41	1.33
2	6	212	ARG	CZ-NH1	7.42	1.43	1.32
2	2	148	TYR	CA-C	-7.42	1.43	1.52
1	E	192	GLY	CA-C	-7.41	1.42	1.51
2	7	59	SER	C-N	7.39	1.43	1.33
1	C	111	GLU	CA-C	-7.39	1.42	1.52
1	C	140	GLY	C-N	7.38	1.42	1.33
2	4	55	THR	CA-C	-7.38	1.43	1.52
2	6	113	GLY	CA-C	-7.37	1.42	1.51
2	4	124	SER	C-N	7.37	1.42	1.33
2	2	44	LYS	CA-C	-7.36	1.42	1.52
1	E	53	ARG	CD-NE	7.36	1.56	1.46
2	5	135	LYS	CA-CB	7.36	1.65	1.53
1	G	163	ALA	N-CA	-7.36	1.36	1.45
1	G	6	MET	N-CA	-7.35	1.36	1.45
1	A	63	THR	CA-C	-7.35	1.44	1.52
2	6	162	ASP	CA-CB	7.34	1.64	1.53
1	C	109	VAL	CA-CB	-7.33	1.45	1.54
2	6	142	SER	C-N	7.32	1.41	1.33
2	2	170	ARG	NE-CZ	7.31	1.41	1.33
1	A	148	TYR	CA-C	-7.29	1.43	1.52
2	5	112	ILE	CA-C	-7.29	1.43	1.52
1	C	112	LEU	C-O	-7.29	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	71	LYS	C-N	7.29	1.43	1.33
1	E	181	ASP	CA-C	-7.29	1.42	1.52
2	2	115	ILE	CA-CB	7.27	1.64	1.54
2	3	18	VAL	C-N	7.26	1.43	1.33
1	G	53	ARG	NE-CZ	7.23	1.41	1.33
2	4	181	ALA	CA-C	-7.23	1.43	1.52
2	5	196	PHE	CA-C	-7.23	1.45	1.53
1	G	235	ARG	CA-C	-7.22	1.42	1.52
2	7	52	MET	C-N	7.21	1.43	1.33
2	4	79	ILE	CA-CB	-7.18	1.46	1.54
2	4	170	ARG	CA-CB	7.17	1.64	1.53
2	5	123	TYR	CA-C	-7.17	1.43	1.52
1	D	197	GLY	CA-C	-7.16	1.44	1.52
1	E	227	GLU	CA-C	-7.16	1.43	1.52
1	F	209	ILE	C-N	7.15	1.43	1.33
1	F	86	ARG	NE-CZ	7.14	1.41	1.33
1	G	31	VAL	N-CA	-7.13	1.37	1.46
1	A	91	ARG	CA-C	-7.13	1.43	1.52
1	E	23	GLN	N-CA	-7.13	1.37	1.46
2	4	153	ASP	C-N	7.13	1.42	1.33
2	4	88	ARG	NE-CZ	7.12	1.40	1.33
2	5	158	GLU	CA-CB	7.09	1.63	1.53
2	6	178	ARG	CD-NE	7.09	1.56	1.46
2	2	66	LEU	CA-C	-7.08	1.43	1.52
2	1	54	MET	N-CA	-7.08	1.37	1.46
1	G	39	GLY	CA-C	-7.08	1.47	1.52
2	1	31	ALA	CA-C	-7.07	1.44	1.52
2	7	151	LEU	CA-C	-7.07	1.43	1.52
1	D	203	GLU	CA-C	7.07	1.61	1.52
2	7	182	SER	CA-C	-7.06	1.44	1.52
1	G	156	LEU	N-CA	-7.05	1.37	1.46
1	B	224	VAL	N-CA	-7.03	1.37	1.46
2	4	158	GLU	CA-C	-7.01	1.42	1.52
1	G	122	GLN	CA-C	-7.01	1.43	1.52
1	A	132	PHE	CA-C	-7.00	1.43	1.52
1	C	172	THR	N-CA	-6.98	1.38	1.46
2	4	124	SER	N-CA	-6.98	1.37	1.46
1	D	131	PRO	N-CA	-6.97	1.38	1.47
2	1	138	VAL	CA-CB	6.96	1.62	1.55
2	5	170	ARG	N-CA	-6.95	1.37	1.46
2	2	24	VAL	CA-C	-6.95	1.44	1.52
2	4	105	PRO	C-N	6.91	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	LYS	CA-C	-6.90	1.44	1.53
2	6	86	THR	N-CA	-6.90	1.37	1.45
3	L	393	LYS	N-CA	-6.90	1.37	1.46
1	C	24	VAL	CA-CB	-6.90	1.45	1.54
1	F	111	GLU	CA-C	-6.89	1.44	1.52
2	4	171	ALA	C-N	6.88	1.42	1.33
2	5	88	ARG	CD-NE	6.88	1.55	1.46
2	5	80	ARG	CZ-NH1	6.84	1.42	1.32
2	2	64	GLN	CA-CB	6.83	1.64	1.53
2	4	170	ARG	CZ-NH1	6.83	1.42	1.32
1	A	168	ARG	CZ-NH2	6.83	1.42	1.33
2	6	159	ILE	N-CA	-6.83	1.39	1.46
2	3	138	VAL	C-N	6.81	1.43	1.33
2	6	156	THR	N-CA	-6.80	1.41	1.46
1	F	93	ARG	NE-CZ	6.79	1.40	1.33
1	B	239	ARG	C-N	6.79	1.42	1.33
2	5	93	LEU	CA-C	-6.79	1.44	1.52
1	F	6	MET	CA-C	-6.78	1.46	1.53
2	1	205	GLU	N-CA	6.78	1.54	1.46
1	D	73	HIS	N-CA	-6.76	1.38	1.46
2	5	153	ASP	N-CA	-6.75	1.38	1.46
1	B	235	ARG	CZ-NH1	6.74	1.42	1.32
1	E	130	ARG	NE-CZ	6.74	1.40	1.33
2	3	15	VAL	CA-CB	-6.72	1.44	1.54
1	A	41	LYS	CA-C	6.71	1.60	1.52
2	3	146	THR	N-CA	-6.70	1.38	1.46
1	D	240	ILE	C-N	6.69	1.42	1.33
2	2	81	ARG	CZ-NH1	6.68	1.42	1.32
2	4	65	PHE	CA-C	-6.68	1.44	1.52
1	A	159	TYR	CA-C	-6.68	1.44	1.52
1	B	149	GLU	N-CA	-6.68	1.37	1.46
1	E	93	ARG	CD-NE	6.68	1.55	1.46
2	1	112	ILE	N-CA	-6.68	1.38	1.46
1	D	217	ASP	CA-CB	6.67	1.64	1.53
1	C	10	ARG	CD-NE	6.67	1.55	1.46
1	A	10	ARG	NE-CZ	6.66	1.40	1.33
2	2	206	GLN	C-N	6.63	1.42	1.33
2	7	152	GLU	C-N	6.63	1.42	1.33
1	D	42	CYS	N-CA	-6.63	1.37	1.46
2	2	30	ARG	CD-NE	6.63	1.55	1.46
1	F	20	ARG	CA-C	-6.62	1.44	1.52
2	7	137	ILE	C-N	6.62	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	20	ARG	NE-CZ	6.62	1.40	1.33
1	B	96	ALA	CA-C	-6.61	1.44	1.52
2	7	51	ARG	CD-NE	6.61	1.55	1.46
1	A	20	ARG	N-CA	-6.59	1.37	1.45
2	7	90	ILE	CA-C	-6.57	1.44	1.52
1	A	44	GLU	CA-C	-6.56	1.43	1.52
1	F	231	PRO	N-CA	-6.56	1.38	1.47
1	A	224	VAL	CA-C	-6.56	1.44	1.52
1	D	119	PHE	C-N	6.56	1.42	1.33
2	1	185	GLY	C-N	6.56	1.41	1.33
1	B	85	ALA	N-CA	-6.56	1.38	1.46
2	6	80	ARG	CD-NE	6.56	1.55	1.46
1	C	131	PRO	CA-CB	-6.55	1.44	1.53
2	1	176	MET	CA-CB	6.55	1.64	1.53
1	E	100	ARG	NE-CZ	6.55	1.40	1.33
2	1	163	GLU	N-CA	-6.54	1.37	1.46
1	E	140	GLY	CA-C	-6.53	1.44	1.51
1	C	142	ASP	CA-C	6.52	1.58	1.52
1	C	191	LEU	CA-C	-6.52	1.44	1.52
2	6	107	LEU	CA-CB	6.52	1.62	1.53
2	3	75	ASN	C-N	6.51	1.42	1.33
1	D	121	GLN	CA-CB	6.50	1.63	1.53
1	G	33	ARG	CA-CB	6.50	1.64	1.53
2	1	146	THR	CA-C	-6.50	1.44	1.52
2	6	36	PHE	CA-C	-6.50	1.44	1.52
1	A	108	THR	N-CA	-6.50	1.38	1.46
1	B	25	GLU	C-N	6.49	1.43	1.33
2	3	156	THR	CA-C	-6.48	1.45	1.52
2	4	45	ILE	CA-C	-6.47	1.44	1.52
1	B	146	LYS	C-N	6.47	1.42	1.33
2	7	154	ARG	CD-NE	6.47	1.55	1.46
2	5	81	ARG	CA-C	-6.47	1.43	1.52
2	2	87	VAL	CA-CB	-6.46	1.46	1.54
1	A	39	GLY	CA-C	-6.46	1.46	1.52
2	1	47	GLN	C-N	6.45	1.39	1.33
1	B	38	ILE	CA-CB	-6.45	1.45	1.54
1	F	9	ASP	N-CA	-6.45	1.37	1.46
2	6	128	ILE	CA-C	-6.42	1.44	1.52
2	3	142	SER	CA-C	-6.42	1.44	1.52
2	3	184	ASP	C-N	6.42	1.42	1.33
1	B	73	HIS	C-N	6.42	1.41	1.33
1	D	163	ALA	CA-C	-6.42	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	ARG	NE-CZ	6.41	1.40	1.33
1	B	126	TYR	C-N	6.41	1.40	1.33
1	G	205	VAL	CA-C	-6.41	1.48	1.52
1	A	222	LYS	N-CA	-6.40	1.37	1.45
1	G	60	GLU	C-N	6.40	1.42	1.33
1	A	61	ALA	C-N	6.39	1.42	1.33
1	F	53	ARG	CD-NE	6.39	1.55	1.46
1	B	103	TYR	CA-C	-6.38	1.44	1.52
1	E	173	GLU	CA-C	-6.37	1.44	1.52
1	G	241	ARG	NE-CZ	6.37	1.40	1.33
1	E	111	GLU	N-CA	-6.37	1.38	1.46
2	6	188	VAL	N-CA	6.35	1.53	1.46
1	B	32	LYS	CA-C	-6.34	1.44	1.52
1	F	107	ILE	CA-CB	-6.33	1.47	1.54
2	1	120	LYS	CA-C	-6.33	1.45	1.52
1	C	15	PHE	CA-C	-6.33	1.44	1.52
2	2	185	GLY	C-N	6.33	1.42	1.33
1	F	129	VAL	N-CA	-6.33	1.38	1.46
1	B	20	ARG	CD-NE	6.33	1.55	1.46
2	7	180	SER	N-CA	-6.33	1.38	1.46
2	2	47	GLN	CA-C	-6.32	1.45	1.52
1	E	209	ILE	N-CA	-6.32	1.39	1.46
2	7	48	ILE	C-N	6.32	1.41	1.33
1	F	130	ARG	CA-CB	6.31	1.62	1.53
1	D	156	LEU	CA-C	-6.30	1.44	1.52
2	4	32	THR	C-N	6.30	1.42	1.33
2	7	50	ASP	CA-CB	6.30	1.64	1.53
1	G	201	GLU	C-N	6.30	1.41	1.33
2	3	188	VAL	N-CA	6.29	1.53	1.46
1	G	67	ILE	CA-C	-6.28	1.45	1.52
2	4	126	ASP	C-N	6.28	1.39	1.33
2	7	105	PRO	C-N	6.28	1.41	1.33
2	1	22	GLY	C-N	6.27	1.41	1.33
2	5	182	SER	C-N	6.27	1.42	1.33
2	3	47	GLN	CA-C	-6.26	1.44	1.52
1	F	86	ARG	C-N	6.26	1.42	1.33
2	3	163	GLU	CA-C	6.25	1.61	1.52
2	4	47	GLN	CA-CB	6.25	1.60	1.52
2	3	187	ASP	C-N	6.25	1.42	1.33
1	F	223	GLU	CA-C	-6.25	1.45	1.52
1	G	53	ARG	CD-NE	6.25	1.54	1.46
1	F	37	ALA	CA-C	-6.24	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	155	PHE	N-CA	-6.24	1.38	1.46
2	5	41	ALA	C-N	6.24	1.41	1.33
1	A	122	GLN	C-N	6.24	1.42	1.33
2	2	88	ARG	NE-CZ	6.23	1.40	1.33
2	2	155	PHE	CA-CB	6.23	1.62	1.53
1	B	8	TYR	CA-C	-6.22	1.45	1.53
1	D	184	SER	C-N	-6.22	1.25	1.33
1	E	115	LYS	CA-C	-6.22	1.44	1.52
2	2	31	ALA	CA-C	-6.21	1.44	1.52
1	F	205	VAL	C-N	6.21	1.40	1.34
2	6	70	ILE	N-CA	-6.21	1.39	1.46
2	1	212	ARG	NE-CZ	6.21	1.39	1.33
2	6	63	ALA	CA-C	-6.21	1.45	1.52
1	C	100	ARG	NE-CZ	6.21	1.39	1.33
1	A	196	MET	CA-C	-6.21	1.44	1.52
2	7	91	ALA	N-CA	-6.21	1.39	1.46
2	5	54	MET	CA-C	-6.20	1.45	1.52
1	G	238	GLU	CA-CB	6.20	1.63	1.53
2	7	178	ARG	NE-CZ	6.20	1.39	1.33
1	F	91	ARG	CZ-NH2	6.20	1.41	1.33
1	C	97	GLN	N-CA	-6.20	1.38	1.46
2	1	43	LYS	N-CA	-6.19	1.38	1.46
2	7	150	VAL	CA-C	-6.19	1.45	1.52
2	2	30	ARG	CZ-NH1	6.18	1.41	1.32
2	4	71	LYS	CA-C	-6.18	1.45	1.52
2	4	55	THR	C-N	6.18	1.41	1.33
2	3	80	ARG	CA-C	6.18	1.61	1.52
1	G	59	LEU	C-N	6.18	1.41	1.33
2	2	74	ALA	CA-C	-6.17	1.44	1.52
1	C	237	ASN	N-CA	-6.17	1.38	1.46
1	B	130	ARG	CA-C	-6.17	1.46	1.52
2	3	55	THR	N-CA	-6.16	1.38	1.46
1	D	85	ALA	CA-C	-6.16	1.44	1.52
1	G	93	ARG	C-N	6.15	1.41	1.33
1	A	9	ASP	N-CA	-6.14	1.38	1.46
1	F	113	ALA	CA-C	-6.14	1.44	1.52
1	G	49	ILE	CB-CG1	6.14	1.65	1.53
2	1	33	MET	CA-C	-6.14	1.45	1.52
1	C	151	ASP	C-N	-6.14	1.27	1.34
1	B	86	ARG	CD-NE	6.13	1.54	1.46
1	B	67	ILE	CB-CG1	6.13	1.65	1.53
1	F	235	ARG	NE-CZ	6.13	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	88	ARG	CD-NE	6.13	1.54	1.46
1	A	216	VAL	N-CA	-6.12	1.39	1.46
2	2	68	ARG	CD-NE	6.12	1.54	1.46
1	F	121	GLN	CA-C	-6.12	1.44	1.52
1	C	130	ARG	NE-CZ	6.11	1.39	1.33
2	7	102	ARG	CZ-NH2	6.11	1.41	1.33
2	2	177	LYS	C-N	6.10	1.41	1.33
2	3	137	ILE	N-CA	-6.10	1.38	1.46
1	F	222	LYS	CA-C	-6.10	1.45	1.52
1	B	8	TYR	N-CA	-6.09	1.39	1.46
1	B	105	GLU	CA-C	-6.09	1.47	1.52
1	D	62	ASP	CA-C	-6.09	1.44	1.52
1	E	223	GLU	CA-C	-6.09	1.45	1.52
3	H	391	ASP	CA-C	-6.09	1.44	1.52
1	D	111	GLU	N-CA	-6.08	1.39	1.46
1	D	124	THR	CA-C	-6.08	1.45	1.52
1	E	143	GLU	CA-C	-6.07	1.44	1.52
2	6	145	LEU	N-CA	-6.07	1.39	1.46
1	G	224	VAL	N-CA	-6.06	1.38	1.46
2	5	43	LYS	CA-C	-6.06	1.45	1.52
1	D	214	VAL	CA-CB	6.04	1.61	1.53
2	6	134	GLU	N-CA	-6.04	1.38	1.46
1	A	202	SER	N-CA	-6.03	1.39	1.46
1	F	132	PHE	CA-C	-6.03	1.45	1.52
1	B	239	ARG	CD-NE	6.03	1.54	1.46
1	A	54	VAL	N-CA	-6.03	1.39	1.46
2	3	158	GLU	CA-C	-6.02	1.45	1.52
2	2	123	TYR	CA-C	-6.02	1.45	1.52
2	5	54	MET	C-N	6.02	1.41	1.33
2	3	148	TYR	N-CA	-6.01	1.38	1.46
1	E	154	GLY	CA-C	6.01	1.59	1.51
2	1	198	GLN	CA-CB	6.01	1.62	1.53
2	4	82	GLU	C-N	6.01	1.41	1.33
1	B	73	HIS	CG-CD2	6.00	1.42	1.35
2	7	131	ALA	CA-C	-5.98	1.45	1.52
2	2	203	GLU	CA-C	-5.97	1.45	1.52
2	1	32	THR	N-CA	-5.97	1.38	1.46
2	3	102	ARG	CA-C	5.97	1.61	1.52
1	G	234	GLU	CA-C	-5.96	1.45	1.52
2	5	147	ALA	CA-C	-5.96	1.44	1.52
2	7	40	LYS	CA-C	-5.96	1.45	1.52
2	6	102	ARG	NE-CZ	5.96	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	39	SER	N-CA	-5.96	1.39	1.46
1	C	168	ARG	NE-CZ	5.95	1.39	1.33
1	C	174	PHE	CA-CB	5.95	1.62	1.53
1	B	90	ASP	CA-C	-5.95	1.45	1.52
2	3	59	SER	CA-C	-5.95	1.45	1.52
2	7	189	VAL	CA-C	-5.95	1.45	1.52
1	C	219	ARG	CD-NE	5.94	1.54	1.46
1	D	107	ILE	C-N	5.94	1.41	1.33
2	1	129	GLY	C-O	-5.94	1.17	1.23
2	4	198	GLN	N-CA	-5.94	1.39	1.46
2	1	74	ALA	N-CA	-5.94	1.39	1.46
2	5	189	VAL	CA-C	-5.93	1.45	1.52
2	3	63	ALA	CA-C	-5.93	1.45	1.52
1	A	212	GLY	C-N	5.92	1.40	1.33
3	H	396	MET	N-CA	-5.92	1.39	1.46
1	B	66	LYS	C-N	5.92	1.41	1.33
2	4	139	ALA	CA-C	-5.92	1.45	1.52
1	G	70	ILE	CA-CB	-5.91	1.46	1.54
1	D	22	PHE	CA-C	-5.91	1.44	1.52
2	1	58	GLY	CA-C	-5.91	1.45	1.52
1	A	179	TYR	CB-CG	-5.90	1.38	1.51
2	6	60	VAL	C-N	5.90	1.41	1.33
2	6	178	ARG	NE-CZ	5.90	1.39	1.33
2	6	91	ALA	C-O	-5.90	1.17	1.24
2	6	48	ILE	CA-C	-5.90	1.45	1.52
2	4	141	GLY	CA-C	-5.89	1.43	1.51
1	B	75	CYS	CA-C	-5.89	1.45	1.52
2	5	207	ILE	CA-C	-5.88	1.45	1.53
1	G	78	THR	CA-C	-5.88	1.45	1.52
1	B	233	VAL	N-CA	-5.88	1.39	1.46
2	4	30	ARG	CA-C	5.88	1.60	1.52
2	7	109	GLN	CA-C	-5.87	1.45	1.52
1	B	53	ARG	NE-CZ	5.86	1.39	1.33
1	F	138	ILE	CA-CB	-5.86	1.47	1.54
1	D	49	ILE	C-N	5.86	1.40	1.33
2	1	13	THR	C-N	5.86	1.40	1.33
2	2	104	PHE	C-N	5.86	1.40	1.33
1	B	73	HIS	N-CA	-5.85	1.41	1.46
1	G	93	ARG	NE-CZ	5.85	1.39	1.33
1	D	214	VAL	CA-C	-5.85	1.45	1.52
2	6	39	SER	N-CA	-5.85	1.38	1.46
1	F	135	SER	CA-C	-5.84	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	200	ILE	CA-CB	-5.84	1.47	1.54
2	3	186	ILE	CA-CB	-5.84	1.47	1.54
1	F	138	ILE	CA-C	-5.84	1.45	1.52
2	2	42	ALA	N-CA	-5.84	1.38	1.45
2	4	113	GLY	N-CA	-5.84	1.38	1.45
1	A	143	GLU	CA-C	-5.83	1.45	1.52
2	1	178	ARG	CZ-NH1	5.83	1.41	1.32
2	5	22	GLY	CA-C	-5.83	1.45	1.52
1	C	94	ILE	CA-C	-5.82	1.45	1.52
1	B	156	LEU	CA-C	-5.82	1.45	1.52
1	G	141	VAL	N-CA	-5.82	1.39	1.46
2	7	30	ARG	CA-CB	5.82	1.62	1.53
2	2	83	ARG	CA-C	-5.81	1.45	1.52
2	1	172	ILE	N-CA	-5.81	1.38	1.46
2	5	131	ALA	N-CA	-5.81	1.38	1.46
2	3	90	ILE	CA-C	-5.81	1.45	1.52
2	4	74	ALA	CA-C	-5.80	1.45	1.52
2	4	175	ALA	N-CA	-5.80	1.38	1.46
2	2	188	VAL	N-CA	-5.80	1.39	1.46
2	1	188	VAL	CA-C	-5.79	1.45	1.52
1	A	117	CYS	N-CA	-5.78	1.39	1.46
2	4	133	GLU	CA-CB	5.78	1.60	1.53
2	1	181	ALA	C-O	-5.78	1.16	1.24
1	G	171	VAL	CA-C	-5.78	1.45	1.52
2	3	203	GLU	C-N	5.78	1.41	1.33
2	7	20	LYS	C-N	5.78	1.42	1.33
1	C	126	TYR	CA-CB	5.78	1.62	1.53
1	F	41	LYS	CA-C	-5.77	1.45	1.52
1	D	53	ARG	N-CA	5.77	1.53	1.46
1	A	17	PRO	C-N	5.76	1.42	1.34
2	1	149	GLY	C-N	5.76	1.41	1.34
1	C	27	ALA	C-N	5.76	1.42	1.33
1	B	193	LEU	CA-C	-5.76	1.45	1.52
1	E	149	GLU	CA-C	-5.76	1.45	1.52
2	5	186	ILE	CA-CB	-5.76	1.49	1.55
2	5	41	ALA	N-CA	5.75	1.53	1.46
1	D	78	THR	CA-C	-5.75	1.45	1.52
3	M	393	LYS	C-N	5.75	1.40	1.34
1	F	209	ILE	CA-CB	-5.75	1.45	1.55
1	A	241	ARG	CZ-NH1	5.74	1.40	1.32
2	2	212	ARG	CZ-NH2	5.74	1.41	1.33
1	A	23	GLN	CA-CB	5.74	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	48	ILE	CA-CB	5.74	1.63	1.54
1	G	119	PHE	CA-CB	5.73	1.62	1.53
2	2	187	ASP	C-N	5.73	1.41	1.33
2	2	32	THR	C-N	5.73	1.41	1.33
1	E	54	VAL	N-CA	-5.73	1.39	1.46
2	5	82	GLU	CA-CB	5.73	1.62	1.53
1	E	112	LEU	CA-CB	5.72	1.62	1.53
1	F	168	ARG	NE-CZ	5.72	1.39	1.33
1	B	195	ALA	N-CA	-5.71	1.39	1.46
1	G	205	VAL	N-CA	-5.71	1.41	1.46
1	C	51	ASP	N-CA	-5.71	1.39	1.46
1	A	219	ARG	CZ-NH1	5.71	1.40	1.32
1	D	20	ARG	CA-C	-5.71	1.45	1.52
1	G	168	ARG	CD-NE	5.71	1.54	1.46
1	F	212	GLY	CA-C	-5.71	1.47	1.52
2	4	47	GLN	N-CA	-5.71	1.39	1.46
2	4	68	ARG	C-N	5.71	1.41	1.33
1	C	222	LYS	N-CA	-5.71	1.38	1.45
1	F	241	ARG	CZ-NH1	5.71	1.40	1.32
2	1	128	ILE	CA-CB	5.70	1.61	1.54
2	1	156	THR	N-CA	5.70	1.51	1.45
1	A	143	GLU	C-N	5.69	1.38	1.33
3	M	394	GLY	CA-C	-5.69	1.44	1.51
1	G	235	ARG	NE-CZ	5.69	1.39	1.33
1	D	126	TYR	CA-C	-5.68	1.45	1.52
2	4	161	VAL	C-N	5.68	1.41	1.33
1	A	218	ASP	C-N	5.68	1.41	1.33
2	4	120	LYS	CA-C	-5.68	1.45	1.52
1	E	159	TYR	CA-C	-5.67	1.45	1.52
2	3	78	GLU	CA-CB	5.67	1.62	1.53
2	4	102	ARG	NE-CZ	5.67	1.39	1.33
2	7	106	TYR	C-N	5.67	1.41	1.33
1	D	222	LYS	CA-C	-5.66	1.45	1.52
2	1	131	ALA	CA-C	-5.66	1.46	1.52
2	4	102	ARG	CD-NE	5.66	1.54	1.46
1	F	84	ASP	CA-C	-5.65	1.45	1.52
2	1	169	VAL	N-CA	5.65	1.53	1.46
1	A	104	ASP	CA-C	-5.65	1.46	1.53
1	F	98	ILE	CA-C	-5.65	1.45	1.52
1	F	227	GLU	C-O	-5.65	1.17	1.24
1	G	8	TYR	CA-C	-5.64	1.45	1.52
2	4	148	TYR	C-N	5.64	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	191	ILE	C-N	5.64	1.41	1.33
1	F	94	ILE	N-CA	-5.64	1.39	1.46
1	G	68	TYR	CA-C	-5.64	1.45	1.52
2	1	49	ALA	CA-C	5.64	1.60	1.53
1	E	138	ILE	N-CA	-5.64	1.39	1.46
1	A	118	ASP	C-N	5.63	1.41	1.34
1	F	75	CYS	N-CA	-5.63	1.37	1.46
1	D	210	GLU	C-N	5.63	1.41	1.33
1	F	14	VAL	C-N	5.63	1.40	1.33
1	G	143	GLU	CA-C	-5.63	1.45	1.52
1	A	130	ARG	NE-CZ	5.63	1.39	1.33
1	A	212	GLY	CA-C	-5.63	1.47	1.52
1	C	74	ILE	CA-C	-5.63	1.45	1.52
1	C	114	LYS	CA-C	5.63	1.60	1.52
1	D	235	ARG	CD-NE	5.63	1.54	1.46
1	F	66	LYS	C-N	5.63	1.40	1.33
2	5	153	ASP	CA-CB	5.63	1.62	1.53
1	E	87	VAL	CA-C	-5.62	1.46	1.52
2	3	32	THR	CA-CB	-5.62	1.45	1.53
2	5	24	VAL	CA-C	-5.62	1.46	1.52
1	E	73	HIS	CE1-NE2	5.62	1.38	1.32
1	G	41	LYS	CA-C	-5.62	1.46	1.52
1	D	72	GLU	N-CA	-5.62	1.39	1.46
2	1	87	VAL	N-CA	-5.62	1.39	1.46
2	4	102	ARG	CA-CB	5.62	1.63	1.53
1	B	81	LEU	CA-C	-5.62	1.45	1.52
1	C	131	PRO	CA-C	-5.62	1.45	1.52
1	C	208	ASN	N-CA	-5.61	1.41	1.46
1	C	12	ILE	C-N	5.61	1.41	1.33
1	E	203	GLU	CA-CB	5.61	1.62	1.53
2	2	132	ILE	C-O	5.61	1.29	1.23
1	E	226	PRO	C-N	5.61	1.41	1.33
2	7	28	GLU	CA-C	-5.61	1.46	1.52
2	7	47	GLN	CA-C	-5.59	1.45	1.52
1	E	156	LEU	CA-C	-5.59	1.46	1.52
3	I	396	MET	CA-C	-5.59	1.45	1.52
2	5	186	ILE	C-N	5.58	1.41	1.33
1	E	58	LEU	CA-C	-5.58	1.45	1.52
2	2	72	ILE	C-N	5.58	1.41	1.34
2	1	110	LEU	CA-C	-5.58	1.45	1.52
2	2	197	TYR	CA-CB	5.58	1.61	1.53
2	7	154	ARG	NE-CZ	5.58	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	THR	C-N	5.58	1.41	1.33
1	B	224	VAL	CA-C	-5.58	1.46	1.52
2	1	120	LYS	N-CA	-5.58	1.39	1.46
1	D	239	ARG	NE-CZ	5.57	1.39	1.33
1	F	126	TYR	CA-CB	5.57	1.62	1.53
2	1	114	GLY	C-O	5.57	1.31	1.23
2	7	108	VAL	CA-CB	-5.57	1.47	1.54
1	E	213	TYR	CA-C	-5.57	1.45	1.52
2	5	98	LEU	CA-C	-5.57	1.45	1.52
1	C	33	ARG	CZ-NH2	5.57	1.40	1.33
2	7	63	ALA	C-N	5.56	1.41	1.33
1	B	180	ARG	N-CA	-5.56	1.38	1.45
1	C	43	LYS	N-CA	-5.56	1.40	1.46
2	4	144	SER	CA-C	-5.56	1.45	1.52
2	1	151	LEU	CB-CG	5.56	1.64	1.53
2	7	86	THR	N-CA	-5.55	1.38	1.45
3	H	393	LYS	C-N	5.55	1.42	1.33
1	B	93	ARG	NE-CZ	5.55	1.39	1.33
1	A	112	LEU	CA-C	-5.55	1.45	1.52
2	4	210	LYS	C-N	5.55	1.41	1.33
1	C	67	ILE	CA-C	-5.54	1.45	1.52
2	4	111	LEU	C-O	-5.54	1.17	1.24
1	C	76	ALA	CA-C	-5.54	1.45	1.52
1	B	22	PHE	CA-CB	5.54	1.62	1.53
1	B	86	ARG	CA-C	-5.54	1.45	1.52
1	E	49	ILE	C-N	5.54	1.41	1.33
1	G	138	ILE	CA-C	-5.54	1.45	1.52
2	6	211	PHE	CA-CB	-5.54	1.45	1.53
1	D	50	ALA	N-CA	-5.54	1.39	1.45
2	1	171	ALA	N-CA	5.54	1.53	1.46
1	A	102	THR	N-CA	-5.54	1.38	1.45
1	A	158	GLU	CA-CB	5.54	1.61	1.53
1	G	86	ARG	CZ-NH1	5.53	1.40	1.32
1	A	239	ARG	NE-CZ	5.53	1.39	1.33
1	D	118	ASP	C-N	5.53	1.41	1.33
1	A	129	VAL	N-CA	-5.53	1.39	1.46
1	C	145	PRO	N-CA	-5.52	1.40	1.47
2	3	51	ARG	CD-NE	5.52	1.53	1.46
1	C	53	ARG	NE-CZ	5.52	1.39	1.33
2	4	68	ARG	NE-CZ	5.51	1.39	1.33
1	E	51	ASP	C-N	5.51	1.40	1.33
2	1	12	THR	C-N	5.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	145	PRO	N-CA	-5.50	1.40	1.47
1	F	54	VAL	CA-C	-5.50	1.45	1.52
2	7	165	VAL	N-CA	-5.50	1.39	1.46
1	A	148	TYR	CZ-OH	5.49	1.49	1.38
1	E	49	ILE	CA-C	-5.49	1.46	1.52
2	1	204	VAL	C-O	-5.49	1.17	1.24
2	7	118	GLU	C-N	5.49	1.41	1.33
1	C	54	VAL	CA-CB	-5.49	1.45	1.55
1	D	62	ASP	CA-CB	5.48	1.61	1.53
1	B	136	LEU	CA-C	-5.48	1.46	1.52
2	2	160	GLY	C-O	-5.48	1.17	1.23
1	D	58	LEU	CA-C	-5.48	1.45	1.52
1	G	180	ARG	CD-NE	5.48	1.53	1.46
2	1	211	PHE	CA-CB	5.47	1.63	1.53
1	A	116	ILE	CA-C	-5.47	1.46	1.52
2	4	210	LYS	CA-CB	5.47	1.63	1.53
2	1	104	PHE	CA-CB	5.46	1.62	1.53
1	E	42	CYS	CA-C	-5.46	1.45	1.52
1	B	180	ARG	CZ-NH2	5.46	1.40	1.33
2	5	119	GLY	C-N	5.46	1.41	1.33
2	3	21	ASP	CA-C	-5.46	1.48	1.52
1	D	71	ASP	CA-C	-5.46	1.45	1.52
2	4	124	SER	CA-CB	5.46	1.61	1.53
1	F	30	ALA	C-N	5.46	1.40	1.33
1	F	211	VAL	N-CA	-5.46	1.40	1.46
1	E	156	LEU	N-CA	-5.46	1.39	1.45
1	A	209	ILE	CB-CG1	5.45	1.64	1.53
2	1	169	VAL	C-N	5.45	1.41	1.34
1	A	219	ARG	NE-CZ	5.45	1.39	1.33
1	B	36	THR	C-N	5.45	1.40	1.33
1	B	104	ASP	CA-CB	5.45	1.61	1.53
1	C	91	ARG	NE-CZ	5.45	1.39	1.33
1	C	211	VAL	CA-C	-5.45	1.46	1.52
1	G	121	GLN	N-CA	-5.45	1.38	1.46
2	1	94	THR	C-O	-5.45	1.17	1.24
2	4	198	GLN	C-N	5.45	1.41	1.34
1	E	35	ALA	CA-C	-5.44	1.45	1.52
1	G	60	GLU	N-CA	-5.44	1.39	1.46
1	G	148	TYR	N-CA	-5.44	1.38	1.45
2	3	68	ARG	NE-CZ	5.44	1.39	1.33
2	1	20	LYS	N-CA	-5.44	1.39	1.46
2	7	36	PHE	CA-C	5.44	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	18	VAL	C-O	-5.43	1.18	1.24
2	6	83	ARG	CD-NE	5.43	1.53	1.46
2	1	191	ILE	N-CA	-5.43	1.39	1.46
1	F	94	ILE	CA-C	-5.43	1.45	1.52
2	1	133	GLU	C-N	5.43	1.40	1.33
2	3	69	ILE	C-N	5.42	1.40	1.33
2	7	83	ARG	N-CA	-5.42	1.39	1.46
1	G	142	ASP	N-CA	-5.42	1.39	1.46
1	A	33	ARG	N-CA	5.42	1.52	1.46
2	4	84	LYS	CA-C	-5.42	1.47	1.53
2	5	166	GLU	CA-C	-5.42	1.45	1.52
2	7	191	ILE	CB-CG1	5.42	1.64	1.53
2	1	38	ALA	CA-CB	5.41	1.61	1.53
2	7	125	ILE	CA-CB	5.41	1.61	1.54
1	C	86	ARG	CZ-NH1	5.41	1.40	1.32
1	A	33	ARG	CZ-NH1	5.41	1.40	1.32
1	G	85	ALA	N-CA	-5.41	1.39	1.46
1	D	33	ARG	NE-CZ	5.41	1.39	1.33
1	A	106	PRO	C-N	5.40	1.40	1.33
2	2	80	ARG	C-O	-5.40	1.17	1.24
2	3	190	LYS	CA-C	-5.40	1.46	1.52
1	B	59	LEU	C-N	5.39	1.40	1.33
1	G	136	LEU	CA-C	-5.39	1.46	1.52
2	1	80	ARG	CZ-NH1	5.39	1.40	1.32
2	5	87	VAL	CA-CB	-5.39	1.46	1.54
1	B	91	ARG	NE-CZ	5.39	1.39	1.33
2	1	123	TYR	CA-C	-5.39	1.46	1.52
1	A	22	PHE	CA-C	-5.39	1.45	1.52
2	5	68	ARG	CZ-NH1	5.39	1.40	1.32
1	E	91	ARG	CA-C	-5.38	1.45	1.52
1	G	148	TYR	CA-C	-5.38	1.46	1.52
2	5	142	SER	C-O	-5.38	1.17	1.24
1	E	193	LEU	CA-C	-5.38	1.45	1.52
2	6	16	GLY	CA-C	-5.38	1.44	1.51
1	C	115	LYS	N-CA	-5.38	1.39	1.46
2	5	198	GLN	CA-C	-5.38	1.46	1.52
2	1	45	ILE	C-N	5.38	1.41	1.33
1	A	91	ARG	C-N	5.37	1.40	1.33
1	G	138	ILE	N-CA	-5.37	1.39	1.46
2	5	186	ILE	CA-C	-5.37	1.46	1.52
1	G	176	GLU	C-N	5.37	1.40	1.33
3	J	392	LEU	N-CA	-5.36	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	60	VAL	N-CA	-5.36	1.39	1.46
2	1	212	ARG	N-CA	-5.36	1.39	1.46
2	6	122	ILE	C-N	5.36	1.40	1.33
2	2	45	ILE	CA-C	-5.35	1.45	1.52
2	2	70	ILE	CA-CB	-5.35	1.47	1.54
2	7	81	ARG	CD-NE	5.35	1.53	1.46
2	2	130	GLY	C-O	-5.35	1.16	1.23
2	4	212	ARG	CA-C	-5.34	1.45	1.52
2	4	191	ILE	C-O	-5.34	1.18	1.24
1	G	24	VAL	N-CA	-5.34	1.39	1.46
1	E	235	ARG	CZ-NH2	5.33	1.40	1.33
1	A	208	ASN	N-CA	-5.33	1.39	1.46
1	G	102	THR	N-CA	-5.33	1.39	1.46
2	2	124	SER	N-CA	-5.33	1.39	1.46
2	7	102	ARG	CD-NE	5.32	1.53	1.46
1	E	105	GLU	N-CA	-5.32	1.40	1.46
2	7	62	ASP	C-N	5.31	1.41	1.33
2	2	63	ALA	N-CA	5.31	1.52	1.46
1	B	91	ARG	N-CA	-5.31	1.40	1.46
1	F	45	GLY	N-CA	-5.31	1.39	1.45
1	A	70	ILE	C-O	-5.31	1.18	1.23
2	4	74	ALA	CA-CB	5.31	1.61	1.53
1	A	80	GLY	CA-C	-5.30	1.46	1.52
2	4	103	TYR	CA-CB	5.30	1.61	1.53
1	F	10	ARG	NE-CZ	5.30	1.38	1.33
1	G	148	TYR	CE1-CZ	5.30	1.50	1.38
2	5	168	ALA	C-N	5.30	1.40	1.33
1	F	219	ARG	CZ-NH1	5.29	1.40	1.32
2	5	29	LYS	N-CA	-5.29	1.39	1.46
2	6	204	VAL	CA-C	-5.29	1.46	1.52
2	7	181	ALA	C-N	5.29	1.40	1.33
3	J	396	MET	CA-C	-5.29	1.45	1.52
1	G	149	GLU	N-CA	-5.29	1.39	1.46
2	3	96	ASN	CA-CB	5.29	1.61	1.53
2	5	34	GLY	N-CA	-5.28	1.37	1.45
2	6	68	ARG	NE-CZ	5.28	1.38	1.33
1	C	170	ALA	CA-C	-5.28	1.46	1.52
1	E	57	LYS	CA-C	-5.28	1.45	1.52
2	5	80	ARG	CD-NE	5.28	1.53	1.46
1	B	69	LYS	N-CA	-5.27	1.39	1.46
2	1	22	GLY	N-CA	-5.27	1.39	1.45
2	7	88	ARG	CA-CB	5.27	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	240	ILE	C-O	5.27	1.30	1.24
1	F	10	ARG	CD-NE	5.26	1.53	1.46
2	4	130	GLY	CA-C	-5.26	1.44	1.51
2	5	80	ARG	N-CA	5.26	1.52	1.46
2	7	179	ASP	CA-C	-5.26	1.46	1.52
1	D	151	ASP	CA-C	-5.26	1.45	1.52
2	2	100	SER	C-N	5.26	1.39	1.33
1	G	187	ASP	C-N	5.26	1.41	1.33
2	4	162	ASP	CA-C	-5.26	1.46	1.52
2	3	58	GLY	CA-C	-5.26	1.44	1.51
2	5	16	GLY	N-CA	-5.26	1.40	1.45
2	6	65	PHE	CA-CB	5.25	1.61	1.53
1	F	23	GLN	C-N	5.25	1.40	1.33
2	5	109	GLN	CA-C	-5.25	1.46	1.52
1	C	189	MET	CA-C	-5.25	1.46	1.52
1	B	128	GLY	CA-C	-5.25	1.44	1.51
2	3	105	PRO	N-CA	-5.25	1.41	1.47
2	7	117	SER	C-O	-5.25	1.17	1.24
2	1	44	LYS	CA-C	5.25	1.59	1.52
2	3	48	ILE	CA-C	-5.25	1.45	1.52
2	5	35	ASN	C-N	5.25	1.40	1.33
1	A	15	PHE	CA-C	-5.24	1.46	1.52
1	E	60	GLU	C-N	5.24	1.40	1.33
1	E	208	ASN	CA-C	-5.24	1.45	1.52
1	F	190	VAL	C-N	5.24	1.41	1.34
2	5	158	GLU	C-N	5.24	1.40	1.33
1	B	164	ILE	CA-C	-5.24	1.46	1.52
1	C	179	TYR	CG-CD1	5.24	1.50	1.39
1	E	161	ALA	CA-C	-5.24	1.46	1.52
2	1	141	GLY	C-N	5.23	1.41	1.34
1	E	188	ALA	CA-C	-5.23	1.46	1.52
2	1	139	ALA	C-N	5.23	1.40	1.33
2	3	98	LEU	CA-CB	5.23	1.61	1.53
2	3	118	GLU	C-N	5.23	1.42	1.33
2	7	210	LYS	N-CA	5.23	1.52	1.46
1	A	86	ARG	CZ-NH2	5.23	1.40	1.33
1	G	166	MET	N-CA	-5.23	1.40	1.46
2	7	23	VAL	C-N	5.23	1.40	1.33
3	I	396	MET	CA-CB	5.22	1.62	1.53
1	D	104	ASP	CA-C	5.22	1.59	1.53
2	3	123	TYR	N-CA	-5.22	1.39	1.46
2	4	204	VAL	CA-C	-5.22	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	16	GLY	CA-C	5.22	1.57	1.51
1	C	10	ARG	CZ-NH1	5.22	1.40	1.32
1	F	67	ILE	CA-C	-5.22	1.46	1.52
2	5	170	ARG	NE-CZ	5.22	1.38	1.33
1	D	111	GLU	C-O	-5.21	1.18	1.24
2	5	50	ASP	N-CA	-5.21	1.40	1.46
1	F	150	THR	CA-CB	-5.21	1.45	1.53
1	A	203	GLU	N-CA	-5.21	1.39	1.46
1	D	110	LYS	CA-CB	5.20	1.61	1.53
2	2	194	ASP	N-CA	-5.20	1.39	1.46
1	G	144	VAL	CA-C	-5.20	1.47	1.52
2	1	75	ASN	CA-C	-5.20	1.46	1.52
1	B	214	VAL	N-CA	-5.20	1.39	1.46
1	G	106	PRO	N-CA	-5.20	1.40	1.47
2	5	158	GLU	N-CA	-5.20	1.40	1.46
1	A	139	ALA	N-CA	-5.19	1.40	1.46
1	D	170	ALA	N-CA	-5.19	1.39	1.46
1	A	61	ALA	N-CA	-5.19	1.39	1.46
1	A	210	GLU	N-CA	-5.19	1.39	1.46
1	C	112	LEU	CA-C	-5.19	1.46	1.52
1	D	90	ASP	CA-C	-5.18	1.46	1.52
1	E	168	ARG	N-CA	-5.18	1.40	1.46
2	5	160	GLY	C-N	5.18	1.40	1.33
1	F	93	ARG	CA-C	-5.17	1.46	1.52
1	G	69	LYS	C-N	5.17	1.40	1.33
1	G	126	TYR	C-N	5.17	1.41	1.33
1	F	22	PHE	CA-C	-5.17	1.45	1.52
2	7	43	LYS	N-CA	-5.17	1.39	1.46
2	2	16	GLY	CA-C	-5.17	1.44	1.51
1	A	93	ARG	C-N	5.17	1.40	1.33
2	1	165	VAL	CA-C	-5.17	1.46	1.52
1	G	20	ARG	CZ-NH2	5.16	1.40	1.33
2	1	115	ILE	CA-CB	-5.16	1.48	1.54
2	2	93	LEU	N-CA	-5.16	1.40	1.46
2	6	66	LEU	CA-C	-5.16	1.46	1.52
2	2	125	ILE	CA-C	-5.16	1.45	1.52
2	1	116	ASP	CA-C	-5.16	1.46	1.52
2	7	198	GLN	CD-NE2	5.16	1.44	1.33
2	3	81	ARG	NE-CZ	5.15	1.38	1.33
2	4	100	SER	CA-CB	5.15	1.61	1.53
1	B	176	GLU	C-N	5.15	1.40	1.33
1	D	19	GLY	CA-C	-5.15	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	121	SER	CA-C	-5.15	1.46	1.52
2	3	174	SER	C-N	5.15	1.40	1.34
3	J	396	MET	N-CA	-5.15	1.39	1.46
2	5	67	ALA	N-CA	5.14	1.52	1.46
1	E	112	LEU	CA-C	-5.14	1.46	1.52
2	1	167	LEU	C-N	5.14	1.40	1.33
1	B	31	VAL	N-CA	5.14	1.52	1.46
2	6	126	ASP	C-N	5.14	1.39	1.34
2	4	85	PRO	CA-C	-5.14	1.46	1.52
2	4	212	ARG	NE-CZ	5.13	1.38	1.33
2	3	139	ALA	N-CA	-5.13	1.39	1.46
2	6	194	ASP	CA-C	-5.13	1.45	1.52
2	7	77	TYR	CZ-OH	5.13	1.48	1.38
1	A	197	GLY	CA-C	5.12	1.57	1.52
2	6	46	TYR	N-CA	-5.12	1.39	1.45
1	C	61	ALA	CA-C	-5.12	1.46	1.52
2	6	198	GLN	CA-CB	5.12	1.61	1.53
2	6	187	ASP	CA-C	-5.12	1.46	1.52
1	F	140	GLY	N-CA	5.11	1.50	1.45
2	5	102	ARG	NE-CZ	5.11	1.38	1.33
2	7	58	GLY	CA-C	-5.11	1.46	1.52
1	C	58	LEU	C-N	5.11	1.40	1.33
2	5	154	ARG	N-CA	-5.11	1.39	1.46
2	7	94	THR	N-CA	-5.11	1.40	1.46
1	F	219	ARG	C-N	5.11	1.40	1.33
1	E	98	ILE	CA-CB	-5.10	1.48	1.54
1	G	215	LYS	C-N	5.10	1.40	1.33
1	A	65	GLU	C-N	5.10	1.40	1.33
1	B	95	GLU	N-CA	-5.10	1.40	1.46
1	C	17	PRO	N-CA	-5.09	1.41	1.47
2	4	15	VAL	CA-C	-5.09	1.46	1.52
2	3	74	ALA	CA-CB	5.09	1.61	1.53
1	D	20	ARG	CZ-NH2	5.09	1.40	1.33
1	F	30	ALA	CA-C	-5.09	1.46	1.52
1	F	53	ARG	CA-C	-5.09	1.46	1.52
2	3	189	VAL	CA-CB	5.09	1.62	1.55
2	5	183	GLY	C-N	5.09	1.40	1.33
1	E	14	VAL	CA-CB	-5.09	1.48	1.54
1	F	235	ARG	CD-NE	5.09	1.53	1.46
1	A	91	ARG	CZ-NH2	5.09	1.40	1.33
1	C	156	LEU	CA-C	-5.09	1.46	1.52
1	G	163	ALA	CA-C	-5.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	114	LYS	CA-C	-5.09	1.46	1.52
2	5	157	PRO	C-N	-5.09	1.27	1.33
2	6	174	SER	C-N	5.09	1.40	1.34
2	4	30	ARG	NE-CZ	5.08	1.38	1.33
1	B	199	SER	C-N	5.08	1.39	1.34
2	1	99	ASN	CA-C	-5.08	1.46	1.52
2	7	75	ASN	CA-C	-5.08	1.46	1.52
2	5	142	SER	C-N	5.08	1.39	1.33
2	7	210	LYS	CA-C	-5.08	1.46	1.52
2	6	193	GLU	CA-CB	5.08	1.60	1.53
1	G	152	PRO	CA-C	-5.08	1.44	1.52
1	G	239	ARG	CD-NE	5.07	1.53	1.46
2	1	162	ASP	CA-CB	5.07	1.61	1.53
2	3	65	PHE	CA-CB	5.07	1.61	1.53
2	6	109	GLN	C-N	5.07	1.40	1.33
1	D	180	ARG	NE-CZ	5.07	1.38	1.33
1	A	123	TYR	N-CA	-5.07	1.39	1.46
2	1	61	GLY	CA-C	5.07	1.57	1.52
2	3	172	ILE	C-N	5.06	1.40	1.34
1	E	154	GLY	C-N	5.06	1.40	1.33
1	D	5	GLN	C-N	5.06	1.40	1.33
2	5	75	ASN	CA-C	-5.05	1.46	1.52
1	C	72	GLU	CA-CB	5.05	1.61	1.53
1	D	100	ARG	CZ-NH2	5.05	1.40	1.33
1	E	131	PRO	CA-CB	-5.05	1.45	1.53
1	D	219	ARG	NE-CZ	5.05	1.38	1.33
2	7	197	TYR	CA-C	-5.05	1.46	1.52
1	A	240	ILE	C-N	5.05	1.40	1.33
1	G	162	THR	CA-C	-5.05	1.46	1.52
2	1	71	LYS	CA-C	5.05	1.59	1.52
1	A	75	CYS	CA-CB	5.05	1.63	1.54
1	B	79	SER	C-N	5.05	1.39	1.33
1	A	239	ARG	CZ-NH1	5.04	1.39	1.32
1	F	146	LYS	CA-C	-5.04	1.46	1.52
1	G	232	TYR	C-N	5.04	1.40	1.33
1	A	193	LEU	C-N	5.04	1.40	1.33
1	A	243	LEU	C-O	-5.04	1.18	1.24
1	E	92	ALA	CA-C	-5.04	1.46	1.52
2	1	165	VAL	CA-CB	-5.04	1.48	1.54
2	4	194	ASP	CA-C	-5.04	1.46	1.52
1	A	159	TYR	CA-CB	5.04	1.61	1.53
2	4	160	GLY	C-N	5.04	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	79	ILE	CA-C	-5.04	1.46	1.52
2	2	65	PHE	C-N	5.04	1.40	1.34
2	7	46	TYR	N-CA	-5.04	1.39	1.46
2	6	195	GLU	N-CA	-5.03	1.39	1.45
1	C	172	THR	C-N	5.03	1.40	1.33
1	G	241	ARG	C-N	5.03	1.40	1.33
1	A	26	TYR	N-CA	-5.03	1.39	1.46
2	7	24	VAL	CA-C	-5.03	1.46	1.52
1	C	86	ARG	NE-CZ	5.03	1.38	1.33
1	D	109	VAL	N-CA	-5.03	1.40	1.46
1	A	228	GLU	C-N	5.03	1.40	1.34
2	7	171	ALA	N-CA	5.02	1.52	1.46
1	E	110	LYS	CA-C	-5.02	1.46	1.52
1	G	177	LYS	C-N	5.02	1.41	1.33
2	2	196	PHE	CA-C	-5.02	1.46	1.53
1	B	243	LEU	CA-CB	5.02	1.62	1.53
1	D	96	ALA	N-CA	5.02	1.52	1.46
2	4	42	ALA	C-N	5.02	1.40	1.33
1	C	241	ARG	CD-NE	5.02	1.53	1.46
2	2	66	LEU	C-N	5.02	1.40	1.33
1	A	209	ILE	CA-CB	-5.01	1.47	1.55
2	4	100	SER	C-N	5.01	1.40	1.33
1	E	163	ALA	CA-C	-5.01	1.46	1.52
2	5	156	THR	C-O	-5.01	1.19	1.24
2	5	168	ALA	N-CA	-5.01	1.40	1.46
1	G	15	PHE	CA-CB	5.01	1.61	1.53
2	1	129	GLY	C-N	5.01	1.40	1.33
2	2	102	ARG	NE-CZ	5.01	1.38	1.33
2	6	34	GLY	C-O	-5.01	1.18	1.24
1	A	199	SER	CA-CB	5.00	1.61	1.53
1	C	239	ARG	CD-NE	5.00	1.53	1.46
1	E	229	LEU	C-N	5.00	1.40	1.33
2	2	201	PRO	N-CA	-5.00	1.41	1.47

