



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:49 PM UTC

PDB ID : 6HE7 / pdb_00006he7
EMDB ID : EMD-0211
Title : 20S proteasome from Archaeoglobus fulgidus
Authors : Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.
Deposited on : 2018-08-20
Resolution : 3.69 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

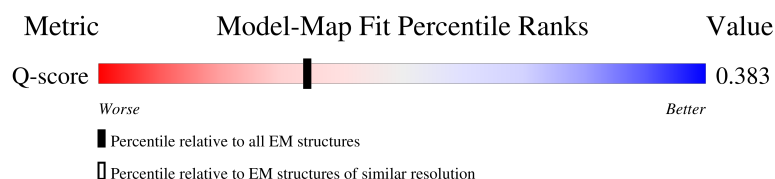
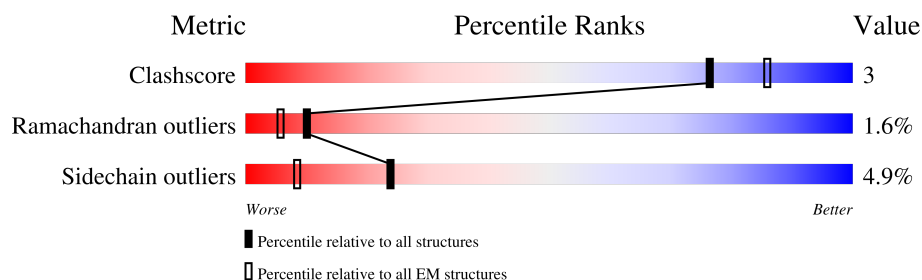
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.69 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	11284 (3.19 - 4.18)

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	235	23% 40% 53% 7%
1	B	235	20% 41% 52% 6%
1	C	235	20% 40% 51% 9%
1	D	235	24% 40% 52% 8%

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Mol	Chain	Length	Quality of chain
1	E	235	
1	F	235	
1	G	235	
2	1	202	
2	2	202	
2	3	202	
2	4	202	
2	5	202	
2	6	202	
2	7	202	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23821 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	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	B	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	C	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	D	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	E	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	F	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		
1	G	235	Total	C	N	O	S	0	0
			1850	1177	310	357	6		

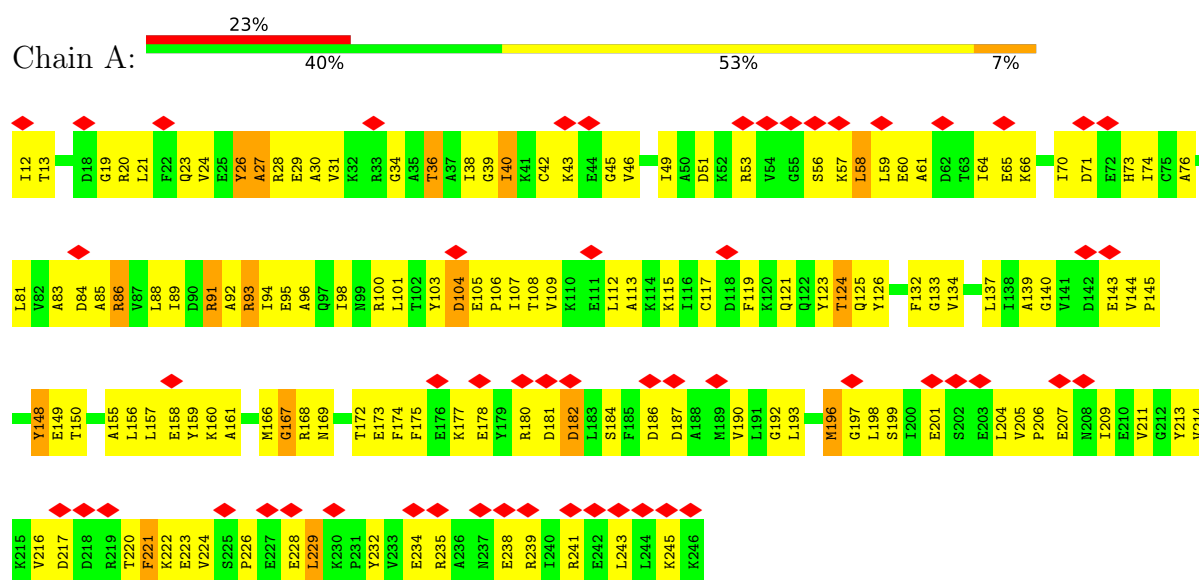
- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	2	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	3	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	4	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	5	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	6	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		
2	7	202	Total	C	N	O	S	0	0
			1553	982	260	305	6		

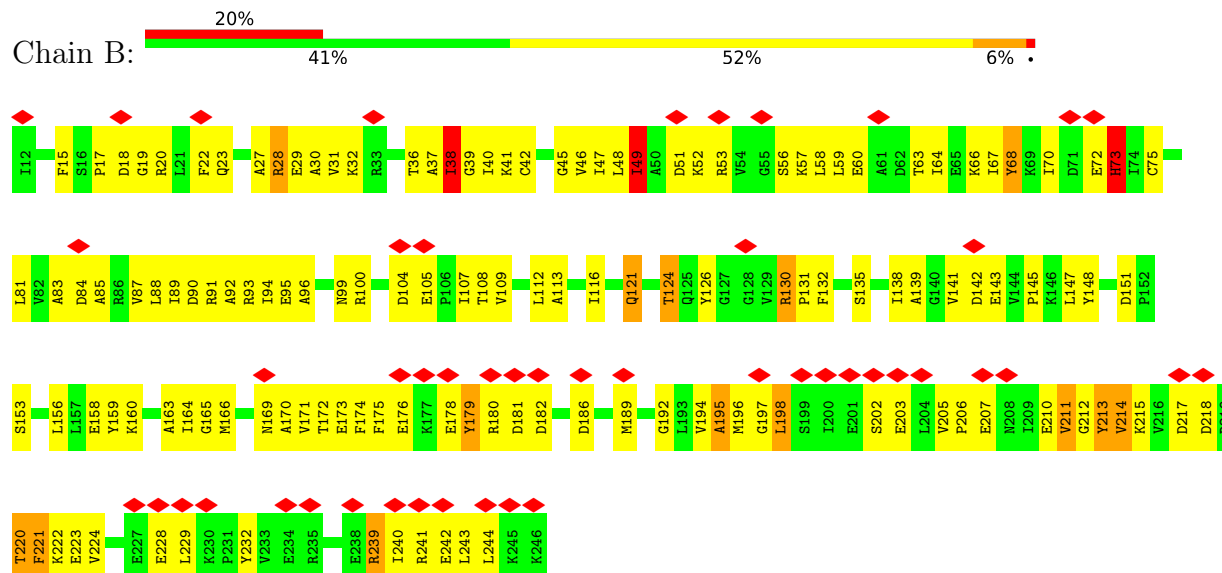
3 Residue-property plots

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

• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha



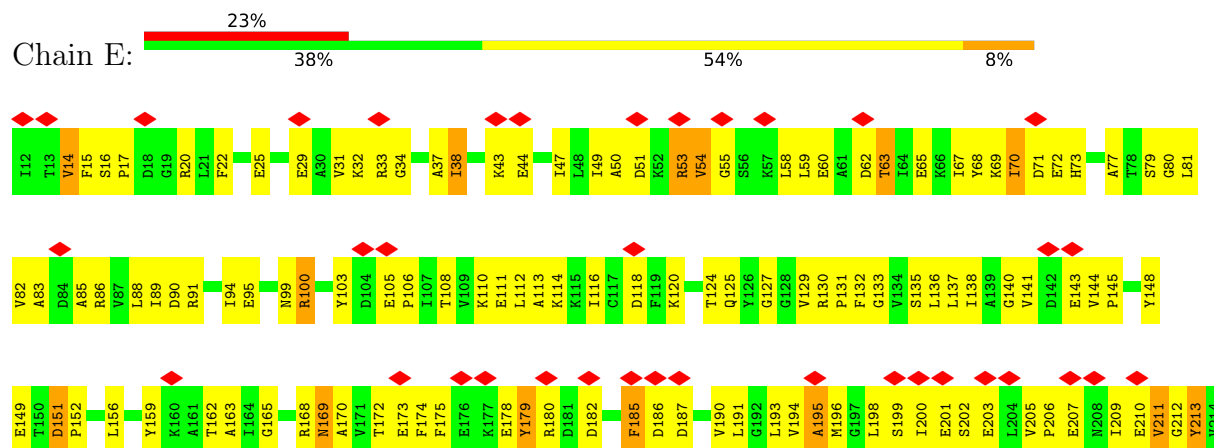
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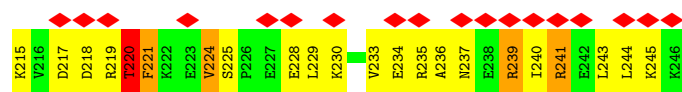


• Molecule 1: Proteasome subunit alpha

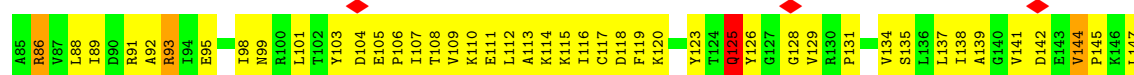
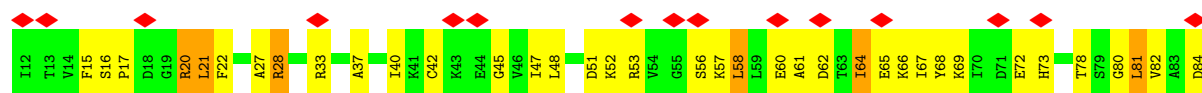
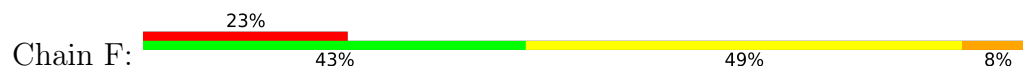


• Molecule 1: Proteasome subunit alpha

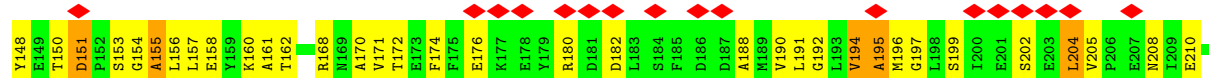
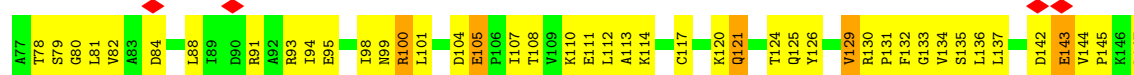
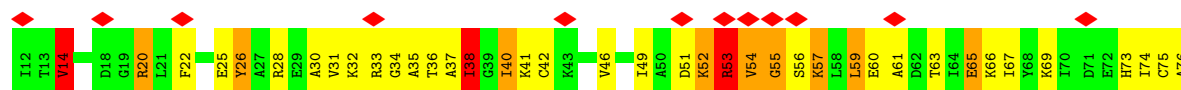
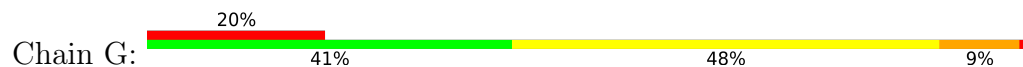