All (1558) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	170	ARG	NE-CZ-NH2	-19.79	101.39	119.20
2	2	40	LYS	N-CA-C	-16.45	95.87	114.62
1	E	65	GLU	CA-C-N	15.58	141.72	120.38
1	E	65	GLU	C-N-CA	15.58	141.72	120.38
1	E	66	LYS	O-C-N	12.98	135.88	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ILE	N-CA-C	-12.57	101.56	112.12
1	E	66	LYS	CA-C-N	-12.24	106.82	123.10
1	E	66	LYS	C-N-CA	-12.24	106.82	123.10
1	E	132	PHE	CA-CB-CG	-11.60	102.20	113.80
2	6	179	ASP	CA-CB-CG	-11.59	101.01	112.60
1	E	65	GLU	O-C-N	-10.95	105.49	123.00
1	G	205	VAL	CA-C-O	-10.88	112.76	119.51
1	G	14	VAL	CA-C-N	10.79	136.20	120.87
1	G	14	VAL	C-N-CA	10.79	136.20	120.87
1	B	208	ASN	CA-CB-CG	10.77	123.37	112.60
2	7	170	ARG	CA-C-N	10.46	134.67	120.44
2	7	170	ARG	C-N-CA	10.46	134.67	120.44
1	B	38	ILE	CA-C-N	10.41	129.36	122.18
1	B	38	ILE	C-N-CA	10.41	129.36	122.18
2	2	78	GLU	N-CA-C	-10.35	100.08	111.36
2	6	70	ILE	CA-C-O	-10.34	110.20	120.95
2	5	103	TYR	N-CA-C	-10.30	98.83	111.40
1	A	144	VAL	O-C-N	-10.15	115.30	121.69
1	D	196	MET	CA-C-N	10.03	131.07	119.94
1	D	196	MET	C-N-CA	10.03	131.07	119.94
2	3	48	ILE	N-CA-C	-9.82	102.34	111.67
1	E	225	SER	CA-C-N	9.80	130.07	119.28
1	E	225	SER	C-N-CA	9.80	130.07	119.28
1	G	8	TYR	N-CA-C	-9.79	98.92	114.09
2	4	211	PHE	CA-CB-CG	-9.76	104.04	113.80
2	1	71	LYS	O-C-N	-9.72	112.06	122.07
1	F	137	LEU	N-CA-C	-9.68	92.64	108.41
1	B	144	VAL	O-C-N	-9.59	115.01	121.72
1	D	53	ARG	N-CA-C	-9.56	94.56	109.76
1	B	175	PHE	CA-CB-CG	9.54	123.34	113.80
1	B	22	PHE	CA-CB-CG	-9.51	104.29	113.80
1	D	208	ASN	CA-CB-CG	9.49	122.09	112.60
2	1	74	ALA	CA-C-N	9.46	132.74	120.44
2	1	74	ALA	C-N-CA	9.46	132.74	120.44
1	C	82	VAL	N-CA-C	-9.41	101.02	110.62
1	C	205	VAL	CA-C-O	-9.40	110.68	121.59
1	D	64	ILE	CA-C-N	9.40	138.62	121.70
1	D	64	ILE	C-N-CA	9.40	138.62	121.70
2	2	147	ALA	CA-C-N	9.39	133.62	120.29
2	2	147	ALA	C-N-CA	9.39	133.62	120.29
2	5	123	TYR	CA-C-O	-9.31	110.64	120.70
1	G	241	ARG	CA-C-N	9.27	132.70	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	241	ARG	C-N-CA	9.27	132.70	120.28
3	L	397	PHE	CA-CB-CG	-9.26	104.54	113.80
3	M	392	LEU	N-CA-C	-9.25	103.09	114.75
1	F	132	PHE	CA-CB-CG	-9.24	104.56	113.80
2	7	70	ILE	CA-C-N	9.21	132.41	120.44
2	7	70	ILE	C-N-CA	9.21	132.41	120.44
2	3	124	SER	N-CA-C	-9.14	94.87	109.59
3	J	395	VAL	N-CA-C	-9.14	103.78	112.83
2	7	60	VAL	CA-C-N	9.09	129.99	120.00
2	7	60	VAL	C-N-CA	9.09	129.99	120.00
1	B	80	GLY	N-CA-C	-9.07	102.40	111.56
1	C	153	SER	N-CA-C	-9.04	100.57	111.69
3	I	395	VAL	N-CA-C	-9.03	104.68	113.53
2	6	64	GLN	OE1-CD-NE2	9.02	131.62	122.60
2	5	179	ASP	CA-C-N	9.01	133.25	120.28
2	5	179	ASP	C-N-CA	9.01	133.25	120.28
1	E	54	VAL	CA-C-N	9.00	129.93	119.94
1	E	54	VAL	C-N-CA	9.00	129.93	119.94
1	C	28	ARG	N-CA-C	-8.99	102.32	113.38
1	G	219	ARG	N-CA-C	-8.98	100.20	113.40
2	5	170	ARG	NE-CZ-NH1	8.97	130.47	121.50
1	C	211	VAL	CA-C-N	8.89	128.46	121.61
1	C	211	VAL	C-N-CA	8.89	128.46	121.61
2	5	143	GLY	CA-C-N	8.89	132.19	120.28
2	5	143	GLY	C-N-CA	8.89	132.19	120.28
1	D	8	TYR	N-CA-C	-8.87	100.44	112.94
2	5	195	GLU	O-C-N	8.86	133.29	123.10
1	D	86	ARG	NE-CZ-NH2	-8.84	111.24	119.20
2	6	45	ILE	N-CA-C	-8.82	96.71	108.35
1	E	205	VAL	CA-C-N	8.78	129.86	120.12
1	E	205	VAL	C-N-CA	8.78	129.86	120.12
2	7	77	TYR	O-C-N	-8.74	112.19	122.15
1	C	105	GLU	CA-C-N	8.73	129.27	119.93
1	C	105	GLU	C-N-CA	8.73	129.27	119.93
1	C	208	ASN	CA-CB-CG	8.70	121.30	112.60
1	D	65	GLU	N-CA-CB	8.67	125.24	110.50
1	A	18	ASP	CA-CB-CG	-8.66	103.94	112.60
1	B	132	PHE	CA-CB-CG	-8.66	105.14	113.80
1	E	141	VAL	O-C-N	-8.65	113.91	123.26
1	F	35	ALA	CA-C-N	8.64	133.40	121.05
1	F	35	ALA	C-N-CA	8.64	133.40	121.05
2	2	166	GLU	CA-C-N	8.61	132.52	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	166	GLU	C-N-CA	8.61	132.52	120.29
2	2	196	PHE	CA-CB-CG	-8.60	105.20	113.80
2	5	188	VAL	CA-C-N	8.60	134.94	122.99
2	5	188	VAL	C-N-CA	8.60	134.94	122.99
2	6	58	GLY	CA-C-O	-8.59	115.37	122.33
1	B	203	GLU	N-CA-CB	8.57	122.64	110.04
1	E	70	ILE	N-CA-C	-8.53	104.95	112.12
2	2	212	ARG	NE-CZ-NH1	8.50	130.00	121.50
1	C	105	GLU	CA-C-O	-8.41	112.06	119.72
2	5	211	PHE	CA-CB-CG	-8.39	105.41	113.80
2	4	13	THR	O-C-N	-8.39	113.85	123.33
2	3	49	ALA	N-CA-C	-8.35	97.66	109.69
1	B	235	ARG	NE-CZ-NH2	8.30	126.67	119.20
1	F	95	GLU	N-CA-CB	8.30	122.32	110.12
1	D	152	PRO	CA-C-N	8.30	131.22	120.44
1	D	152	PRO	C-N-CA	8.30	131.22	120.44
2	4	35	ASN	OD1-CG-ND2	8.29	130.89	122.60
2	5	156	THR	O-C-N	-8.28	116.41	121.71
1	F	216	VAL	N-CA-C	-8.26	102.80	110.82
2	2	30	ARG	NE-CZ-NH2	8.26	126.63	119.20
2	2	88	ARG	CA-C-N	8.26	131.17	120.44
2	2	88	ARG	C-N-CA	8.26	131.17	120.44
1	F	70	ILE	CB-CA-C	-8.24	102.88	110.63
2	6	113	GLY	CA-C-O	8.23	129.12	121.38
2	2	163	GLU	N-CA-C	-8.23	103.26	113.38
1	B	18	ASP	CA-CB-CG	-8.21	104.39	112.60
1	G	104	ASP	N-CA-CB	8.19	124.36	111.91
2	1	103	TYR	N-CA-C	-8.18	102.33	112.88
2	5	83	ARG	CA-C-N	8.16	131.73	120.39
2	5	83	ARG	C-N-CA	8.16	131.73	120.39
2	7	211	PHE	N-CA-C	-8.11	101.87	112.41
1	G	243	LEU	N-CA-C	-8.10	103.18	113.23
1	A	88	LEU	N-CA-C	8.10	121.02	111.71
2	6	89	ALA	N-CA-C	8.10	119.73	111.07
1	E	109	VAL	CA-C-N	8.08	130.94	120.44
1	E	109	VAL	C-N-CA	8.08	130.94	120.44
1	D	173	GLU	CA-C-N	8.06	130.92	120.44
1	D	173	GLU	C-N-CA	8.06	130.92	120.44
1	G	149	GLU	N-CA-C	-8.04	96.29	109.40
1	D	59	LEU	CA-C-O	-8.03	111.77	120.92
2	2	202	GLU	N-CA-C	8.03	119.66	111.07
2	5	36	PHE	CA-CB-CG	-8.02	105.78	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	70	ILE	CA-C-N	8.01	131.66	120.29
2	6	70	ILE	C-N-CA	8.01	131.66	120.29
1	G	15	PHE	CA-CB-CG	-7.99	105.81	113.80
1	D	196	MET	N-CA-C	7.99	120.89	111.71
2	4	106	TYR	CA-C-O	7.99	129.69	120.75
1	C	190	VAL	CA-C-N	7.98	131.62	120.29
1	C	190	VAL	C-N-CA	7.98	131.62	120.29
2	6	86	THR	CA-CB-OG1	7.98	121.57	109.60
2	3	210	LYS	N-CA-C	-7.97	102.83	114.39
1	B	144	VAL	N-CA-CB	7.97	120.64	111.87
2	2	44	LYS	CA-C-N	7.95	133.67	123.10
2	2	44	LYS	C-N-CA	7.95	133.67	123.10
2	6	97	LEU	N-CA-C	7.94	119.94	111.28
1	D	84	ASP	CA-CB-CG	7.92	120.53	112.60
1	B	150	THR	N-CA-C	-7.88	96.06	108.90
2	7	198	GLN	CA-C-N	7.83	131.41	120.29
2	7	198	GLN	C-N-CA	7.83	131.41	120.29
1	C	118	ASP	N-CA-C	-7.82	102.83	111.36
1	D	205	VAL	CA-C-O	-7.82	114.66	119.51
2	2	83	ARG	NE-CZ-NH2	7.81	126.22	119.20
1	B	201	GLU	CB-CG-CD	-7.79	99.35	112.60
1	G	196	MET	CA-C-N	7.79	128.79	119.99
1	G	196	MET	C-N-CA	7.79	128.79	119.99
2	5	90	ILE	CA-C-N	7.78	130.71	120.28
2	5	90	ILE	C-N-CA	7.78	130.71	120.28
1	B	26	TYR	N-CA-C	-7.78	103.81	113.38
2	6	171	ALA	CA-C-N	7.77	132.97	120.55
2	6	171	ALA	C-N-CA	7.77	132.97	120.55
1	E	230	LYS	CA-C-O	-7.76	111.15	118.44
2	1	147	ALA	N-CA-C	7.75	119.72	111.28
1	G	146	LYS	N-CA-C	-7.74	96.84	108.99
1	E	218	ASP	N-CA-C	-7.73	102.18	111.69
1	E	104	ASP	CA-CB-CG	7.72	120.33	112.60
1	F	227	GLU	O-C-N	7.71	130.30	122.12
2	4	144	SER	N-CA-C	7.71	120.57	111.71
3	K	397	PHE	N-CA-C	-7.71	97.57	109.52
1	B	27	ALA	CA-C-N	7.70	131.22	120.29
1	B	27	ALA	C-N-CA	7.70	131.22	120.29
1	G	180	ARG	N-CA-C	-7.70	97.62	109.24
1	E	194	VAL	CA-C-N	7.69	130.90	120.44
1	E	194	VAL	C-N-CA	7.69	130.90	120.44
1	A	39	GLY	O-C-N	-7.69	116.25	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	THR	CA-C-N	7.68	130.43	120.44
1	A	172	THR	C-N-CA	7.68	130.43	120.44
1	C	57	LYS	CA-C-N	7.67	130.56	120.28
1	C	57	LYS	C-N-CA	7.67	130.56	120.28
2	1	156	THR	N-CA-C	-7.66	99.36	108.25
2	5	180	SER	N-CA-C	7.66	120.52	111.71
2	3	62	ASP	CA-C-N	7.65	130.53	120.28
2	3	62	ASP	C-N-CA	7.65	130.53	120.28
1	B	9	ASP	N-CA-C	-7.65	101.90	112.30
2	2	59	SER	CA-C-N	7.64	130.19	120.56
2	2	59	SER	C-N-CA	7.64	130.19	120.56
1	F	218	ASP	CA-C-N	7.64	133.48	122.40
1	F	218	ASP	C-N-CA	7.64	133.48	122.40
1	D	128	GLY	CA-C-N	7.62	130.65	122.11
1	D	128	GLY	C-N-CA	7.62	130.65	122.11
1	F	20	ARG	NE-CZ-NH2	7.62	126.06	119.20
2	1	181	ALA	O-C-N	7.60	131.30	122.25
2	4	162	ASP	CA-CB-CG	7.60	120.20	112.60
1	D	74	ILE	N-CA-CB	7.59	122.60	111.52
1	F	212	GLY	O-C-N	-7.59	116.52	123.42
1	D	211	VAL	CA-C-N	7.58	127.41	122.18
1	D	211	VAL	C-N-CA	7.58	127.41	122.18
2	7	65	PHE	CA-C-N	7.58	131.06	120.29
2	7	65	PHE	C-N-CA	7.58	131.06	120.29
1	A	245	LYS	N-CA-C	-7.58	103.14	113.30
2	4	21	ASP	N-CA-C	-7.57	104.94	114.56
2	4	84	LYS	CA-C-N	7.57	128.59	120.11
2	4	84	LYS	C-N-CA	7.57	128.59	120.11
1	D	88	LEU	N-CA-C	7.56	119.52	111.28
2	1	106	TYR	N-CA-C	-7.55	95.97	108.34
2	3	96	ASN	CA-CB-CG	7.54	120.14	112.60
1	B	151	ASP	O-C-N	-7.53	113.83	120.99
1	G	84	ASP	CA-C-N	7.52	130.35	120.28
1	G	84	ASP	C-N-CA	7.52	130.35	120.28
1	A	144	VAL	N-CA-C	-7.51	103.03	109.19
2	3	75	ASN	N-CA-C	-7.51	103.18	111.36
3	H	394	GLY	O-C-N	-7.44	115.70	122.77
2	5	112	ILE	N-CA-C	-7.43	96.77	107.77
1	C	231	PRO	O-C-N	7.43	130.57	122.17
2	1	59	SER	CA-C-N	7.43	129.79	120.72
2	1	59	SER	C-N-CA	7.43	129.79	120.72
1	B	208	ASN	N-CA-C	-7.43	103.29	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	84	LYS	CA-C-N	7.42	127.34	119.85
2	3	84	LYS	C-N-CA	7.42	127.34	119.85
1	D	205	VAL	N-CA-C	-7.41	98.79	107.61
1	C	94	ILE	CA-C-N	7.37	130.75	120.29
1	C	94	ILE	C-N-CA	7.37	130.75	120.29
2	6	156	THR	CA-C-N	7.37	126.88	118.85
2	6	156	THR	C-N-CA	7.37	126.88	118.85
1	E	16	SER	CA-C-N	7.33	126.97	119.56
1	E	16	SER	C-N-CA	7.33	126.97	119.56
2	3	23	VAL	N-CA-C	-7.33	97.60	108.45
1	C	204	LEU	CA-C-N	7.33	132.01	121.68
1	C	204	LEU	C-N-CA	7.33	132.01	121.68
1	G	237	ASN	CA-C-N	7.33	130.70	120.29
1	G	237	ASN	C-N-CA	7.33	130.70	120.29
1	A	80	GLY	O-C-N	7.32	129.19	122.90
2	6	59	SER	N-CA-C	7.31	120.30	110.35
2	3	150	VAL	CA-C-O	-7.30	112.36	120.46
1	B	205	VAL	N-CA-C	-7.28	100.78	109.01
2	1	107	LEU	N-CA-CB	7.28	118.72	110.35
1	D	150	THR	N-CA-C	-7.28	97.87	109.59
1	E	124	THR	CA-C-N	7.27	129.89	120.44
1	E	124	THR	C-N-CA	7.27	129.89	120.44
1	F	212	GLY	N-CA-C	-7.27	99.99	111.18
1	A	154	GLY	N-CA-C	-7.27	104.09	116.01
1	G	123	TYR	CA-C-N	7.26	129.88	120.44
1	G	123	TYR	C-N-CA	7.26	129.88	120.44
2	7	210	LYS	CA-C-O	7.25	128.14	119.59
1	G	125	GLN	N-CA-C	7.24	119.25	111.36
2	3	68	ARG	N-CA-CB	7.24	120.76	110.12
2	4	124	SER	CA-C-O	-7.23	112.78	120.80
1	C	54	VAL	CB-CA-C	7.22	122.24	110.69
2	5	176	MET	CA-C-N	7.21	130.53	120.29
2	5	176	MET	C-N-CA	7.21	130.53	120.29
1	G	102	THR	N-CA-C	-7.21	104.06	112.92
1	C	180	ARG	NE-CZ-NH2	7.20	125.68	119.20
1	B	181	ASP	N-CA-C	-7.18	104.54	113.38
2	4	158	GLU	N-CA-C	-7.18	104.53	112.72
1	D	202	SER	N-CA-CB	7.17	123.64	111.66
1	D	126	TYR	N-CA-CB	7.17	121.85	110.23
2	4	109	GLN	N-CA-CB	7.17	121.82	110.57
2	4	80	ARG	N-CA-CB	7.17	120.77	110.16
2	6	168	ALA	CA-C-N	7.17	130.59	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	168	ALA	C-N-CA	7.17	130.59	120.42
2	4	102	ARG	NE-CZ-NH2	7.16	125.64	119.20
1	F	87	VAL	N-CA-C	-7.15	103.21	111.00
1	B	62	ASP	CA-CB-CG	-7.14	105.45	112.60
1	D	184	SER	CA-C-N	7.14	129.72	120.44
1	D	184	SER	C-N-CA	7.14	129.72	120.44
1	G	144	VAL	CA-C-O	-7.14	110.39	119.95
2	5	112	ILE	N-CA-CB	7.13	121.52	111.82
2	6	51	ARG	NE-CZ-NH1	-7.13	114.37	121.50
2	6	153	ASP	CA-C-O	-7.13	112.99	120.55
2	6	67	ALA	CA-C-N	7.12	129.82	120.28
2	6	67	ALA	C-N-CA	7.12	129.82	120.28
1	F	109	VAL	CA-C-N	7.12	129.82	120.28
1	F	109	VAL	C-N-CA	7.12	129.82	120.28
1	E	19	GLY	N-CA-C	-7.12	104.33	116.01
1	C	145	PRO	N-CA-CB	7.12	109.95	103.19
2	3	33	MET	N-CA-C	-7.11	104.48	113.72
2	3	139	ALA	CA-C-N	7.10	134.49	121.70
2	3	139	ALA	C-N-CA	7.10	134.49	121.70
3	I	397	PHE	CA-CB-CG	-7.10	106.70	113.80
2	1	82	GLU	N-CA-CB	7.10	123.61	112.46
1	C	241	ARG	NE-CZ-NH2	7.10	125.59	119.20
1	A	61	ALA	N-CA-C	-7.09	104.51	113.02
2	6	140	THR	N-CA-CB	7.09	123.55	111.50
2	7	44	LYS	N-CA-C	-7.09	103.87	114.64
2	6	91	ALA	O-C-N	7.07	129.35	122.07
2	4	196	PHE	N-CA-CB	7.06	123.89	110.82
2	5	71	LYS	CA-C-O	-7.05	113.41	120.82
1	B	52	LYS	N-CA-C	-7.05	103.34	113.21
1	C	22	PHE	CA-CB-CG	-7.04	106.76	113.80
3	M	397	PHE	CA-CB-CG	-7.04	106.76	113.80
2	2	122	ILE	CA-C-O	7.02	128.08	120.43
1	E	33	ARG	NE-CZ-NH2	7.02	125.52	119.20
2	7	191	ILE	N-CA-C	-7.02	94.75	109.34
1	D	9	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	92	ALA	CA-C-N	7.01	129.67	120.28
1	A	92	ALA	C-N-CA	7.01	129.67	120.28
2	6	165	VAL	N-CA-CB	7.01	121.09	110.58
1	G	228	GLU	N-CA-C	-7.01	104.54	113.23
2	4	83	ARG	NE-CZ-NH1	-7.01	114.49	121.50
3	M	397	PHE	N-CA-C	-7.00	97.98	109.40
1	G	124	THR	O-C-N	6.99	129.27	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	29	LYS	N-CA-C	-6.99	103.94	113.30
2	2	62	ASP	CA-C-N	6.99	130.21	120.29
2	2	62	ASP	C-N-CA	6.99	130.21	120.29
1	B	218	ASP	N-CA-C	-6.98	101.99	112.04
1	E	87	VAL	N-CA-C	6.98	117.09	110.53
1	C	16	SER	CA-C-N	6.96	126.44	118.85
1	C	16	SER	C-N-CA	6.96	126.44	118.85
1	E	114	LYS	CA-C-N	6.96	130.17	120.29
1	E	114	LYS	C-N-CA	6.96	130.17	120.29
1	A	121	GLN	CA-C-N	6.95	129.91	120.38
1	A	121	GLN	C-N-CA	6.95	129.91	120.38
2	6	102	ARG	NE-CZ-NH2	6.95	125.46	119.20
2	7	172	ILE	CA-C-O	-6.95	113.48	120.85
2	3	195	GLU	N-CA-C	-6.95	97.78	108.76
1	A	186	ASP	CA-CB-CG	6.95	119.55	112.60
1	C	112	LEU	CA-C-N	6.94	129.46	120.44
1	C	112	LEU	C-N-CA	6.94	129.46	120.44
1	F	215	LYS	CA-C-N	6.94	130.66	120.74
1	F	215	LYS	C-N-CA	6.94	130.66	120.74
2	5	81	ARG	NE-CZ-NH2	6.94	125.44	119.20
1	E	47	ILE	N-CA-C	-6.93	98.47	108.17
3	I	391	ASP	CB-CA-C	-6.93	107.54	115.79
2	5	150	VAL	N-CA-CB	6.93	119.96	110.54
1	A	65	GLU	CB-CG-CD	-6.91	100.85	112.60
2	5	102	ARG	N-CA-C	-6.91	104.51	114.12
2	2	179	ASP	N-CA-C	-6.91	98.58	109.50
2	6	139	ALA	CA-C-N	6.91	134.14	121.70
2	6	139	ALA	C-N-CA	6.91	134.14	121.70
2	7	182	SER	CA-C-O	-6.91	113.20	121.56
1	D	134	VAL	CA-C-O	-6.91	114.42	121.67
1	A	172	THR	O-C-N	6.90	129.18	122.07
1	F	83	ALA	CA-C-N	6.90	129.53	120.28
1	F	83	ALA	C-N-CA	6.90	129.53	120.28
1	G	192	GLY	N-CA-C	-6.90	106.11	114.66
1	C	210	GLU	N-CA-C	-6.89	98.16	109.40
1	E	130	ARG	NE-CZ-NH2	-6.89	113.00	119.20
2	3	207	ILE	N-CA-C	-6.89	102.21	111.44
1	F	145	PRO	N-CA-CB	6.88	109.73	103.33
2	6	88	ARG	NE-CZ-NH2	6.88	125.39	119.20
1	B	32	LYS	CA-C-N	6.87	132.35	120.68
1	B	32	LYS	C-N-CA	6.87	132.35	120.68
1	A	67	ILE	N-CA-CB	6.86	122.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ILE	N-CA-C	-6.86	95.06	109.34
1	B	82	VAL	CA-C-N	6.86	129.35	120.44
1	B	82	VAL	C-N-CA	6.86	129.35	120.44
1	E	226	PRO	CA-C-N	6.86	129.47	120.28
1	E	226	PRO	C-N-CA	6.86	129.47	120.28
1	G	106	PRO	N-CA-CB	6.86	110.45	103.25
1	D	121	GLN	CA-C-O	-6.84	113.30	120.55
2	2	139	ALA	N-CA-C	-6.84	96.22	110.80
2	5	72	ILE	CA-CB-CG2	6.84	122.13	110.50
2	3	172	ILE	CA-C-N	6.84	130.13	120.28
2	3	172	ILE	C-N-CA	6.84	130.13	120.28
1	D	86	ARG	NE-CZ-NH1	6.84	128.34	121.50
2	5	132	ILE	CB-CA-C	6.84	120.69	111.19
1	B	44	GLU	N-CA-C	-6.83	102.84	113.02
2	1	102	ARG	NE-CZ-NH2	6.83	125.35	119.20
2	7	39	SER	N-CA-CB	6.83	122.03	110.49
2	6	139	ALA	N-CA-C	-6.83	96.26	110.80
2	1	132	ILE	CA-CB-CG2	-6.82	98.90	110.50
1	G	200	ILE	CA-C-N	6.82	131.82	122.07
1	G	200	ILE	C-N-CA	6.82	131.82	122.07
2	7	38	ALA	O-C-N	6.82	129.35	122.12
1	D	80	GLY	N-CA-C	-6.82	102.02	111.76
1	E	184	SER	CA-C-N	6.82	129.97	120.29
1	E	184	SER	C-N-CA	6.82	129.97	120.29
2	3	51	ARG	NE-CZ-NH2	6.82	125.33	119.20
1	G	135	SER	N-CA-C	-6.81	99.09	109.85
1	G	118	ASP	CA-C-N	6.81	129.40	120.28
1	G	118	ASP	C-N-CA	6.81	129.40	120.28
1	B	10	ARG	N-CA-C	-6.80	105.02	113.38
1	C	120	LYS	N-CA-C	6.80	119.53	111.71
1	E	42	CYS	N-CA-C	-6.79	99.28	108.86
2	2	111	LEU	N-CA-C	-6.79	97.83	108.90
2	3	20	LYS	N-CA-CB	-6.79	99.42	110.42
2	5	170	ARG	NH1-CZ-NH2	6.79	128.13	119.30
1	G	229	LEU	CA-C-O	6.79	127.80	119.79
1	C	9	ASP	CA-CB-CG	6.79	119.39	112.60
2	4	116	ASP	CA-C-N	6.79	132.05	120.72
2	4	116	ASP	C-N-CA	6.79	132.05	120.72
1	D	118	ASP	N-CA-CB	6.78	120.78	110.28
1	B	190	VAL	N-CA-CB	6.78	119.76	110.54
1	E	40	ILE	N-CA-C	-6.77	98.28	108.17
3	L	390	PRO	N-CA-CB	6.77	110.45	103.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ASN	CA-C-N	6.77	129.24	120.44
1	A	169	ASN	C-N-CA	6.77	129.24	120.44
1	G	39	GLY	O-C-N	-6.77	117.57	123.80
2	3	133	GLU	CB-CA-C	-6.76	101.39	110.79
2	3	178	ARG	NE-CZ-NH1	6.76	128.26	121.50
2	4	14	THR	CA-C-O	6.75	129.03	121.40
2	4	109	GLN	N-CA-C	-6.75	98.20	109.07
1	F	43	LYS	N-CA-C	-6.75	105.81	112.97
1	F	205	VAL	CA-C-N	6.75	126.44	119.82
1	F	205	VAL	C-N-CA	6.75	126.44	119.82
2	2	154	ARG	NE-CZ-NH1	-6.72	114.78	121.50
2	4	158	GLU	CB-CG-CD	-6.72	101.18	112.60
2	1	142	SER	N-CA-C	6.71	119.43	111.71
1	A	202	SER	CA-C-N	6.71	130.28	120.82
1	A	202	SER	C-N-CA	6.71	130.28	120.82
1	D	205	VAL	CA-C-N	6.71	126.97	119.32
1	D	205	VAL	C-N-CA	6.71	126.97	119.32
1	G	240	ILE	CA-C-N	6.71	129.27	120.28
1	G	240	ILE	C-N-CA	6.71	129.27	120.28
1	F	105	GLU	CA-C-N	6.71	128.22	119.84
1	F	105	GLU	C-N-CA	6.71	128.22	119.84
1	F	70	ILE	N-CA-C	-6.70	107.34	113.71
1	C	20	ARG	N-CA-C	-6.70	96.52	110.80
2	1	160	GLY	N-CA-C	-6.70	102.35	112.60
2	7	13	THR	N-CA-CB	6.70	122.84	110.99
2	1	37	ILE	O-C-N	6.69	130.30	123.20
1	B	241	ARG	NE-CZ-NH2	6.69	125.22	119.20
1	A	187	ASP	N-CA-CB	6.69	119.95	110.12
2	1	172	ILE	N-CA-C	-6.69	102.73	111.09
2	1	188	VAL	O-C-N	-6.69	115.96	123.18
2	6	158	GLU	CA-C-N	6.68	131.15	121.80
2	6	158	GLU	C-N-CA	6.68	131.15	121.80
2	6	76	LEU	CA-C-N	6.68	129.12	120.44
2	6	76	LEU	C-N-CA	6.68	129.12	120.44
2	7	180	SER	N-CA-C	-6.68	104.27	112.88
1	D	5	GLN	CB-CG-CD	-6.67	101.26	112.60
1	D	81	LEU	N-CA-CB	6.67	119.81	109.48
1	F	60	GLU	CA-C-N	6.66	129.75	120.29
1	F	60	GLU	C-N-CA	6.66	129.75	120.29
2	7	112	ILE	CA-C-O	6.66	127.31	120.39
1	E	105	GLU	CB-CA-C	-6.65	100.88	109.92
1	E	197	GLY	CA-C-N	6.65	129.73	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	197	GLY	C-N-CA	6.65	129.73	120.29
1	F	120	LYS	CA-C-N	6.65	130.41	120.31
1	F	120	LYS	C-N-CA	6.65	130.41	120.31
1	B	53	ARG	CA-C-N	6.63	129.45	120.63
1	B	53	ARG	C-N-CA	6.63	129.45	120.63
2	7	38	ALA	N-CA-C	6.63	118.51	111.28
2	3	139	ALA	N-CA-C	-6.63	96.68	110.80
2	4	80	ARG	O-C-N	-6.63	114.60	122.15
1	F	28	ARG	N-CA-C	-6.62	103.88	112.23
2	4	120	LYS	CA-C-O	-6.62	113.70	121.44
2	1	96	ASN	CA-C-N	6.62	129.15	120.28
2	1	96	ASN	C-N-CA	6.62	129.15	120.28
2	4	205	GLU	CB-CG-CD	6.62	123.85	112.60
2	7	186	ILE	N-CA-CB	6.62	118.10	110.49
2	6	69	ILE	N-CA-CB	6.60	118.27	110.55
1	C	93	ARG	CA-C-N	6.60	129.79	120.42
1	C	93	ARG	C-N-CA	6.60	129.79	120.42
2	4	127	PRO	N-CA-C	-6.60	105.43	114.80