• Molecule 1: Proteasome subunit alpha

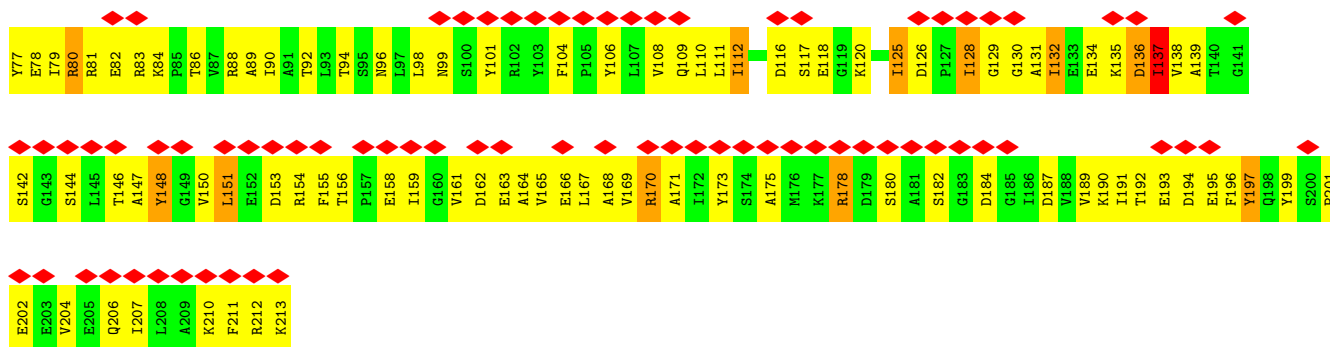


• Molecule 1: Proteasome subunit alpha

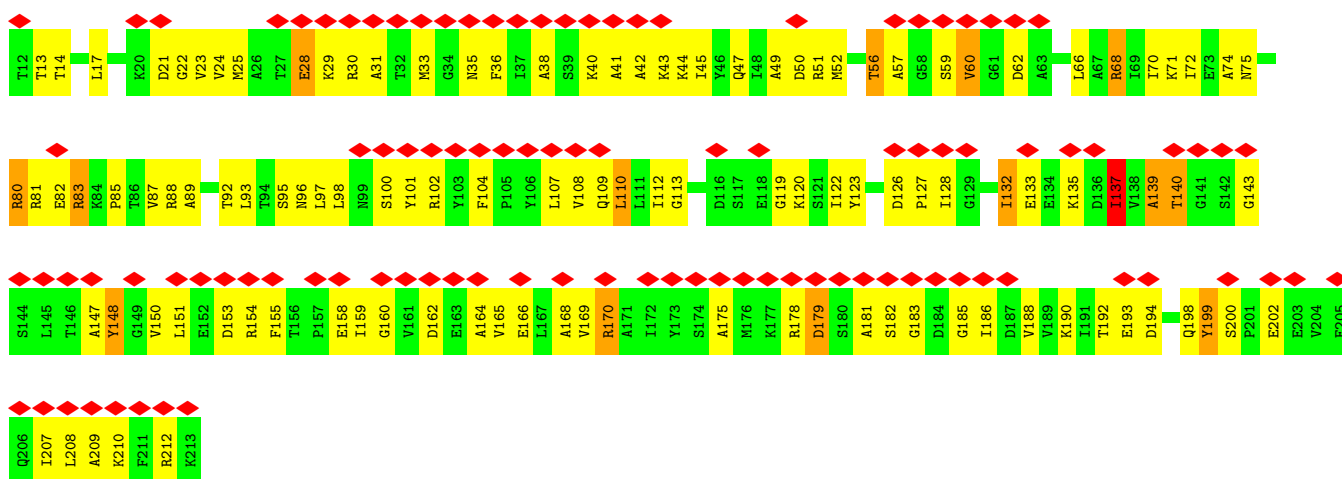


• Molecule 2: Proteasome subunit beta

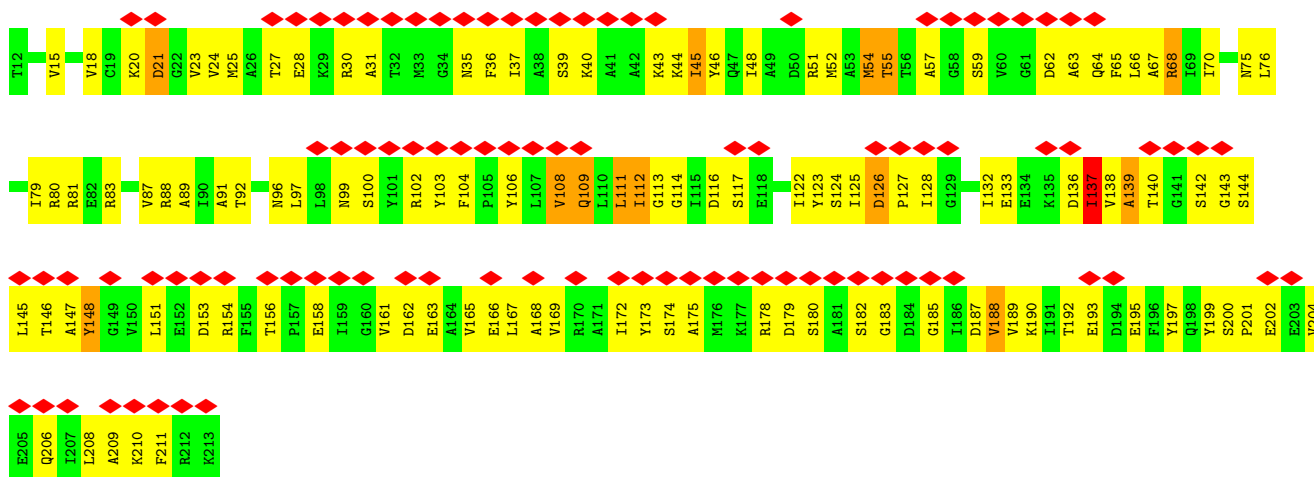




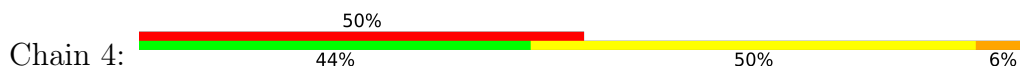
• Molecule 2: Proteasome subunit beta

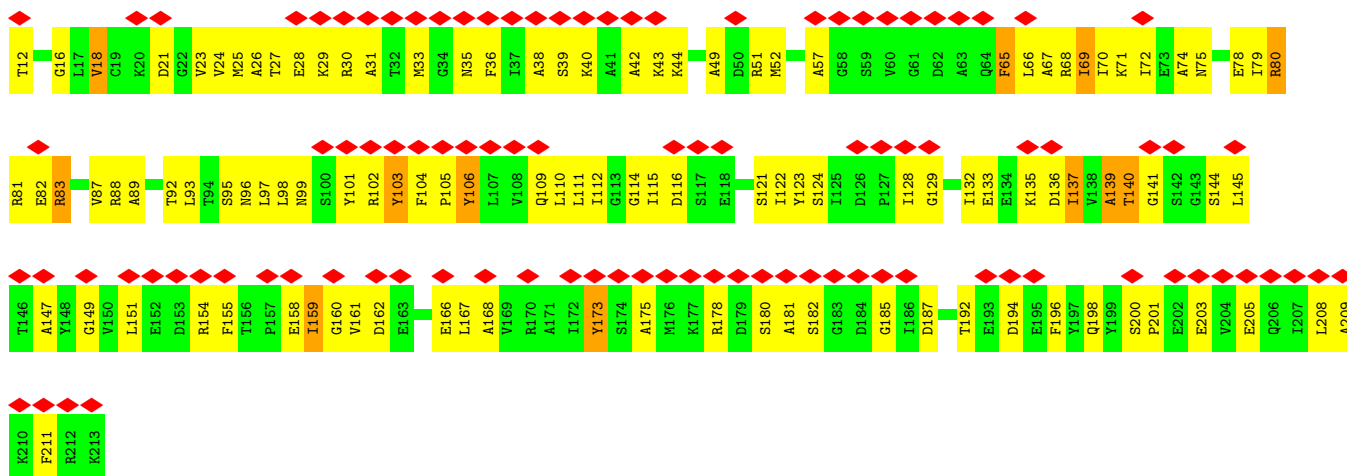


• Molecule 2: Proteasome subunit beta

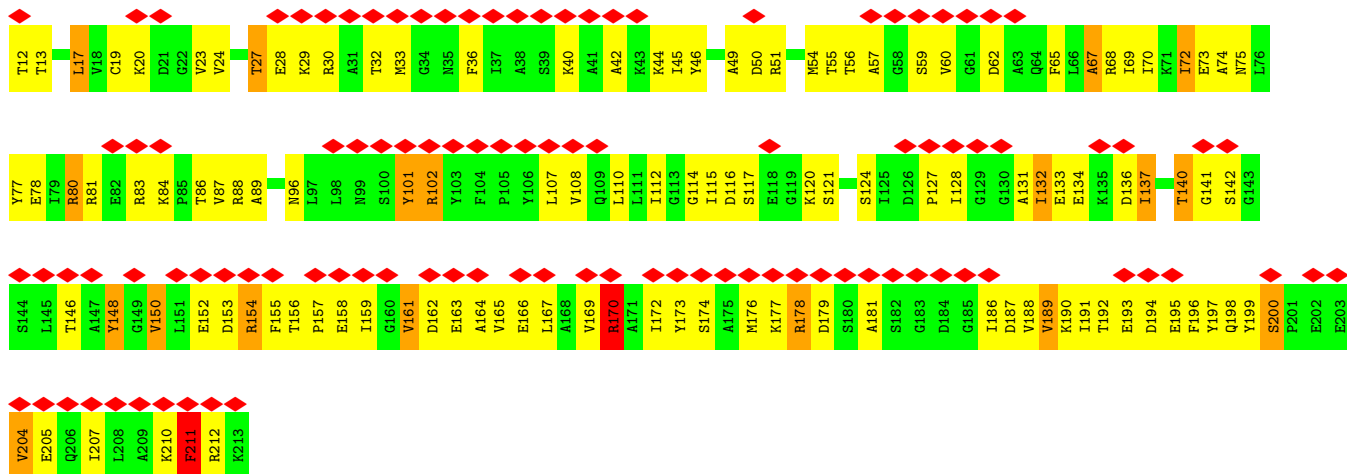


• Molecule 2: Proteasome subunit beta

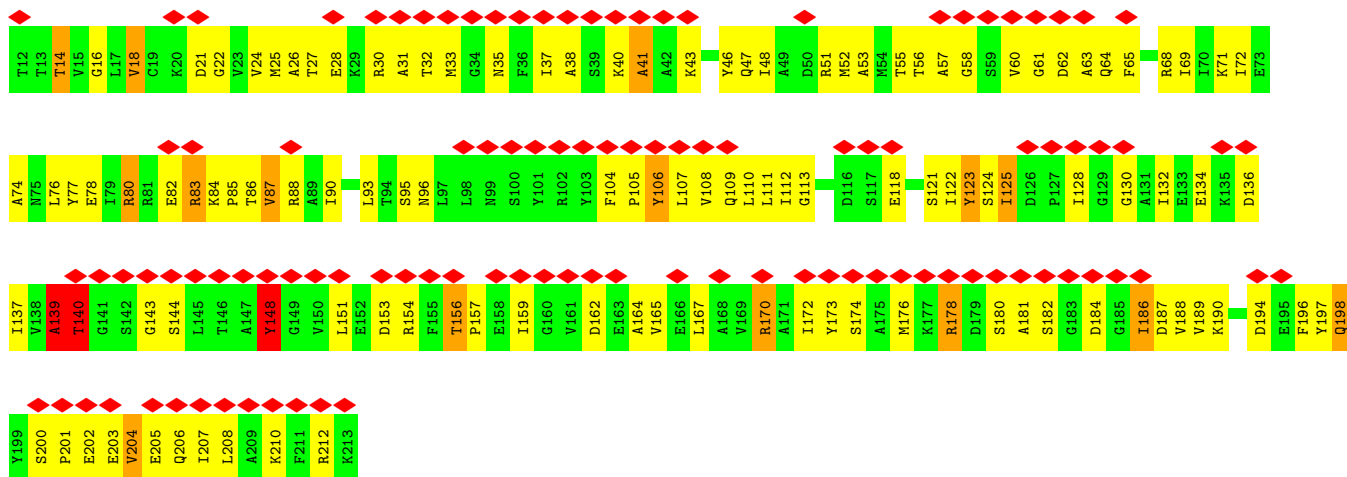
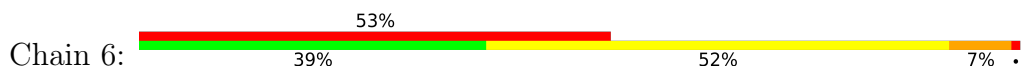




• Molecule 2: Proteasome subunit beta

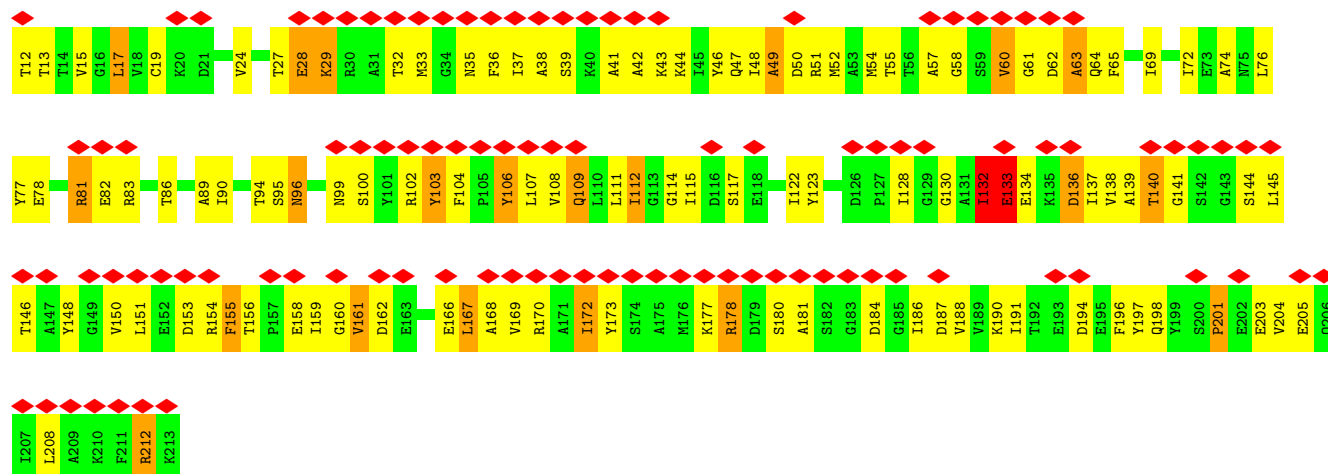


• Molecule 2: Proteasome subunit beta



● Molecule 2: Proteasome subunit beta

Chain 7: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	105384	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	0.509	Depositor
Minimum map value	-0.339	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	2.29	77/1876 (4.1%)	2.42	115/2528 (4.5%)
1	B	2.26	78/1876 (4.2%)	2.49	135/2528 (5.3%)
1	C	2.25	67/1876 (3.6%)	2.55	129/2528 (5.1%)
1	D	2.31	86/1876 (4.6%)	2.45	122/2528 (4.8%)
1	E	2.31	74/1876 (3.9%)	2.51	145/2528 (5.7%)
1	F	2.25	68/1876 (3.6%)	2.51	137/2528 (5.4%)
1	G	2.31	80/1876 (4.3%)	2.48	125/2528 (4.9%)
2	1	2.36	73/1573 (4.6%)	2.56	128/2121 (6.0%)
2	2	2.40	70/1573 (4.5%)	2.49	112/2121 (5.3%)
2	3	2.38	76/1573 (4.8%)	2.53	116/2121 (5.5%)
2	4	2.30	55/1573 (3.5%)	2.41	90/2121 (4.2%)
2	5	3.46	81/1573 (5.1%)	2.47	109/2121 (5.1%)
2	6	2.33	77/1573 (4.9%)	2.49	116/2121 (5.5%)
2	7	2.32	65/1573 (4.1%)	2.52	117/2121 (5.5%)
All	All	2.40	1027/24143 (4.3%)	2.49	1696/32543 (5.2%)

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	5
1	C	0	10
1	D	0	10
1	E	0	11
1	F	0	9
1	G	0	12
2	1	0	5
2	2	0	8
2	3	0	4
2	4	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	5	0	10
2	6	0	8
2	7	0	6
All	All	0	115