1	B	65	GLU	N-CA-CB	6.59	121.71	110.50
1	D	24	VAL	CA-CB-CG2	-6.59	99.20	110.40
1	D	144	VAL	CA-C-N	6.59	126.98	119.93
1	D	144	VAL	C-N-CA	6.59	126.98	119.93
1	F	185	PHE	CA-CB-CG	-6.59	107.21	113.80
1	B	217	ASP	CA-CB-CG	6.58	119.18	112.60
2	6	179	ASP	N-CA-C	-6.58	100.23	110.17
1	B	62	ASP	CA-C-N	6.58	130.50	120.82
1	B	62	ASP	C-N-CA	6.58	130.50	120.82
1	B	94	ILE	CA-C-N	6.58	129.10	120.28
1	B	94	ILE	C-N-CA	6.58	129.10	120.28
1	C	52	LYS	CA-C-N	6.57	130.17	120.90
1	C	52	LYS	C-N-CA	6.57	130.17	120.90
1	B	60	GLU	CA-C-N	6.56	129.07	120.28
1	B	60	GLU	C-N-CA	6.56	129.07	120.28
2	2	188	VAL	N-CA-C	-6.56	98.01	108.90
2	3	151	LEU	CA-C-O	6.56	127.50	120.55
1	C	20	ARG	N-CA-CB	6.55	121.57	110.49
2	2	141	GLY	N-CA-C	-6.55	105.35	112.04
1	A	97	GLN	CA-C-N	6.55	129.43	120.46
1	A	97	GLN	C-N-CA	6.55	129.43	120.46
1	C	99	ASN	OD1-CG-ND2	6.55	129.15	122.60
1	G	69	LYS	N-CA-CB	6.55	119.61	109.85
2	5	61	GLY	N-CA-C	6.53	120.55	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	ARG	CB-CA-C	-6.53	99.95	110.79
1	E	175	PHE	CA-CB-CG	6.52	120.32	113.80
2	5	49	ALA	CA-C-N	6.52	129.34	120.54
2	5	49	ALA	C-N-CA	6.52	129.34	120.54
1	C	99	ASN	CA-C-N	6.51	131.59	120.72
1	C	99	ASN	C-N-CA	6.51	131.59	120.72
2	2	36	PHE	CA-C-N	6.51	129.29	120.63
2	2	36	PHE	C-N-CA	6.51	129.29	120.63
1	C	23	GLN	CA-C-N	6.51	129.66	120.42
1	C	23	GLN	C-N-CA	6.51	129.66	120.42
2	6	32	THR	N-CA-C	-6.50	98.00	109.06
2	7	77	TYR	CA-C-O	6.50	127.31	120.42
2	1	68	ARG	CA-C-N	6.50	129.36	120.46
2	1	68	ARG	C-N-CA	6.50	129.36	120.46
1	D	169	ASN	CA-C-O	-6.50	113.66	120.55
1	E	7	GLY	N-CA-C	-6.50	106.11	115.27
2	2	156	THR	N-CA-C	-6.50	100.72	108.25
1	E	58	LEU	O-C-N	6.49	129.10	122.09
2	2	135	LYS	N-CA-C	-6.49	103.87	113.61
1	F	227	GLU	CA-C-O	-6.49	113.67	120.55
1	C	205	VAL	O-C-N	6.48	125.78	121.69
2	7	62	ASP	CA-C-N	6.48	129.50	120.29
2	7	62	ASP	C-N-CA	6.48	129.50	120.29
1	D	9	ASP	N-CA-C	-6.48	104.14	113.21
1	E	31	VAL	CA-C-O	-6.48	113.98	120.85
2	1	95	SER	CB-CA-C	-6.48	99.84	110.85
1	F	47	ILE	N-CA-C	-6.48	98.81	108.46
1	B	31	VAL	CB-CA-C	-6.47	103.28	112.22
1	D	244	LEU	N-CA-C	-6.47	105.34	112.72
2	7	91	ALA	CA-C-N	6.47	129.49	120.29
2	7	91	ALA	C-N-CA	6.47	129.49	120.29
2	5	199	TYR	N-CA-C	6.47	119.15	111.71
1	B	50	ALA	CA-C-N	6.46	130.50	120.75
1	B	50	ALA	C-N-CA	6.46	130.50	120.75
2	3	199	TYR	CA-C-O	-6.46	114.51	121.94
1	G	187	ASP	CA-CB-CG	-6.45	106.15	112.60
1	F	104	ASP	CA-CB-CG	6.45	119.05	112.60
2	3	193	GLU	N-CA-CB	6.45	121.38	110.49
2	1	156	THR	O-C-N	-6.44	116.95	121.65
2	3	178	ARG	NE-CZ-NH2	-6.44	113.41	119.20
1	B	222	LYS	N-CA-C	-6.43	99.26	109.23
1	A	67	ILE	N-CA-C	-6.43	95.97	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	124	SER	N-CA-C	-6.43	98.04	108.52
1	A	10	ARG	NE-CZ-NH2	6.43	124.98	119.20
1	G	81	LEU	CA-C-O	-6.43	113.42	120.81
1	A	185	PHE	CA-CB-CG	-6.43	107.37	113.80
1	C	223	GLU	CA-C-O	-6.42	113.25	120.32
1	A	103	TYR	N-CA-C	-6.42	106.66	114.75
2	6	93	LEU	O-C-N	6.42	128.93	122.12
1	D	63	THR	CA-C-N	6.42	133.53	121.97
1	D	63	THR	C-N-CA	6.42	133.53	121.97
2	1	144	SER	N-CA-C	6.42	118.28	111.28
1	F	114	LYS	N-CA-CB	6.41	119.55	110.12
2	5	161	VAL	N-CA-C	6.41	117.16	110.62
2	2	153	ASP	CA-C-O	6.41	127.34	120.10
1	A	153	SER	N-CA-C	-6.41	104.22	111.14
2	3	182	SER	N-CA-C	-6.40	101.90	110.55
2	2	153	ASP	O-C-N	-6.40	114.73	122.22
2	6	106	TYR	N-CA-C	-6.40	103.65	112.03
2	5	87	VAL	O-C-N	6.39	128.33	121.87
1	F	33	ARG	N-CA-C	-6.39	104.40	111.36
1	D	85	ALA	CA-C-N	6.38	128.83	120.28
1	D	85	ALA	C-N-CA	6.38	128.83	120.28
2	7	143	GLY	CA-C-N	6.38	128.83	120.28
2	7	143	GLY	C-N-CA	6.38	128.83	120.28
1	F	13	THR	N-CA-C	-6.37	105.46	112.72
1	E	186	ASP	CA-C-N	6.37	129.99	120.31
1	E	186	ASP	C-N-CA	6.37	129.99	120.31
1	F	66	LYS	N-CA-C	-6.37	106.10	114.31
1	B	55	GLY	N-CA-C	-6.36	104.64	112.33
1	B	36	THR	N-CA-C	6.35	118.50	110.24
2	6	142	SER	N-CA-C	-6.35	105.57	113.38
2	6	83	ARG	NE-CZ-NH1	-6.35	115.15	121.50
2	7	136	ASP	O-C-N	6.35	131.03	122.59
2	4	39	SER	N-CA-C	-6.34	97.29	110.80
2	6	147	ALA	CA-C-N	6.33	128.77	120.28
2	6	147	ALA	C-N-CA	6.33	128.77	120.28
3	J	391	ASP	CA-C-O	6.33	127.69	120.54
2	5	116	ASP	CA-CB-CG	6.33	118.93	112.60
2	6	54	MET	CG-SD-CE	-6.33	86.98	100.90
2	5	106	TYR	CB-CG-CD2	6.33	130.29	120.80
1	B	147	LEU	N-CA-C	-6.32	97.50	108.69
2	2	127	PRO	CA-C-O	-6.32	110.94	118.90
2	7	129	GLY	N-CA-C	-6.32	101.38	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	78	GLU	CA-C-N	6.31	128.64	120.56
2	1	78	GLU	C-N-CA	6.31	128.64	120.56
2	6	127	PRO	CB-CA-C	-6.31	101.91	111.44
1	B	31	VAL	N-CA-C	-6.31	104.34	110.72
2	4	154	ARG	NE-CZ-NH1	-6.31	115.19	121.50
2	6	207	ILE	N-CA-C	-6.31	104.12	111.00
1	C	8	TYR	N-CA-C	-6.30	102.88	110.44
2	3	169	VAL	CA-CB-CG2	-6.30	99.69	110.40
2	5	35	ASN	CA-CB-CG	-6.30	106.30	112.60
2	5	158	GLU	CB-CA-C	-6.30	100.87	111.02
2	4	51	ARG	N-CA-C	-6.29	103.78	112.03
2	7	24	VAL	CA-CB-CG2	-6.29	99.70	110.40
2	7	177	LYS	N-CA-C	-6.29	105.88	112.93
1	A	59	LEU	N-CA-CB	6.29	119.23	110.17
1	B	8	TYR	N-CA-C	-6.29	103.00	111.87
1	F	44	GLU	CB-CA-C	-6.29	97.90	110.42
2	4	88	ARG	O-C-N	6.29	128.79	122.12
2	5	30	ARG	N-CA-C	-6.29	99.15	109.40
2	7	156	THR	CA-CB-OG1	-6.29	100.17	109.60
1	A	151	ASP	CA-C-O	-6.28	114.19	120.66
2	1	49	ALA	N-CA-C	-6.28	99.94	108.24
2	6	44	LYS	N-CA-C	-6.28	102.75	110.61
1	B	184	SER	N-CA-C	-6.28	100.65	109.69
1	B	185	PHE	CA-CB-CG	-6.28	107.52	113.80
1	G	29	GLU	CA-CB-CG	-6.27	101.55	114.10
1	A	24	VAL	CA-C-N	6.27	129.31	120.28
1	A	24	VAL	C-N-CA	6.27	129.31	120.28
1	E	73	HIS	CE1-NE2-CD2	-6.27	102.73	109.00
2	1	75	ASN	O-C-N	-6.26	115.62	122.07
1	E	151	ASP	CA-CB-CG	-6.26	106.34	112.60
2	7	104	PHE	N-CA-C	-6.26	102.19	110.07
2	4	153	ASP	CA-CB-CG	-6.25	106.35	112.60
1	B	69	LYS	CA-C-N	6.25	129.33	122.77
1	B	69	LYS	C-N-CA	6.25	129.33	122.77
1	G	78	THR	CA-CB-OG1	6.25	118.98	109.60
2	2	112	ILE	N-CA-C	-6.25	98.52	107.77
2	6	80	ARG	O-C-N	-6.25	114.58	122.27
2	4	142	SER	O-C-N	6.25	128.72	122.10
2	6	125	ILE	N-CA-C	-6.24	99.43	108.17
1	E	86	ARG	NE-CZ-NH1	-6.24	115.26	121.50
2	4	35	ASN	N-CA-CB	6.24	121.04	110.49
1	D	199	SER	CB-CA-C	-6.24	100.44	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	167	LEU	CA-C-N	6.23	128.63	120.28
2	1	167	LEU	C-N-CA	6.23	128.63	120.28
1	D	225	SER	CA-C-O	-6.23	114.22	120.64
1	E	182	ASP	N-CA-C	-6.23	103.09	111.87
2	2	141	GLY	O-C-N	-6.22	115.80	123.21
1	E	244	LEU	CA-C-N	6.22	131.60	122.08
1	E	244	LEU	C-N-CA	6.22	131.60	122.08
2	5	184	ASP	N-CA-C	-6.22	99.26	109.40
1	F	208	ASN	CA-CB-CG	6.22	118.82	112.60
2	3	38	ALA	O-C-N	-6.22	114.41	122.37
2	4	160	GLY	CA-C-N	6.22	130.50	120.30
2	4	160	GLY	C-N-CA	6.22	130.50	120.30
2	6	143	GLY	N-CA-C	-6.22	104.98	115.80
2	2	64	GLN	CA-C-N	6.22	129.12	120.29
2	2	64	GLN	C-N-CA	6.22	129.12	120.29
2	1	156	THR	CA-C-N	6.21	125.84	119.56
2	1	156	THR	C-N-CA	6.21	125.84	119.56
1	A	228	GLU	N-CA-C	6.21	118.05	111.28
1	A	232	TYR	CA-C-N	6.21	130.28	120.47
1	A	232	TYR	C-N-CA	6.21	130.28	120.47
1	B	193	LEU	CA-C-N	6.21	128.61	120.60
1	B	193	LEU	C-N-CA	6.21	128.61	120.60
2	1	92	THR	CA-C-O	6.21	127.00	120.42
1	G	63	THR	N-CA-CB	6.20	119.27	110.46
1	D	82	VAL	CB-CA-C	-6.20	102.06	112.16
2	7	174	SER	CA-C-N	6.19	128.57	120.28
2	7	174	SER	C-N-CA	6.19	128.57	120.28
2	5	203	GLU	CA-C-N	6.19	129.21	120.42
2	5	203	GLU	C-N-CA	6.19	129.21	120.42
1	B	146	LYS	N-CA-C	-6.19	99.64	109.23
1	D	73	HIS	CA-CB-CG	6.18	119.98	113.80
2	3	29	LYS	CA-C-O	6.18	127.37	120.70
2	7	13	THR	CA-C-N	6.18	133.00	122.37
2	7	13	THR	C-N-CA	6.18	133.00	122.37
2	1	129	GLY	N-CA-C	-6.17	105.74	112.04
2	3	46	TYR	CB-CA-C	-6.17	98.42	109.71
1	B	151	ASP	CA-C-N	6.17	126.35	119.32
1	B	151	ASP	C-N-CA	6.17	126.35	119.32
1	E	83	ALA	N-CA-C	6.16	117.66	111.07
3	M	396	MET	N-CA-C	-6.16	104.26	112.94
2	1	43	LYS	N-CA-CB	6.16	121.02	110.68
2	5	191	ILE	N-CA-CB	6.16	121.39	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	38	ALA	O-C-N	6.15	128.74	122.09
1	A	241	ARG	NE-CZ-NH2	6.15	124.74	119.20
2	6	180	SER	N-CA-C	-6.15	105.29	114.64
1	D	172	THR	CA-C-N	6.15	129.02	120.29
1	D	172	THR	C-N-CA	6.15	129.02	120.29
2	1	36	PHE	CA-C-N	6.15	131.28	123.10
2	1	36	PHE	C-N-CA	6.15	131.28	123.10
1	C	198	LEU	CA-C-N	6.14	129.01	120.29
1	C	198	LEU	C-N-CA	6.14	129.01	120.29
2	4	185	GLY	CA-C-N	6.14	131.48	122.94
2	4	185	GLY	C-N-CA	6.14	131.48	122.94
2	4	67	ALA	N-CA-CB	6.14	119.15	110.12
2	6	183	GLY	N-CA-C	-6.14	98.63	113.18
1	G	133	GLY	N-CA-C	-6.14	98.64	113.18
2	1	115	ILE	CA-C-N	6.13	131.86	122.11
2	1	115	ILE	C-N-CA	6.13	131.86	122.11
1	C	132	PHE	CA-CB-CG	-6.12	107.69	113.80
2	2	146	THR	N-CA-C	-6.12	104.69	111.36
2	6	99	ASN	OD1-CG-ND2	6.11	128.71	122.60
2	1	156	THR	N-CA-CB	6.10	119.85	111.25
2	7	61	GLY	CA-C-N	6.10	128.96	120.29
2	7	61	GLY	C-N-CA	6.10	128.96	120.29
2	3	150	VAL	CA-C-N	6.10	128.45	120.28
2	3	150	VAL	C-N-CA	6.10	128.45	120.28
1	C	233	VAL	CA-C-O	-6.10	113.89	120.47
2	3	44	LYS	N-CA-C	-6.09	104.26	113.89
1	G	206	PRO	N-CA-C	-6.09	106.74	114.35
2	6	206	GLN	OE1-CD-NE2	6.09	128.69	122.60
1	A	41	LYS	N-CA-C	-6.09	99.79	109.59
1	D	68	TYR	CA-C-N	6.08	130.12	121.42
1	D	68	TYR	C-N-CA	6.08	130.12	121.42
1	E	115	LYS	CA-C-O	-6.08	113.97	120.42
2	2	101	TYR	CB-CG-CD2	-6.08	111.68	120.80
1	D	87	VAL	N-CA-C	-6.08	104.37	111.00
1	F	88	LEU	O-C-N	-6.08	115.68	122.12
1	B	14	VAL	CA-C-N	6.08	133.15	121.54
1	B	14	VAL	C-N-CA	6.08	133.15	121.54
1	F	169	ASN	CA-CB-CG	-6.07	106.53	112.60
1	A	117	CYS	N-CA-CB	6.07	119.04	110.12
1	C	242	GLU	CB-CA-C	6.07	120.86	110.79
2	7	103	TYR	N-CA-C	-6.06	104.75	111.36
1	C	239	ARG	CA-C-O	6.05	126.84	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	243	LEU	N-CA-C	6.05	117.95	111.36
2	1	109	GLN	CA-C-O	6.05	126.93	120.46
1	E	120	LYS	CB-CA-C	-6.05	101.39	110.88
2	3	88	ARG	CB-CA-C	-6.05	100.75	110.79
1	F	5	GLN	CA-C-N	6.04	131.97	122.78
1	F	5	GLN	C-N-CA	6.04	131.97	122.78
1	F	64	ILE	CA-C-O	6.04	128.33	120.78
2	3	75	ASN	N-CA-CB	6.04	119.10	110.16
2	7	209	ALA	CA-C-O	6.04	126.81	119.38
2	3	212	ARG	CG-CD-NE	-6.03	98.72	112.00
1	F	64	ILE	CA-C-N	6.03	133.06	121.54
1	F	64	ILE	C-N-CA	6.03	133.06	121.54
2	6	135	LYS	N-CA-CB	6.03	119.62	110.28
1	G	179	TYR	N-CA-CB	6.03	118.83	109.97
1	G	181	ASP	CA-C-N	6.01	132.67	122.26
1	G	181	ASP	C-N-CA	6.01	132.67	122.26
2	3	49	ALA	CA-C-N	6.01	128.94	120.28
2	3	49	ALA	C-N-CA	6.01	128.94	120.28
2	5	45	ILE	N-CA-CB	6.01	119.24	111.67
2	3	135	LYS	CB-CA-C	-6.01	101.02	110.94
2	6	49	ALA	CA-C-N	6.01	128.61	120.38
2	6	49	ALA	C-N-CA	6.01	128.61	120.38
1	D	115	LYS	O-C-N	-6.01	115.88	122.07
2	4	192	THR	N-CA-C	-6.01	105.25	113.30
1	C	207	GLU	N-CA-C	-6.00	105.54	112.92
2	2	101	TYR	CB-CG-CD1	6.00	129.80	120.80
1	B	57	LYS	N-CA-C	-6.00	105.82	113.02
2	1	149	GLY	CA-C-N	6.00	128.99	120.53
2	1	149	GLY	C-N-CA	6.00	128.99	120.53
1	B	224	VAL	N-CA-CB	5.99	118.47	110.26
2	4	126	ASP	CA-CB-CG	-5.99	106.61	112.60
1	F	204	LEU	N-CA-C	-5.99	100.43	109.95
2	1	35	ASN	OD1-CG-ND2	-5.99	116.61	122.60
2	5	204	VAL	CA-C-N	5.99	128.90	120.28
2	5	204	VAL	C-N-CA	5.99	128.90	120.28
1	A	98	ILE	N-CA-CB	5.98	118.68	110.54
2	2	84	LYS	CA-C-N	5.98	125.89	119.85
2	2	84	LYS	C-N-CA	5.98	125.89	119.85
2	6	212	ARG	N-CA-C	-5.98	107.80	114.62
1	F	235	ARG	CD-NE-CZ	-5.98	116.03	124.40
2	7	87	VAL	CA-C-N	5.98	128.29	120.28
2	7	87	VAL	C-N-CA	5.98	128.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	144	VAL	N-CA-CB	5.97	119.57	111.21
1	D	187	ASP	CA-CB-CG	-5.97	106.63	112.60
2	6	29	LYS	N-CA-CB	5.97	119.00	110.16
2	1	173	TYR	CA-CB-CG	5.97	124.65	113.90
1	G	52	LYS	CA-CB-CG	5.96	126.03	114.10
2	4	78	GLU	CA-C-N	5.96	128.07	120.56
2	4	78	GLU	C-N-CA	5.96	128.07	120.56
2	7	187	ASP	N-CA-C	-5.96	100.47	109.95
2	2	202	GLU	O-C-N	-5.96	115.93	122.07
1	B	128	GLY	O-C-N	5.96	130.43	122.27
2	3	83	ARG	CD-NE-CZ	-5.96	116.06	124.40
2	1	206	GLN	OE1-CD-NE2	5.95	128.55	122.60
1	B	165	GLY	CA-C-N	5.95	128.25	120.28
1	B	165	GLY	C-N-CA	5.95	128.25	120.28
2	2	120	LYS	CA-C-O	-5.95	114.40	120.71
2	3	140	THR	N-CA-CB	5.94	121.60	111.50
1	E	240	ILE	CA-C-N	5.94	128.24	120.28
1	E	240	ILE	C-N-CA	5.94	128.24	120.28
2	3	42	ALA	N-CA-CB	5.94	119.82	110.56
2	3	120	LYS	N-CA-CB	5.94	121.76	111.13
2	5	33	MET	N-CA-C	-5.94	105.62	114.64
2	6	205	GLU	N-CA-C	5.94	118.54	111.71
1	B	205	VAL	CA-C-N	5.93	125.63	119.64
1	B	205	VAL	C-N-CA	5.93	125.63	119.64
2	7	21	ASP	N-CA-C	-5.93	104.70	112.41
2	1	67	ALA	N-CA-CB	5.93	119.35	110.22
1	G	68	TYR	CA-C-N	5.93	129.25	120.95
1	G	68	TYR	C-N-CA	5.93	129.25	120.95
1	G	100	ARG	NE-CZ-NH1	-5.93	115.57	121.50
2	7	186	ILE	CA-CB-CG1	5.93	120.48	110.40
1	D	233	VAL	CA-C-N	5.93	128.22	120.28
1	D	233	VAL	C-N-CA	5.93	128.22	120.28
2	5	122	ILE	N-CA-CB	5.92	120.17	111.52
2	6	90	ILE	O-C-N	5.92	127.93	121.83
2	1	45	ILE	CB-CA-C	5.92	119.39	110.63
1	C	211	VAL	N-CA-C	-5.92	99.53	108.17
2	3	165	VAL	N-CA-CB	5.92	119.46	110.58
2	6	156	THR	CA-C-O	-5.92	114.96	120.94
1	E	83	ALA	O-C-N	5.92	128.16	122.07
1	F	241	ARG	O-C-N	-5.92	115.85	122.12
1	C	35	ALA	O-C-N	-5.91	116.11	122.85
2	2	212	ARG	NH1-CZ-NH2	-5.91	111.61	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	24	VAL	CA-CB-CG2	-5.91	100.35	110.40
1	G	93	ARG	CA-C-O	5.91	126.69	120.42
2	1	170	ARG	NH1-CZ-NH2	-5.91	111.62	119.30
2	3	67	ALA	CA-C-N	5.91	128.19	120.28
2	3	67	ALA	C-N-CA	5.91	128.19	120.28
2	5	116	ASP	CA-C-N	5.91	130.58	120.72
2	5	116	ASP	C-N-CA	5.91	130.58	120.72
2	5	129	GLY	CA-C-N	5.90	132.97	121.41
2	5	129	GLY	C-N-CA	5.90	132.97	121.41
2	7	28	GLU	N-CA-C	-5.90	98.79	108.41
2	4	212	ARG	N-CA-C	-5.90	106.62	113.88
1	B	22	PHE	CA-C-N	5.90	128.66	120.29
1	B	22	PHE	C-N-CA	5.90	128.66	120.29
2	2	91	ALA	CA-C-O	5.90	126.80	120.55
1	C	238	GLU	CA-C-N	5.89	128.66	120.29
1	C	238	GLU	C-N-CA	5.89	128.66	120.29
2	1	126	ASP	CA-C-N	5.89	125.51	119.56
2	1	126	ASP	C-N-CA	5.89	125.51	119.56
2	7	126	ASP	CA-C-O	-5.89	112.09	120.16
2	7	145	LEU	CA-C-N	5.89	128.18	120.28
2	7	145	LEU	C-N-CA	5.89	128.18	120.28
1	F	196	MET	CA-C-N	5.89	127.50	120.14
1	F	196	MET	C-N-CA	5.89	127.50	120.14
1	C	106	PRO	N-CA-CB	5.89	108.49	103.19
2	6	104	PHE	CA-CB-CG	-5.89	107.91	113.80
1	C	160	LYS	CB-CA-C	-5.88	99.95	109.13
2	6	60	VAL	CA-C-N	5.88	126.47	119.94
2	6	60	VAL	C-N-CA	5.88	126.47	119.94
1	B	187	ASP	CA-C-N	5.88	128.09	120.44
1	B	187	ASP	C-N-CA	5.88	128.09	120.44
1	G	130	ARG	CA-C-O	-5.88	114.55	120.96
2	4	160	GLY	N-CA-C	-5.88	101.34	111.57
1	E	152	PRO	CA-C-N	5.88	131.43	121.14
1	E	152	PRO	C-N-CA	5.88	131.43	121.14
1	B	107	ILE	O-C-N	-5.87	115.23	122.57
2	3	135	LYS	CA-C-N	5.87	130.92	122.23
2	3	135	LYS	C-N-CA	5.87	130.92	122.23
2	4	41	ALA	CA-C-O	5.87	127.97	121.11
2	6	17	LEU	CA-C-N	5.87	129.94	122.37
2	6	17	LEU	C-N-CA	5.87	129.94	122.37
2	4	86	THR	CA-C-N	5.87	128.75	120.42
2	4	86	THR	C-N-CA	5.87	128.75	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	90	ILE	CB-CA-C	-5.87	104.12	112.22
1	B	130	ARG	CA-C-N	5.86	125.84	120.21
1	B	130	ARG	C-N-CA	5.86	125.84	120.21
1	A	143	GLU	CB-CG-CD	-5.86	102.63	112.60
2	4	161	VAL	CA-C-N	5.86	128.61	120.29
2	4	161	VAL	C-N-CA	5.86	128.61	120.29
2	1	117	SER	CA-C-N	5.86	128.06	120.44
2	1	117	SER	C-N-CA	5.86	128.06	120.44
2	7	161	VAL	N-CA-CB	5.86	118.51	110.54
1	F	153	SER	N-CA-C	-5.86	104.25	111.40
3	K	395	VAL	N-CA-C	-5.86	105.14	110.82
2	7	17	LEU	CA-C-N	5.85	130.73	123.12
2	7	17	LEU	C-N-CA	5.85	130.73	123.12
1	F	9	ASP	CA-CB-CG	5.85	118.45	112.60
1	F	56	SER	N-CA-C	-5.85	100.24	108.96
1	D	46	VAL	N-CA-C	-5.85	99.79	108.45
2	2	57	ALA	N-CA-C	-5.85	98.75	108.34
2	7	132	ILE	O-C-N	5.85	129.88	122.57
2	1	35	ASN	N-CA-C	-5.84	105.34	112.88
1	B	27	ALA	N-CA-CB	5.84	119.92	110.40
1	A	222	LYS	CA-C-O	-5.84	114.97	121.51
1	C	231	PRO	CA-C-O	-5.84	111.57	120.03
2	2	134	GLU	N-CA-CB	5.84	120.61	110.81
1	G	194	VAL	N-CA-C	-5.83	104.67	110.62
2	7	86	THR	N-CA-C	-5.83	102.68	110.55
1	G	59	LEU	N-CA-CB	5.83	118.86	110.06
1	E	100	ARG	NE-CZ-NH2	5.82	124.44	119.20
2	2	122	ILE	N-CA-C	-5.82	99.67	108.17
1	G	134	VAL	N-CA-C	-5.82	100.10	108.42
2	3	86	THR	CA-CB-OG1	5.81	118.32	109.60
2	4	172	ILE	O-C-N	5.81	128.36	121.80
1	G	244	LEU	N-CA-C	-5.81	106.19	113.28
1	A	21	LEU	CA-C-O	-5.80	114.37	120.58
1	G	74	ILE	N-CA-C	-5.80	99.86	108.45
1	C	17	PRO	N-CA-C	-5.80	105.62	113.40
1	E	118	ASP	N-CA-CB	5.80	118.75	110.16
2	7	81	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	F	62	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	35	ALA	CA-C-N	5.80	128.94	120.71
1	A	35	ALA	C-N-CA	5.80	128.94	120.71
2	3	62	ASP	O-C-N	5.79	128.26	122.12
1	E	8	TYR	CB-CG-CD1	-5.79	112.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	PRO	N-CA-CB	5.79	109.42	103.23
2	6	82	GLU	CA-C-N	5.79	131.70	121.80
2	6	82	GLU	C-N-CA	5.79	131.70	121.80
2	5	155	PHE	CB-CA-C	-5.79	101.83	110.16
1	F	99	ASN	CA-C-N	5.79	129.10	120.31
1	F	99	ASN	C-N-CA	5.79	129.10	120.31
1	G	130	ARG	CD-NE-CZ	-5.79	116.30	124.40
2	1	108	VAL	CB-CA-C	5.79	119.41	110.50
2	6	161	VAL	CA-C-N	5.79	127.96	120.44
2	6	161	VAL	C-N-CA	5.79	127.96	120.44
2	7	194	ASP	CB-CA-C	-5.79	98.91	110.42
2	2	113	GLY	O-C-N	5.78	128.63	123.60
2	5	106	TYR	CB-CG-CD1	-5.78	112.12	120.80
1	B	20	ARG	NH1-CZ-NH2	-5.78	111.78	119.30
1	E	107	ILE	O-C-N	-5.78	116.36	122.95
1	C	149	GLU	N-CA-C	-5.78	98.87	108.34
2	1	105	PRO	CB-CA-C	-5.77	103.53	111.21
1	E	229	LEU	N-CA-C	-5.77	106.37	113.41
2	7	52	MET	CG-SD-CE	-5.77	88.20	100.90
2	7	164	ALA	CB-CA-C	-5.77	101.04	110.85
2	2	93	LEU	N-CA-C	5.77	117.57	111.28
2	5	147	ALA	CA-C-N	5.76	127.93	120.44
2	5	147	ALA	C-N-CA	5.76	127.93	120.44
1	A	239	ARG	CA-C-O	5.76	126.59	119.79
1	A	200	ILE	N-CA-C	-5.76	105.18	113.07
1	F	203	GLU	N-CA-CB	5.76	118.50	110.04
2	3	102	ARG	N-CA-CB	5.76	119.25	110.44
2	7	142	SER	O-C-N	5.76	129.96	122.42
1	B	150	THR	O-C-N	-5.75	116.45	123.30
1	B	157	LEU	N-CA-C	-5.75	99.29	109.06
1	E	12	ILE	O-C-N	-5.75	115.40	122.18
2	2	128	ILE	N-CA-C	-5.75	106.80	111.91
2	3	153	ASP	CA-C-O	-5.74	114.79	120.70
3	J	394	GLY	CA-C-N	5.74	130.64	122.09
3	J	394	GLY	C-N-CA	5.74	130.64	122.09
1	A	108	THR	CA-C-N	5.74	127.79	120.56
1	A	108	THR	C-N-CA	5.74	127.79	120.56
1	A	15	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	79	SER	N-CA-C	-5.73	99.99	108.99
1	D	238	GLU	CA-C-N	5.73	128.23	120.44
1	D	238	GLU	C-N-CA	5.73	128.23	120.44
2	1	116	ASP	N-CA-C	-5.73	100.83	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	394	GLY	CA-C-N	5.73	132.28	121.97
3	H	394	GLY	C-N-CA	5.73	132.28	121.97
1	D	70	ILE	CB-CA-C	-5.73	101.90	111.29
2	1	165	VAL	N-CA-CB	5.73	119.17	110.58
1	D	87	VAL	N-CA-CB	5.72	120.12	110.56
1	D	85	ALA	CA-C-O	-5.72	114.49	120.55
2	1	111	LEU	O-C-N	-5.72	116.58	123.27
2	7	134	GLU	N-CA-CB	5.72	121.37	111.13
1	B	170	ALA	CB-CA-C	-5.72	101.30	110.79
1	A	5	GLN	CA-C-N	5.71	131.99	121.70
1	A	5	GLN	C-N-CA	5.71	131.99	121.70
1	B	189	MET	O-C-N	-5.71	116.07	122.12
2	7	56	THR	CA-CB-OG1	5.71	118.16	109.60
3	K	397	PHE	N-CA-CB	5.71	121.48	111.55
2	7	195	GLU	N-CA-CB	5.70	121.15	111.57
1	F	233	VAL	CB-CA-C	-5.70	104.35	112.22
2	4	40	LYS	CA-C-N	5.70	131.51	122.62
2	4	40	LYS	C-N-CA	5.70	131.51	122.62
2	5	23	VAL	CA-CB-CG1	5.70	120.09	110.40
2	7	28	GLU	N-CA-CB	5.70	119.54	110.65
2	2	49	ALA	CA-C-N	5.69	128.23	120.54
2	2	49	ALA	C-N-CA	5.69	128.23	120.54
1	E	73	HIS	CG-CD2-NE2	5.69	112.89	107.20
1	F	54	VAL	CA-C-N	5.69	127.51	120.34
1	F	54	VAL	C-N-CA	5.69	127.51	120.34
2	1	28	GLU	N-CA-CB	5.69	119.45	110.23
1	C	39	GLY	N-CA-C	-5.69	101.51	111.46
1	G	233	VAL	CA-C-N	5.69	127.90	120.28
1	G	233	VAL	C-N-CA	5.69	127.90	120.28
1	B	219	ARG	NE-CZ-NH2	5.69	124.32	119.20
2	5	148	TYR	CA-C-N	5.69	126.42	119.99
2	5	148	TYR	C-N-CA	5.69	126.42	119.99
2	2	182	SER	N-CA-CB	5.68	120.10	110.49
2	3	69	ILE	CA-C-N	5.68	128.49	120.42
2	3	69	ILE	C-N-CA	5.68	128.49	120.42
1	D	59	LEU	N-CA-CB	5.68	118.38	109.69
1	A	204	LEU	CA-C-N	5.68	132.64	122.13
1	A	204	LEU	C-N-CA	5.68	132.64	122.13
2	3	89	ALA	CA-C-N	5.68	128.24	120.46
2	3	89	ALA	C-N-CA	5.68	128.24	120.46
2	4	93	LEU	CB-CA-C	-5.68	101.36	110.79
1	E	226	PRO	O-C-N	5.68	129.54	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	141	VAL	N-CA-C	-5.67	99.89	108.17
1	E	16	SER	CA-C-O	-5.67	114.78	120.96
2	1	87	VAL	N-CA-C	-5.67	104.99	110.72
2	3	200	SER	CA-C-N	5.67	126.93	119.84
2	3	200	SER	C-N-CA	5.67	126.93	119.84
1	E	115	LYS	CA-C-N	5.67	128.47	120.42
1	E	115	LYS	C-N-CA	5.67	128.47	120.42
2	4	195	GLU	CA-C-N	5.67	131.96	123.23
2	4	195	GLU	C-N-CA	5.67	131.96	123.23
2	6	51	ARG	NE-CZ-NH2	5.67	124.30	119.20
2	1	148	TYR	CB-CA-C	-5.67	101.38	110.79
2	6	123	TYR	CB-CA-C	-5.67	99.74	109.65
2	1	23	VAL	N-CA-C	-5.66	100.87	108.35
1	E	31	VAL	CA-CB-CG2	-5.66	100.78	110.40
2	5	177	LYS	CA-C-O	-5.66	114.42	120.42
1	C	163	ALA	CA-C-N	5.66	130.38	122.23
1	C	163	ALA	C-N-CA	5.66	130.38	122.23
2	1	24	VAL	N-CA-C	-5.66	100.03	108.46
2	5	30	ARG	NE-CZ-NH2	5.66	124.29	119.20
2	2	153	ASP	CA-CB-CG	-5.66	106.94	112.60
2	5	212	ARG	NE-CZ-NH2	-5.66	114.11	119.20
1	B	220	THR	N-CA-C	-5.65	99.68	108.90
1	E	35	ALA	CA-C-N	5.65	129.29	120.75
1	E	35	ALA	C-N-CA	5.65	129.29	120.75
1	C	161	ALA	N-CA-C	-5.65	99.40	108.55
2	1	171	ALA	N-CA-C	5.65	117.52	111.36
1	F	76	ALA	CB-CA-C	-5.65	100.11	110.62
2	7	144	SER	O-C-N	5.65	128.11	122.12
1	D	129	VAL	N-CA-C	-5.65	99.73	107.75
1	B	225	SER	CA-C-O	-5.64	115.40	121.27
2	3	121	SER	CA-C-N	5.64	130.99	122.98
2	3	121	SER	C-N-CA	5.64	130.99	122.98
2	3	162	ASP	CA-CB-CG	5.64	118.24	112.60
1	G	25	GLU	N-CA-C	-5.64	106.36	113.18
2	2	88	ARG	NE-CZ-NH1	-5.64	115.86	121.50
2	3	156	THR	N-CA-CB	5.64	119.20	111.25
1	G	235	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	B	23	GLN	CA-C-N	5.64	129.54	120.30
1	B	23	GLN	C-N-CA	5.64	129.54	120.30
1	B	182	ASP	CA-C-O	5.63	126.52	119.59
1	G	184	SER	CA-C-N	5.63	127.83	120.28
1	G	184	SER	C-N-CA	5.63	127.83	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	63	ALA	N-CA-CB	5.63	118.18	110.01
1	G	51	ASP	CA-C-N	5.63	129.64	120.23
1	G	51	ASP	C-N-CA	5.63	129.64	120.23
1	B	193	LEU	N-CA-C	-5.63	105.22	111.36
3	L	393	LYS	CA-C-N	5.63	129.59	121.54
3	L	393	LYS	C-N-CA	5.63	129.59	121.54
2	4	94	THR	CA-C-N	5.63	127.82	120.28
2	4	94	THR	C-N-CA	5.63	127.82	120.28
2	4	100	SER	O-C-N	5.63	128.17	122.09
1	C	12	ILE	N-CA-C	-5.62	105.42	113.07
1	E	188	ALA	N-CA-C	5.62	117.21	111.14
2	2	163	GLU	N-CA-CB	5.62	118.91	110.53
2	4	208	LEU	N-CA-CB	5.62	118.91	110.53
2	6	118	GLU	N-CA-C	-5.62	107.06	114.31
2	2	75	ASN	CA-CB-CG	-5.61	106.99	112.60
2	4	48	ILE	CA-C-O	-5.61	115.11	120.95
1	F	137	LEU	CA-C-O	-5.61	114.30	120.30
2	3	154	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	5	91	ALA	O-C-N	5.61	128.07	122.12
1	B	91	ARG	CA-C-N	5.61	127.79	120.28
1	B	91	ARG	C-N-CA	5.61	127.79	120.28
1	C	104	ASP	CA-CB-CG	5.61	118.21	112.60
2	7	159	ILE	N-CA-C	-5.61	100.40	108.53
2	6	61	GLY	CA-C-N	5.60	128.25	120.29
2	6	61	GLY	C-N-CA	5.60	128.25	120.29
1	C	212	GLY	N-CA-C	-5.60	102.25	111.38
1	F	201	GLU	CB-CG-CD	-5.60	103.09	112.60
1	C	79	SER	N-CA-CB	5.59	121.25	111.13
1	E	215	LYS	O-C-N	-5.59	116.95	123.27
1	F	84	ASP	N-CA-C	-5.59	105.19	111.28
1	E	221	PHE	N-CA-C	5.58	122.70	110.80
1	G	150	THR	N-CA-C	-5.58	99.80	108.90
1	E	217	ASP	N-CA-CB	5.58	118.42	110.16
1	A	12	ILE	O-C-N	5.58	127.55	122.14
1	B	47	ILE	N-CA-C	-5.58	100.02	108.17
2	6	192	THR	CA-CB-OG1	5.58	117.97	109.60
1	E	38	ILE	CA-C-N	-5.58	117.86	121.65
1	E	38	ILE	C-N-CA	-5.58	117.86	121.65
2	7	27	THR	CA-C-N	5.58	130.87	123.00
2	7	27	THR	C-N-CA	5.58	130.87	123.00
2	7	196	PHE	CA-C-N	5.58	130.42	122.72
2	7	196	PHE	C-N-CA	5.58	130.42	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	29	LYS	CA-C-O	5.58	126.84	120.54
2	3	143	GLY	N-CA-C	-5.58	108.40	115.31
1	B	49	ILE	N-CA-C	-5.57	100.45	108.48
1	E	125	GLN	CB-CA-C	-5.57	102.13	110.88
2	2	129	GLY	N-CA-C	-5.57	104.71	112.18
2	5	148	TYR	O-C-N	-5.57	116.33	122.07
2	7	127	PRO	N-CA-CB	5.57	108.90	102.33
2	1	65	PHE	CA-C-O	-5.57	114.52	120.42
1	E	232	TYR	CA-C-N	5.56	127.57	120.56
1	E	232	TYR	C-N-CA	5.56	127.57	120.56
1	F	235	ARG	NE-CZ-NH1	-5.56	115.94	121.50
2	7	88	ARG	CD-NE-CZ	-5.56	116.61	124.40
1	G	207	GLU	N-CA-C	-5.56	105.71	112.88
2	1	200	SER	CA-C-N	5.56	126.79	119.84
2	1	200	SER	C-N-CA	5.56	126.79	119.84
1	A	65	GLU	CA-C-N	5.56	129.78	122.06
1	A	65	GLU	C-N-CA	5.56	129.78	122.06
2	5	157	PRO	N-CA-CB	5.56	108.48	103.20
1	E	59	LEU	N-CA-CB	5.55	118.81	109.92
1	F	234	GLU	O-C-N	5.55	128.01	122.12
2	3	185	GLY	N-CA-C	-5.55	100.02	113.18
1	A	118	ASP	N-CA-CB	5.55	118.38	110.16
1	E	169	ASN	CA-CB-CG	-5.55	107.05	112.60
1	F	86	ARG	N-CA-CB	5.55	118.88	110.28
1	G	79	SER	N-CA-C	-5.55	100.28	108.99
1	G	186	ASP	CA-CB-CG	5.55	118.15	112.60
2	4	61	GLY	CA-C-O	5.55	126.54	120.66
1	D	221	PHE	CA-C-N	5.55	131.27	122.62
1	D	221	PHE	C-N-CA	5.55	131.27	122.62
1	G	141	VAL	N-CA-C	-5.55	99.56	107.77
1	C	49	ILE	CB-CA-C	5.54	118.89	110.90
1	E	235	ARG	O-C-N	5.54	128.00	122.12
2	4	108	VAL	O-C-N	-5.54	118.15	122.97
2	4	208	LEU	N-CA-C	-5.54	106.57	113.38
2	5	201	PRO	N-CA-C	5.54	123.88	112.47
1	F	232	TYR	O-C-N	5.54	128.46	122.15
2	4	102	ARG	NH1-CZ-NH2	-5.54	112.10	119.30
2	4	64	GLN	CA-C-N	5.54	128.15	120.29
2	4	64	GLN	C-N-CA	5.54	128.15	120.29
1	F	29	GLU	N-CA-CB	5.53	119.57	110.39
2	2	166	GLU	CB-CA-C	-5.53	102.16	110.90
2	7	87	VAL	O-C-N	5.53	127.31	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	PHE	N-CA-CB	5.53	119.83	110.49
2	3	188	VAL	O-C-N	-5.53	116.90	123.04
1	E	74	ILE	N-CA-C	-5.53	100.16	108.12
1	B	170	ALA	O-C-N	5.52	127.97	122.12
1	C	235	ARG	NE-CZ-NH2	5.52	124.17	119.20
2	4	106	TYR	CB-CG-CD1	5.52	129.08	120.80
1	C	63	THR	CA-C-N	5.52	129.28	121.66
1	C	63	THR	C-N-CA	5.52	129.28	121.66
1	E	15	PHE	CA-CB-CG	-5.52	108.28	113.80
1	C	35	ALA	CA-C-N	5.51	128.54	120.71
1	C	35	ALA	C-N-CA	5.51	128.54	120.71
2	5	179	ASP	CA-CB-CG	-5.51	107.09	112.60
1	F	130	ARG	CA-C-O	-5.51	114.81	120.87
2	4	120	LYS	N-CA-C	-5.51	100.98	109.52
2	3	115	ILE	CA-C-O	5.51	126.32	120.48
2	3	30	ARG	N-CA-C	-5.51	100.06	108.76
1	E	93	ARG	O-C-N	-5.50	116.40	122.07
2	2	66	LEU	CA-C-N	5.50	127.66	120.28
2	2	66	LEU	C-N-CA	5.50	127.66	120.28
2	5	36	PHE	N-CA-CB	5.50	120.54	111.62
1	F	235	ARG	CA-C-N	5.50	128.10	120.29
1	F	235	ARG	C-N-CA	5.50	128.10	120.29
2	3	204	VAL	N-CA-C	-5.50	105.16	110.72
2	3	209	ALA	N-CA-C	-5.50	106.45	112.72
2	4	170	ARG	O-C-N	-5.50	116.41	122.07
2	2	200	SER	CA-C-N	5.50	124.96	119.24
2	2	200	SER	C-N-CA	5.50	124.96	119.24
1	G	172	THR	CA-C-N	5.49	128.19	120.28
1	G	172	THR	C-N-CA	5.49	128.19	120.28
1	D	42	CYS	CA-C-N	5.49	131.60	122.54
1	D	42	CYS	C-N-CA	5.49	131.60	122.54
2	3	131	ALA	N-CA-C	-5.49	99.46	108.41
1	A	62	ASP	N-CA-C	-5.49	99.46	108.41
1	D	200	ILE	CA-C-N	5.48	130.64	122.74
1	D	200	ILE	C-N-CA	5.48	130.64	122.74
2	1	165	VAL	CA-C-O	-5.48	115.04	120.85
1	D	27	ALA	N-CA-C	-5.48	106.55	113.18
1	A	175	PHE	N-CA-C	-5.48	106.64	113.38
2	6	92	THR	CA-C-O	5.48	126.23	120.42
1	C	167	GLY	CA-C-N	5.48	127.93	120.54
1	C	167	GLY	C-N-CA	5.48	127.93	120.54
1	G	216	VAL	CB-CA-C	-5.47	104.85	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	220	THR	CA-C-O	-5.47	112.69	120.51
2	3	47	GLN	N-CA-CB	5.47	118.43	109.95
2	4	158	GLU	CA-C-N	5.47	128.74	120.75
2	4	158	GLU	C-N-CA	5.47	128.74	120.75
2	4	36	PHE	CA-C-N	5.47	127.91	120.63
2	4	36	PHE	C-N-CA	5.47	127.91	120.63
1	F	108	THR	CB-CA-C	5.47	119.41	109.62
1	D	12	ILE	N-CA-C	-5.46	107.03	113.42
2	5	62	ASP	CA-CB-CG	-5.46	107.14	112.60
2	3	15	VAL	N-CA-C	-5.46	100.83	108.80
1	G	240	ILE	N-CA-C	-5.46	105.05	110.62
1	D	82	VAL	CA-C-N	5.46	127.59	120.28
1	D	82	VAL	C-N-CA	5.46	127.59	120.28
1	E	90	ASP	CA-C-N	5.46	127.59	120.28
1	E	90	ASP	C-N-CA	5.46	127.59	120.28
1	F	46	VAL	CA-C-N	5.45	130.52	122.94
1	F	46	VAL	C-N-CA	5.45	130.52	122.94
2	2	30	ARG	NE-CZ-NH1	-5.45	116.05	121.50
2	7	126	ASP	CA-CB-CG	5.45	118.05	112.60
1	F	54	VAL	CA-CB-CG1	-5.45	101.13	110.40
2	1	40	LYS	N-CA-C	-5.45	106.22	112.92
2	6	21	ASP	N-CA-C	-5.45	104.50	113.50
1	G	53	ARG	O-C-N	5.45	128.36	122.15
2	7	107	LEU	N-CA-CB	5.45	119.25	110.65
1	A	216	VAL	N-CA-C	-5.44	107.50	113.43
1	E	73	HIS	N-CA-C	-5.44	106.10	114.16
2	2	139	ALA	N-CA-CB	5.44	119.69	110.49
2	6	39	SER	N-CA-CB	5.44	119.95	110.81
1	A	224	VAL	N-CA-C	-5.44	99.41	107.51
1	C	79	SER	N-CA-C	-5.44	99.45	108.75
1	F	217	ASP	N-CA-C	5.44	119.17	112.54
2	6	21	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	14	VAL	N-CA-C	5.43	114.56	106.85
2	7	67	ALA	N-CA-C	-5.43	105.36	111.28
2	2	88	ARG	NE-CZ-NH2	5.42	124.08	119.20
2	4	98	LEU	N-CA-C	5.42	116.87	111.07
1	B	127	GLY	O-C-N	5.42	127.12	121.97
1	C	158	GLU	N-CA-CB	5.42	118.24	110.06
1	E	194	VAL	N-CA-C	5.42	116.14	110.62
2	5	77	TYR	O-C-N	-5.42	116.38	122.12
1	G	219	ARG	N-CA-CB	5.41	122.58	113.10
2	6	73	GLU	CA-C-O	5.41	126.02	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	153	ASP	O-C-N	-5.41	115.20	122.23
1	D	213	TYR	CB-CG-CD1	5.41	128.91	120.80
1	F	26	TYR	CA-C-O	-5.41	114.69	120.42
1	F	72	GLU	N-CA-C	-5.41	106.88	112.93
1	B	225	SER	CA-C-N	5.40	125.74	119.47
1	B	225	SER	C-N-CA	5.40	125.74	119.47
1	F	44	GLU	N-CA-CB	5.40	119.62	110.49
1	A	224	VAL	CA-C-N	5.40	129.67	121.03
1	A	224	VAL	C-N-CA	5.40	129.67	121.03
3	J	393	LYS	N-CA-C	-5.40	106.06	113.30
1	G	67	ILE	O-C-N	5.40	127.95	122.71
2	6	128	ILE	CA-CB-CG1	5.40	119.58	110.40
3	H	396	MET	N-CA-CB	5.40	119.89	110.98
1	F	136	LEU	CB-CA-C	-5.39	99.19	109.66
1	G	215	LYS	CA-C-N	5.39	127.46	120.56
1	G	215	LYS	C-N-CA	5.39	127.46	120.56
3	K	394	GLY	N-CA-C	-5.39	107.97	114.66
2	6	35	ASN	O-C-N	-5.39	115.24	122.19
1	E	204	LEU	CA-C-O	5.39	127.25	121.16
1	E	243	LEU	N-CA-C	-5.38	105.58	111.82
1	C	173	GLU	CA-C-N	5.38	127.75	120.65
1	C	173	GLU	C-N-CA	5.38	127.75	120.65
2	4	33	MET	N-CA-C	-5.38	99.34	110.80
1	A	34	GLY	CA-C-N	5.38	128.73	120.82
1	A	34	GLY	C-N-CA	5.38	128.73	120.82
2	1	184	ASP	N-CA-C	-5.38	101.24	109.41
1	D	16	SER	CA-C-N	5.38	125.70	119.47
1	D	16	SER	C-N-CA	5.38	125.70	119.47
1	G	225	SER	N-CA-CB	5.37	117.29	110.04
2	3	99	ASN	OD1-CG-ND2	5.37	127.97	122.60
2	6	55	THR	N-CA-C	-5.37	101.41	109.95
2	6	145	LEU	CA-C-O	5.37	126.25	120.55
1	G	108	THR	N-CA-C	-5.37	102.53	110.48
1	G	109	VAL	CA-C-N	5.37	127.48	120.28
1	G	109	VAL	C-N-CA	5.37	127.48	120.28
1	G	177	LYS	CG-CD-CE	5.37	123.64	111.30
1	A	85	ALA	CA-C-N	5.36	127.78	120.54
1	A	85	ALA	C-N-CA	5.36	127.78	120.54
1	C	183	LEU	O-C-N	5.36	129.19	122.86
2	7	62	ASP	CA-C-O	-5.36	114.73	120.42
2	5	68	ARG	CB-CA-C	-5.36	101.89	110.79
1	C	112	LEU	CB-CA-C	-5.36	102.43	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	117	CYS	CB-CA-C	-5.36	101.89	110.79
1	D	49	ILE	O-C-N	-5.36	117.39	123.18
3	K	391	ASP	CA-C-N	5.36	131.77	121.54
3	K	391	ASP	C-N-CA	5.36	131.77	121.54
1	F	126	TYR	CB-CG-CD1	5.35	128.83	120.80
2	2	156	THR	O-C-N	-5.35	117.74	121.65
2	5	188	VAL	CA-C-O	-5.35	114.87	120.76
2	7	156	THR	N-CA-C	-5.35	100.11	109.48
2	4	191	ILE	CA-CB-CG2	-5.35	101.41	110.50
1	E	166	MET	N-CA-CB	5.35	118.07	110.16
1	F	11	ALA	N-CA-CB	5.35	119.69	111.46
1	G	117	CYS	O-C-N	-5.35	116.45	122.12
2	2	37	ILE	CA-C-O	-5.35	114.93	121.13
2	5	21	ASP	N-CA-C	-5.35	104.38	112.99
1	B	149	GLU	O-C-N	-5.35	117.06	123.31
1	E	220	THR	O-C-N	5.35	129.70	122.59
1	G	174	PHE	CA-C-N	5.34	130.49	121.14
1	G	174	PHE	C-N-CA	5.34	130.49	121.14
2	6	143	GLY	CA-C-N	5.34	127.70	120.38
2	6	143	GLY	C-N-CA	5.34	127.70	120.38
2	7	202	GLU	O-C-N	5.34	127.59	122.03
1	A	230	LYS	CA-C-N	5.34	125.16	119.28
1	A	230	LYS	C-N-CA	5.34	125.16	119.28
1	C	196	MET	CA-C-N	5.34	125.91	119.98
1	C	196	MET	C-N-CA	5.34	125.91	119.98
2	2	37	ILE	O-C-N	5.34	128.12	122.67
1	G	90	ASP	CA-C-N	5.34	127.43	120.28
1	G	90	ASP	C-N-CA	5.34	127.43	120.28
1	G	102	THR	CA-C-O	-5.34	113.32	119.56
2	1	71	LYS	CB-CA-C	-5.34	102.50	110.88
2	1	80	ARG	CG-CD-NE	-5.34	100.26	112.00
2	2	198	GLN	CA-C-N	5.34	127.38	120.44
2	2	198	GLN	C-N-CA	5.34	127.38	120.44
2	5	122	ILE	N-CA-C	-5.34	100.44	108.12
1	B	245	LYS	CA-C-O	-5.33	114.39	120.58
2	5	15	VAL	CA-C-O	-5.33	116.35	121.63
2	2	69	ILE	CA-C-O	5.33	126.82	121.17
1	E	143	GLU	N-CA-C	-5.33	105.92	112.90
1	A	228	GLU	CA-C-N	5.33	127.95	120.28
1	A	228	GLU	C-N-CA	5.33	127.95	120.28
2	6	175	ALA	CA-C-N	5.33	127.42	120.28
2	6	175	ALA	C-N-CA	5.33	127.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	74	ALA	N-CA-C	5.32	117.16	111.36
2	7	132	ILE	CA-C-N	5.32	131.71	121.54
2	7	132	ILE	C-N-CA	5.32	131.71	121.54
1	C	67	ILE	N-CA-CB	5.32	120.00	111.23
2	2	199	TYR	CA-CB-CG	-5.32	104.33	113.90
2	5	48	ILE	N-CA-C	5.31	116.79	111.00
2	7	185	GLY	CA-C-O	5.31	123.77	118.77
1	C	116	ILE	N-CA-CB	5.31	118.55	110.58
1	E	129	VAL	N-CA-C	-5.31	99.86	107.78
2	6	26	ALA	CA-C-N	5.31	131.29	121.94
2	6	26	ALA	C-N-CA	5.31	131.29	121.94
2	6	136	ASP	N-CA-CB	5.31	119.47	110.49
2	1	118	GLU	CA-C-O	5.31	126.39	120.82
1	A	211	VAL	CA-C-N	5.31	126.28	121.82
1	A	211	VAL	C-N-CA	5.31	126.28	121.82
1	D	230	LYS	CA-C-O	-5.31	113.75	118.63
1	F	124	THR	OG1-CB-CG2	-5.31	98.69	109.30
1	C	186	ASP	CA-C-O	5.30	126.04	120.42
2	5	149	GLY	CA-C-N	5.30	127.72	120.46
2	5	149	GLY	C-N-CA	5.30	127.72	120.46
2	3	155	PHE	O-C-N	5.30	129.35	122.89
2	3	205	GLU	CB-CG-CD	5.30	121.61	112.60
1	E	170	ALA	CA-C-O	-5.30	114.94	120.55
2	5	77	TYR	CA-C-N	5.30	128.36	120.31
2	5	77	TYR	C-N-CA	5.30	128.36	120.31
1	D	185	PHE	CA-C-O	-5.29	115.26	120.82
2	7	55	THR	CA-CB-OG1	5.29	117.54	109.60
1	A	200	ILE	CA-C-O	5.29	125.60	119.36
2	1	178	ARG	O-C-N	-5.29	116.12	122.15
2	4	71	LYS	N-CA-C	5.29	116.73	111.07
2	4	97	LEU	CA-C-O	-5.29	115.26	120.82
2	6	96	ASN	N-CA-C	-5.29	105.59	111.36
2	6	111	LEU	CA-C-O	-5.29	114.45	120.32
2	1	210	LYS	N-CA-C	-5.29	106.51	113.17
2	6	201	PRO	N-CA-C	5.29	123.37	112.47
1	B	82	VAL	CB-CA-C	-5.29	103.69	112.26
1	F	36	THR	CA-C-N	5.29	131.24	121.94
1	F	36	THR	C-N-CA	5.29	131.24	121.94
2	3	111	LEU	CB-CA-C	-5.28	100.14	109.70
1	A	30	ALA	CA-C-O	5.28	125.86	119.31
1	A	230	LYS	CA-C-O	-5.28	112.93	120.16
1	E	149	GLU	N-CA-C	-5.28	99.92	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	86	THR	N-CA-CB	5.28	118.79	110.56
2	3	112	ILE	O-C-N	-5.28	117.61	123.20
1	E	120	LYS	CA-CB-CG	-5.28	103.55	114.10
1	F	192	GLY	CA-C-O	-5.28	114.44	120.09
2	3	29	LYS	CB-CA-C	-5.28	99.29	109.37
1	F	46	VAL	N-CA-C	-5.27	100.26	108.86
1	A	129	VAL	CA-C-N	5.27	128.69	120.68
1	A	129	VAL	C-N-CA	5.27	128.69	120.68
1	A	57	LYS	N-CA-C	-5.27	106.11	112.54
1	B	16	SER	CA-C-O	-5.27	113.68	121.27
1	E	113	ALA	CA-C-O	-5.27	114.96	120.55
2	3	190	LYS	N-CA-CB	5.27	118.87	110.65
2	1	48	ILE	N-CA-C	-5.27	107.28	111.81
1	G	18	ASP	N-CA-C	-5.26	105.60	112.23
1	G	154	GLY	N-CA-C	-5.26	107.30	115.67
2	4	70	ILE	N-CA-C	-5.26	105.41	110.72
1	C	144	VAL	CA-C-N	5.26	125.67	119.99
1	C	144	VAL	C-N-CA	5.26	125.67	119.99
2	2	86	THR	O-C-N	-5.26	117.09	123.03
1	A	184	SER	CA-C-N	5.25	127.27	120.44
1	A	184	SER	C-N-CA	5.25	127.27	120.44
1	A	80	GLY	CA-C-O	-5.25	115.13	122.43
2	4	143	GLY	N-CA-C	-5.25	106.64	115.62
1	D	83	ALA	O-C-N	5.24	127.68	122.12
1	D	104	ASP	O-C-N	5.24	129.31	122.86
2	6	181	ALA	N-CA-C	-5.24	106.72	113.01
1	B	64	ILE	CA-C-N	5.24	131.13	121.70
1	B	64	ILE	C-N-CA	5.24	131.13	121.70
1	E	233	VAL	N-CA-CB	5.24	116.68	110.55
1	C	151	ASP	N-CA-C	-5.24	102.09	110.10
1	D	229	LEU	O-C-N	5.24	128.12	122.15
2	3	102	ARG	N-CA-C	-5.24	106.67	113.16
1	F	42	CYS	N-CA-C	-5.24	101.45	109.41
1	A	90	ASP	N-CA-C	-5.23	105.66	111.36
1	C	82	VAL	O-C-N	-5.23	116.80	121.87
1	F	189	MET	CB-CA-C	-5.23	102.11	110.79
2	1	140	THR	O-C-N	-5.23	117.00	123.44
2	7	37	ILE	CA-C-O	5.23	126.03	120.48
1	F	192	GLY	O-C-N	5.23	128.35	122.34
2	2	79	ILE	CA-C-O	-5.23	115.31	120.85
2	7	151	LEU	N-CA-C	5.23	117.06	111.36
2	5	87	VAL	CA-C-N	5.23	127.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	87	VAL	C-N-CA	5.23	127.29	120.28
1	E	120	LYS	CA-C-N	5.23	127.81	120.28
1	E	120	LYS	C-N-CA	5.23	127.81	120.28
1	F	8	TYR	N-CA-C	-5.23	99.67	110.80
2	1	163	GLU	CB-CG-CD	-5.23	103.71	112.60
2	2	165	VAL	CA-C-N	5.23	127.55	120.44
2	2	165	VAL	C-N-CA	5.23	127.55	120.44
2	4	113	GLY	N-CA-C	-5.23	101.88	110.56
1	C	219	ARG	NE-CZ-NH2	-5.22	114.50	119.20
2	3	205	GLU	N-CA-C	5.22	117.72	111.71
2	1	169	VAL	O-C-N	-5.22	116.80	121.87
1	E	34	GLY	CA-C-N	5.22	128.28	120.87
1	E	34	GLY	C-N-CA	5.22	128.28	120.87
1	B	28	ARG	CA-C-O	-5.22	114.89	120.42
1	D	105	GLU	CA-C-N	5.21	126.36	119.84
1	D	105	GLU	C-N-CA	5.21	126.36	119.84
2	6	204	VAL	CA-C-O	-5.21	115.32	120.85
2	7	60	VAL	CB-CA-C	-5.21	105.21	112.04
3	H	392	LEU	CA-C-O	5.21	126.06	120.38
2	1	144	SER	CA-C-N	5.21	127.22	120.44
2	1	144	SER	C-N-CA	5.21	127.22	120.44
2	5	81	ARG	CA-C-O	5.21	125.77	119.31
2	5	139	ALA	O-C-N	-5.21	116.86	123.17
1	B	168	ARG	N-CA-C	5.21	116.64	111.07
1	D	179	TYR	N-CA-C	5.21	117.01	110.24
2	5	154	ARG	NE-CZ-NH1	-5.21	116.29	121.50