All (1027) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	211	PHE	CG-CD1	75.44	2.97	1.38
2	5	211	PHE	CG-CD2	38.01	2.18	1.38
2	5	211	PHE	CE2-CZ	29.40	2.26	1.38
2	5	211	PHE	CD1-CE1	28.09	2.23	1.38
2	5	211	PHE	CE1-CZ	27.27	2.20	1.38
2	5	211	PHE	CD2-CE2	27.09	2.19	1.38
1	A	119	PHE	N-CA	-11.45	1.32	1.46
2	3	133	GLU	CA-C	-11.21	1.39	1.52
2	7	187	ASP	C-N	10.62	1.48	1.33
2	3	83	ARG	CD-NE	9.97	1.60	1.46
2	2	137	ILE	C-N	9.77	1.45	1.33
1	E	91	ARG	NE-CZ	9.66	1.43	1.33
1	D	113	ALA	CA-C	-9.51	1.40	1.52
1	D	124	THR	CA-C	-9.48	1.40	1.52
2	2	110	LEU	CA-C	-9.16	1.41	1.52
1	B	205	VAL	CA-C	-9.09	1.43	1.52
2	4	68	ARG	NE-CZ	9.05	1.43	1.33
2	6	51	ARG	NE-CZ	8.99	1.43	1.33
1	B	52	LYS	CA-C	-8.96	1.41	1.53
2	6	167	LEU	CA-CB	8.95	1.67	1.53
1	E	67	ILE	CA-CB	-8.91	1.43	1.54
1	E	44	GLU	C-N	8.91	1.46	1.32
1	G	105	GLU	CA-C	-8.82	1.43	1.52
2	5	199	TYR	CA-C	-8.82	1.41	1.52
2	2	42	ALA	CA-C	-8.77	1.41	1.52
1	E	58	LEU	N-CA	-8.76	1.33	1.45
2	3	154	ARG	CD-NE	8.75	1.58	1.46
1	F	104	ASP	CA-CB	8.68	1.66	1.53
1	B	51	ASP	CA-CB	8.66	1.63	1.52
1	F	53	ARG	CA-CB	8.66	1.67	1.53
1	E	200	ILE	CA-CB	-8.65	1.44	1.54
1	E	60	GLU	CA-CB	8.61	1.63	1.52
2	6	173	TYR	CA-CB	8.54	1.66	1.53
1	A	24	VAL	CA-CB	-8.51	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	ARG	NE-CZ	8.50	1.42	1.33
2	1	212	ARG	NE-CZ	8.49	1.42	1.33
2	4	96	ASN	CA-CB	8.45	1.66	1.53
1	A	31	VAL	CA-C	-8.42	1.42	1.52
2	2	36	PHE	C-N	8.41	1.43	1.33
1	E	234	GLU	N-CA	8.40	1.56	1.46
2	5	72	ILE	CA-CB	8.37	1.64	1.54
2	1	144	SER	CA-C	-8.32	1.41	1.52
1	D	158	GLU	CA-C	-8.31	1.42	1.52
1	A	223	GLU	CA-C	-8.28	1.42	1.52
1	C	86	ARG	NE-CZ	8.28	1.42	1.33
1	D	160	LYS	C-N	8.27	1.43	1.33
2	2	107	LEU	CA-CB	8.26	1.63	1.52
2	2	155	PHE	C-N	8.23	1.43	1.33
2	1	43	LYS	N-CA	-8.20	1.36	1.46
1	C	212	GLY	CA-C	-8.20	1.42	1.51
2	2	154	ARG	CA-C	-8.18	1.41	1.52
1	C	33	ARG	NE-CZ	8.17	1.42	1.33
2	1	148	TYR	N-CA	-8.17	1.36	1.46
2	3	59	SER	CA-C	-8.10	1.42	1.52
2	1	126	ASP	C-N	-8.09	1.25	1.34
1	E	182	ASP	N-CA	-8.08	1.36	1.46
1	A	239	ARG	CD-NE	8.03	1.57	1.46
2	2	113	GLY	N-CA	-7.99	1.37	1.45
1	G	133	GLY	CA-C	-7.99	1.40	1.51
1	B	105	GLU	CA-C	-7.97	1.46	1.52
1	B	70	ILE	CA-C	-7.96	1.45	1.52
1	A	115	LYS	N-CA	-7.96	1.36	1.46
1	D	84	ASP	CA-C	-7.93	1.42	1.52
1	G	241	ARG	NE-CZ	7.93	1.41	1.33
1	E	77	ALA	CA-C	-7.93	1.43	1.52
1	G	75	CYS	CA-C	-7.93	1.42	1.52
1	G	192	GLY	CA-C	-7.93	1.43	1.52
1	E	190	VAL	CA-CB	-7.93	1.44	1.54
2	5	137	ILE	CA-C	-7.93	1.43	1.52
1	F	42	CYS	CA-CB	7.91	1.65	1.53
1	B	203	GLU	CA-C	-7.89	1.42	1.52
1	G	67	ILE	N-CA	-7.88	1.36	1.46
1	A	243	LEU	CA-C	-7.87	1.42	1.52
1	G	233	VAL	CA-CB	-7.87	1.44	1.54
2	2	192	THR	N-CA	7.85	1.54	1.46
1	E	156	LEU	N-CA	-7.84	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	35	ASN	CA-C	-7.84	1.43	1.53
1	G	241	ARG	C-N	7.82	1.43	1.33
1	C	115	LYS	N-CA	-7.81	1.36	1.46
2	3	190	LYS	CA-C	-7.79	1.43	1.52
2	3	80	ARG	CA-CB	7.79	1.65	1.53
2	3	202	GLU	CA-C	-7.76	1.42	1.52
2	1	142	SER	CA-C	7.76	1.63	1.52
2	7	86	THR	CA-C	-7.75	1.43	1.52
2	7	203	GLU	N-CA	-7.75	1.36	1.46
2	5	45	ILE	CA-C	-7.74	1.43	1.52
1	G	161	ALA	CA-C	-7.74	1.42	1.52
2	5	148	TYR	CA-CB	7.73	1.65	1.53
1	D	144	VAL	CA-C	-7.73	1.44	1.52
1	G	174	PHE	CA-C	-7.72	1.43	1.52
1	A	148	TYR	CA-C	-7.69	1.43	1.52
2	1	166	GLU	N-CA	-7.68	1.37	1.46
2	1	151	LEU	CA-C	-7.67	1.43	1.52
1	B	192	GLY	N-CA	-7.66	1.35	1.45
1	E	20	ARG	C-O	7.66	1.33	1.23
2	5	60	VAL	C-N	7.66	1.42	1.33
1	A	91	ARG	NE-CZ	7.65	1.41	1.33
1	D	146	LYS	N-CA	-7.65	1.36	1.46
1	D	163	ALA	CA-C	-7.65	1.43	1.52
2	7	46	TYR	CA-C	-7.59	1.43	1.52
2	7	15	VAL	CA-C	-7.59	1.43	1.52
2	1	55	THR	CA-C	-7.54	1.43	1.52
2	1	137	ILE	C-N	7.53	1.40	1.33
1	G	69	LYS	CA-C	-7.53	1.43	1.52
1	G	73	HIS	CA-CB	7.53	1.64	1.53
1	C	171	VAL	CA-CB	-7.53	1.45	1.54
2	5	96	ASN	CA-CB	7.51	1.65	1.53
2	7	123	TYR	CA-CB	7.50	1.64	1.53
2	5	196	PHE	CA-C	-7.47	1.43	1.53
2	2	93	LEU	C-N	7.45	1.44	1.33
1	B	66	LYS	CA-C	7.45	1.61	1.52
1	C	91	ARG	C-N	7.44	1.44	1.33
2	7	159	ILE	CA-C	-7.42	1.44	1.52
2	3	75	ASN	CA-C	-7.42	1.43	1.52
1	E	86	ARG	NE-CZ	7.41	1.41	1.33
2	3	83	ARG	CA-C	-7.40	1.42	1.52
2	4	12	THR	C-N	7.40	1.43	1.33
2	6	68	ARG	N-CA	-7.38	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	131	PRO	N-CA	-7.38	1.38	1.47
1	A	133	GLY	CA-C	-7.37	1.41	1.51
1	D	30	ALA	CA-C	-7.37	1.43	1.52
2	2	23	VAL	CA-C	-7.37	1.43	1.52
1	F	86	ARG	NE-CZ	7.35	1.41	1.33
1	G	91	ARG	CD-NE	7.35	1.56	1.46
2	6	106	TYR	N-CA	-7.35	1.36	1.46
1	C	214	VAL	CA-C	-7.35	1.43	1.52
2	3	54	MET	CA-C	-7.33	1.43	1.52
2	7	197	TYR	N-CA	-7.33	1.37	1.46
2	5	88	ARG	N-CA	-7.32	1.37	1.46
2	7	108	VAL	C-N	7.29	1.43	1.33
1	D	111	GLU	CA-C	-7.28	1.43	1.52
2	4	123	TYR	CA-C	-7.27	1.44	1.52
1	F	60	GLU	CA-C	-7.25	1.43	1.52
2	2	31	ALA	CA-C	-7.24	1.43	1.52
2	5	50	ASP	CA-C	-7.24	1.42	1.52
2	5	116	ASP	N-CA	-7.24	1.37	1.46
1	F	141	VAL	CA-C	-7.22	1.43	1.52
2	7	134	GLU	CA-C	-7.22	1.43	1.52
2	1	98	LEU	CA-C	-7.21	1.43	1.52
1	B	174	PHE	N-CA	7.21	1.54	1.46
1	A	65	GLU	CA-C	-7.19	1.43	1.52
1	D	141	VAL	CA-C	-7.19	1.43	1.52
1	G	42	CYS	CA-C	-7.19	1.43	1.53
2	1	65	PHE	CA-CB	7.17	1.64	1.53
2	4	88	ARG	CD-NE	7.17	1.56	1.46
2	6	190	LYS	CA-C	-7.17	1.44	1.52
2	1	83	ARG	NE-CZ	7.16	1.41	1.33
2	3	127	PRO	C-N	7.15	1.41	1.33
1	E	206	PRO	CA-C	-7.15	1.45	1.52
2	2	170	ARG	NE-CZ	7.14	1.41	1.33
1	G	41	LYS	CA-C	-7.13	1.44	1.52
2	5	51	ARG	CZ-NH1	7.12	1.42	1.32
2	6	144	SER	CA-CB	7.12	1.64	1.53
2	5	196	PHE	N-CA	-7.12	1.37	1.46
2	7	13	THR	C-N	7.11	1.42	1.33
2	4	122	ILE	CA-CB	7.10	1.63	1.54
1	A	64	ILE	CA-CB	-7.10	1.45	1.54
2	1	130	GLY	CA-C	-7.09	1.41	1.51
1	D	112	LEU	N-CA	-7.07	1.37	1.46
2	1	92	THR	N-CA	-7.06	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	148	TYR	CA-C	-7.05	1.43	1.52
2	5	120	LYS	C-N	7.05	1.42	1.33
1	D	60	GLU	CA-CB	7.04	1.61	1.52
1	E	130	ARG	CZ-NH2	7.03	1.42	1.33
2	1	193	GLU	CA-CB	7.03	1.65	1.53
1	A	53	ARG	NE-CZ	7.02	1.40	1.33
1	A	214	VAL	CA-CB	-7.02	1.46	1.54
2	2	120	LYS	N-CA	-7.02	1.37	1.46
2	3	87	VAL	C-N	7.02	1.43	1.33
1	D	52	LYS	CA-C	-7.01	1.46	1.53
2	6	207	ILE	N-CA	-6.97	1.37	1.46
1	E	205	VAL	C-N	6.96	1.39	1.33
1	G	78	THR	CA-C	-6.96	1.44	1.52
2	7	169	VAL	C-N	6.93	1.43	1.33
2	6	212	ARG	CD-NE	6.93	1.55	1.46
1	A	98	ILE	N-CA	6.92	1.54	1.46
1	D	213	TYR	N-CA	-6.92	1.36	1.45
2	6	157	PRO	CA-CB	6.91	1.61	1.53
1	B	85	ALA	N-CA	-6.91	1.38	1.46
1	B	164	ILE	N-CA	-6.91	1.38	1.46
1	F	198	LEU	N-CA	6.91	1.54	1.46
1	E	94	ILE	CA-CB	-6.90	1.46	1.54
2	5	121	SER	CA-C	-6.90	1.44	1.52
1	C	224	VAL	CA-C	-6.89	1.44	1.52
1	D	219	ARG	NE-CZ	6.89	1.40	1.33
1	D	134	VAL	CA-CB	-6.89	1.45	1.54
1	E	20	ARG	CA-C	-6.88	1.44	1.52
2	2	113	GLY	CA-C	-6.88	1.44	1.51
1	A	57	LYS	C-N	6.88	1.43	1.33
2	6	132	ILE	N-CA	-6.87	1.38	1.46
2	4	168	ALA	C-N	6.87	1.42	1.33
2	4	106	TYR	C-N	6.87	1.43	1.33
2	5	114	GLY	CA-C	-6.87	1.42	1.51
2	4	80	ARG	CD-NE	6.86	1.55	1.46
2	6	77	TYR	CA-CB	6.86	1.64	1.53
1	A	239	ARG	NE-CZ	6.85	1.40	1.33
2	2	190	LYS	N-CA	-6.85	1.37	1.46
2	2	139	ALA	C-N	6.85	1.42	1.33
1	G	91	ARG	C-N	6.83	1.42	1.33
2	3	210	LYS	CA-C	-6.83	1.43	1.52
1	E	168	ARG	NE-CZ	6.83	1.40	1.33
2	6	113	GLY	CA-C	-6.83	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	124	SER	CA-CB	6.83	1.63	1.53
2	6	78	GLU	C-N	6.82	1.42	1.33
2	2	127	PRO	CA-C	-6.81	1.46	1.52
2	2	80	ARG	NE-CZ	6.81	1.40	1.33
1	F	37	ALA	CA-C	-6.80	1.44	1.52
2	6	148	TYR	N-CA	-6.79	1.38	1.46
1	E	83	ALA	CA-C	-6.79	1.44	1.52
2	3	36	PHE	CA-C	-6.79	1.44	1.52
2	3	45	ILE	CA-CB	-6.79	1.46	1.54
2	6	30	ARG	N-CA	-6.78	1.38	1.46
1	E	141	VAL	CA-CB	6.77	1.63	1.54
2	1	80	ARG	CD-NE	6.77	1.55	1.46
1	F	47	ILE	CA-CB	-6.76	1.45	1.54
2	2	81	ARG	NE-CZ	6.76	1.40	1.33
1	B	20	ARG	NE-CZ	6.75	1.40	1.33
1	D	33	ARG	NE-CZ	6.74	1.40	1.33
2	3	15	VAL	CA-C	-6.74	1.44	1.52
2	6	52	MET	CA-C	-6.74	1.44	1.52
1	G	214	VAL	CA-CB	-6.73	1.46	1.54
1	F	52	LYS	N-CA	-6.73	1.37	1.46
2	1	79	ILE	CA-C	6.72	1.61	1.52
1	A	105	GLU	CA-C	-6.71	1.45	1.52
2	7	158	GLU	CA-CB	6.71	1.62	1.53
1	D	112	LEU	C-N	6.70	1.43	1.33
1	C	100	ARG	NE-CZ	6.70	1.40	1.33
2	7	107	LEU	CA-C	-6.70	1.44	1.53
2	7	148	TYR	CA-C	-6.69	1.44	1.52
2	5	141	GLY	C-O	-6.68	1.20	1.24
2	6	198	GLN	CA-C	-6.68	1.44	1.52
1	F	81	LEU	CA-CB	6.68	1.62	1.53
2	1	48	ILE	CA-C	-6.68	1.43	1.52
2	6	156	THR	C-N	-6.67	1.28	1.33
1	G	56	SER	C-N	6.67	1.43	1.33
2	7	155	PHE	CA-CB	6.67	1.62	1.53
2	4	187	ASP	CA-CB	6.66	1.63	1.53
2	7	150	VAL	CA-CB	-6.66	1.46	1.54
2	3	106	TYR	CA-C	-6.66	1.45	1.53
2	6	172	ILE	CA-C	6.64	1.61	1.52
1	D	103	TYR	CA-C	-6.64	1.43	1.52
1	G	204	LEU	C-N	6.62	1.40	1.33
2	1	16	GLY	CA-C	-6.62	1.42	1.51
2	4	181	ALA	CA-C	-6.61	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	PRO	N-CA	-6.60	1.39	1.47
1	G	60	GLU	CA-C	-6.60	1.45	1.53
1	G	120	LYS	CA-C	-6.60	1.44	1.52
2	5	178	ARG	NE-CZ	6.60	1.40	1.33
2	1	64	GLN	CA-C	-6.59	1.44	1.52
2	5	88	ARG	CD-NE	6.59	1.55	1.46
1	A	139	ALA	C-N	6.59	1.40	1.33
1	D	134	VAL	CA-C	-6.59	1.44	1.52
2	5	74	ALA	CA-C	-6.59	1.44	1.52
1	D	222	LYS	CA-C	-6.58	1.44	1.52
2	5	86	THR	N-CA	-6.58	1.38	1.45
1	D	133	GLY	CA-C	-6.57	1.42	1.51
1	G	228	GLU	CA-CB	6.57	1.64	1.53
2	6	90	ILE	CA-C	-6.56	1.44	1.52
1	F	93	ARG	NE-CZ	6.56	1.40	1.33
2	7	146	THR	N-CA	-6.56	1.38	1.46
2	1	151	LEU	CA-CB	6.55	1.63	1.53
2	6	189	VAL	CA-CB	-6.55	1.46	1.54
2	2	148	TYR	N-CA	-6.55	1.38	1.46
1	E	211	VAL	CA-CB	-6.54	1.46	1.54
1	F	117	CYS	CA-C	-6.54	1.44	1.52
2	3	81	ARG	C-N	6.54	1.42	1.33
1	B	130	ARG	NE-CZ	6.53	1.40	1.33
2	7	35	ASN	CA-C	6.53	1.61	1.52
1	E	212	GLY	CA-C	-6.53	1.46	1.52
1	C	245	LYS	CA-C	-6.52	1.44	1.52
2	3	102	ARG	CZ-NH2	6.52	1.42	1.33
1	D	148	TYR	CA-C	-6.51	1.44	1.52
2	1	23	VAL	CA-C	-6.51	1.44	1.52
2	5	42	ALA	CA-C	-6.51	1.44	1.52
2	2	123	TYR	CA-C	-6.51	1.45	1.52
1	G	38	ILE	CA-C	-6.51	1.44	1.52
1	E	241	ARG	CZ-NH2	6.50	1.41	1.33
2	7	96	ASN	N-CA	-6.50	1.38	1.46
1	C	62	ASP	CA-C	-6.50	1.43	1.52
2	7	180	SER	C-N	6.50	1.42	1.33
1	D	70	ILE	CA-C	-6.49	1.45	1.52
1	G	28	ARG	NE-CZ	6.49	1.40	1.33
1	C	24	VAL	C-N	6.49	1.42	1.33
2	5	178	ARG	C-N	6.49	1.42	1.33
2	5	188	VAL	CA-C	-6.49	1.44	1.52
2	5	164	ALA	N-CA	-6.48	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	88	ARG	CD-NE	6.47	1.55	1.46
2	7	47	GLN	N-CA	-6.47	1.38	1.46
2	4	31	ALA	N-CA	-6.47	1.38	1.46
1	D	227	GLU	CA-C	-6.46	1.44	1.52
1	D	235	ARG	C-N	6.46	1.42	1.33
2	3	166	GLU	N-CA	-6.46	1.38	1.46
2	6	96	ASN	CA-C	-6.46	1.44	1.52
1	D	235	ARG	CD-NE	6.45	1.55	1.46
1	B	171	VAL	N-CA	-6.44	1.38	1.46
1	A	60	GLU	CA-C	-6.43	1.44	1.52
1	C	234	GLU	N-CA	-6.43	1.38	1.46
1	F	51	ASP	CA-CB	6.43	1.61	1.53
1	B	195	ALA	CA-CB	6.43	1.63	1.53
1	G	157	LEU	CA-C	-6.42	1.44	1.52
2	7	168	ALA	CA-C	-6.41	1.44	1.52
1	D	191	LEU	C-N	6.41	1.42	1.33
1	C	70	ILE	CA-CB	6.41	1.63	1.54
1	G	135	SER	CA-C	-6.40	1.44	1.52
1	D	20	ARG	CD-NE	6.39	1.55	1.46
1	B	72	GLU	CA-CB	6.39	1.62	1.53
2	2	88	ARG	N-CA	-6.39	1.38	1.46
1	C	205	VAL	C-N	-6.38	1.27	1.34
2	1	21	ASP	CA-C	-6.38	1.44	1.52
1	A	107	ILE	CA-CB	-6.38	1.47	1.54
1	E	141	VAL	CA-C	-6.37	1.44	1.52
1	E	159	TYR	CA-C	-6.37	1.45	1.52
2	1	68	ARG	CA-C	-6.37	1.44	1.52
2	5	128	ILE	CA-CB	6.37	1.62	1.54
2	2	24	VAL	CA-CB	-6.37	1.45	1.54
2	3	96	ASN	CA-CB	6.37	1.63	1.53
1	E	47	ILE	N-CA	-6.36	1.38	1.46
2	3	96	ASN	C-N	6.35	1.42	1.34
2	7	15	VAL	N-CA	-6.34	1.39	1.46
1	D	141	VAL	CA-CB	-6.34	1.46	1.54
1	B	241	ARG	CZ-NH1	6.33	1.41	1.32
2	2	198	GLN	C-N	6.33	1.42	1.33
2	3	68	ARG	CZ-NH1	6.33	1.41	1.32
2	3	70	ILE	C-N	6.33	1.42	1.33
2	7	90	ILE	CA-C	-6.33	1.45	1.52
2	2	35	ASN	N-CA	-6.32	1.37	1.46
2	1	25	MET	N-CA	-6.32	1.38	1.45
2	5	83	ARG	NE-CZ	6.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	215	LYS	CA-C	-6.32	1.45	1.52
1	E	240	ILE	C-N	6.31	1.41	1.33
2	4	52	MET	N-CA	-6.30	1.38	1.46
2	1	180	SER	CA-C	6.30	1.61	1.52
2	1	134	GLU	CA-C	-6.30	1.45	1.52
1	F	193	LEU	C-N	6.29	1.41	1.33
1	G	147	LEU	CA-C	-6.29	1.44	1.52
1	B	68	TYR	CA-C	-6.29	1.45	1.52
1	A	106	PRO	C-N	6.29	1.41	1.33
1	B	37	ALA	N-CA	-6.28	1.38	1.46
2	2	85	PRO	CA-C	-6.27	1.44	1.52
2	4	208	LEU	CA-C	-6.27	1.44	1.52
2	7	24	VAL	C-N	6.26	1.41	1.33
1	B	18	ASP	CA-C	-6.26	1.44	1.52
1	A	64	ILE	CA-C	-6.26	1.45	1.52
2	3	64	GLN	CA-C	-6.26	1.44	1.52
1	E	133	GLY	C-N	6.25	1.41	1.33
1	G	33	ARG	N-CA	-6.25	1.37	1.46
2	6	30	ARG	NE-CZ	6.25	1.40	1.33
2	6	181	ALA	N-CA	-6.25	1.38	1.46
1	B	147	LEU	CA-C	-6.25	1.45	1.52
1	E	33	ARG	CZ-NH2	6.24	1.41	1.33
2	6	107	LEU	C-N	6.24	1.39	1.33
2	4	74	ALA	C-N	6.24	1.42	1.33
2	5	191	ILE	CA-CB	-6.24	1.46	1.54
1	E	162	THR	C-N	6.24	1.41	1.33
1	B	242	GLU	CA-CB	6.23	1.63	1.53
2	3	156	THR	C-N	-6.23	1.27	1.34
1	C	202	SER	C-N	6.23	1.42	1.33
2	3	197	TYR	CA-C	-6.23	1.45	1.52
2	2	51	ARG	CD-NE	6.22	1.54	1.46
1	F	101	LEU	CA-C	-6.21	1.45	1.52
2	6	125	ILE	N-CA	-6.21	1.38	1.46
1	B	210	GLU	CA-C	-6.21	1.44	1.52
2	4	168	ALA	CA-C	-6.20	1.44	1.52
1	G	34	GLY	N-CA	6.20	1.51	1.44
1	B	126	TYR	CZ-OH	6.19	1.51	1.38
2	6	58	GLY	C-N	6.19	1.41	1.33
1	F	166	MET	CA-C	-6.18	1.44	1.52
2	6	78	GLU	CA-C	-6.18	1.45	1.52
2	7	48	ILE	N-CA	-6.18	1.38	1.46
1	B	148	TYR	CA-C	-6.17	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	ASP	C-O	6.17	1.31	1.24
1	E	230	LYS	CA-C	6.17	1.58	1.52
2	2	22	GLY	N-CA	-6.17	1.35	1.45
1	C	211	VAL	CA-C	-6.16	1.44	1.52
1	A	187	ASP	C-N	6.16	1.42	1.33
2	6	178	ARG	NE-CZ	6.15	1.39	1.33
2	1	154	ARG	NE-CZ	6.15	1.39	1.33
2	1	163	GLU	CA-C	-6.15	1.44	1.52
1	A	96	ALA	N-CA	-6.14	1.38	1.46
1	A	206	PRO	C-N	6.14	1.42	1.33
2	2	137	ILE	N-CA	-6.14	1.39	1.46
2	3	104	PHE	CA-CB	6.14	1.63	1.54
1	D	33	ARG	C-N	6.14	1.40	1.33
2	7	160	GLY	N-CA	6.14	1.52	1.45
2	1	207	ILE	C-N	6.13	1.41	1.33
1	F	174	PHE	CA-CB	6.13	1.62	1.53
1	E	116	ILE	C-N	6.13	1.42	1.33
2	3	25	MET	N-CA	-6.12	1.39	1.46
1	A	172	THR	C-N	6.12	1.42	1.33
2	3	112	ILE	CA-C	-6.12	1.45	1.52
2	4	105	PRO	C-N	6.12	1.42	1.33
2	5	112	ILE	CA-CB	-6.11	1.46	1.54
2	4	116	ASP	N-CA	-6.11	1.38	1.46
1	C	111	GLU	N-CA	-6.11	1.38	1.46
2	3	79	ILE	N-CA	-6.11	1.39	1.46
1	G	40	ILE	N-CA	-6.11	1.39	1.46
1	D	123	TYR	CZ-OH	6.10	1.50	1.38
2	4	70	ILE	C-N	6.10	1.41	1.33
1	F	190	VAL	CA-C	-6.10	1.44	1.52
2	4	180	SER	CA-C	-6.09	1.45	1.53
2	1	88	ARG	NE-CZ	6.09	1.39	1.33
2	2	199	TYR	N-CA	-6.09	1.39	1.46
1	G	74	ILE	CA-C	-6.09	1.45	1.52
1	D	151	ASP	C-N	6.09	1.41	1.33
1	D	208	ASN	CA-C	-6.08	1.45	1.52
1	E	130	ARG	N-CA	-6.08	1.36	1.45
2	1	51	ARG	CA-CB	6.08	1.61	1.53
1	F	213	TYR	CA-C	-6.08	1.45	1.52
2	7	99	ASN	C-N	6.08	1.42	1.33
1	G	205	VAL	C-O	-6.08	1.16	1.24
2	6	72	ILE	N-CA	-6.07	1.39	1.46
2	7	44	LYS	N-CA	-6.07	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	69	ILE	CA-C	-6.07	1.45	1.52
1	C	97	GLN	CA-C	-6.06	1.45	1.52
1	A	29	GLU	C-N	6.06	1.41	1.33
1	B	28	ARG	CD-NE	6.06	1.54	1.46
2	7	44	LYS	CA-C	-6.06	1.46	1.52
1	A	85	ALA	N-CA	-6.05	1.39	1.46
1	A	193	LEU	C-N	6.05	1.41	1.33
2	2	21	ASP	C-N	6.05	1.41	1.33
2	4	198	GLN	C-N	6.05	1.42	1.34
2	7	109	GLN	N-CA	-6.05	1.38	1.46
1	F	106	PRO	CA-C	-6.05	1.45	1.52
2	6	51	ARG	CD-NE	6.04	1.54	1.46
1	E	201	GLU	CA-CB	6.04	1.62	1.53
1	D	204	LEU	CA-C	-6.04	1.45	1.53
2	2	212	ARG	CZ-NH2	6.04	1.41	1.33
2	3	132	ILE	CA-C	-6.04	1.45	1.52
1	A	155	ALA	N-CA	-6.03	1.38	1.46
2	6	143	GLY	C-N	6.03	1.41	1.33
1	G	154	GLY	CA-C	-6.03	1.43	1.51
2	6	48	ILE	C-O	-6.03	1.18	1.24
1	A	51	ASP	C-N	6.03	1.41	1.33
1	F	198	LEU	CA-C	-6.03	1.45	1.52
2	3	28	GLU	N-CA	6.02	1.53	1.46
2	3	108	VAL	N-CA	-6.02	1.38	1.46
1	F	47	ILE	CA-C	-6.01	1.45	1.52
1	F	192	GLY	CA-C	-6.01	1.45	1.52
1	C	185	PHE	CA-C	-6.01	1.45	1.52
1	A	187	ASP	CA-C	-6.01	1.45	1.52
1	F	239	ARG	NE-CZ	6.00	1.39	1.33
1	B	22	PHE	CA-C	-6.00	1.45	1.52
1	D	32	LYS	CA-C	-6.00	1.44	1.52
1	G	51	ASP	CA-C	-5.99	1.45	1.52
1	D	241	ARG	CD-NE	5.99	1.54	1.46
2	4	23	VAL	CA-C	-5.99	1.45	1.52
1	G	154	GLY	C-N	5.99	1.42	1.33
1	C	143	GLU	C-N	5.98	1.40	1.33
1	F	180	ARG	CA-C	-5.98	1.45	1.52
2	4	124	SER	CA-CB	5.98	1.62	1.53
2	7	178	ARG	CD-NE	5.97	1.54	1.46
1	B	88	LEU	C-O	-5.97	1.17	1.24
1	G	176	GLU	C-N	5.97	1.41	1.33
2	2	83	ARG	CZ-NH1	5.96	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	225	SER	CA-C	-5.96	1.45	1.52
2	3	114	GLY	CA-C	-5.96	1.43	1.51
2	1	40	LYS	CA-CB	5.96	1.63	1.53
1	B	60	GLU	CA-C	-5.96	1.44	1.52
1	G	137	LEU	C-O	-5.95	1.17	1.24
1	G	148	TYR	CA-C	-5.95	1.45	1.52
2	1	70	ILE	CA-C	-5.95	1.45	1.52
1	D	168	ARG	NE-CZ	5.95	1.39	1.33
2	4	211	PHE	CA-CB	5.95	1.63	1.53
2	5	131	ALA	CA-C	-5.95	1.45	1.52
2	6	55	THR	N-CA	-5.95	1.38	1.45
1	E	55	GLY	CA-C	-5.94	1.43	1.51
1	G	84	ASP	CA-C	-5.94	1.45	1.52
2	5	207	ILE	C-N	5.94	1.41	1.33
2	2	178	ARG	NE-CZ	5.94	1.39	1.33
1	A	43	LYS	CA-C	-5.94	1.44	1.52
1	C	91	ARG	CA-C	-5.94	1.45	1.52
2	7	173	TYR	C-N	5.94	1.41	1.33
2	4	135	LYS	CA-C	-5.93	1.45	1.52
1	C	135	SER	CA-C	-5.93	1.45	1.52
2	3	46	TYR	CA-C	-5.92	1.45	1.52
1	F	53	ARG	CD-NE	5.92	1.54	1.46
1	D	93	ARG	NE-CZ	5.92	1.39	1.33
1	D	239	ARG	CZ-NH2	5.91	1.41	1.33
2	7	166	GLU	CA-CB	5.91	1.62	1.53
2	1	153	ASP	CA-C	-5.91	1.45	1.52
2	5	211	PHE	C-N	5.91	1.42	1.33
1	G	239	ARG	CZ-NH1	5.91	1.41	1.32
2	2	147	ALA	CA-C	-5.91	1.45	1.52
1	D	65	GLU	CA-C	-5.91	1.45	1.52
1	D	108	THR	CA-C	-5.90	1.44	1.53
1	E	140	GLY	CA-C	-5.90	1.44	1.51
2	6	123	TYR	CA-C	-5.89	1.45	1.52
2	3	51	ARG	CA-C	-5.89	1.46	1.53
1	F	66	LYS	CA-C	-5.89	1.45	1.52
2	1	108	VAL	N-CA	-5.89	1.39	1.46
2	6	25	MET	CA-C	-5.89	1.45	1.52
1	C	38	ILE	C-N	5.88	1.39	1.33
2	1	109	GLN	CA-C	-5.88	1.45	1.53
2	4	200	SER	CA-CB	5.88	1.62	1.53
2	6	71	LYS	C-N	5.88	1.41	1.33
2	3	35	ASN	CA-CB	5.88	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	TYR	N-CA	5.88	1.53	1.46
2	6	109	GLN	C-N	5.87	1.41	1.33
2	6	111	LEU	CA-CB	5.87	1.62	1.53
2	4	147	ALA	C-N	5.87	1.41	1.33
1	D	177	LYS	C-N	5.87	1.42	1.33
1	A	125	GLN	C-N	5.86	1.41	1.33
1	C	68	TYR	N-CA	-5.86	1.38	1.45
2	5	32	THR	N-CA	-5.86	1.39	1.46
2	7	122	ILE	C-N	5.86	1.41	1.33
1	B	220	THR	CA-C	-5.86	1.46	1.52
2	2	25	MET	CA-C	-5.85	1.45	1.52
2	5	12	THR	N-CA	5.85	1.57	1.46
2	1	71	LYS	N-CA	5.84	1.53	1.46
1	B	28	ARG	CZ-NH2	5.84	1.41	1.33
2	7	138	VAL	N-CA	-5.84	1.39	1.46
1	A	56	SER	N-CA	-5.84	1.39	1.46
1	D	28	ARG	NE-CZ	5.84	1.39	1.33
1	D	172	THR	C-N	5.84	1.41	1.33
2	3	142	SER	CA-CB	5.84	1.62	1.54
1	G	197	GLY	CA-C	-5.83	1.45	1.52
2	4	24	VAL	CA-C	-5.83	1.45	1.52
1	B	158	GLU	C-N	5.83	1.41	1.33
1	G	133	GLY	C-N	5.83	1.39	1.33
2	3	106	TYR	N-CA	-5.83	1.39	1.46
1	B	160	LYS	CA-C	-5.82	1.45	1.52
2	2	38	ALA	C-N	5.82	1.40	1.33
1	B	85	ALA	C-O	-5.81	1.17	1.24
1	C	93	ARG	CD-NE	5.81	1.54	1.46
2	3	137	ILE	CB-CG1	5.81	1.65	1.53
1	C	14	VAL	CA-CB	-5.81	1.46	1.54
1	D	100	ARG	NE-CZ	5.81	1.39	1.33
1	F	128	GLY	C-N	5.80	1.39	1.33
2	6	107	LEU	CA-CB	5.80	1.61	1.53
1	G	155	ALA	C-N	5.80	1.41	1.33
2	5	83	ARG	CA-C	-5.80	1.45	1.52
2	5	170	ARG	NE-CZ	5.80	1.39	1.33
2	2	186	ILE	N-CA	-5.80	1.38	1.46
1	D	224	VAL	CA-C	-5.80	1.47	1.53
2	5	204	VAL	CA-CB	-5.80	1.47	1.54
1	E	67	ILE	CA-C	-5.79	1.45	1.52
2	2	212	ARG	NE-CZ	5.79	1.39	1.33
1	A	158	GLU	N-CA	-5.79	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	213	TYR	C-N	5.79	1.40	1.33
2	2	30	ARG	CZ-NH2	5.79	1.41	1.33
2	3	81	ARG	CD-NE	5.78	1.54	1.46
2	5	56	THR	CA-C	-5.78	1.45	1.52
1	G	38	ILE	C-N	5.78	1.42	1.33
2	7	151	LEU	N-CA	5.78	1.53	1.46
2	3	183	GLY	N-CA	5.77	1.50	1.45
2	3	102	ARG	CD-NE	5.77	1.54	1.46
1	B	45	GLY	CA-C	-5.76	1.46	1.52
1	E	151	ASP	C-N	5.76	1.40	1.33
2	5	68	ARG	C-N	5.76	1.41	1.33
1	B	206	PRO	CA-C	5.76	1.61	1.52
1	B	224	VAL	N-CA	-5.76	1.39	1.46
2	6	170	ARG	NE-CZ	5.76	1.39	1.33
1	D	140	GLY	N-CA	5.76	1.51	1.45
2	3	35	ASN	C-N	5.76	1.40	1.33
2	3	44	LYS	CA-CB	5.75	1.63	1.53
1	C	207	GLU	N-CA	-5.75	1.39	1.46
2	6	182	SER	C-N	5.75	1.42	1.33
1	B	179	TYR	N-CA	-5.75	1.38	1.46
2	5	101	TYR	CA-CB	5.75	1.61	1.53
1	A	167	GLY	C-O	-5.75	1.16	1.23
1	F	173	GLU	N-CA	-5.75	1.39	1.46
2	3	89	ALA	N-CA	-5.75	1.39	1.46
1	G	95	GLU	CA-CB	5.74	1.62	1.53
1	D	98	ILE	CA-CB	-5.74	1.47	1.54
1	F	98	ILE	N-CA	5.73	1.53	1.46
2	6	80	ARG	NE-CZ	5.73	1.39	1.33
2	6	37	ILE	CA-C	5.73	1.59	1.52
2	5	55	THR	CA-C	-5.73	1.45	1.52
1	D	157	LEU	N-CA	-5.72	1.39	1.46
1	G	221	PHE	CA-CB	5.72	1.63	1.53
1	A	20	ARG	NE-CZ	5.72	1.39	1.33
1	G	245	LYS	C-N	5.72	1.41	1.33
1	A	74	ILE	N-CA	-5.72	1.39	1.46
1	F	172	THR	N-CA	5.72	1.53	1.46
1	C	126	TYR	CA-CB	5.71	1.61	1.53
1	C	73	HIS	N-CA	-5.71	1.42	1.47
2	1	159	ILE	CA-C	-5.70	1.45	1.52
2	4	57	ALA	N-CA	-5.70	1.39	1.46
2	1	211	PHE	C-N	5.70	1.40	1.33
1	B	138	ILE	N-CA	-5.70	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	157	LEU	N-CA	-5.70	1.39	1.46
2	2	102	ARG	NE-CZ	5.70	1.39	1.33
2	6	110	LEU	N-CA	-5.69	1.39	1.45
1	A	101	LEU	N-CA	-5.69	1.39	1.46
1	C	20	ARG	NE-CZ	5.69	1.39	1.33
2	6	52	MET	CA-CB	5.69	1.63	1.53
1	G	38	ILE	N-CA	-5.68	1.39	1.46
1	A	178	GLU	C-N	5.68	1.41	1.33
2	3	197	TYR	N-CA	-5.68	1.39	1.46
1	E	49	ILE	C-O	-5.68	1.18	1.24
2	6	194	ASP	CA-C	-5.68	1.45	1.52
1	B	53	ARG	NE-CZ	5.68	1.39	1.33
2	2	104	PHE	C-O	-5.68	1.18	1.24
2	6	128	ILE	C-N	5.68	1.40	1.33
1	E	137	LEU	CA-C	-5.67	1.45	1.52
2	7	160	GLY	C-N	5.67	1.40	1.33
1	F	225	SER	CA-CB	5.67	1.61	1.53
2	2	168	ALA	C-N	-5.67	1.26	1.33
2	7	28	GLU	N-CA	5.67	1.52	1.46
2	7	55	THR	CA-C	-5.67	1.46	1.52
2	3	80	ARG	CZ-NH1	5.66	1.40	1.32
2	5	159	ILE	CA-CB	-5.66	1.47	1.54
1	G	210	GLU	CA-C	-5.66	1.45	1.52
2	1	153	ASP	N-CA	-5.66	1.39	1.46
2	1	164	ALA	C-N	5.66	1.40	1.33
1	B	38	ILE	C-N	5.65	1.40	1.32
1	E	132	PHE	CA-C	-5.65	1.45	1.52
1	D	80	GLY	CA-C	-5.65	1.44	1.52
1	E	50	ALA	C-N	5.65	1.41	1.33
2	2	112	ILE	N-CA	-5.65	1.39	1.46
1	G	223	GLU	N-CA	-5.65	1.39	1.46
1	F	219	ARG	NE-CZ	5.65	1.39	1.33
1	B	223	GLU	CA-C	-5.64	1.45	1.52
1	D	125	GLN	N-CA	-5.64	1.39	1.46
1	G	194	VAL	CA-C	-5.64	1.45	1.52
1	C	13	THR	N-CA	-5.64	1.39	1.46
1	A	140	GLY	C-N	5.62	1.40	1.33
1	C	131	PRO	CA-C	-5.62	1.45	1.52
2	2	35	ASN	CA-CB	5.62	1.63	1.53
1	E	205	VAL	CA-CB	-5.62	1.47	1.54
1	A	51	ASP	CA-C	-5.61	1.46	1.52
1	E	152	PRO	N-CD	-5.61	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	45	GLY	CA-C	-5.61	1.45	1.52
2	1	132	ILE	CA-C	-5.61	1.45	1.52
2	7	107	LEU	C-N	5.61	1.39	1.33
1	A	51	ASP	CA-CB	5.60	1.60	1.53
1	E	236	ALA	CA-CB	5.60	1.62	1.53
1	B	107	ILE	CA-CB	-5.59	1.48	1.54
1	D	161	ALA	N-CA	-5.59	1.39	1.46
1	A	76	ALA	CA-C	-5.59	1.45	1.52
1	G	41	LYS	N-CA	-5.59	1.39	1.46
2	2	200	SER	CA-CB	5.59	1.62	1.53
2	6	178	ARG	CD-NE	5.59	1.54	1.46
2	3	154	ARG	NE-CZ	5.59	1.39	1.33
1	C	79	SER	CA-C	-5.59	1.45	1.52
1	C	157	LEU	CA-C	-5.59	1.45	1.52
2	6	61	GLY	CA-C	-5.59	1.46	1.52
2	6	128	ILE	CB-CG1	5.58	1.64	1.53
2	4	43	LYS	CA-C	-5.58	1.46	1.52
1	A	92	ALA	N-CA	-5.58	1.39	1.46
1	C	156	LEU	CA-C	-5.57	1.45	1.52
1	G	235	ARG	NE-CZ	5.57	1.39	1.33
2	5	212	ARG	CD-NE	5.57	1.54	1.46
2	4	137	ILE	C-N	5.57	1.40	1.33
2	5	80	ARG	CZ-NH1	5.57	1.40	1.32
1	G	107	ILE	CA-CB	-5.56	1.48	1.54
1	B	180	ARG	CD-NE	5.56	1.54	1.46
1	A	86	ARG	CA-C	-5.56	1.45	1.52
2	7	49	ALA	C-O	-5.55	1.16	1.23
2	5	101	TYR	N-CA	-5.55	1.40	1.46
1	G	238	GLU	N-CA	5.54	1.52	1.46
2	4	25	MET	N-CA	-5.54	1.38	1.45
1	A	159	TYR	N-CA	-5.54	1.39	1.45
2	3	21	ASP	C-N	5.54	1.40	1.32
2	3	102	ARG	NE-CZ	5.54	1.39	1.33
1	D	212	GLY	CA-C	-5.54	1.47	1.51
1	F	92	ALA	C-N	5.54	1.41	1.33
2	3	20	LYS	CA-C	-5.54	1.45	1.52
1	C	20	ARG	CD-NE	5.53	1.53	1.46
2	6	87	VAL	N-CA	-5.53	1.39	1.46
2	4	141	GLY	C-O	5.52	1.30	1.24
2	2	207	ILE	CA-C	-5.52	1.46	1.52
2	5	136	ASP	N-CA	-5.52	1.39	1.46
1	G	136	LEU	CA-C	-5.52	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	81	ARG	CD-NE	5.52	1.53	1.46
2	4	79	ILE	CA-C	5.52	1.59	1.52
2	2	52	MET	N-CA	-5.52	1.39	1.46
2	2	89	ALA	N-CA	-5.52	1.39	1.46
2	3	55	THR	CB-OG1	-5.52	1.34	1.43
1	F	170	ALA	CA-C	-5.52	1.45	1.52
1	B	143	GLU	C-O	-5.51	1.17	1.24
1	F	233	VAL	CA-CB	-5.51	1.47	1.54
2	1	196	PHE	N-CA	-5.51	1.40	1.46
1	D	47	ILE	CA-C	-5.51	1.46	1.52
2	1	28	GLU	CA-C	-5.51	1.46	1.52
1	G	53	ARG	CZ-NH2	5.51	1.40	1.33
1	G	204	LEU	N-CA	-5.51	1.38	1.45
2	1	173	TYR	CA-CB	5.51	1.62	1.53
1	C	137	LEU	C-N	5.50	1.41	1.33
1	F	209	ILE	CB-CG1	-5.50	1.42	1.53
1	G	168	ARG	NE-CZ	5.50	1.39	1.33
2	7	37	ILE	C-N	5.50	1.41	1.33
1	A	235	ARG	C-O	-5.50	1.17	1.24