2	7	151	LEU	CA-C-N	5.21	127.69	120.29
2	7	151	LEU	C-N-CA	5.21	127.69	120.29
2	7	191	ILE	CA-C-O	5.21	127.29	120.78
1	A	78	THR	O-C-N	5.20	129.64	123.24
1	E	213	TYR	CA-CB-CG	5.20	123.27	113.90
2	4	133	GLU	CA-C-O	5.20	125.95	120.54
1	C	240	ILE	CB-CA-C	-5.20	105.12	112.14
1	F	230	LYS	CA-C-N	5.20	125.00	119.28
1	F	230	LYS	C-N-CA	5.20	125.00	119.28
2	2	196	PHE	N-CA-C	-5.20	95.57	107.48
1	D	90	ASP	CA-C-N	5.20	127.25	120.28
1	D	90	ASP	C-N-CA	5.20	127.25	120.28
1	F	218	ASP	CA-CB-CG	-5.20	107.40	112.60
1	E	92	ALA	O-C-N	5.20	128.07	122.15
2	1	87	VAL	CA-C-N	5.20	127.67	120.29
2	1	87	VAL	C-N-CA	5.20	127.67	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	150	VAL	N-CA-CB	5.20	120.01	110.40
2	4	19	CYS	N-CA-C	-5.20	102.21	109.69
1	G	23	GLN	CG-CD-NE2	5.19	124.19	116.40
2	5	134	GLU	N-CA-CB	5.19	118.33	109.87
2	3	125	ILE	CA-C-N	5.19	130.89	122.48
2	3	125	ILE	C-N-CA	5.19	130.89	122.48
1	C	223	GLU	N-CA-C	-5.19	100.06	108.52
2	4	161	VAL	CA-CB-CG1	-5.19	101.58	110.40
1	C	182	ASP	N-CA-C	-5.18	106.20	112.88
1	F	51	ASP	N-CA-C	-5.18	102.19	109.96
2	2	122	ILE	O-C-N	-5.18	117.48	123.07
2	7	189	VAL	CA-C-O	5.18	126.73	120.67
1	C	119	PHE	CA-CB-CG	-5.17	108.62	113.80
2	4	170	ARG	CB-CG-CD	5.17	123.20	111.30
1	C	98	ILE	CA-CB-CG2	5.17	119.29	110.50
2	3	52	MET	N-CA-C	-5.17	99.91	108.75
2	6	133	GLU	CA-CB-CG	5.17	124.44	114.10
2	6	188	VAL	N-CA-CB	5.17	120.39	111.39
2	1	178	ARG	CA-C-O	5.17	125.90	120.42
1	A	21	LEU	CA-C-N	5.17	127.20	120.28
1	A	21	LEU	C-N-CA	5.17	127.20	120.28
1	B	190	VAL	CA-C-N	5.17	127.20	120.28
1	B	190	VAL	C-N-CA	5.17	127.20	120.28
2	4	98	LEU	O-C-N	5.17	127.39	122.07
2	6	177	LYS	O-C-N	5.17	128.04	122.15
1	D	212	GLY	N-CA-C	-5.16	102.15	111.19
1	F	225	SER	N-CA-CB	5.16	117.52	110.03
1	A	129	VAL	CA-C-O	5.16	126.06	120.43
1	D	28	ARG	N-CA-C	-5.16	106.83	113.23
1	D	113	ALA	CA-C-N	5.16	127.15	120.44
1	D	113	ALA	C-N-CA	5.16	127.15	120.44
1	B	109	VAL	O-C-N	5.16	127.14	121.83
2	1	206	GLN	N-CA-C	-5.16	106.49	112.89
2	2	65	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	51	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	236	ALA	N-CA-C	5.15	116.98	111.36
2	3	60	VAL	CB-CA-C	-5.15	105.18	112.14
2	6	102	ARG	NH1-CZ-NH2	-5.15	112.61	119.30
1	B	37	ALA	CA-C-N	5.15	130.09	122.94
1	B	37	ALA	C-N-CA	5.15	130.09	122.94
1	G	202	SER	CA-C-N	5.15	128.52	120.75
1	G	202	SER	C-N-CA	5.15	128.52	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	149	GLY	N-CA-C	5.15	118.47	112.50
1	B	240	ILE	N-CA-C	-5.14	105.37	110.62
1	G	29	GLU	CA-C-N	5.14	127.17	120.28
1	G	29	GLU	C-N-CA	5.14	127.17	120.28
1	G	148	TYR	CB-CA-C	-5.14	98.75	110.07
2	1	151	LEU	CB-CA-C	-5.14	102.77	110.90
2	3	114	GLY	CA-C-N	5.14	129.57	123.19
2	3	114	GLY	C-N-CA	5.14	129.57	123.19
2	6	157	PRO	O-C-N	5.14	128.66	122.23
2	5	143	GLY	N-CA-C	-5.14	107.08	115.46
1	E	156	LEU	N-CA-CB	5.14	119.07	110.85
3	I	396	MET	N-CA-C	-5.14	107.06	113.38
2	3	46	TYR	CA-CB-CG	-5.14	104.65	113.90
2	3	17	LEU	O-C-N	-5.13	117.41	123.41
1	A	136	LEU	N-CA-C	-5.13	101.79	109.95
2	6	199	TYR	CB-CG-CD1	5.13	128.50	120.80
1	E	124	THR	N-CA-C	-5.13	105.32	112.45
1	B	11	ALA	O-C-N	-5.13	117.54	123.33
2	7	45	ILE	N-CA-C	-5.13	100.27	107.75
1	E	67	ILE	N-CA-C	-5.12	100.27	107.75
2	3	200	SER	CA-C-O	-5.12	113.89	120.04
2	1	81	ARG	CA-C-O	5.12	124.77	119.14
1	C	95	GLU	N-CA-C	-5.12	105.78	111.36
2	3	162	ASP	CA-C-N	5.12	130.10	121.14
2	3	162	ASP	C-N-CA	5.12	130.10	121.14
1	A	116	ILE	CA-C-N	5.12	127.14	120.28
1	A	116	ILE	C-N-CA	5.12	127.14	120.28
1	C	127	GLY	CA-C-N	5.12	131.44	121.41
1	C	127	GLY	C-N-CA	5.12	131.44	121.41
2	2	142	SER	CA-C-O	5.11	125.47	119.28
1	A	111	GLU	N-CA-C	5.11	117.75	111.82
2	6	29	LYS	CB-CA-C	-5.11	102.17	110.85
1	F	30	ALA	N-CA-C	-5.10	105.80	111.36
2	3	23	VAL	CA-CB-CG2	-5.10	101.73	110.40
2	4	109	GLN	CG-CD-NE2	5.10	124.05	116.40
2	5	26	ALA	CA-C-N	5.10	130.52	122.36
2	5	26	ALA	C-N-CA	5.10	130.52	122.36
1	A	179	TYR	N-CA-CB	5.10	117.45	109.85
2	2	71	LYS	CG-CD-CE	5.10	123.03	111.30
2	7	180	SER	CA-C-N	5.10	131.22	122.09
2	7	180	SER	C-N-CA	5.10	131.22	122.09
1	G	198	LEU	N-CA-C	5.10	116.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	LEU	N-CA-CB	5.09	118.30	110.61
1	G	240	ILE	N-CA-CB	5.09	117.47	110.54
1	B	126	TYR	O-C-N	-5.09	117.21	122.96
1	C	68	TYR	N-CA-C	-5.09	101.00	108.99
2	6	162	ASP	O-C-N	-5.09	116.83	122.07
1	C	155	ALA	CA-C-O	-5.09	115.40	121.56
1	G	144	VAL	N-CA-C	-5.09	97.89	108.88
2	6	58	GLY	CA-C-N	5.09	128.43	120.75
2	6	58	GLY	C-N-CA	5.09	128.43	120.75
2	6	200	SER	CA-C-N	5.09	126.20	119.84
2	6	200	SER	C-N-CA	5.09	126.20	119.84
2	5	105	PRO	O-C-N	5.08	129.20	123.10
2	6	15	VAL	CA-CB-CG2	5.08	119.04	110.40
2	6	43	LYS	O-C-N	5.08	128.65	122.85
2	6	196	PHE	CA-CB-CG	5.08	118.88	113.80
2	1	86	THR	CA-C-N	5.08	127.64	120.42
2	1	86	THR	C-N-CA	5.08	127.64	120.42
2	1	18	VAL	CA-CB-CG1	5.08	119.04	110.40
2	1	139	ALA	N-CA-C	-5.08	101.36	109.23
2	6	195	GLU	N-CA-CB	5.08	120.97	111.52
1	B	49	ILE	O-C-N	-5.08	117.70	123.18
2	4	86	THR	N-CA-C	-5.08	102.04	109.81
1	G	169	ASN	CA-CB-CG	-5.07	107.53	112.60
2	1	159	ILE	CA-C-O	-5.07	116.51	121.58
1	E	75	CYS	N-CA-C	-5.07	101.66	109.52
2	4	123	TYR	CA-C-O	-5.07	114.88	120.36
2	1	77	TYR	CA-C-O	5.07	125.93	120.55
2	2	201	PRO	O-C-N	5.07	127.66	122.18
1	A	112	LEU	CA-C-N	5.07	128.01	120.31
1	A	112	LEU	C-N-CA	5.07	128.01	120.31
1	D	214	VAL	O-C-N	-5.07	117.57	122.99
1	F	221	PHE	CA-CB-CG	-5.07	108.73	113.80
1	G	118	ASP	N-CA-C	5.07	116.80	111.28
2	6	18	VAL	N-CA-CB	5.07	116.24	110.72
1	G	64	ILE	CA-CB-CG2	5.07	119.11	110.50
1	E	190	VAL	CA-C-O	-5.06	115.68	120.95
1	G	200	ILE	N-CA-C	-5.06	108.04	112.90
2	6	101	TYR	CB-CA-C	-5.06	101.18	109.53
1	D	136	LEU	N-CA-CB	5.06	120.36	111.55
1	D	184	SER	N-CA-C	-5.06	102.52	110.36
2	2	95	SER	O-C-N	5.06	127.48	122.12
2	3	159	ILE	CB-CA-C	5.06	118.87	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ASP	N-CA-C	5.06	116.87	111.36
1	C	85	ALA	N-CA-CB	5.06	117.34	110.01
1	A	186	ASP	CA-C-N	5.06	127.06	120.28
1	A	186	ASP	C-N-CA	5.06	127.06	120.28
1	G	218	ASP	O-C-N	5.06	128.81	122.19
2	2	154	ARG	CA-C-O	5.06	125.48	120.32
2	3	93	LEU	CA-C-N	5.06	127.47	120.29
2	3	93	LEU	C-N-CA	5.06	127.47	120.29
1	B	64	ILE	O-C-N	-5.05	116.25	122.57
2	4	140	THR	N-CA-C	-5.05	100.04	110.80
1	C	85	ALA	CB-CA-C	-5.05	102.95	110.88
1	C	236	ALA	CA-C-O	-5.05	115.07	120.42
1	A	85	ALA	N-CA-CB	5.05	117.54	110.12
1	D	139	ALA	N-CA-C	-5.05	100.67	108.90
1	F	119	PHE	N-CA-C	-5.05	105.86	111.36
2	7	108	VAL	N-CA-C	-5.05	101.68	108.35
1	B	117	CYS	O-C-N	-5.05	116.77	122.12
2	1	107	LEU	N-CA-C	-5.05	104.29	110.65
1	D	120	LYS	N-CA-CB	5.05	117.54	110.12
1	D	161	ALA	CB-CA-C	-5.05	100.38	110.42
2	4	195	GLU	N-CA-C	-5.05	100.79	108.76
1	C	113	ALA	CA-C-N	5.04	127.04	120.28
1	C	113	ALA	C-N-CA	5.04	127.04	120.28
1	C	81	LEU	N-CA-CB	5.04	117.95	110.29
1	C	214	VAL	CA-C-N	5.04	130.69	122.07
1	C	214	VAL	C-N-CA	5.04	130.69	122.07
1	F	99	ASN	O-C-N	-5.04	116.78	122.12
2	5	75	ASN	N-CA-CB	5.04	117.53	110.12
1	A	99	ASN	N-CA-C	-5.04	105.87	111.36
1	B	9	ASP	N-CA-CB	5.04	119.86	111.49
1	C	135	SER	N-CA-C	-5.04	101.54	109.50
2	3	86	THR	CA-C-O	-5.04	115.51	121.66
1	B	84	ASP	CA-C-N	5.04	127.44	120.29
1	B	84	ASP	C-N-CA	5.04	127.44	120.29
2	3	117	SER	O-C-N	-5.04	116.30	122.34
2	5	27	THR	CA-C-O	5.03	127.15	121.51
2	5	163	GLU	N-CA-C	-5.03	106.99	113.23
1	B	66	LYS	CA-C-O	5.03	124.43	118.90
1	B	170	ALA	CA-C-N	5.03	128.94	120.29
1	B	170	ALA	C-N-CA	5.03	128.94	120.29
2	5	172	ILE	O-C-N	5.03	127.96	122.12
2	6	169	VAL	CA-C-O	-5.03	115.52	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	GLU	CA-C-N	5.03	129.25	121.71
1	B	223	GLU	C-N-CA	5.03	129.25	121.71
1	G	25	GLU	O-C-N	-5.03	115.09	122.43
2	3	99	ASN	CA-CB-CG	-5.03	107.57	112.60
2	5	13	THR	CA-C-O	-5.03	115.90	121.33
1	A	224	VAL	CG1-CB-CG2	-5.03	99.74	110.80
1	B	91	ARG	NE-CZ-NH2	5.03	123.72	119.20
2	1	195	GLU	CB-CG-CD	-5.03	104.06	112.60
1	E	105	GLU	CA-C-N	5.02	126.12	119.84
1	E	105	GLU	C-N-CA	5.02	126.12	119.84
1	B	182	ASP	N-CA-C	-5.02	107.31	112.93
1	F	224	VAL	CA-CB-CG1	5.02	118.93	110.40
2	2	55	THR	N-CA-C	-5.02	101.69	109.72
2	3	87	VAL	CA-C-N	5.02	127.01	120.28
2	3	87	VAL	C-N-CA	5.02	127.01	120.28
2	4	65	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	33	ARG	CA-C-N	5.02	125.91	120.44
1	A	33	ARG	C-N-CA	5.02	125.91	120.44
1	A	211	VAL	O-C-N	5.02	128.47	123.10
1	D	127	GLY	N-CA-C	-5.02	104.97	112.89
2	3	87	VAL	N-CA-CB	5.01	117.36	110.54
2	3	179	ASP	CA-C-O	-5.01	115.76	121.58
1	B	93	ARG	CA-C-N	5.01	126.88	120.56
1	B	93	ARG	C-N-CA	5.01	126.88	120.56
1	E	33	ARG	CA-C-O	5.01	125.73	120.42
1	C	33	ARG	CA-C-N	-5.01	116.70	122.77
1	C	33	ARG	C-N-CA	-5.01	116.70	122.77
1	E	66	LYS	N-CA-CB	5.01	117.58	110.06
1	B	169	ASN	CB-CA-C	-5.01	102.47	110.79
1	G	160	LYS	N-CA-C	-5.01	105.90	111.36
2	3	36	PHE	CA-CB-CG	-5.01	108.79	113.80
2	5	47	GLN	OE1-CD-NE2	5.01	127.61	122.60
2	6	103	TYR	N-CA-C	-5.01	104.83	112.04
1	E	216	VAL	CA-CB-CG2	-5.01	101.89	110.40
2	3	109	GLN	N-CA-C	-5.00	100.30	108.76
2	7	96	ASN	CA-C-O	-5.00	115.11	120.42
1	G	212	GLY	N-CA-C	-5.00	103.84	111.14
2	2	89	ALA	CA-C-N	5.00	127.53	120.42
2	2	89	ALA	C-N-CA	5.00	127.53	120.42
2	6	188	VAL	N-CA-C	-5.00	101.27	108.48
1	G	182	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (114) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	199	TYR	Sidechain
2	1	211	PHE	Sidechain
2	1	77	TYR	Sidechain
2	1	80	ARG	Sidechain
2	2	101	TYR	Sidechain
2	2	139	ALA	Peptide,Mainchain
2	2	148	TYR	Sidechain
2	2	173	TYR	Sidechain
2	2	197	TYR	Sidechain
2	2	77	TYR	Sidechain
2	2	81	ARG	Sidechain
2	3	101	TYR	Sidechain
2	3	148	TYR	Sidechain
2	3	212	ARG	Sidechain
2	3	68	ARG	Sidechain
2	4	103	TYR	Sidechain
2	4	123	TYR	Sidechain
2	4	139	ALA	Peptide
2	4	155	PHE	Sidechain
2	4	68	ARG	Sidechain
2	4	83	ARG	Sidechain
2	5	106	TYR	Sidechain
2	5	132	ILE	Peptide
2	5	139	ALA	Mainchain
2	5	154	ARG	Sidechain
2	5	170	ARG	Sidechain
2	5	199	TYR	Sidechain
2	5	81	ARG	Sidechain
2	5	88	ARG	Sidechain
2	6	101	TYR	Sidechain
2	6	103	TYR	Sidechain
2	6	139	ALA	Peptide
2	6	148	TYR	Sidechain
2	6	173	TYR	Sidechain
2	6	36	PHE	Sidechain
2	6	46	TYR	Sidechain
2	6	77	TYR	Sidechain
2	6	88	ARG	Sidechain
2	7	132	ILE	Peptide
2	7	139	ALA	Peptide
2	7	199	TYR	Sidechain
2	7	51	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	7	77	TYR	Sidechain
2	7	83	ARG	Sidechain
2	7	88	ARG	Sidechain
1	A	123	TYR	Sidechain
1	A	148	TYR	Sidechain
1	A	213	TYR	Sidechain
1	A	220	THR	Peptide
1	A	221	PHE	Sidechain
1	A	65	GLU	Peptide
1	A	86	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	14	VAL	Peptide
1	B	179	TYR	Sidechain
1	B	22	PHE	Sidechain
1	B	220	THR	Peptide
1	B	232	TYR	Sidechain
1	B	235	ARG	Sidechain
1	B	86	ARG	Sidechain
1	C	10	ARG	Sidechain
1	C	148	TYR	Sidechain
1	C	159	TYR	Sidechain
1	C	179	TYR	Sidechain
1	C	20	ARG	Sidechain
1	C	213	TYR	Sidechain
1	C	220	THR	Peptide
1	C	221	PHE	Sidechain
1	C	235	ARG	Sidechain
1	C	65	GLU	Peptide
1	C	66	LYS	Peptide
1	C	91	ARG	Sidechain
1	C	93	ARG	Sidechain
1	D	105	GLU	Peptide
1	D	174	PHE	Sidechain
1	D	179	TYR	Sidechain
1	D	213	TYR	Sidechain
1	D	220	THR	Peptide
1	D	239	ARG	Sidechain
1	E	103	TYR	Sidechain
1	E	123	TYR	Sidechain
1	E	159	TYR	Sidechain
1	E	168	ARG	Sidechain
1	E	175	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	E	179	TYR	Sidechain
1	E	20	ARG	Sidechain
1	E	215	LYS	Peptide
1	E	220	THR	Peptide
1	E	221	PHE	Sidechain
1	E	28	ARG	Sidechain
1	F	103	TYR	Sidechain
1	F	14	VAL	Peptide
1	F	159	TYR	Sidechain
1	F	213	TYR	Sidechain
1	F	220	THR	Peptide
1	F	53	ARG	Sidechain
1	F	8	TYR	Sidechain
1	F	86	ARG	Sidechain
1	G	123	TYR	Sidechain
1	G	126	TYR	Sidechain
1	G	148	TYR	Sidechain
1	G	159	TYR	Sidechain
1	G	179	TYR	Sidechain
1	G	220	THR	Peptide
1	G	235	ARG	Sidechain
1	G	34	GLY	Peptide
1	G	35	ALA	Peptide
1	G	5	GLN	Peptide
3	H	394	GLY	Peptide
3	I	394	GLY	Peptide
3	I	397	PHE	Sidechain
3	J	397	PHE	Sidechain
3	L	394	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1941	6	0
1	B	1907	0	1941	5	0
1	C	1907	0	1941	9	0
1	D	1907	0	1941	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1907	0	1940	19	0
1	F	1907	0	1941	2	0
1	G	1907	0	1941	7	0
2	1	1552	0	1580	6	0
2	2	1552	0	1580	2	0
2	3	1552	0	1580	2	0
2	4	1552	0	1580	3	0
2	5	1552	0	1580	27	0
2	6	1552	0	1580	7	0
2	7	1552	0	1580	10	0
3	H	70	0	74	1	0
3	I	70	0	74	0	0
3	J	70	0	74	0	0
3	K	70	0	74	1	0
3	L	70	0	74	1	0
3	M	70	0	74	0	0
All	All	24633	0	25090	104	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 (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:LYS:C	1:E:67:ILE:N	1.71	1.49
2:5:211:PHE:CE1	2:5:211:PHE:CZ	2.02	1.46
2:5:211:PHE:CZ	2:5:211:PHE:CE2	2.03	1.46
2:5:211:PHE:CG	2:5:211:PHE:CD1	2.04	1.45
2:5:211:PHE:CE1	2:5:211:PHE:CD1	2.04	1.43
2:5:211:PHE:CE2	2:5:211:PHE:CD2	2.08	1.41
2:5:211:PHE:CG	2:5:211:PHE:CD2	2.10	1.37
2:5:170:ARG:CZ	2:5:211:PHE:CE2	2.34	1.11
2:5:170:ARG:CZ	2:5:170:ARG:NH1	2.15	1.10
2:5:170:ARG:CZ	2:5:211:PHE:CD1	2.36	1.08
2:5:170:ARG:CZ	2:5:211:PHE:CE1	2.37	1.07
2:5:170:ARG:NH1	2:5:211:PHE:CD1	2.24	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CG	2.24	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CE1	2.25	1.05
2:5:170:ARG:NH1	2:5:211:PHE:CE2	2.24	1.04
2:5:170:ARG:NH1	2:5:211:PHE:CD2	2.25	1.04
2:5:170:ARG:CZ	2:5:211:PHE:CD2	2.42	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:170:ARG:NH1	2:5:211:PHE:CZ	2.25	1.03
2:5:170:ARG:CZ	2:5:211:PHE:CZ	2.42	1.03
2:5:170:ARG:CZ	2:5:211:PHE:CG	2.47	0.98
2:5:170:ARG:NE	2:5:211:PHE:CZ	2.43	0.86
2:5:170:ARG:NH2	2:5:211:PHE:CG	2.46	0.84
1:E:35:ALA:HB3	1:E:66:LYS:NZ	1.93	0.83
1:E:66:LYS:C	1:E:67:ILE:CA	2.53	0.81
2:5:170:ARG:NE	2:5:211:PHE:CE1	2.52	0.78
1:E:35:ALA:HB3	1:E:66:LYS:HZ2	1.48	0.78
2:5:170:ARG:NH2	2:5:211:PHE:CD2	2.51	0.77
1:E:66:LYS:CA	1:E:67:ILE:N	2.49	0.75
2:7:64:GLN:HE22	2:7:68:ARG:HE	1.39	0.71
1:A:163:ALA:HB2	1:A:171:VAL:HG11	1.78	0.65
1:E:36:THR:HG23	1:E:196:MET:HE2	1.80	0.64
1:A:13:THR:HA	1:B:130:ARG:HB3	1.83	0.60
2:1:154:ARG:HH12	2:1:166:GLU:HG2	1.71	0.56
1:G:237:ASN:HA	1:G:240:ILE:HD12	1.91	0.53
1:A:65:GLU:H	1:A:66:LYS:HA	1.74	0.52
1:C:80:GLY:HA3	1:C:134:VAL:HG12	1.90	0.52
2:1:68:ARG:HH22	2:2:131:ALA:H	1.54	0.52
1:D:79:SER:HB3	1:D:164:ILE:HD12	1.92	0.51
1:G:143:GLU:HA	1:G:219:ARG:HH12	1.77	0.49
1:B:28:ARG:HA	1:B:152:PRO:HG2	1.94	0.48
2:7:173:TYR:HA	2:7:176:MET:HE3	1.94	0.48
1:C:229:LEU:O	1:C:233:VAL:HG23	2.13	0.48
2:4:94:THR:HG21	2:4:110:LEU:HD22	1.94	0.48
2:5:56:THR:HG21	2:5:63:ALA:HB1	1.94	0.48
2:4:68:ARG:HH22	2:5:131:ALA:HB3	1.78	0.48
1:G:102:THR:HG23	1:G:103:TYR:CD2	2.49	0.48
1:E:35:ALA:HB3	1:E:66:LYS:HZ3	1.78	0.47
1:G:227:GLU:CD	1:G:227:GLU:H	2.22	0.47
2:7:54:MET:HE2	2:7:112:ILE:HD11	1.97	0.47
2:7:137:ILE:HD11	2:7:155:PHE:CD1	2.48	0.47
1:E:66:LYS:O	1:E:78:THR:HG22	2.14	0.47
2:6:45:ILE:HD12	2:6:189:VAL:HG11	1.97	0.47
1:B:64:ILE:HG21	3:K:398:VAL:HG11	1.97	0.47
2:3:56:THR:HG23	2:3:110:LEU:HD23	1.97	0.47
2:7:20:LYS:HD3	2:7:158:GLU:HA	1.97	0.46
1:E:33:ARG:HB3	3:H:397:PHE:CD2	2.50	0.46
2:5:78:GLU:HB2	2:5:85:PRO:HD3	1.95	0.46
1:G:81:LEU:HD11	3:L:397:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HD12	1:A:131:PRO:HD3	1.98	0.45
1:C:238:GLU:HA	1:C:241:ARG:HE	1.82	0.45
2:1:137:ILE:HD11	2:1:155:PHE:CD1	2.52	0.45
1:C:190:VAL:O	1:C:194:VAL:HG23	2.16	0.45
1:D:200:ILE:HD11	1:D:204:LEU:HD23	1.98	0.45
2:6:36:PHE:CD1	2:7:140:THR:HA	2.52	0.44
1:D:148:TYR:CD1	1:D:156:LEU:HD11	2.53	0.44
2:2:169:VAL:HA	2:2:186:ILE:HD11	1.99	0.44
2:7:64:GLN:NE2	2:7:68:ARG:HE	2.09	0.44
1:E:35:ALA:CB	1:E:66:LYS:HZ3	2.31	0.44
1:E:66:LYS:N	1:E:67:ILE:N	2.66	0.44
1:A:78:THR:HG21	1:A:85:ALA:CB	2.48	0.44
1:E:194:VAL:HG11	1:E:239:ARG:HG2	2.00	0.43
2:6:86:THR:HG23	2:6:89:ALA:H	1.83	0.43
2:1:165:VAL:O	2:1:169:VAL:HG23	2.18	0.43
1:D:155:ALA:HB2	1:E:83:ALA:HB2	2.01	0.43
1:F:47:ILE:HD13	1:F:189:MET:HA	2.00	0.43
2:7:207:ILE:HG22	2:7:211:PHE:CZ	2.54	0.43
2:4:125:ILE:HD12	2:4:125:ILE:N	2.34	0.43
2:5:64:GLN:HG2	2:6:131:ALA:H	1.84	0.43
2:7:14:THR:HG22	2:7:27:THR:HG22	2.01	0.43
2:7:179:ASP:HB3	2:7:181:ALA:H	1.83	0.42
1:C:193:LEU:HD23	1:C:233:VAL:HA	2.01	0.42
2:1:137:ILE:HD13	2:1:137:ILE:HA	1.92	0.42
1:C:193:LEU:CD2	1:C:233:VAL:HG22	2.50	0.42
1:D:74:ILE:HG21	1:D:112:LEU:HD23	2.02	0.42
1:E:51:ASP:O	1:E:66:LYS:HG3	2.20	0.42
2:6:122:ILE:HG21	2:6:138:VAL:HG11	2.01	0.42
1:E:59:LEU:HD12	1:E:59:LEU:H	1.84	0.42
1:C:190:VAL:HG21	1:C:235:ARG:HH11	1.85	0.42
1:E:74:ILE:HG21	1:E:112:LEU:HD23	2.02	0.42
1:E:141:VAL:HG11	1:E:216:VAL:HG22	2.02	0.42
1:C:193:LEU:HD21	1:C:233:VAL:HG22	2.02	0.41
1:E:205:VAL:HG22	1:E:208:ASN:HD21	1.84	0.41
1:G:31:VAL:HA	1:G:80:GLY:HA2	2.02	0.41
2:6:12:THR:HG21	2:6:58:GLY:H	1.85	0.41
1:G:132:PHE:HB3	1:G:134:VAL:HG12	2.02	0.41
1:E:70:ILE:HG21	1:E:112:LEU:HD21	2.03	0.41
1:B:181:ASP:C	1:B:183:LEU:H	2.29	0.41
1:C:17:PRO:HA	1:D:26:TYR:CE1	2.56	0.41
1:F:141:VAL:HG11	1:F:216:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:70:ILE:HD11	2:6:94:THR:HA	2.03	0.41
2:1:95:SER:HB3	2:1:130:GLY:H	1.86	0.40
1:A:205:VAL:HG12	1:A:207:GLU:H	1.87	0.40
1:B:163:ALA:HB3	1:B:168:ARG:HA	2.03	0.40
2:3:154:ARG:HD3	2:3:167:LEU:HD13	2.03	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	240/247 (97%)	227 (95%)	10 (4%)	3 (1%)	9	41
1	B	240/247 (97%)	223 (93%)	12 (5%)	5 (2%)	5	32
1	C	240/247 (97%)	222 (92%)	11 (5%)	7 (3%)	3	26
1	D	240/247 (97%)	223 (93%)	13 (5%)	4 (2%)	7	36
1	E	240/247 (97%)	226 (94%)	13 (5%)	1 (0%)	30	65
1	F	240/247 (97%)	224 (93%)	11 (5%)	5 (2%)	5	32
1	G	240/247 (97%)	225 (94%)	9 (4%)	6 (2%)	4	29
2	1	200/210 (95%)	191 (96%)	5 (2%)	4 (2%)	6	33
2	2	200/210 (95%)	182 (91%)	12 (6%)	6 (3%)	3	25
2	3	200/210 (95%)	181 (90%)	14 (7%)	5 (2%)	4	29
2	4	200/210 (95%)	185 (92%)	12 (6%)	3 (2%)	8	39
2	5	200/210 (95%)	185 (92%)	10 (5%)	5 (2%)	4	29
2	6	200/210 (95%)	180 (90%)	14 (7%)	6 (3%)	3	25
2	7	200/210 (95%)	182 (91%)	15 (8%)	3 (2%)	8	39
3	H	7/401 (2%)	4 (57%)	2 (29%)	1 (14%)	0	3
3	I	7/401 (2%)	5 (71%)	1 (14%)	1 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	7/401 (2%)	7 (100%)	0	0	100	100
3	K	7/401 (2%)	5 (71%)	1 (14%)	1 (14%)	0	3
3	L	7/401 (2%)	5 (71%)	0	2 (29%)	0	0
3	M	7/401 (2%)	6 (86%)	1 (14%)	0	100	100
All	All	3122/5605 (56%)	2888 (92%)	166 (5%)	68 (2%)	7	31