1	B	91	ARG	N-CA	-5.50	1.39	1.46
2	4	26	ALA	N-CA	5.50	1.52	1.46
2	1	29	LYS	CA-C	-5.50	1.45	1.52
2	3	174	SER	CA-CB	5.50	1.61	1.53
1	D	36	THR	N-CA	-5.49	1.39	1.46
1	E	32	LYS	CA-CB	5.49	1.62	1.53
2	3	116	ASP	CA-C	5.49	1.59	1.52
1	C	211	VAL	CA-CB	-5.49	1.46	1.54
2	2	47	GLN	N-CA	-5.49	1.39	1.46
1	E	73	HIS	CG-CD2	-5.49	1.29	1.35
1	B	41	LYS	CA-C	-5.49	1.46	1.52
1	B	73	HIS	CE1-NE2	5.49	1.38	1.32
1	C	74	ILE	CA-C	5.49	1.59	1.52
2	1	199	TYR	CA-CB	5.48	1.61	1.53
1	C	123	TYR	N-CA	-5.48	1.38	1.46
2	7	155	PHE	N-CA	-5.48	1.39	1.46
2	1	154	ARG	CD-NE	5.47	1.53	1.46
2	4	75	ASN	CA-CB	5.47	1.61	1.53
1	A	161	ALA	CA-C	-5.47	1.45	1.52
1	B	91	ARG	NE-CZ	5.47	1.39	1.33
1	B	239	ARG	NE-CZ	5.47	1.39	1.33
1	E	25	GLU	CA-C	-5.47	1.45	1.52
1	A	65	GLU	CA-CB	5.47	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	48	ILE	C-N	5.46	1.40	1.33
2	5	210	LYS	N-CA	-5.46	1.39	1.46
1	A	234	GLU	CA-C	-5.46	1.45	1.52
2	7	100	SER	C-N	5.45	1.39	1.33
1	C	201	GLU	CA-CB	5.45	1.61	1.53
2	1	66	LEU	C-N	5.45	1.41	1.33
1	B	100	ARG	CZ-NH1	5.45	1.40	1.32
1	D	94	ILE	CA-C	-5.45	1.46	1.52
1	E	209	ILE	N-CA	-5.45	1.39	1.46
1	G	204	LEU	CA-C	-5.45	1.45	1.53
2	1	34	GLY	N-CA	5.45	1.53	1.45
2	3	89	ALA	C-N	5.45	1.40	1.33
2	1	15	VAL	CA-C	-5.45	1.45	1.52
1	B	20	ARG	CZ-NH2	5.44	1.40	1.33
2	3	63	ALA	CA-C	-5.44	1.46	1.52
2	4	140	THR	N-CA	-5.44	1.39	1.46
2	5	89	ALA	N-CA	-5.44	1.39	1.46
2	2	122	ILE	C-N	5.44	1.40	1.33
2	6	148	TYR	C-N	5.44	1.40	1.33
1	A	71	ASP	CA-C	-5.44	1.45	1.53
1	B	30	ALA	CA-C	-5.44	1.45	1.52
1	C	64	ILE	C-N	5.44	1.40	1.33
1	D	161	ALA	CA-CB	5.44	1.62	1.53
1	F	236	ALA	C-N	5.44	1.41	1.33
1	G	99	ASN	C-O	-5.44	1.17	1.24
1	B	214	VAL	CA-C	-5.43	1.45	1.52
2	5	19	CYS	CA-CB	5.43	1.62	1.53
2	5	132	ILE	C-N	-5.43	1.26	1.33
2	6	35	ASN	CA-C	-5.43	1.46	1.53
2	7	82	GLU	CA-CB	-5.43	1.45	1.53
1	C	24	VAL	CA-CB	-5.43	1.47	1.54
1	A	197	GLY	CA-C	-5.42	1.46	1.52
2	5	136	ASP	CA-CB	5.42	1.62	1.53
1	F	33	ARG	CZ-NH1	5.42	1.40	1.32
2	5	60	VAL	CA-CB	-5.42	1.47	1.54
2	3	48	ILE	CA-C	-5.42	1.45	1.52
2	3	158	GLU	CA-C	-5.42	1.46	1.53
2	4	109	GLN	N-CA	-5.42	1.39	1.46
1	D	230	LYS	CA-CB	-5.41	1.49	1.54
2	2	108	VAL	CA-C	-5.41	1.46	1.52
2	2	192	THR	C-N	5.41	1.40	1.33
1	B	49	ILE	N-CA	-5.41	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	GLN	N-CA	-5.41	1.39	1.46
1	F	123	TYR	CA-CB	5.41	1.62	1.53
1	B	27	ALA	C-N	5.40	1.41	1.33
1	C	28	ARG	NE-CZ	5.40	1.39	1.33
1	B	57	LYS	CA-C	-5.39	1.45	1.52
2	2	202	GLU	N-CA	-5.39	1.40	1.46
2	7	111	LEU	C-N	5.39	1.40	1.33
1	F	206	PRO	N-CD	5.39	1.55	1.47
1	A	150	THR	CA-C	-5.38	1.46	1.52
2	6	46	TYR	CA-C	-5.38	1.46	1.52
1	A	73	HIS	ND1-CE1	5.38	1.38	1.32
1	B	23	GLN	CA-C	-5.38	1.45	1.52
1	F	82	VAL	N-CA	-5.38	1.40	1.46
1	G	202	SER	N-CA	-5.38	1.39	1.46
2	4	96	ASN	C-O	-5.38	1.17	1.24
2	1	206	GLN	C-N	5.38	1.40	1.33
2	2	181	ALA	CA-C	-5.37	1.45	1.52
2	3	178	ARG	CA-C	-5.37	1.45	1.52
1	D	168	ARG	CZ-NH2	5.37	1.40	1.33
2	6	83	ARG	CA-C	-5.37	1.46	1.52
1	C	241	ARG	NE-CZ	5.37	1.39	1.33
2	1	37	ILE	CB-CG1	5.37	1.64	1.53
2	4	82	GLU	CA-CB	5.36	1.62	1.53
1	A	91	ARG	N-CA	-5.36	1.39	1.46
2	2	71	LYS	C-O	-5.36	1.18	1.24
2	4	145	LEU	CA-CB	5.36	1.61	1.53
1	B	109	VAL	C-N	5.36	1.41	1.33
1	F	58	LEU	CA-C	-5.36	1.45	1.52
1	E	63	THR	C-N	5.35	1.38	1.33
1	A	39	GLY	CA-C	-5.35	1.44	1.51
1	A	93	ARG	NE-CZ	5.35	1.39	1.33
2	5	187	ASP	CA-C	-5.35	1.46	1.52
2	6	148	TYR	CA-CB	5.35	1.61	1.53
1	C	104	ASP	N-CA	-5.34	1.38	1.46
1	E	69	LYS	CA-C	-5.34	1.46	1.52
2	4	139	ALA	C-O	-5.34	1.17	1.23
1	E	99	ASN	N-CA	-5.34	1.39	1.46
1	B	213	TYR	N-CA	-5.34	1.39	1.46
2	5	127	PRO	C-N	5.34	1.39	1.33
1	G	196	MET	N-CA	-5.34	1.39	1.46
1	B	135	SER	N-CA	-5.34	1.39	1.46
1	D	91	ARG	CD-NE	5.34	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	174	PHE	N-CA	-5.34	1.40	1.46
1	F	152	PRO	N-CA	-5.33	1.40	1.47
1	G	108	THR	CA-C	-5.33	1.46	1.53
2	7	139	ALA	CA-C	5.33	1.58	1.52
1	A	169	ASN	CA-CB	5.33	1.61	1.53
1	C	91	ARG	CZ-NH2	5.33	1.40	1.33
2	1	213	LYS	C-O	5.33	1.34	1.23
2	7	83	ARG	CD-NE	5.33	1.53	1.46
1	G	94	ILE	C-N	5.33	1.40	1.33
2	7	172	ILE	CA-CB	5.33	1.61	1.54
2	6	173	TYR	C-N	5.33	1.41	1.33
1	D	85	ALA	CA-C	-5.32	1.46	1.52
1	E	130	ARG	CZ-NH1	5.32	1.40	1.32
2	5	24	VAL	C-O	-5.32	1.18	1.24
2	6	57	ALA	C-N	5.32	1.41	1.32
2	6	159	ILE	N-CA	5.32	1.52	1.46
1	E	163	ALA	CA-C	-5.32	1.46	1.52
2	5	141	GLY	N-CA	-5.32	1.39	1.45
1	B	32	LYS	N-CA	-5.31	1.39	1.46
1	B	158	GLU	CA-C	-5.31	1.46	1.52
2	4	103	TYR	CE2-CZ	5.31	1.50	1.38
1	D	98	ILE	CA-C	-5.31	1.46	1.52
1	E	111	GLU	CA-C	-5.31	1.46	1.52
2	5	69	ILE	CA-CB	5.31	1.60	1.54
1	C	214	VAL	CA-CB	5.31	1.60	1.54
1	D	114	LYS	N-CA	-5.31	1.40	1.46
2	4	132	ILE	CA-CB	-5.31	1.47	1.54
2	5	108	VAL	CA-C	-5.31	1.47	1.52
1	B	160	LYS	C-O	-5.30	1.17	1.24
2	4	128	ILE	C-N	5.30	1.41	1.33
1	A	234	GLU	C-N	5.30	1.41	1.33
1	E	135	SER	CA-C	-5.30	1.46	1.52
2	1	162	ASP	C-N	5.30	1.41	1.33
1	B	176	GLU	CA-C	5.29	1.59	1.52
1	C	140	GLY	C-N	5.29	1.40	1.33
1	E	33	ARG	CZ-NH1	5.29	1.40	1.32
1	F	139	ALA	CA-C	-5.29	1.46	1.52
2	6	139	ALA	C-N	5.29	1.40	1.33
2	3	81	ARG	CZ-NH2	5.29	1.40	1.33
1	F	219	ARG	CZ-NH2	5.29	1.40	1.33
2	1	135	LYS	CA-CB	5.29	1.61	1.53
2	7	76	LEU	CA-C	-5.29	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	184	ASP	C-N	5.29	1.39	1.32
2	5	154	ARG	CA-CB	5.29	1.61	1.53
1	F	89	ILE	N-CA	-5.28	1.40	1.46
1	B	240	ILE	C-N	5.28	1.40	1.33
1	F	111	GLU	N-CA	5.28	1.52	1.46
1	A	46	VAL	CA-C	5.27	1.59	1.52
1	C	86	ARG	CA-C	-5.27	1.46	1.52
2	6	123	TYR	N-CA	-5.27	1.39	1.46
1	A	213	TYR	N-CA	5.27	1.52	1.46
2	2	140	THR	C-N	5.27	1.42	1.33
2	6	83	ARG	CD-NE	5.27	1.53	1.46
1	C	100	ARG	C-O	-5.27	1.18	1.24
1	F	179	TYR	CG-CD2	5.27	1.50	1.39
2	4	133	GLU	CA-C	-5.27	1.46	1.52
1	D	43	LYS	C-O	-5.26	1.18	1.24
1	E	14	VAL	CA-C	5.26	1.58	1.52
1	E	17	PRO	CA-C	-5.26	1.45	1.52
2	2	158	GLU	CA-CB	5.26	1.60	1.52
1	B	95	GLU	CA-C	-5.26	1.46	1.52
1	E	168	ARG	C-O	5.26	1.30	1.24
1	B	108	THR	CA-C	-5.26	1.45	1.53
1	G	91	ARG	CZ-NH2	5.26	1.40	1.33
2	1	128	ILE	C-N	5.26	1.38	1.32
1	E	186	ASP	CA-C	5.26	1.59	1.52
1	A	86	ARG	C-N	5.25	1.40	1.33
1	G	129	VAL	CA-C	-5.25	1.46	1.52
2	7	123	TYR	C-N	5.25	1.40	1.33
1	E	210	GLU	CA-CB	5.25	1.61	1.53
2	4	70	ILE	CA-CB	-5.25	1.48	1.54
2	5	33	MET	CA-C	-5.25	1.45	1.52
1	F	40	ILE	C-O	-5.25	1.18	1.24
2	7	136	ASP	CA-CB	5.25	1.62	1.53
1	C	21	LEU	C-N	5.24	1.41	1.33
1	D	135	SER	CA-C	-5.24	1.46	1.52
2	4	159	ILE	N-CA	-5.24	1.39	1.46
1	D	127	GLY	C-N	5.24	1.40	1.33
1	F	67	ILE	CA-CB	-5.24	1.47	1.54
1	F	235	ARG	CD-NE	5.24	1.53	1.46
1	D	39	GLY	N-CA	5.23	1.51	1.45
1	D	69	LYS	CA-C	-5.23	1.46	1.52
2	1	153	ASP	C-N	5.23	1.40	1.33
2	5	81	ARG	NE-CZ	5.23	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	173	TYR	CA-C	5.23	1.59	1.52
1	A	167	GLY	C-N	5.22	1.40	1.33
1	B	180	ARG	C-N	5.22	1.41	1.33
1	D	214	VAL	C-N	5.22	1.40	1.33
1	B	85	ALA	CA-C	-5.22	1.46	1.52
2	3	162	ASP	N-CA	-5.22	1.40	1.46
2	6	121	SER	CA-C	-5.22	1.46	1.52
2	7	77	TYR	CA-CB	5.21	1.61	1.53
1	E	50	ALA	CA-C	-5.21	1.46	1.52
1	D	168	ARG	CD-NE	5.21	1.53	1.46
2	2	166	GLU	N-CA	-5.20	1.40	1.46
2	6	121	SER	CA-CB	5.20	1.62	1.53
1	F	65	GLU	CA-C	-5.20	1.46	1.52
1	C	110	LYS	C-O	-5.19	1.18	1.24
1	D	84	ASP	CA-CB	5.19	1.61	1.53
1	G	36	THR	CA-C	-5.19	1.46	1.52
2	2	102	ARG	CD-NE	5.19	1.53	1.46
1	C	93	ARG	CZ-NH1	5.19	1.40	1.32
2	6	24	VAL	CA-CB	-5.19	1.48	1.54
1	C	111	GLU	CA-C	-5.19	1.46	1.52
2	2	89	ALA	CA-C	-5.19	1.46	1.52
1	C	222	LYS	N-CA	-5.18	1.39	1.45
2	5	154	ARG	NE-CZ	5.18	1.38	1.33
1	B	141	VAL	CA-C	-5.18	1.46	1.52
2	2	193	GLU	C-N	5.18	1.41	1.33
2	3	81	ARG	CA-C	-5.18	1.45	1.52
2	6	53	ALA	CA-C	-5.18	1.46	1.52
2	4	30	ARG	CA-C	-5.18	1.45	1.52
2	5	70	ILE	CA-CB	5.18	1.60	1.54
1	D	196	MET	CA-CB	5.17	1.61	1.53
2	3	165	VAL	CA-C	-5.17	1.46	1.52
1	A	95	GLU	CA-C	-5.17	1.46	1.52
2	1	116	ASP	CA-C	-5.17	1.46	1.52
1	C	18	ASP	N-CA	-5.17	1.39	1.46
2	5	179	ASP	N-CA	-5.17	1.39	1.46
1	B	93	ARG	CZ-NH2	5.17	1.40	1.33
2	6	154	ARG	CA-C	-5.17	1.45	1.52
2	7	177	LYS	CA-C	5.17	1.59	1.52
1	F	118	ASP	C-N	5.17	1.40	1.33
1	G	14	VAL	CA-C	-5.16	1.46	1.52
1	G	161	ALA	N-CA	-5.16	1.39	1.46
2	7	168	ALA	C-N	5.16	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	39	SER	CA-C	-5.16	1.46	1.52
1	D	71	ASP	N-CA	-5.15	1.38	1.46
1	F	168	ARG	C-N	5.15	1.40	1.33
2	3	113	GLY	N-CA	-5.15	1.39	1.45
1	G	65	GLU	CA-C	-5.15	1.46	1.52
1	B	156	LEU	N-CA	-5.15	1.39	1.46
2	1	155	PHE	N-CA	5.15	1.52	1.46
1	A	88	LEU	N-CA	5.14	1.52	1.46
2	3	24	VAL	C-O	-5.14	1.18	1.24
2	7	133	GLU	CA-C	-5.14	1.45	1.52
1	D	243	LEU	C-N	5.14	1.40	1.33
1	F	223	GLU	N-CA	-5.14	1.39	1.46
2	4	44	LYS	CA-C	-5.13	1.46	1.53
1	F	20	ARG	CZ-NH2	5.13	1.40	1.33
1	G	144	VAL	CA-C	-5.13	1.47	1.52
2	1	81	ARG	NE-CZ	5.13	1.38	1.33
2	4	39	SER	C-N	-5.13	1.26	1.33
1	A	166	MET	CA-CB	5.12	1.61	1.53
2	2	92	THR	C-N	5.12	1.41	1.33
1	D	223	GLU	CA-C	-5.12	1.46	1.52
2	6	208	LEU	CA-CB	5.12	1.62	1.53
1	E	210	GLU	N-CA	5.12	1.52	1.46
1	D	219	ARG	CZ-NH1	5.12	1.40	1.32
1	E	73	HIS	CA-C	5.12	1.58	1.52
1	F	86	ARG	C-N	5.12	1.40	1.33
1	D	133	GLY	C-N	5.12	1.39	1.33
2	1	56	THR	CA-C	-5.12	1.46	1.52
2	2	35	ASN	C-N	5.12	1.40	1.33
2	1	37	ILE	C-N	5.11	1.41	1.33
2	3	80	ARG	CD-NE	5.11	1.53	1.46
2	5	110	LEU	CA-C	-5.11	1.46	1.52
1	C	140	GLY	C-O	-5.11	1.18	1.23
2	3	206	GLN	CA-CB	5.11	1.62	1.53
1	A	180	ARG	CZ-NH2	5.11	1.40	1.33
2	4	137	ILE	N-CA	-5.11	1.40	1.46
1	C	169	ASN	CG-ND2	5.10	1.44	1.33
1	C	29	GLU	C-N	5.10	1.40	1.33
2	7	158	GLU	N-CA	-5.10	1.40	1.46
1	E	131	PRO	C-N	5.10	1.40	1.33
1	F	33	ARG	NE-CZ	5.10	1.38	1.33
2	3	197	TYR	CZ-OH	5.10	1.48	1.38
2	7	64	GLN	CA-CB	5.10	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	VAL	C-N	5.10	1.41	1.33
1	F	234	GLU	C-N	5.10	1.40	1.33
1	C	14	VAL	CA-C	-5.09	1.46	1.52
1	C	39	GLY	N-CA	-5.09	1.40	1.45
2	4	149	GLY	C-N	5.09	1.40	1.33
2	7	155	PHE	CA-C	-5.09	1.46	1.52
1	F	48	LEU	C-N	5.09	1.40	1.33
2	1	194	ASP	CA-C	-5.09	1.46	1.52
2	2	60	VAL	N-CA	-5.09	1.40	1.46
2	4	97	LEU	N-CA	5.09	1.52	1.46
1	D	241	ARG	NE-CZ	5.08	1.38	1.33
2	5	77	TYR	CA-C	-5.08	1.46	1.52
2	5	140	THR	C-N	5.08	1.37	1.33
2	6	104	PHE	CA-C	-5.08	1.47	1.52
1	A	59	LEU	CA-CB	5.08	1.59	1.53
2	1	104	PHE	CA-CB	5.08	1.58	1.53
1	C	224	VAL	N-CA	-5.08	1.40	1.46
1	A	199	SER	C-O	-5.08	1.18	1.24
1	A	224	VAL	N-CA	-5.07	1.40	1.46
2	6	14	THR	N-CA	-5.07	1.39	1.45
2	5	156	THR	N-CA	-5.07	1.41	1.45
1	A	144	VAL	N-CA	-5.07	1.40	1.46
1	D	86	ARG	CZ-NH1	5.07	1.39	1.32
1	E	120	LYS	C-O	-5.07	1.18	1.24
2	1	35	ASN	C-N	5.07	1.40	1.33
2	6	106	TYR	CA-CB	5.07	1.62	1.53
2	2	170	ARG	C-O	-5.06	1.18	1.24
2	7	94	THR	C-O	-5.06	1.18	1.24
1	E	169	ASN	C-N	5.06	1.40	1.33
1	E	235	ARG	CA-C	5.06	1.59	1.52
1	G	66	LYS	N-CA	-5.06	1.39	1.46
2	5	163	GLU	C-O	-5.06	1.18	1.24
2	4	102	ARG	CZ-NH2	5.05	1.40	1.33
2	5	81	ARG	C-N	5.05	1.40	1.33
1	B	197	GLY	CA-C	-5.05	1.46	1.52
1	E	149	GLU	CA-C	-5.05	1.46	1.52
2	5	177	LYS	CA-C	5.05	1.59	1.52
1	G	151	ASP	CA-CB	5.05	1.60	1.54
1	G	76	ALA	N-CA	-5.04	1.39	1.46
2	2	74	ALA	C-O	-5.04	1.18	1.24
2	5	81	ARG	CA-C	-5.04	1.46	1.52
2	7	54	MET	CA-C	-5.04	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	94	ILE	C-N	5.04	1.40	1.33
1	F	222	LYS	CA-C	-5.04	1.46	1.52
2	3	193	GLU	N-CA	-5.04	1.39	1.46
1	F	109	VAL	C-N	5.04	1.40	1.33
1	F	119	PHE	C-N	5.03	1.40	1.33
2	6	151	LEU	C-N	5.03	1.41	1.33
2	2	120	LYS	C-N	5.03	1.39	1.33
2	5	117	SER	CA-C	-5.03	1.46	1.52
2	5	159	ILE	N-CA	-5.03	1.39	1.46
1	D	16	SER	CA-CB	5.03	1.60	1.53
1	D	106	PRO	C-N	5.03	1.39	1.33
1	A	168	ARG	CA-C	-5.02	1.45	1.52
2	6	200	SER	CA-C	5.02	1.59	1.52
1	D	230	LYS	CA-C	5.02	1.57	1.52
1	C	42	CYS	CA-CB	5.02	1.61	1.53
1	G	49	ILE	CA-CB	5.02	1.61	1.54
2	5	40	LYS	C-N	5.02	1.40	1.33
1	C	86	ARG	CZ-NH2	5.01	1.40	1.33
1	G	144	VAL	CA-CB	5.01	1.60	1.54
1	F	179	TYR	CA-CB	5.01	1.61	1.53
2	2	71	LYS	N-CA	-5.01	1.40	1.46
1	F	173	GLU	CA-CB	5.01	1.61	1.53
2	3	81	ARG	NE-CZ	5.01	1.38	1.33
1	B	121	GLN	C-N	5.00	1.40	1.33
2	1	66	LEU	CA-C	-5.00	1.46	1.52
2	6	184	ASP	CA-C	-5.00	1.46	1.52
2	1	22	GLY	C-N	5.00	1.40	1.33