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	B	64	ILE
1	C	20	ARG
1	C	67	ILE
1	E	221	PHE
1	F	64	ILE
1	G	20	ARG
2	2	41	ALA
2	2	106	TYR
2	3	139	ALA
2	4	35	ASN
2	4	140	THR
2	6	139	ALA
2	7	39	SER
3	H	395	VAL
1	B	143	GLU
1	C	66	LYS
1	C	221	PHE
1	C	245	LYS
1	D	34	GLY
1	D	65	GLU
1	D	161	ALA
1	F	9	ASP
1	G	221	PHE
2	2	139	ALA
2	2	182	SER
2	2	212	ARG
2	3	41	ALA
2	6	140	THR
2	7	83	ARG
3	K	392	LEU
1	A	9	ASP

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Mol	Chain	Res	Type
1	A	143	GLU
1	B	221	PHE
1	C	9	ASP
1	F	221	PHE
1	G	54	VAL
1	G	184	SER
2	1	136	ASP
2	2	140	THR
2	3	140	THR
2	3	181	ALA
2	5	191	ILE
2	5	212	ARG
2	6	20	LYS
2	6	136	ASP
2	7	133	GLU
3	I	393	LYS
3	L	395	VAL
1	B	65	GLU
1	F	106	PRO
1	G	143	GLU
2	1	183	GLY
2	1	185	GLY
2	5	136	ASP
2	6	41	ALA
2	1	212	ARG
2	3	193	GLU
2	5	133	GLU
2	6	40	LYS
3	L	391	ASP
1	G	71	ASP
2	4	136	ASP
1	D	64	ILE
1	F	105	GLU
2	5	185	GLY
1	C	55	GLY
1	B	7	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	203/207 (98%)	198 (98%)	5 (2%)	42	62
1	B	203/207 (98%)	197 (97%)	6 (3%)	36	57
1	C	203/207 (98%)	194 (96%)	9 (4%)	25	48
1	D	203/207 (98%)	196 (97%)	7 (3%)	32	55
1	E	203/207 (98%)	191 (94%)	12 (6%)	18	42
1	F	203/207 (98%)	192 (95%)	11 (5%)	20	44
1	G	203/207 (98%)	195 (96%)	8 (4%)	28	51
2	1	164/171 (96%)	155 (94%)	9 (6%)	19	44
2	2	164/171 (96%)	153 (93%)	11 (7%)	15	39
2	3	164/171 (96%)	160 (98%)	4 (2%)	43	63
2	4	164/171 (96%)	155 (94%)	9 (6%)	19	44
2	5	164/171 (96%)	156 (95%)	8 (5%)	22	46
2	6	164/171 (96%)	155 (94%)	9 (6%)	19	44
2	7	164/171 (96%)	159 (97%)	5 (3%)	36	57
3	H	8/346 (2%)	8 (100%)	0	100	100
3	I	8/346 (2%)	7 (88%)	1 (12%)	4	19
3	J	8/346 (2%)	5 (62%)	3 (38%)	0	1
3	K	8/346 (2%)	7 (88%)	1 (12%)	4	19
3	L	8/346 (2%)	8 (100%)	0	100	100
3	M	8/346 (2%)	7 (88%)	1 (12%)	4	19
All	All	2617/4722 (55%)	2498 (96%)	119 (4%)	26	47