All (1696) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	181	ASP	O-C-N	32.95	166.42	122.59
1	C	181	ASP	CA-C-O	-24.94	84.84	120.51
1	B	180	ARG	NE-CZ-NH2	13.27	131.14	119.20
1	E	180	ARG	NE-CZ-NH2	12.54	130.48	119.20
1	C	182	ASP	N-CA-CB	12.48	133.77	110.56
1	A	66	LYS	N-CA-C	-12.29	100.61	114.62
2	5	211	PHE	CG-CD1-CE1	-11.69	100.83	120.70
1	D	63	THR	N-CA-C	-10.88	100.05	113.97
1	D	70	ILE	N-CA-C	-10.87	102.46	111.81
2	1	167	LEU	CA-C-O	-10.79	109.49	120.82
1	F	80	GLY	N-CA-C	-10.57	100.88	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	140	THR	CA-C-N	10.43	136.61	122.42
2	3	140	THR	C-N-CA	10.43	136.61	122.42
1	E	80	GLY	N-CA-C	-10.35	101.10	111.56
2	5	128	ILE	N-CA-C	-10.26	102.43	112.17
2	1	150	VAL	CA-C-N	10.24	133.75	120.44
2	1	150	VAL	C-N-CA	10.24	133.75	120.44
1	C	195	ALA	CA-C-N	10.20	133.94	120.28
1	C	195	ALA	C-N-CA	10.20	133.94	120.28
2	2	132	ILE	N-CA-C	-10.19	94.31	108.27
2	6	71	LYS	CA-C-N	10.15	133.35	120.56
2	6	71	LYS	C-N-CA	10.15	133.35	120.56
2	1	195	GLU	CA-C-N	10.11	137.63	122.47
2	1	195	GLU	C-N-CA	10.11	137.63	122.47
2	6	139	ALA	CA-C-N	9.98	139.67	121.70
2	6	139	ALA	C-N-CA	9.98	139.67	121.70
2	1	201	PRO	CA-C-N	9.89	133.71	120.65
2	1	201	PRO	C-N-CA	9.89	133.71	120.65
2	3	139	ALA	CA-C-N	9.86	139.44	121.70
2	3	139	ALA	C-N-CA	9.86	139.44	121.70
1	F	211	VAL	N-CA-C	-9.76	93.92	108.17
2	6	128	ILE	N-CA-C	-9.75	103.13	112.29
1	A	186	ASP	CA-C-N	9.72	133.66	120.44
1	A	186	ASP	C-N-CA	9.72	133.66	120.44
1	D	22	PHE	CA-CB-CG	-9.70	104.11	113.80
2	6	173	TYR	O-C-N	9.65	132.35	122.12
1	G	57	LYS	N-CA-C	-9.57	101.11	113.17
1	F	15	PHE	CA-CB-CG	9.54	123.34	113.80
2	3	201	PRO	CA-C-N	9.50	133.40	120.38
2	3	201	PRO	C-N-CA	9.50	133.40	120.38
2	3	99	ASN	CA-CB-CG	-9.42	103.18	112.60
1	D	181	ASP	N-CA-C	-9.30	104.02	114.62
1	B	81	LEU	CA-C-N	9.29	132.26	120.56
1	B	81	LEU	C-N-CA	9.29	132.26	120.56
1	G	22	PHE	CA-C-N	9.21	132.62	120.28
1	G	22	PHE	C-N-CA	9.21	132.62	120.28
2	5	142	SER	N-CA-C	-9.18	102.23	113.97
1	G	196	MET	CA-C-N	9.15	130.14	119.98
1	G	196	MET	C-N-CA	9.15	130.14	119.98
2	7	194	ASP	N-CA-C	-9.10	104.25	114.62
2	5	75	ASN	CA-C-O	9.04	130.14	120.55
1	F	142	ASP	N-CA-C	-8.98	102.46	113.41
1	F	67	ILE	N-CA-C	-8.95	94.45	107.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	56	THR	CA-C-N	8.95	135.34	123.00
2	2	56	THR	C-N-CA	8.95	135.34	123.00
2	2	49	ALA	N-CA-C	-8.92	97.21	108.45
1	A	73	HIS	CG-CD2-NE2	8.88	116.08	107.20
2	4	27	THR	O-C-N	-8.86	113.56	123.48
1	F	17	PRO	N-CA-C	-8.84	103.15	114.03
2	5	140	THR	CA-C-O	-8.84	111.61	121.51
2	3	116	ASP	CA-CB-CG	-8.79	103.81	112.60
2	4	65	PHE	CA-C-N	8.77	132.03	120.28
2	4	65	PHE	C-N-CA	8.77	132.03	120.28
1	A	108	THR	N-CA-CB	8.76	122.89	110.36
1	G	31	VAL	CA-C-O	-8.75	111.89	121.17
1	B	171	VAL	N-CA-C	8.73	119.54	110.72
1	E	218	ASP	N-CA-C	-8.72	101.56	112.72
2	5	197	TYR	N-CA-C	-8.68	95.62	109.59
2	4	111	LEU	N-CA-C	-8.65	94.31	108.41
1	C	132	PHE	CA-CB-CG	-8.64	105.16	113.80
2	1	162	ASP	N-CA-C	8.61	120.66	111.28
2	3	182	SER	N-CA-C	-8.58	102.83	113.38
1	F	230	LYS	CA-C-O	-8.52	108.48	120.16
2	3	128	ILE	N-CA-C	-8.52	104.28	112.29
1	F	105	GLU	CA-C-N	8.51	128.83	119.90
1	F	105	GLU	C-N-CA	8.51	128.83	119.90
2	6	111	LEU	CA-C-N	8.47	133.61	122.93
2	6	111	LEU	C-N-CA	8.47	133.61	122.93
2	2	128	ILE	N-CA-C	-8.46	102.91	111.88
1	B	169	ASN	CA-C-N	8.44	131.79	120.65
1	B	169	ASN	C-N-CA	8.44	131.79	120.65
2	3	136	ASP	CA-CB-CG	8.42	121.02	112.60
1	D	91	ARG	CA-C-N	8.42	131.56	120.28
1	D	91	ARG	C-N-CA	8.42	131.56	120.28
2	1	75	ASN	CA-CB-CG	-8.39	104.20	112.60
2	2	96	ASN	CA-CB-CG	-8.39	104.21	112.60
1	C	182	ASP	N-CA-C	-8.38	90.48	107.41
2	3	137	ILE	N-CA-CB	-8.38	96.06	110.13
2	2	60	VAL	CB-CA-C	-8.37	101.26	111.97
2	6	148	TYR	CA-C-N	8.36	129.43	119.99
2	6	148	TYR	C-N-CA	8.36	129.43	119.99
1	E	180	ARG	NE-CZ-NH1	-8.34	113.16	121.50
1	A	125	GLN	N-CA-CB	8.33	122.61	110.20
2	7	156	THR	CA-C-O	-8.33	111.05	120.46
2	6	104	PHE	CA-C-O	-8.33	113.47	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ILE	CA-C-O	-8.33	112.45	121.28
2	2	98	LEU	CA-C-N	8.28	132.04	120.29
2	2	98	LEU	C-N-CA	8.28	132.04	120.29
1	D	184	SER	CA-C-N	8.25	131.67	120.54
1	D	184	SER	C-N-CA	8.25	131.67	120.54
2	3	57	ALA	N-CA-C	-8.24	95.80	109.07
2	2	45	ILE	N-CA-C	-8.22	96.28	108.12
1	E	16	SER	CA-C-O	-8.21	112.02	120.96
2	6	106	TYR	N-CA-C	-8.19	93.36	110.80
1	E	124	THR	N-CA-C	-8.17	103.44	113.41
2	5	73	GLU	CA-C-N	8.17	131.06	120.44
2	5	73	GLU	C-N-CA	8.17	131.06	120.44
1	G	52	LYS	CA-C-O	-8.16	110.88	120.10
1	F	216	VAL	CA-C-N	8.16	131.21	120.28
1	F	216	VAL	C-N-CA	8.16	131.21	120.28
1	A	181	ASP	N-CA-C	8.13	119.78	111.07
1	A	187	ASP	N-CA-CB	8.13	121.86	110.07
1	E	245	LYS	N-CA-C	-8.11	102.32	114.64
1	D	216	VAL	N-CA-C	8.09	118.64	110.23
2	2	60	VAL	N-CA-C	8.06	118.16	110.42
2	2	22	GLY	CA-C-O	-8.03	115.37	120.91
1	F	211	VAL	CA-C-N	8.02	128.55	121.82
1	F	211	VAL	C-N-CA	8.02	128.55	121.82
1	F	73	HIS	N-CA-C	-8.01	103.31	113.72
2	1	104	PHE	CA-C-N	7.99	127.99	119.76
2	1	104	PHE	C-N-CA	7.99	127.99	119.76
2	6	196	PHE	CA-CB-CG	-7.98	105.82	113.80
2	3	204	VAL	N-CA-C	-7.97	102.31	111.00
2	3	31	ALA	N-CA-CB	7.97	123.28	110.77
1	C	216	VAL	N-CA-CB	7.95	120.75	110.57
2	5	112	ILE	N-CA-C	-7.95	96.14	107.75
1	E	196	MET	CA-C-N	7.93	128.79	119.98
1	E	196	MET	C-N-CA	7.93	128.79	119.98
2	2	140	THR	N-CA-C	7.90	121.64	110.50
2	4	115	ILE	CA-C-N	7.88	134.65	122.11
2	4	115	ILE	C-N-CA	7.88	134.65	122.11
2	4	21	ASP	CA-CB-CG	-7.87	104.73	112.60
2	2	126	ASP	CA-CB-CG	-7.85	104.75	112.60
1	E	236	ALA	CA-C-N	7.84	130.78	120.28
1	E	236	ALA	C-N-CA	7.84	130.78	120.28
2	1	142	SER	N-CA-C	-7.84	102.63	112.90
2	3	143	GLY	N-CA-C	-7.82	102.71	115.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GLU	N-CA-C	7.82	119.80	111.28
2	7	61	GLY	CA-C-N	7.81	130.75	120.28
2	7	61	GLY	C-N-CA	7.81	130.75	120.28
2	7	204	VAL	CA-C-N	7.81	131.53	120.28
2	7	204	VAL	C-N-CA	7.81	131.53	120.28
1	D	241	ARG	CA-C-N	7.81	130.74	120.28
1	D	241	ARG	C-N-CA	7.81	130.74	120.28
2	7	140	THR	O-C-N	-7.80	114.52	123.42
2	6	143	GLY	CA-C-N	7.80	132.52	120.82
2	6	143	GLY	C-N-CA	7.80	132.52	120.82
2	6	88	ARG	CA-C-N	7.80	130.57	120.44
2	6	88	ARG	C-N-CA	7.80	130.57	120.44
1	F	185	PHE	O-C-N	7.79	130.37	122.12
1	A	40	ILE	N-CA-C	-7.78	96.93	108.45
2	1	76	LEU	CA-C-N	7.77	131.03	120.54
2	1	76	LEU	C-N-CA	7.77	131.03	120.54
2	5	173	TYR	N-CA-CB	7.76	121.65	110.16
1	G	32	LYS	CA-C-O	-7.75	111.52	120.20
2	4	167	LEU	CA-C-N	7.75	130.67	120.28
2	4	167	LEU	C-N-CA	7.75	130.67	120.28
2	5	32	THR	N-CA-C	-7.75	96.66	108.67
1	A	105	GLU	O-C-N	-7.75	115.80	121.84
2	6	33	MET	N-CA-C	-7.75	102.34	112.41
2	7	35	ASN	CA-CB-CG	-7.73	104.87	112.60
1	B	89	ILE	N-CA-CB	7.69	124.69	110.77
1	G	217	ASP	CA-CB-CG	7.69	120.29	112.60
1	G	170	ALA	N-CA-C	7.69	119.29	111.07
2	7	89	ALA	CA-C-N	7.67	130.22	120.56
2	7	89	ALA	C-N-CA	7.67	130.22	120.56
2	1	171	ALA	CA-C-N	7.66	131.30	120.42
2	1	171	ALA	C-N-CA	7.66	131.30	120.42
2	3	80	ARG	NE-CZ-NH1	-7.64	113.86	121.50
2	5	20	LYS	N-CA-C	-7.64	103.79	113.72
2	1	161	VAL	N-CA-C	7.63	118.40	110.62
1	A	229	LEU	N-CA-C	-7.63	103.05	111.36
1	G	112	LEU	CA-C-N	7.63	130.50	120.28
1	G	112	LEU	C-N-CA	7.63	130.50	120.28
2	1	55	THR	CA-C-O	-7.62	112.63	120.71
2	3	111	LEU	N-CA-CB	7.62	122.53	110.65
1	F	126	TYR	N-CA-C	-7.59	95.93	108.76
2	1	42	ALA	N-CA-C	-7.58	94.67	110.80
1	A	58	LEU	N-CA-C	-7.57	104.19	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	176	MET	CA-C-N	7.57	131.81	120.31
2	6	176	MET	C-N-CA	7.57	131.81	120.31
1	D	185	PHE	CA-C-O	-7.56	112.81	120.90
2	7	111	LEU	N-CA-C	-7.54	96.12	108.41
1	G	113	ALA	CA-C-N	7.53	130.23	120.44
1	G	113	ALA	C-N-CA	7.53	130.23	120.44
1	F	170	ALA	CB-CA-C	-7.53	99.06	110.88
1	G	162	THR	N-CA-C	-7.53	98.21	108.38
2	2	198	GLN	N-CA-C	-7.53	96.14	108.41
2	2	209	ALA	N-CA-C	-7.53	103.68	113.17
1	B	31	VAL	O-C-N	-7.53	114.08	121.83
1	F	28	ARG	NE-CZ-NH1	-7.52	113.98	121.50
1	E	185	PHE	CA-C-N	7.52	133.44	120.58
1	E	185	PHE	C-N-CA	7.52	133.44	120.58
1	G	105	GLU	O-C-N	-7.51	114.05	121.94
2	2	150	VAL	O-C-N	7.51	129.45	121.87
2	6	60	VAL	CA-C-N	7.49	128.25	119.94
2	6	60	VAL	C-N-CA	7.49	128.25	119.94
2	2	154	ARG	NE-CZ-NH1	-7.49	114.01	121.50
2	7	198	GLN	N-CA-C	-7.48	96.22	108.41
1	G	52	LYS	N-CA-C	7.48	120.31	111.71
1	E	120	LYS	CA-C-O	-7.48	112.62	120.55
2	3	96	ASN	CA-CB-CG	-7.47	105.13	112.60
2	2	80	ARG	N-CA-C	7.45	119.19	111.14
2	2	153	ASP	N-CA-CB	7.44	121.28	110.20
2	5	29	LYS	N-CA-C	7.44	119.39	111.28
1	C	88	LEU	CA-C-O	7.43	128.43	120.55
1	F	108	THR	CA-C-N	7.42	129.91	120.56
1	F	108	THR	C-N-CA	7.42	129.91	120.56
1	B	40	ILE	N-CA-CB	7.41	122.34	111.52
1	F	114	LYS	CA-C-N	7.41	130.52	120.44
1	F	114	LYS	C-N-CA	7.41	130.52	120.44
1	F	119	PHE	CA-CB-CG	7.41	121.21	113.80
1	E	165	GLY	CA-C-N	7.40	130.94	120.28
1	E	165	GLY	C-N-CA	7.40	130.94	120.28
2	7	112	ILE	N-CA-C	-7.40	96.95	107.75
2	7	187	ASP	CA-CB-CG	7.38	119.98	112.60
2	1	184	ASP	CA-CB-CG	-7.37	105.23	112.60
1	G	52	LYS	CA-C-N	7.36	135.60	121.54
1	G	52	LYS	C-N-CA	7.36	135.60	121.54
1	B	217	ASP	CA-CB-CG	7.36	119.96	112.60
1	G	135	SER	N-CA-C	-7.35	96.97	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	176	MET	CA-C-N	7.33	130.11	120.28
2	5	176	MET	C-N-CA	7.33	130.11	120.28
2	1	190	LYS	N-CA-C	-7.33	97.29	109.24
1	F	52	LYS	N-CA-C	-7.33	103.43	112.88
2	5	146	THR	CA-C-O	7.32	128.69	121.00
2	4	42	ALA	CA-C-O	7.31	130.00	121.44
2	2	60	VAL	CA-C-N	7.30	128.24	119.99
2	2	60	VAL	C-N-CA	7.30	128.24	119.99
2	4	74	ALA	N-CA-C	7.30	119.32	111.36
2	6	72	ILE	CA-C-N	7.30	130.66	120.29
2	6	72	ILE	C-N-CA	7.30	130.66	120.29
2	3	199	TYR	CA-CB-CG	-7.30	100.76	113.90
2	1	80	ARG	N-CA-C	7.30	119.31	111.36
1	B	181	ASP	CA-CB-CG	-7.29	105.31	112.60
1	C	21	LEU	N-CA-C	-7.29	97.81	109.76
2	6	41	ALA	N-CA-C	-7.29	104.34	112.57
1	A	198	LEU	CA-C-N	7.28	130.04	120.28
1	A	198	LEU	C-N-CA	7.28	130.04	120.28
2	4	70	ILE	CB-CA-C	-7.28	102.65	111.97
2	4	201	PRO	CA-C-N	7.28	130.91	120.79
2	4	201	PRO	C-N-CA	7.28	130.91	120.79
1	G	79	SER	CA-C-N	7.28	130.12	122.63
1	G	79	SER	C-N-CA	7.28	130.12	122.63
2	7	108	VAL	CB-CA-C	7.27	121.91	111.80
2	4	97	LEU	CA-C-N	7.27	129.89	120.44
2	4	97	LEU	C-N-CA	7.27	129.89	120.44
2	6	62	ASP	CA-C-N	7.27	129.89	120.44
2	6	62	ASP	C-N-CA	7.27	129.89	120.44
1	B	70	ILE	CB-CA-C	-7.26	103.79	110.91
1	D	156	LEU	N-CA-C	-7.26	97.11	109.24
1	G	245	LYS	N-CA-C	-7.26	102.42	113.89
1	C	88	LEU	O-C-N	-7.26	114.43	122.12
2	6	165	VAL	N-CA-CB	7.26	119.04	110.55
1	A	100	ARG	CA-C-N	7.25	129.86	120.44
1	A	100	ARG	C-N-CA	7.25	129.86	120.44
2	1	197	TYR	N-CA-C	-7.25	97.93	109.59
2	6	22	GLY	CA-C-N	7.25	133.92	122.33
2	6	22	GLY	C-N-CA	7.25	133.92	122.33
1	G	81	LEU	CA-C-N	7.23	129.68	120.56
1	G	81	LEU	C-N-CA	7.23	129.68	120.56
1	E	194	VAL	O-C-N	7.23	129.42	121.90
2	5	67	ALA	CA-C-N	7.23	129.83	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	67	ALA	C-N-CA	7.23	129.83	120.44
1	A	235	ARG	CA-C-N	7.22	130.54	120.29
1	A	235	ARG	C-N-CA	7.22	130.54	120.29
1	B	198	LEU	CA-C-N	7.22	129.83	120.44
1	B	198	LEU	C-N-CA	7.22	129.83	120.44
1	D	173	GLU	N-CA-C	7.22	120.07	111.33
1	B	124	THR	CA-C-N	7.22	129.83	120.44
1	B	124	THR	C-N-CA	7.22	129.83	120.44
1	F	61	ALA	N-CA-C	-7.21	102.77	112.94
1	F	184	SER	N-CA-C	-7.21	99.81	110.48
2	2	143	GLY	CA-C-N	7.21	129.94	120.28
2	2	143	GLY	C-N-CA	7.21	129.94	120.28
1	A	241	ARG	NE-CZ-NH1	-7.18	114.32	121.50