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PRO
1	A	24	VAL
1	A	49	ILE
1	A	86	ARG
1	A	144	VAL
1	B	48	LEU
1	B	151	ASP
1	B	178	GLU

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Mol	Chain	Res	Type
1	B	205	VAL
1	B	207	GLU
1	B	220	THR
1	C	42	CYS
1	C	66	LYS
1	C	67	ILE
1	C	69	LYS
1	C	101	LEU
1	C	125	GLN
1	C	156	LEU
1	C	208	ASN
1	C	239	ARG
1	D	46	VAL
1	D	54	VAL
1	D	65	GLU
1	D	82	VAL
1	D	189	MET
1	D	229	LEU
1	D	231	PRO
1	E	33	ARG
1	E	51	ASP
1	E	56	SER
1	E	57	LYS
1	E	89	ILE
1	E	98	ILE
1	E	102	THR
1	E	106	PRO
1	E	142	ASP
1	E	190	VAL
1	E	213	TYR
1	E	245	LYS
1	F	21	LEU
1	F	82	VAL
1	F	97	GLN
1	F	121	GLN
1	F	125	GLN
1	F	129	VAL
1	F	142	ASP
1	F	160	LYS
1	F	208	ASN
1	F	229	LEU
1	F	238	GLU

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Mol	Chain	Res	Type
1	G	5	GLN
1	G	14	VAL
1	G	57	LYS
1	G	98	ILE
1	G	152	PRO
1	G	164	ILE
1	G	166	MET
1	G	220	THR
2	1	27	THR
2	1	28	GLU
2	1	45	ILE
2	1	50	ASP
2	1	107	LEU
2	1	120	LYS
2	1	161	VAL
2	1	186	ILE
2	1	202	GLU
2	2	23	VAL
2	2	44	LYS
2	2	45	ILE
2	2	71	LYS
2	2	72	ILE
2	2	84	LYS
2	2	110	LEU
2	2	111	LEU
2	2	132	ILE
2	2	137	ILE
2	2	179	ASP
2	3	19	CYS
2	3	156	THR
2	3	182	SER
2	3	205	GLU
2	4	56	THR
2	4	72	ILE
2	4	109	GLN
2	4	125	ILE
2	4	128	ILE
2	4	134	GLU
2	4	140	THR
2	4	192	THR
2	4	205	GLU
2	5	17	LEU

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Mol	Chain	Res	Type
2	5	19	CYS
2	5	23	VAL
2	5	45	ILE
2	5	72	ILE
2	5	77	TYR
2	5	202	GLU
2	5	205	GLU
2	6	17	LEU
2	6	28	GLU
2	6	45	ILE
2	6	72	ILE
2	6	95	SER
2	6	132	ILE
2	6	136	ASP
2	6	161	VAL
2	6	205	GLU
2	7	45	ILE
2	7	60	VAL
2	7	132	ILE
2	7	133	GLU
2	7	189	VAL
3	I	392	LEU
3	K	398	VAL
3	M	398	VAL
3	J	395	VAL
3	J	396	MET
3	J	398	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	B	97	GLN
1	B	121	GLN
1	C	73	HIS
1	C	237	ASN
1	D	121	GLN
1	E	97	GLN
1	E	208	ASN
1	F	122	GLN
1	F	125	GLN
1	G	97	GLN

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Mol	Chain	Res	Type
1	G	121	GLN
1	G	125	GLN
1	G	237	ASN
2	1	99	ASN
2	2	75	ASN
2	4	99	ASN
2	5	96	ASN
2	5	99	ASN
2	6	109	GLN
2	7	64	GLN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	66:LYS	C	67:ILE	N	1.71

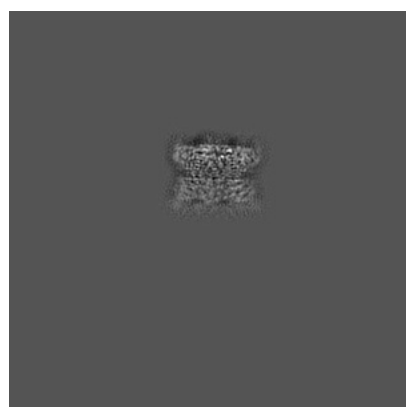
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0210. These allow visual inspection of the internal detail of the map and identification of artifacts.