1	B	46	VAL	O-C-N	7.17	131.01	123.05
1	G	236	ALA	CA-C-N	7.17	130.61	120.28
1	G	236	ALA	C-N-CA	7.17	130.61	120.28
2	1	148	TYR	CA-C-N	7.17	127.76	119.94
2	1	148	TYR	C-N-CA	7.17	127.76	119.94
1	A	123	TYR	CB-CG-CD2	-7.17	110.05	120.80
2	3	27	THR	N-CA-C	-7.16	98.14	108.60
2	1	51	ARG	CA-C-O	7.16	127.46	121.02
1	D	67	ILE	N-CA-CB	7.15	121.26	112.10
1	B	66	LYS	CA-C-N	7.15	132.71	123.13
1	B	66	LYS	C-N-CA	7.15	132.71	123.13
2	6	30	ARG	NE-CZ-NH1	-7.15	114.35	121.50
1	G	144	VAL	O-C-N	-7.14	112.95	121.10
2	7	156	THR	CA-C-N	7.14	128.05	120.12
2	7	156	THR	C-N-CA	7.14	128.05	120.12
2	1	199	TYR	CB-CA-C	-7.14	98.72	110.85
1	D	184	SER	N-CA-C	-7.14	101.33	110.53
2	2	198	GLN	CB-CA-C	7.14	122.00	110.16
2	7	106	TYR	N-CA-C	-7.13	95.61	110.80
2	3	200	SER	CA-C-O	-7.12	114.19	120.60
2	1	129	GLY	CA-C-O	7.12	127.58	122.45
2	2	88	ARG	CA-C-N	7.12	129.81	120.28
2	2	88	ARG	C-N-CA	7.12	129.81	120.28
1	A	123	TYR	CB-CG-CD1	7.11	131.46	120.80
2	1	136	ASP	CA-CB-CG	7.11	119.71	112.60
1	D	145	PRO	CA-C-O	-7.10	112.96	121.48
1	G	95	GLU	CA-C-N	7.09	129.78	120.28
1	G	95	GLU	C-N-CA	7.09	129.78	120.28
2	5	116	ASP	CA-C-N	7.08	129.77	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	116	ASP	C-N-CA	7.08	129.77	120.28
2	7	35	ASN	N-CA-C	-7.08	104.28	114.12
2	3	136	ASP	CA-C-N	7.08	129.98	120.50
2	3	136	ASP	C-N-CA	7.08	129.98	120.50
1	D	42	CYS	N-CA-C	-7.07	99.14	109.18
2	3	156	THR	CA-C-O	-7.07	112.47	120.46
1	D	182	ASP	O-C-N	7.07	132.42	123.23
1	B	90	ASP	CA-C-N	7.06	129.74	120.28
1	B	90	ASP	C-N-CA	7.06	129.74	120.28
2	7	145	LEU	CA-C-N	7.05	130.30	120.29
2	7	145	LEU	C-N-CA	7.05	130.30	120.29
1	A	104	ASP	CA-CB-CG	-7.04	105.56	112.60
1	B	145	PRO	N-CA-CB	7.04	109.89	103.34
1	B	195	ALA	N-CA-CB	7.04	120.58	110.16
1	C	223	GLU	N-CA-C	-7.04	97.74	109.07
1	B	20	ARG	N-CA-C	-7.03	99.20	109.18
1	C	149	GLU	N-CA-C	-7.03	96.95	108.41
2	5	86	THR	N-CA-C	-7.03	99.53	110.42
1	G	160	LYS	N-CA-CB	7.02	122.35	110.49
2	7	81	ARG	CA-C-N	7.01	132.08	122.19
2	7	81	ARG	C-N-CA	7.01	132.08	122.19
1	C	141	VAL	O-C-N	7.01	129.28	122.97
1	B	22	PHE	CA-C-O	-7.01	113.48	120.70
1	A	196	MET	CA-C-N	7.01	127.71	120.00
1	A	196	MET	C-N-CA	7.01	127.71	120.00
1	G	55	GLY	O-C-N	7.00	131.80	122.70
1	C	21	LEU	N-CA-CB	7.00	122.07	110.52
1	F	62	ASP	CA-C-O	6.99	127.45	119.27
2	7	63	ALA	N-CA-C	6.99	118.55	111.07
2	7	168	ALA	CB-CA-C	-6.99	99.19	110.79
1	B	22	PHE	O-C-N	6.99	129.63	122.09
1	E	110	LYS	CA-C-N	6.97	130.19	120.29
1	E	110	LYS	C-N-CA	6.97	130.19	120.29
2	7	17	LEU	CA-C-N	6.97	131.28	121.66
2	7	17	LEU	C-N-CA	6.97	131.28	121.66
2	1	196	PHE	N-CA-C	-6.97	93.99	107.44
1	G	80	GLY	CA-C-O	6.97	130.64	120.89
1	G	132	PHE	CA-CB-CG	-6.97	106.83	113.80
2	7	158	GLU	CA-C-N	6.96	130.58	120.91
2	7	158	GLU	C-N-CA	6.96	130.58	120.91
2	6	180	SER	N-CA-C	-6.96	101.91	110.61
2	5	124	SER	CA-C-O	-6.95	112.68	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	96	ASN	OD1-CG-ND2	6.95	129.55	122.60
2	7	151	LEU	CA-C-N	6.94	130.28	120.28
2	7	151	LEU	C-N-CA	6.94	130.28	120.28
2	1	156	THR	CA-C-N	6.93	128.51	119.84
2	1	156	THR	C-N-CA	6.93	128.51	119.84
1	D	211	VAL	CA-C-N	6.93	126.95	121.61
1	D	211	VAL	C-N-CA	6.93	126.95	121.61
1	B	182	ASP	N-CA-C	-6.92	103.95	112.88
1	E	190	VAL	CA-C-O	-6.92	113.75	120.95
1	F	60	GLU	CB-CA-C	6.92	121.15	109.80
1	C	19	GLY	O-C-N	-6.91	113.16	122.35
2	5	17	LEU	CA-C-N	6.91	131.01	122.37
2	5	17	LEU	C-N-CA	6.91	131.01	122.37
1	C	166	MET	N-CA-C	-6.91	104.67	113.23
1	E	240	ILE	N-CA-CB	6.90	118.63	110.55
2	1	117	SER	CA-C-N	6.90	129.53	120.28
2	1	117	SER	C-N-CA	6.90	129.53	120.28
2	1	147	ALA	N-CA-C	6.90	118.80	111.28
2	7	76	LEU	CA-C-N	6.90	129.86	120.54
2	7	76	LEU	C-N-CA	6.90	129.86	120.54
1	D	181	ASP	N-CA-CB	6.90	122.08	111.18
2	5	55	THR	N-CA-CB	6.90	122.88	111.08
1	C	99	ASN	CA-C-O	6.89	127.86	120.55
1	C	210	GLU	N-CA-C	-6.89	98.17	109.40
1	G	197	GLY	CA-C-O	-6.89	113.66	120.75
1	G	208	ASN	N-CA-CB	6.89	120.69	110.49
1	G	188	ALA	N-CA-C	6.88	118.78	111.28
2	1	35	ASN	CA-C-N	6.88	130.58	120.95
2	1	35	ASN	C-N-CA	6.88	130.58	120.95
2	6	162	ASP	CB-CA-C	-6.88	99.16	110.85
1	B	194	VAL	O-C-N	6.87	128.53	121.87
2	1	147	ALA	O-C-N	6.87	129.40	122.12
2	2	52	MET	CA-C-O	-6.87	110.94	120.21
1	D	51	ASP	CA-CB-CG	6.86	119.46	112.60
1	E	29	GLU	O-C-N	-6.86	113.83	122.27
2	1	101	TYR	CB-CG-CD1	-6.84	110.53	120.80
1	B	218	ASP	CA-CB-CG	-6.84	105.76	112.60
1	B	243	LEU	N-CA-C	6.83	118.73	111.28
2	5	59	SER	CA-C-N	6.83	129.82	120.46
2	5	59	SER	C-N-CA	6.83	129.82	120.46
1	C	110	LYS	CA-C-N	6.83	129.98	120.29
1	C	110	LYS	C-N-CA	6.83	129.98	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	198	GLN	CA-CB-CG	-6.83	100.45	114.10
1	B	94	ILE	CA-C-O	-6.82	113.86	120.95
1	F	152	PRO	CA-C-N	6.81	129.29	120.44
1	F	152	PRO	C-N-CA	6.81	129.29	120.44
1	D	238	GLU	CB-CA-C	-6.81	99.27	110.85
2	5	161	VAL	N-CA-CB	6.81	119.29	110.57
1	B	186	ASP	N-CA-CB	6.80	120.12	110.12
1	F	155	ALA	N-CA-C	6.80	120.71	110.64
1	A	73	HIS	CE1-NE2-CD2	-6.80	102.20	109.00
1	B	151	ASP	CA-C-O	-6.79	113.66	120.66
2	3	75	ASN	CA-C-N	6.79	129.69	120.38
2	3	75	ASN	C-N-CA	6.79	129.69	120.38
2	7	74	ALA	CB-CA-C	-6.79	99.51	110.79
1	D	35	ALA	CA-C-N	6.79	130.39	120.82
1	D	35	ALA	C-N-CA	6.79	130.39	120.82
1	E	106	PRO	CA-C-N	6.79	129.60	120.50
1	E	106	PRO	C-N-CA	6.79	129.60	120.50
1	E	240	ILE	CA-C-N	6.78	129.26	120.44
1	E	240	ILE	C-N-CA	6.78	129.26	120.44
2	4	198	GLN	N-CA-CB	6.77	121.41	110.77
1	B	113	ALA	CA-C-O	-6.77	113.37	120.55
1	D	61	ALA	CA-C-N	6.77	134.47	121.54
1	D	61	ALA	C-N-CA	6.77	134.47	121.54
1	A	173	GLU	CA-C-N	6.77	129.24	120.44
1	A	173	GLU	C-N-CA	6.77	129.24	120.44
2	1	35	ASN	CA-CB-CG	-6.76	105.84	112.60
2	6	122	ILE	N-CA-CB	6.75	122.51	111.44
2	6	170	ARG	O-C-N	6.75	129.27	122.12
2	6	74	ALA	CA-C-N	6.74	129.21	120.44
2	6	74	ALA	C-N-CA	6.74	129.21	120.44
1	C	23	GLN	CA-C-N	6.74	130.38	120.74
1	C	23	GLN	C-N-CA	6.74	130.38	120.74
1	D	204	LEU	N-CA-CB	6.74	120.00	110.36
2	1	129	GLY	N-CA-C	-6.73	105.17	112.04
2	3	76	LEU	CA-C-N	6.73	129.29	120.28
2	3	76	LEU	C-N-CA	6.73	129.29	120.28
1	A	190	VAL	CA-C-N	6.72	129.29	120.28
1	A	190	VAL	C-N-CA	6.72	129.29	120.28
1	B	232	TYR	CA-C-O	-6.72	112.78	120.24
2	3	173	TYR	CA-C-N	6.72	129.17	120.44
2	3	173	TYR	C-N-CA	6.72	129.17	120.44
2	1	51	ARG	O-C-N	-6.72	115.53	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	59	SER	CA-C-O	6.72	128.88	121.56
1	E	228	GLU	N-CA-CB	6.71	120.09	110.16
2	1	169	VAL	O-C-N	6.71	128.38	121.87
2	5	84	LYS	CA-C-O	-6.71	112.85	119.49
1	F	224	VAL	O-C-N	6.70	129.62	122.45
2	4	203	GLU	N-CA-C	6.70	118.67	111.36
2	3	37	ILE	CA-C-N	6.69	129.54	120.44
2	3	37	ILE	C-N-CA	6.69	129.54	120.44
2	3	59	SER	N-CA-C	6.69	120.08	110.24
2	4	178	ARG	NE-CZ-NH1	6.69	128.19	121.50
2	3	148	TYR	CA-C-N	6.68	127.36	119.94
2	3	148	TYR	C-N-CA	6.68	127.36	119.94
2	5	29	LYS	CA-C-O	6.68	127.63	120.55
1	B	47	ILE	N-CA-C	-6.68	98.56	108.85
2	7	190	LYS	CA-C-N	6.68	131.98	123.10
2	7	190	LYS	C-N-CA	6.68	131.98	123.10
1	C	182	ASP	CA-CB-CG	6.68	119.28	112.60
1	F	220	THR	N-CA-C	-6.68	96.87	108.69
1	E	230	LYS	CA-C-N	6.67	126.93	119.32
1	E	230	LYS	C-N-CA	6.67	126.93	119.32
2	1	89	ALA	CB-CA-C	-6.65	100.43	110.88
1	C	132	PHE	CA-C-N	6.65	134.45	121.41
1	C	132	PHE	C-N-CA	6.65	134.45	121.41
1	D	32	LYS	N-CA-C	6.65	119.36	111.71
1	E	149	GLU	N-CA-C	-6.65	98.06	108.90
2	2	35	ASN	N-CA-C	-6.65	105.17	113.28
2	5	83	ARG	CA-C-O	-6.65	111.24	120.21
2	1	84	LYS	N-CA-C	-6.64	101.70	110.07
2	4	69	ILE	N-CA-C	6.64	116.80	110.42
1	E	58	LEU	N-CA-C	-6.64	105.08	113.72
1	F	104	ASP	N-CA-CB	6.63	122.39	112.30
2	1	58	GLY	N-CA-C	-6.62	104.87	111.56
1	G	35	ALA	CA-C-N	6.62	130.51	121.05
1	G	35	ALA	C-N-CA	6.62	130.51	121.05
1	D	242	GLU	CA-C-N	6.62	130.37	120.31
1	D	242	GLU	C-N-CA	6.62	130.37	120.31
1	E	202	SER	CA-C-N	6.62	131.33	120.94
1	E	202	SER	C-N-CA	6.62	131.33	120.94
1	C	83	ALA	CA-C-N	6.61	129.14	120.28
1	C	83	ALA	C-N-CA	6.61	129.14	120.28
1	A	216	VAL	CA-C-N	6.61	130.36	120.31
1	A	216	VAL	C-N-CA	6.61	130.36	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	ALA	CA-C-N	6.61	129.68	120.29
1	C	96	ALA	C-N-CA	6.61	129.68	120.29
1	F	138	ILE	CA-CB-CG1	6.61	121.63	110.40
2	4	147	ALA	CA-C-N	6.61	129.13	120.28
2	4	147	ALA	C-N-CA	6.61	129.13	120.28
1	E	118	ASP	N-CA-CB	6.60	119.93	110.16
2	1	125	ILE	N-CA-C	6.60	117.39	107.75
2	2	208	LEU	N-CA-CB	6.60	120.26	110.49
2	6	68	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	C	205	VAL	N-CA-CB	-6.59	107.28	111.83
1	D	230	LYS	CA-C-O	-6.59	112.25	118.44
1	F	116	ILE	CA-C-N	6.58	129.64	120.29
1	F	116	ILE	C-N-CA	6.58	129.64	120.29
1	E	151	ASP	CA-C-N	6.58	126.27	119.56
1	E	151	ASP	C-N-CA	6.58	126.27	119.56
2	1	111	LEU	O-C-N	-6.57	115.58	123.27
1	G	73	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
1	G	230	LYS	CA-C-N	6.56	126.50	119.28
1	G	230	LYS	C-N-CA	6.56	126.50	119.28
2	1	45	ILE	CA-C-O	6.56	127.32	120.36
2	7	160	GLY	O-C-N	-6.56	114.19	122.84
1	E	194	VAL	CA-C-O	-6.55	113.77	121.05
1	G	100	ARG	NE-CZ-NH2	6.55	125.10	119.20
1	E	195	ALA	CA-C-N	6.55	129.59	120.29
1	E	195	ALA	C-N-CA	6.55	129.59	120.29
2	5	13	THR	N-CA-C	-6.55	97.55	108.75
2	2	178	ARG	N-CA-C	6.55	118.08	111.07
2	2	95	SER	CA-C-N	6.54	129.58	120.29
2	2	95	SER	C-N-CA	6.54	129.58	120.29
1	B	39	GLY	CA-C-N	6.54	132.09	122.99
1	B	39	GLY	C-N-CA	6.54	132.09	122.99
2	7	102	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	G	142	ASP	CA-CB-CG	6.54	119.14	112.60
2	1	27	THR	N-CA-C	-6.54	99.72	108.74
1	D	99	ASN	CA-CB-CG	-6.53	106.07	112.60
1	E	239	ARG	CA-C-N	6.53	128.78	120.56
1	E	239	ARG	C-N-CA	6.53	128.78	120.56
1	D	109	VAL	CA-C-N	6.52	129.02	120.28
1	D	109	VAL	C-N-CA	6.52	129.02	120.28
1	D	225	SER	N-CA-C	-6.52	98.07	109.48
2	5	200	SER	CA-C-N	6.52	126.02	119.24
2	5	200	SER	C-N-CA	6.52	126.02	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	92	THR	O-C-N	6.51	128.78	122.07
1	B	153	SER	N-CA-C	-6.51	104.82	112.89
1	C	57	LYS	N-CA-C	-6.51	105.09	113.16
2	1	138	VAL	O-C-N	6.51	128.63	122.97
1	F	220	THR	CA-C-N	6.50	133.96	121.54
1	F	220	THR	C-N-CA	6.50	133.96	121.54
2	1	173	TYR	CA-C-N	6.50	128.98	120.28
2	1	173	TYR	C-N-CA	6.50	128.98	120.28
1	D	185	PHE	O-C-N	6.49	128.84	122.09
1	E	145	PRO	CA-C-O	-6.49	114.16	121.43
2	6	156	THR	N-CA-C	-6.49	99.73	108.11
1	B	46	VAL	CB-CA-C	6.49	121.94	110.71
2	5	96	ASN	CA-CB-CG	-6.49	106.11	112.60
2	5	44	LYS	N-CA-C	-6.48	103.98	112.41
2	3	23	VAL	N-CA-C	-6.48	98.80	108.46
1	A	84	ASP	CA-C-N	6.48	128.86	120.44
1	A	84	ASP	C-N-CA	6.48	128.86	120.44
2	6	118	GLU	N-CA-C	-6.48	105.41	113.38
2	6	154	ARG	NE-CZ-NH2	6.48	125.03	119.20
1	E	199	SER	N-CA-C	6.48	118.42	111.36
1	C	36	THR	N-CA-CB	6.47	119.59	109.69
2	7	134	GLU	N-CA-CB	6.47	122.84	111.13
2	2	162	ASP	O-C-N	6.47	129.52	122.15
2	6	112	ILE	N-CA-C	-6.47	99.11	108.36
1	F	170	ALA	O-C-N	6.46	128.72	122.07
2	4	175	ALA	CA-C-O	-6.46	113.58	120.42
2	1	210	LYS	N-CA-C	-6.45	106.36	114.56
2	1	204	VAL	N-CA-CB	6.45	119.31	110.54
1	G	220	THR	N-CA-CB	6.45	120.96	110.90
2	2	170	ARG	CA-C-N	6.45	129.45	120.29
2	2	170	ARG	C-N-CA	6.45	129.45	120.29
2	4	203	GLU	CB-CG-CD	-6.45	101.64	112.60
2	3	179	ASP	CA-CB-CG	-6.45	106.15	112.60
1	B	244	LEU	N-CA-C	6.45	119.30	111.82
1	G	114	LYS	O-C-N	-6.45	115.43	122.07
1	E	138	ILE	N-CA-C	-6.44	97.84	107.37
2	1	99	ASN	N-CA-C	6.44	118.30	111.28
1	C	69	LYS	N-CA-C	-6.44	99.20	109.76