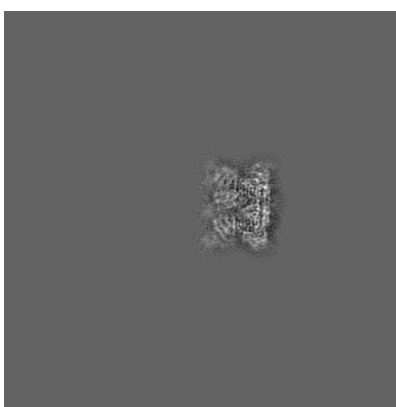
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

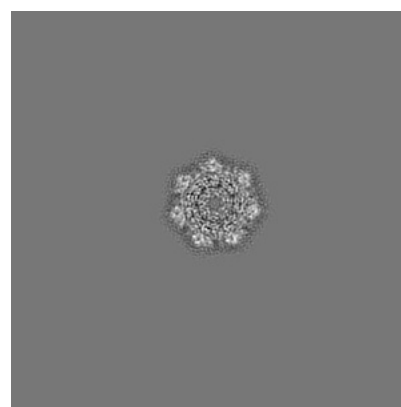
6.1.1 Primary map



X



Y

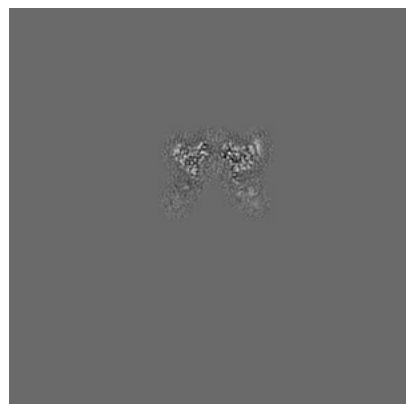


Z

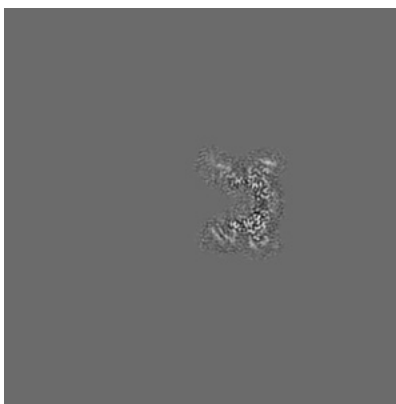
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

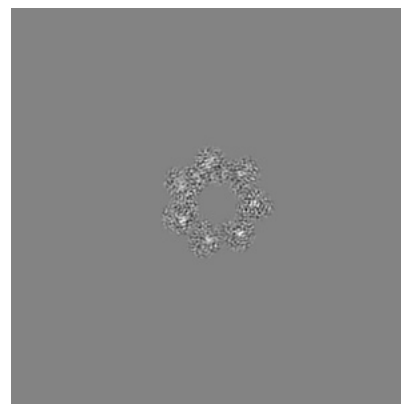
6.2.1 Primary map



X Index: 192



Y Index: 192

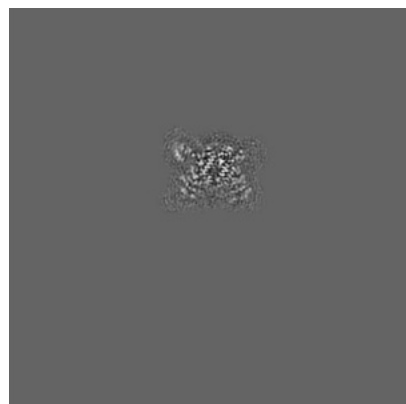


Z Index: 192

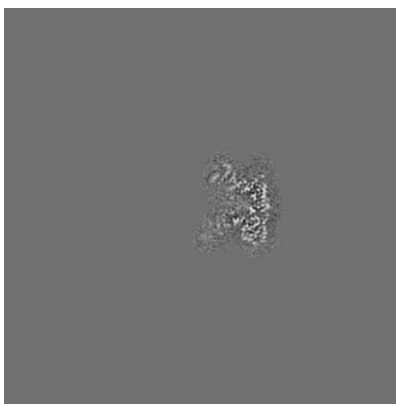
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

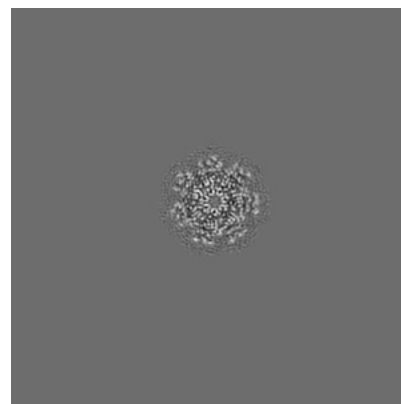
6.3.1 Primary map



X Index: 177



Y Index: 212

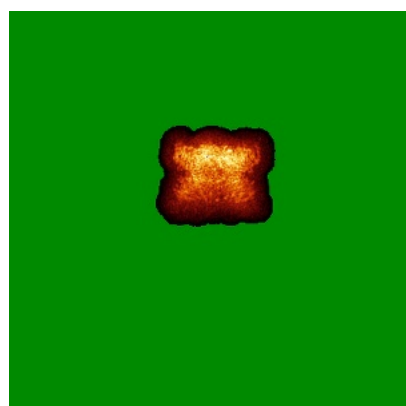


Z Index: 243

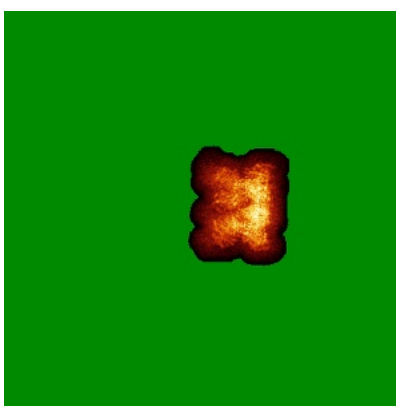
The images above show the largest variance slices of the map in three orthogonal directions.

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

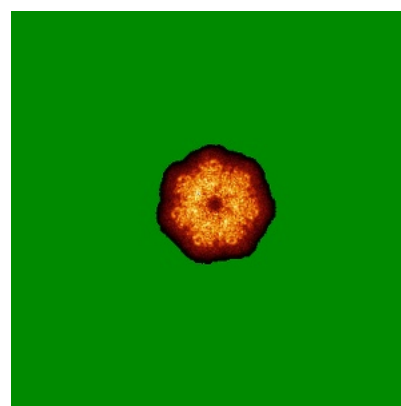
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0372. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

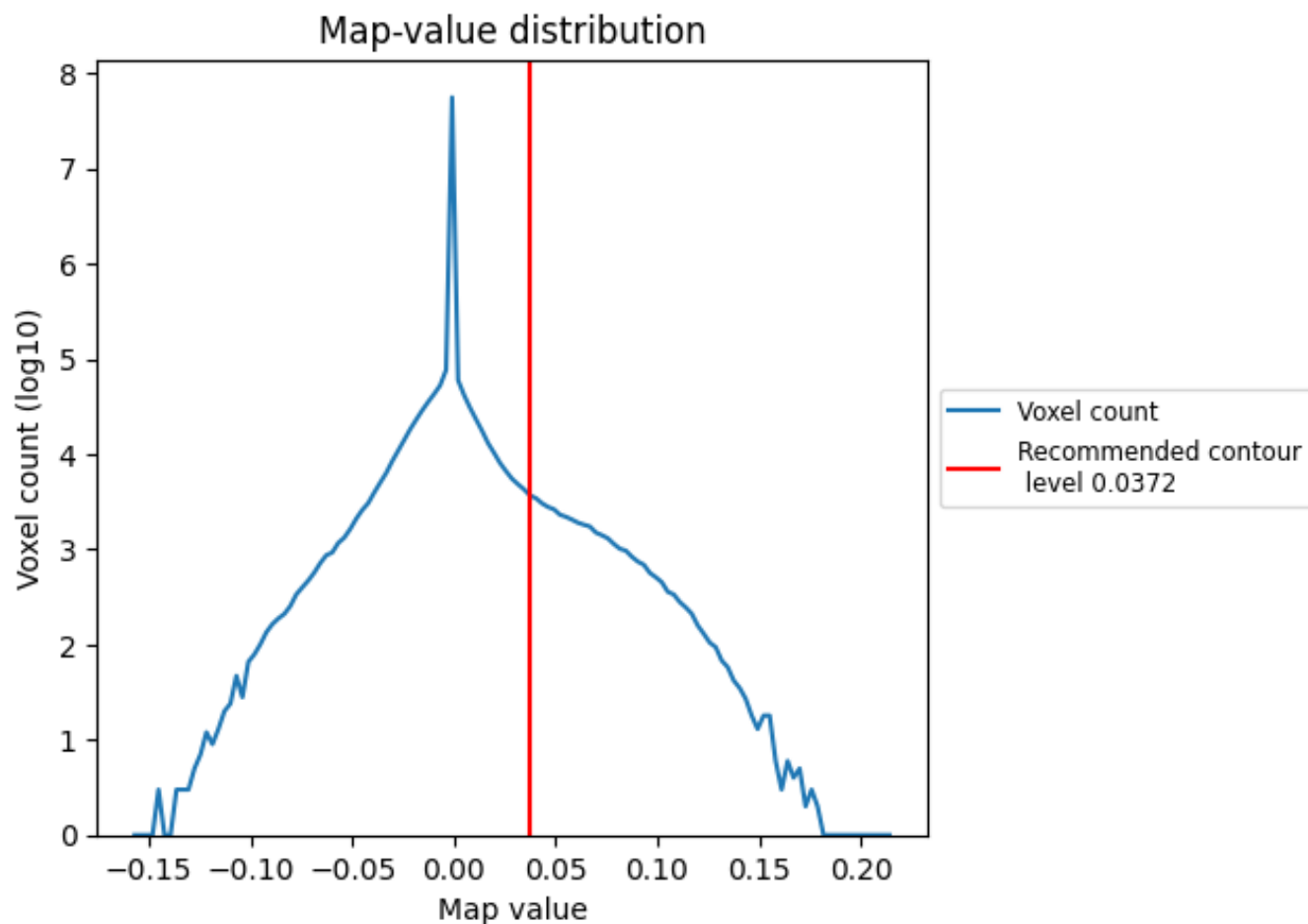
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

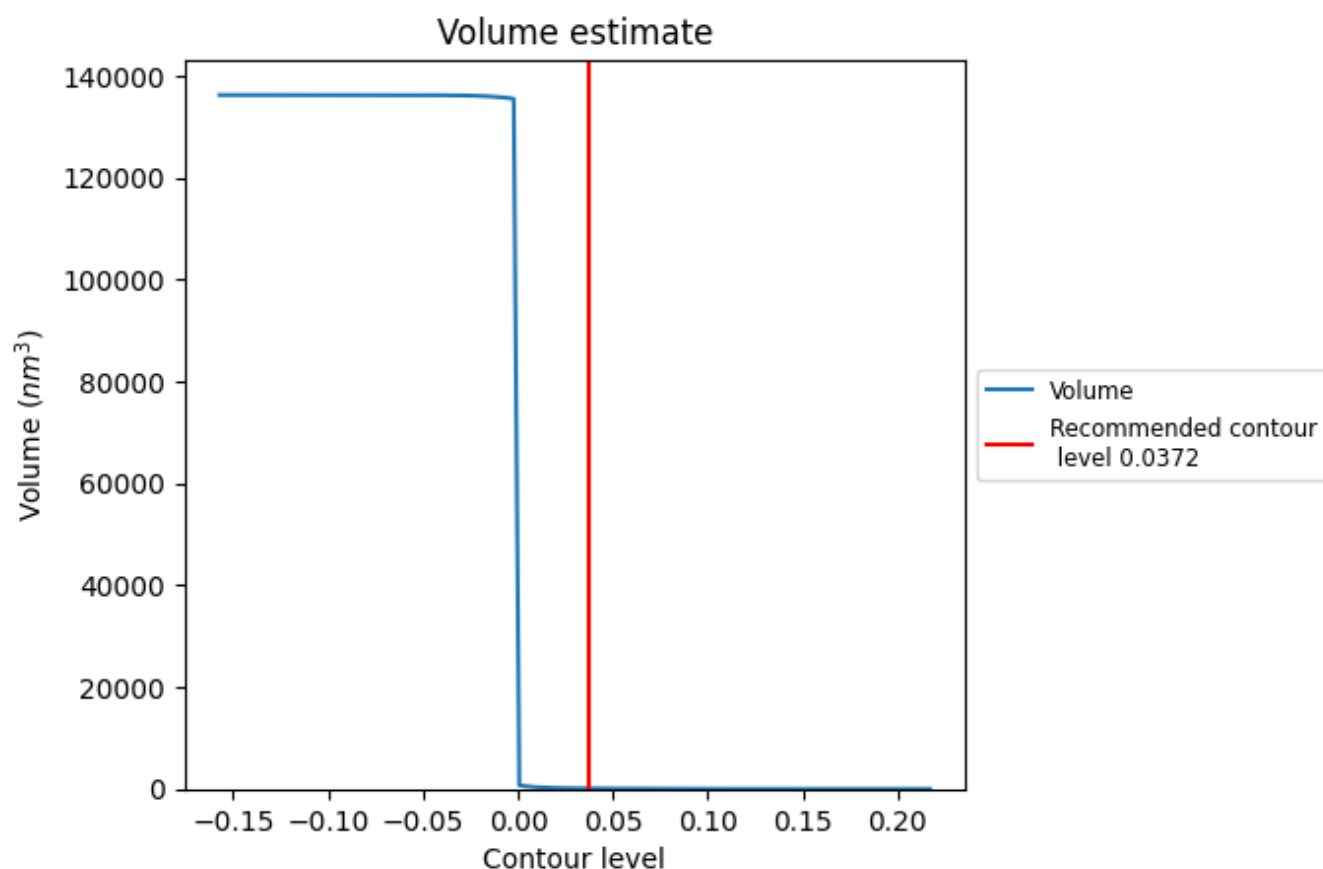
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

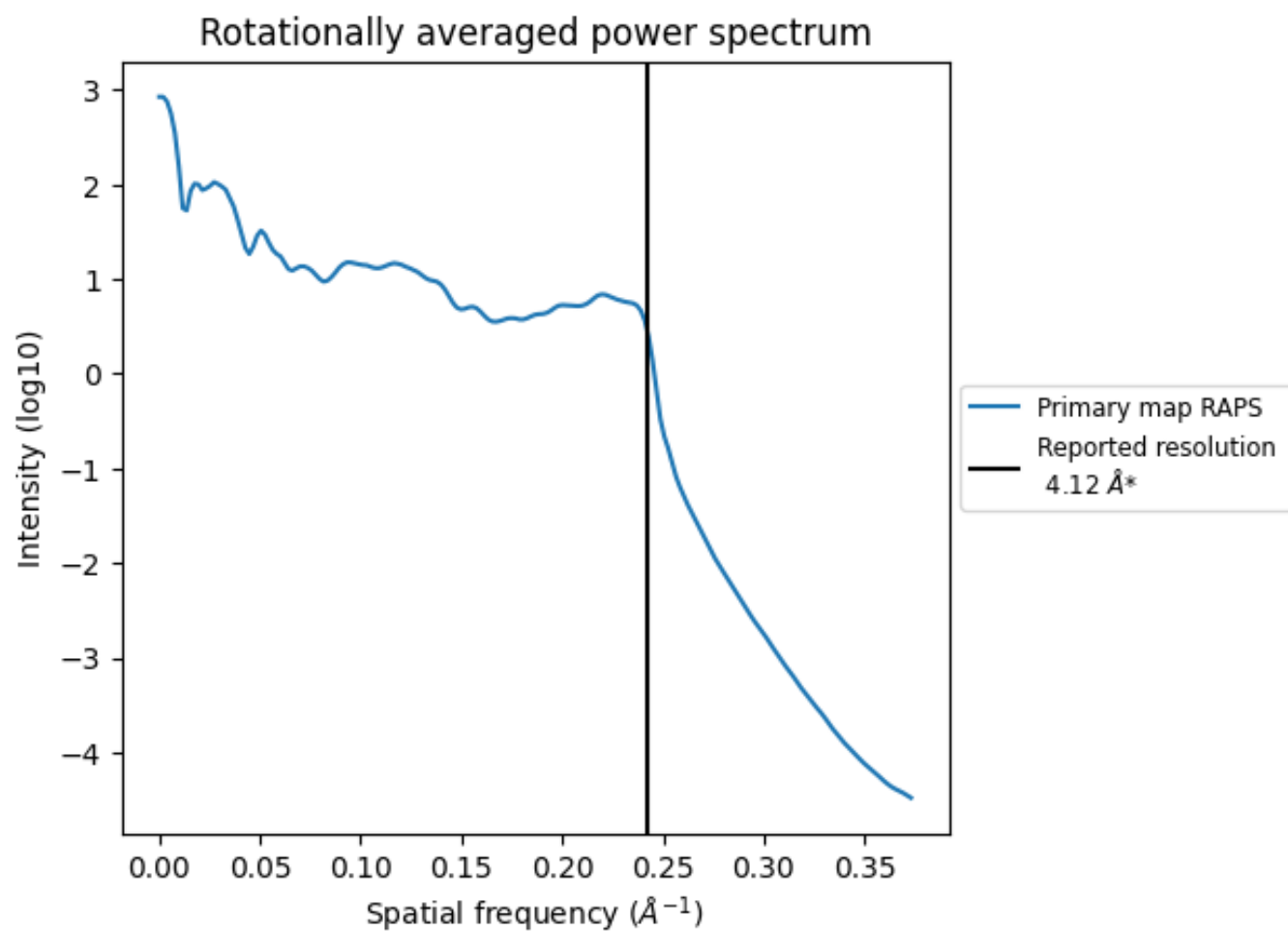
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm^3 ; this corresponds to an approximate mass of 90 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.243 Å⁻¹

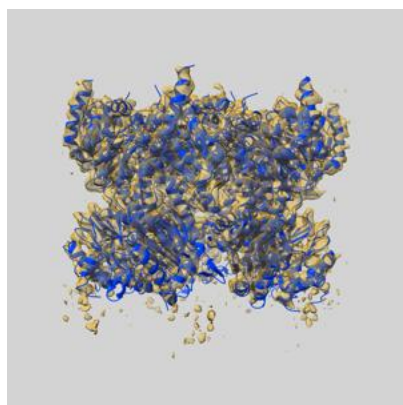
8 Fourier-Shell correlation

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

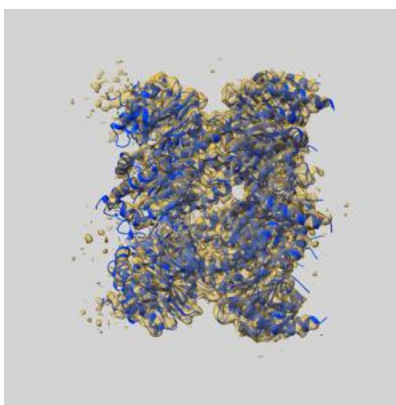
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0210 and PDB model 6HE5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

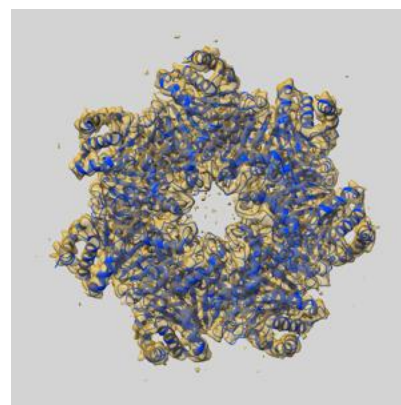
9.1 Map-model overlay [i](#)



X



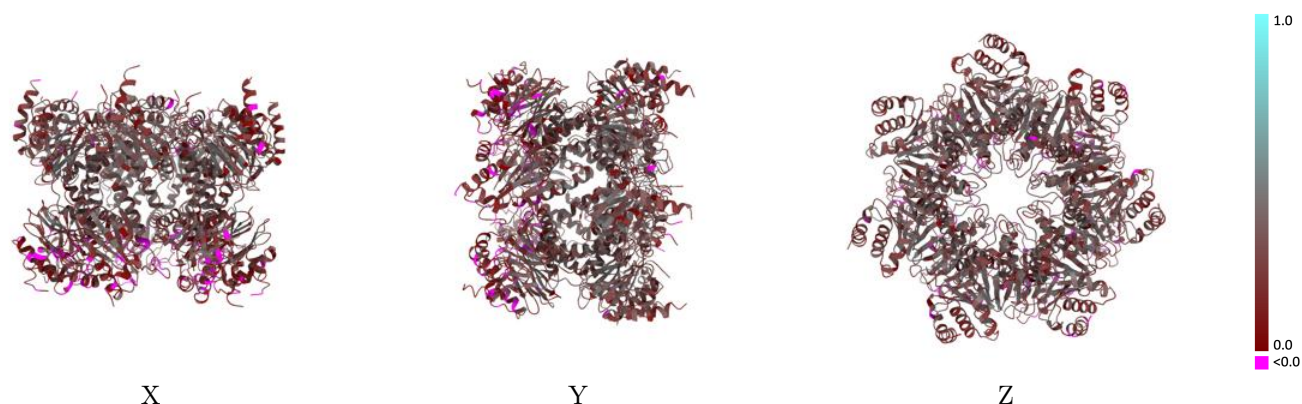
Y



Z

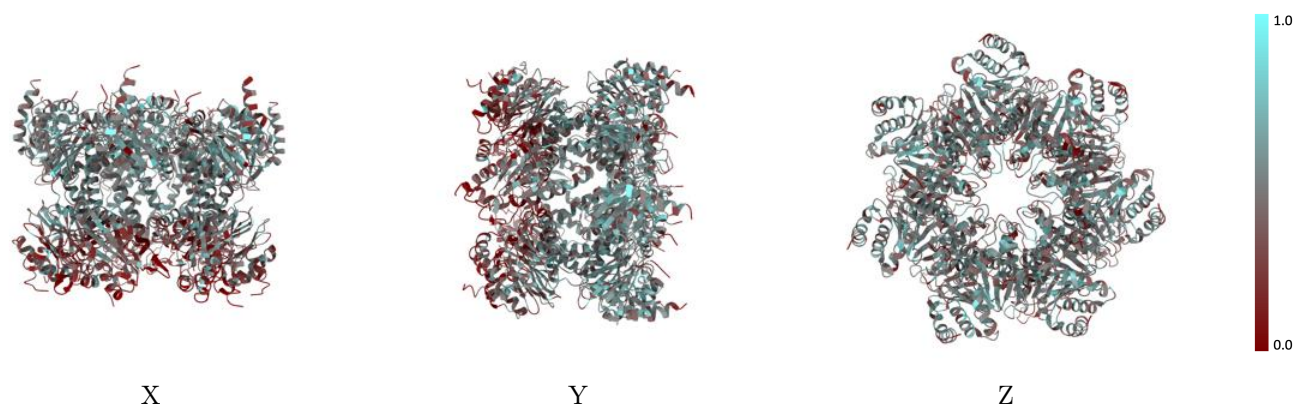
The images above show the 3D surface view of the map at the recommended contour level 0.0372 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



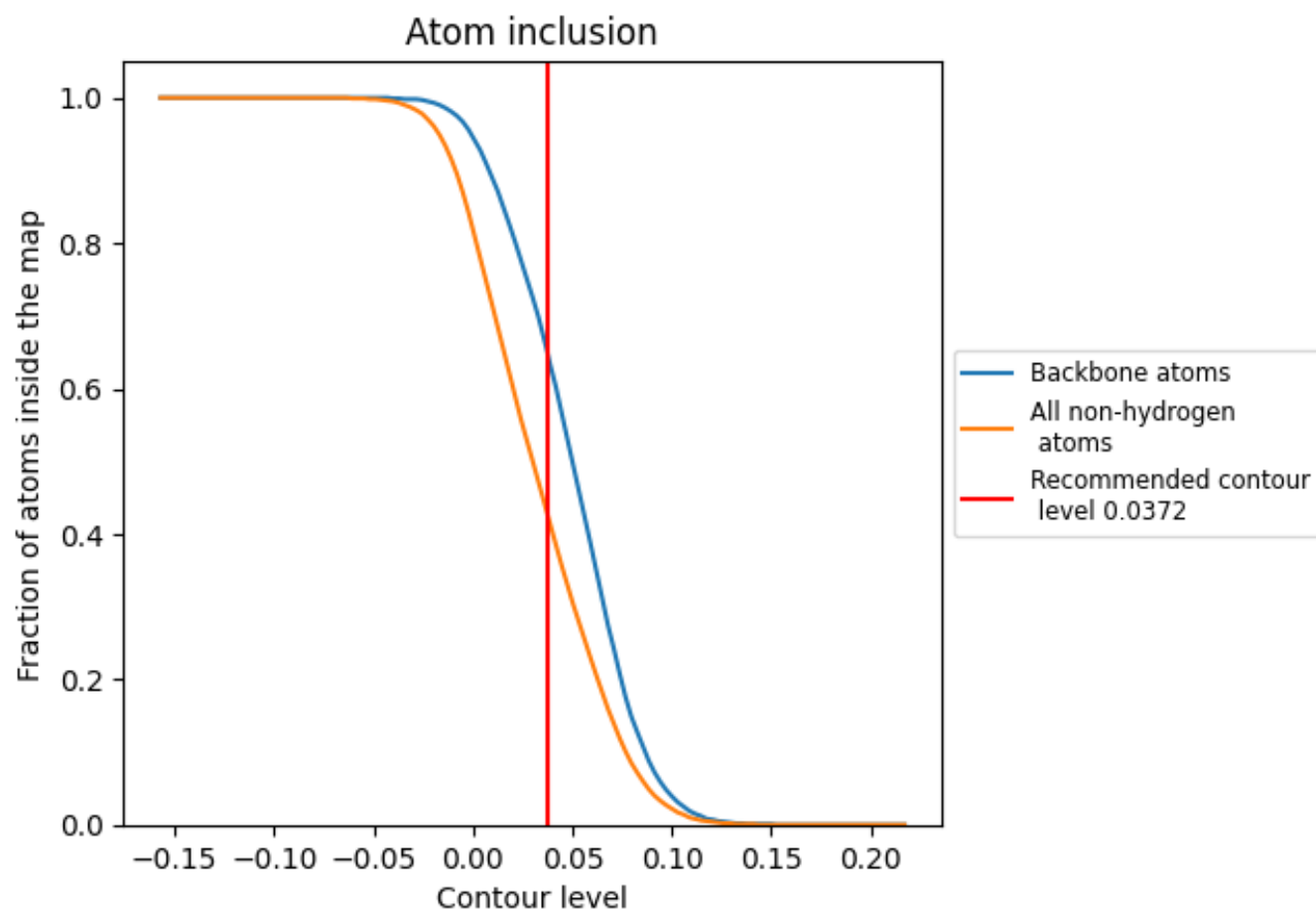
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0372).

9.4 Atom inclusion ⓘ



At the recommended contour level, 65% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0372) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4290	 0.2660
1	 0.3180	 0.2210
2	 0.3370	 0.2170
3	 0.3220	 0.2070
4	 0.3240	 0.2090
5	 0.3220	 0.2000
6	 0.3220	 0.2240
7	 0.3120	 0.2000
A	 0.5200	 0.3060
B	 0.5340	 0.3150
C	 0.5250	 0.3280
D	 0.5280	 0.3110
E	 0.5220	 0.3130
F	 0.5350	 0.3210
G	 0.5020	 0.2970
H	 0.1860	 0.0680
I	 0.2290	 0.2200
J	 0.2140	 0.2510
K	 0.2000	 0.1630
L	 0.0710	 0.1190
M	 0.1860	 0.1990