1	D	130	ARG	CB-CA-C	6.44	118.46	108.61
1	A	125	GLN	CA-C-O	-6.44	113.09	120.24
1	B	131	PRO	CA-C-O	-6.43	113.84	122.08
2	2	137	ILE	CA-CB-CG1	6.43	121.34	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	146	THR	CA-C-N	6.43	128.90	120.28
2	3	146	THR	C-N-CA	6.43	128.90	120.28
1	B	58	LEU	N-CA-C	-6.43	105.43	113.28
2	3	139	ALA	O-C-N	-6.43	114.03	122.59
1	F	222	LYS	O-C-N	-6.43	114.86	122.96
1	A	168	ARG	CA-C-O	-6.42	113.73	120.92
2	3	103	TYR	N-CA-C	-6.42	105.45	113.28
2	1	178	ARG	CA-C-N	6.42	132.04	121.39
2	1	178	ARG	C-N-CA	6.42	132.04	121.39
1	G	101	LEU	N-CA-C	-6.41	104.21	111.07
1	A	174	PHE	CA-C-O	-6.41	114.09	120.82
1	A	172	THR	N-CA-CB	6.41	119.64	110.16
1	G	20	ARG	NE-CZ-NH2	-6.41	113.43	119.20
2	5	198	GLN	N-CA-C	-6.40	96.63	108.02
1	C	241	ARG	NE-CZ-NH2	6.40	124.96	119.20
2	6	130	GLY	N-CA-C	-6.40	104.74	112.48
1	B	38	ILE	CA-C-N	6.39	126.00	121.65
1	B	38	ILE	C-N-CA	6.39	126.00	121.65
2	3	66	LEU	CA-C-N	6.39	128.85	120.28
2	3	66	LEU	C-N-CA	6.39	128.85	120.28
2	4	205	GLU	CA-C-O	-6.39	113.77	120.55
1	A	216	VAL	N-CA-CB	6.39	121.23	110.56
1	B	42	CYS	N-CA-C	-6.39	100.11	109.18
2	7	83	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	A	86	ARG	O-C-N	6.38	128.88	122.12
1	A	166	MET	N-CA-C	-6.38	103.84	111.69
1	D	30	ALA	CA-C-O	-6.38	113.66	120.42
1	B	48	LEU	CB-CA-C	6.38	119.55	110.24
1	B	180	ARG	NE-CZ-NH1	-6.38	115.12	121.50
1	G	88	LEU	CA-C-N	6.38	129.20	120.46
1	G	88	LEU	C-N-CA	6.38	129.20	120.46
1	B	85	ALA	O-C-N	6.38	128.64	122.07
1	G	20	ARG	CA-C-N	6.37	130.42	121.24
1	G	20	ARG	C-N-CA	6.37	130.42	121.24
1	E	169	ASN	CA-C-O	-6.37	113.67	120.42
2	1	139	ALA	N-CA-C	-6.37	99.36	109.23
1	A	124	THR	N-CA-CB	6.37	119.59	110.16
2	1	118	GLU	N-CA-CB	6.37	119.48	110.12
1	B	159	TYR	N-CA-C	-6.36	99.74	109.41
1	G	32	LYS	O-C-N	6.36	129.46	122.20
2	3	153	ASP	N-CA-C	6.36	118.29	111.36
2	7	69	ILE	CB-CA-C	-6.36	103.83	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	220	THR	N-CA-C	-6.35	97.28	110.80
1	C	153	SER	CA-C-O	6.35	127.15	120.42
2	7	170	ARG	CA-C-N	6.34	128.69	120.44
2	7	170	ARG	C-N-CA	6.34	128.69	120.44
1	D	23	GLN	CA-C-N	6.34	129.42	120.42
1	D	23	GLN	C-N-CA	6.34	129.42	120.42
1	D	144	VAL	N-CA-C	-6.34	101.85	109.01
1	A	177	LYS	N-CA-C	-6.34	104.25	112.68
1	B	212	GLY	CA-C-O	-6.34	115.23	121.76
2	1	44	LYS	CA-C-N	6.33	131.79	122.99
2	1	44	LYS	C-N-CA	6.33	131.79	122.99
2	3	43	LYS	N-CA-C	-6.33	98.58	108.90
2	4	40	LYS	N-CA-C	-6.33	105.14	112.92
1	B	105	GLU	CA-C-O	-6.33	113.79	119.86
2	5	55	THR	N-CA-C	-6.33	99.60	109.72
1	D	105	GLU	CA-C-N	6.32	126.66	119.83
1	D	105	GLU	C-N-CA	6.32	126.66	119.83
1	C	27	ALA	CA-C-O	6.32	127.25	120.55
1	C	90	ASP	CA-C-N	6.32	128.65	120.44
1	C	90	ASP	C-N-CA	6.32	128.65	120.44
1	A	19	GLY	N-CA-C	-6.32	106.52	115.43
2	3	200	SER	CA-C-N	6.31	127.73	119.84
2	3	200	SER	C-N-CA	6.31	127.73	119.84
1	B	39	GLY	O-C-N	-6.31	118.44	123.49
2	1	112	ILE	N-CA-C	-6.31	99.28	108.11
2	1	167	LEU	O-C-N	6.31	128.57	122.07
2	4	33	MET	CA-C-N	6.30	133.76	121.41
2	4	33	MET	C-N-CA	6.30	133.76	121.41
2	1	86	THR	N-CA-C	-6.29	101.15	110.46
1	G	216	VAL	CA-CB-CG1	6.29	121.08	110.40
1	B	49	ILE	N-CA-C	-6.28	99.43	108.48
2	3	122	ILE	CB-CA-C	-6.28	101.94	110.42
2	7	60	VAL	N-CA-C	6.28	116.45	110.42
1	F	170	ALA	N-CA-C	6.26	117.77	111.07
2	2	102	ARG	N-CA-C	6.26	119.61	112.97
1	E	47	ILE	N-CA-C	-6.26	99.21	108.85
1	E	219	ARG	CB-CA-C	6.25	120.13	111.63
2	3	117	SER	CA-C-N	6.25	131.38	121.44
2	3	117	SER	C-N-CA	6.25	131.38	121.44
1	B	211	VAL	CA-C-N	6.25	126.95	121.58
1	B	211	VAL	C-N-CA	6.25	126.95	121.58
1	D	118	ASP	N-CA-C	-6.25	104.36	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	135	LYS	N-CA-C	-6.25	104.93	113.30
2	6	77	TYR	CA-C-N	6.24	128.55	120.44
2	6	77	TYR	C-N-CA	6.24	128.55	120.44
1	A	245	LYS	N-CA-C	-6.24	106.30	114.04
1	E	94	ILE	CA-C-N	6.23	128.63	120.28
1	E	94	ILE	C-N-CA	6.23	128.63	120.28
2	6	21	ASP	CA-C-O	6.23	125.66	118.55
1	A	216	VAL	CA-CB-CG1	6.23	120.99	110.40
1	B	222	LYS	N-CA-C	-6.22	99.58	109.23
2	1	147	ALA	CA-C-O	-6.22	113.95	120.55
1	C	109	VAL	CB-CA-C	-6.22	103.64	112.22
2	1	169	VAL	CA-C-O	-6.22	114.48	120.95
1	E	135	SER	N-CA-C	-6.21	99.78	109.72
1	D	30	ALA	CA-C-N	6.21	128.96	120.46
1	D	30	ALA	C-N-CA	6.21	128.96	120.46
1	F	108	THR	N-CA-C	-6.21	101.33	110.52
1	C	81	LEU	CA-C-N	6.21	128.96	120.46
1	C	81	LEU	C-N-CA	6.21	128.96	120.46
2	6	174	SER	CA-C-O	-6.20	113.97	120.55
2	5	50	ASP	N-CA-C	6.20	119.69	111.75
2	6	74	ALA	N-CA-C	6.20	117.83	111.14
1	B	175	PHE	N-CA-CB	-6.20	100.68	110.28
1	D	232	TYR	N-CA-CB	6.20	119.62	110.33
2	4	162	ASP	CA-CB-CG	-6.19	106.41	112.60
2	7	132	ILE	CA-C-N	6.19	133.37	121.54
2	7	132	ILE	C-N-CA	6.19	133.37	121.54
1	E	137	LEU	N-CA-CB	6.19	120.48	110.77
1	C	174	PHE	CA-CB-CG	6.18	119.98	113.80
2	1	158	GLU	N-CA-CB	6.18	120.57	110.37
1	D	14	VAL	CA-CB-CG2	6.18	120.91	110.40
2	2	168	ALA	CA-C-N	6.17	128.92	120.46
2	2	168	ALA	C-N-CA	6.17	128.92	120.46
2	6	47	GLN	CA-C-O	-6.17	113.54	120.32
2	4	18	VAL	N-CA-C	-6.17	99.59	108.53
2	6	178	ARG	CA-C-O	-6.16	112.32	119.59
2	6	76	LEU	CA-C-N	6.16	128.85	120.54
2	6	76	LEU	C-N-CA	6.16	128.85	120.54
2	7	139	ALA	CA-C-N	6.16	132.11	121.64
2	7	139	ALA	C-N-CA	6.16	132.11	121.64
2	7	161	VAL	CA-C-N	6.16	129.03	120.29
2	7	161	VAL	C-N-CA	6.16	129.03	120.29
1	C	235	ARG	CB-CA-C	-6.16	100.39	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	172	THR	CA-C-N	6.16	128.53	120.28
1	G	172	THR	C-N-CA	6.16	128.53	120.28
2	4	87	VAL	O-C-N	-6.15	115.90	121.87
2	5	45	ILE	N-CA-C	-6.15	99.26	108.12
1	D	37	ALA	N-CA-C	-6.15	100.45	109.18
1	C	175	PHE	CA-C-N	6.14	129.13	120.28
1	C	175	PHE	C-N-CA	6.14	129.13	120.28
1	E	221	PHE	CA-CB-CG	-6.14	107.66	113.80
2	4	57	ALA	N-CA-C	-6.14	99.39	109.40
2	5	134	GLU	N-CA-CB	6.14	120.48	110.17
1	B	228	GLU	CA-C-N	6.14	128.79	120.44
1	B	228	GLU	C-N-CA	6.14	128.79	120.44
1	D	62	ASP	N-CA-CB	6.14	120.86	110.49
2	5	162	ASP	N-CA-C	6.14	117.97	111.28
2	5	148	TYR	N-CA-CB	6.13	118.90	110.01
2	7	194	ASP	CA-CB-CG	-6.12	106.47	112.60
2	1	166	GLU	CA-C-N	6.12	128.40	120.44
2	1	166	GLU	C-N-CA	6.12	128.40	120.44
2	2	70	ILE	CA-C-O	-6.12	114.36	120.85
2	2	210	LYS	N-CA-C	-6.12	105.85	113.38
1	F	134	VAL	CA-C-O	6.12	126.10	120.96
1	C	20	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	F	99	ASN	CA-C-N	6.11	129.60	120.31
1	F	99	ASN	C-N-CA	6.11	129.60	120.31
2	6	124	SER	O-C-N	-6.11	116.25	123.22
1	F	89	ILE	CA-C-N	6.11	128.47	120.28
1	F	89	ILE	C-N-CA	6.11	128.47	120.28
2	2	59	SER	CA-C-N	6.11	128.25	120.56
2	2	59	SER	C-N-CA	6.11	128.25	120.56
1	D	52	LYS	CA-C-N	6.11	130.52	120.94
1	D	52	LYS	C-N-CA	6.11	130.52	120.94
1	C	177	LYS	CA-C-N	6.10	131.01	120.58
1	C	177	LYS	C-N-CA	6.10	131.01	120.58
2	1	89	ALA	N-CA-C	6.10	117.60	111.07
1	G	40	ILE	N-CA-C	-6.09	98.71	107.78
2	1	110	LEU	CB-CA-C	-6.09	99.18	109.83
1	E	172	THR	N-CA-CB	6.08	119.17	110.16
2	4	185	GLY	O-C-N	6.08	128.99	122.60
2	7	55	THR	CA-CB-OG1	6.08	118.72	109.60
2	3	144	SER	CA-C-N	6.08	128.42	120.28
2	3	144	SER	C-N-CA	6.08	128.42	120.28
2	6	197	TYR	CA-C-O	6.08	127.26	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	238	GLU	CA-C-N	6.07	128.91	120.29
1	G	238	GLU	C-N-CA	6.07	128.91	120.29
2	5	161	VAL	N-CA-C	-6.07	104.82	110.53
2	2	13	THR	N-CA-C	-6.07	99.17	108.76
2	1	165	VAL	CA-C-O	6.06	126.80	120.25
2	6	170	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	F	221	PHE	CA-C-N	6.06	132.06	122.36
1	F	221	PHE	C-N-CA	6.06	132.06	122.36
2	4	166	GLU	N-CA-C	6.06	117.89	111.28
1	G	100	ARG	CD-NE-CZ	-6.05	115.92	124.40
2	5	116	ASP	O-C-N	6.05	129.47	122.99
1	F	245	LYS	N-CA-C	-6.05	105.94	113.38
2	7	203	GLU	N-CA-C	6.05	117.88	111.28
1	A	83	ALA	CA-C-N	6.05	128.30	120.44
1	A	83	ALA	C-N-CA	6.05	128.30	120.44
1	C	161	ALA	N-CA-C	-6.05	97.92	110.80
2	2	56	THR	CA-CB-CG2	-6.05	100.22	110.50
1	G	143	GLU	CB-CA-C	-6.04	98.39	110.42
1	G	151	ASP	CA-CB-CG	-6.04	106.56	112.60
1	F	125	GLN	N-CA-C	6.04	123.67	110.80
2	6	162	ASP	N-CA-CB	6.04	119.10	110.16
1	D	46	VAL	N-CA-C	-6.04	99.43	108.12
2	4	66	LEU	O-C-N	-6.03	115.72	122.12
2	4	106	TYR	N-CA-CB	6.03	120.26	110.43
1	A	205	VAL	N-CA-C	-6.03	95.85	108.88
1	D	59	LEU	CB-CA-C	-6.03	99.91	109.80
1	D	182	ASP	N-CA-C	-6.03	99.57	109.40
1	E	83	ALA	CA-C-N	6.02	128.35	120.28
1	E	83	ALA	C-N-CA	6.02	128.35	120.28
2	7	167	LEU	CA-C-N	6.02	128.35	120.28
2	7	167	LEU	C-N-CA	6.02	128.35	120.28
2	4	106	TYR	O-C-N	-6.01	116.48	123.27
2	4	144	SER	CA-C-N	6.01	128.25	120.44
2	4	144	SER	C-N-CA	6.01	128.25	120.44
2	5	46	TYR	O-C-N	-6.01	115.34	123.15
2	6	30	ARG	CA-C-N	-6.01	112.91	122.29
2	6	30	ARG	C-N-CA	-6.01	112.91	122.29
2	7	77	TYR	CA-C-N	6.01	128.25	120.44
2	7	77	TYR	C-N-CA	6.01	128.25	120.44
1	C	166	MET	N-CA-CB	6.01	119.81	110.44
1	E	207	GLU	CB-CA-C	-6.00	101.29	111.02
2	7	184	ASP	CA-CB-CG	-6.00	106.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	44	LYS	CA-C-N	6.00	131.34	122.99
2	2	44	LYS	C-N-CA	6.00	131.34	122.99
1	F	225	SER	CA-C-N	6.00	126.16	119.32
1	F	225	SER	C-N-CA	6.00	126.16	119.32
2	3	132	ILE	N-CA-CB	5.99	121.12	111.23
2	5	153	ASP	N-CA-C	5.99	121.26	111.37
2	2	183	GLY	CA-C-O	-5.99	114.07	122.58
1	A	228	GLU	CA-C-N	5.99	128.80	120.29
1	A	228	GLU	C-N-CA	5.99	128.80	120.29
1	C	129	VAL	CA-C-O	-5.99	115.38	121.67
1	E	203	GLU	CA-C-N	5.98	131.32	121.39
1	E	203	GLU	C-N-CA	5.98	131.32	121.39
1	C	205	VAL	CA-C-O	-5.98	113.31	120.90
1	E	81	LEU	O-C-N	5.98	130.96	123.01
2	3	97	LEU	CA-C-N	5.97	130.70	120.72
2	3	97	LEU	C-N-CA	5.97	130.70	120.72
1	C	190	VAL	CB-CA-C	-5.97	103.98	112.22
2	2	164	ALA	CA-C-N	5.97	128.90	120.42
2	2	164	ALA	C-N-CA	5.97	128.90	120.42
1	F	164	ILE	O-C-N	-5.97	116.41	123.04
1	G	67	ILE	CA-C-O	-5.96	114.10	120.59
2	6	204	VAL	N-CA-CB	5.96	118.19	110.57
1	D	215	LYS	CA-C-N	5.95	128.57	120.77
1	D	215	LYS	C-N-CA	5.95	128.57	120.77
2	6	156	THR	N-CA-CB	5.95	119.04	110.77
1	D	219	ARG	CB-CA-C	5.95	119.72	111.63
1	G	147	LEU	N-CA-C	-5.95	98.16	108.69
2	7	32	THR	CA-C-O	5.95	127.50	120.66
2	7	32	THR	O-C-N	-5.95	116.02	123.27
1	E	105	GLU	N-CA-C	-5.94	96.67	109.81
1	F	137	LEU	N-CA-CB	5.94	120.04	110.65
2	4	78	GLU	CA-C-O	-5.94	114.54	120.90
2	2	169	VAL	O-C-N	5.94	127.63	121.87
1	D	218	ASP	CA-C-N	5.94	131.02	122.35
1	D	218	ASP	C-N-CA	5.94	131.02	122.35
1	E	241	ARG	CA-C-O	-5.94	114.59	120.82
1	B	135	SER	N-CA-C	-5.94	99.72	109.40
2	1	187	ASP	CA-CB-CG	-5.93	106.67	112.60
2	5	124	SER	N-CA-CB	5.93	119.87	110.55
2	6	86	THR	N-CA-C	-5.93	101.22	110.42
1	E	86	ARG	NE-CZ-NH2	-5.93	113.86	119.20
1	B	170	ALA	O-C-N	5.93	128.19	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	186	ASP	N-CA-CB	5.93	118.93	110.16
2	1	15	VAL	N-CA-CB	5.93	122.43	112.47
1	C	239	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	B	85	ALA	N-CA-C	5.92	117.41	111.07
2	1	92	THR	CA-C-N	5.92	128.21	120.28
2	1	92	THR	C-N-CA	5.92	128.21	120.28
1	E	14	VAL	CA-C-O	-5.92	115.84	121.64
2	3	20	LYS	CA-C-O	5.92	125.50	118.69
1	D	238	GLU	CA-C-N	5.92	128.69	120.29
1	D	238	GLU	C-N-CA	5.92	128.69	120.29
1	A	115	LYS	N-CA-C	5.92	117.81	111.36
1	B	179	TYR	CB-CG-CD1	5.91	129.67	120.80
2	1	101	TYR	CB-CG-CD2	5.91	129.67	120.80
1	G	73	HIS	ND1-CE1-NE2	5.91	114.31	108.40
1	E	114	LYS	N-CA-C	-5.91	104.84	111.28
1	D	93	ARG	CA-C-N	5.91	128.12	120.56
1	D	93	ARG	C-N-CA	5.91	128.12	120.56
2	4	68	ARG	CA-C-N	5.90	128.00	120.56
2	4	68	ARG	C-N-CA	5.90	128.00	120.56
1	G	25	GLU	N-CA-C	5.90	117.71	111.28
2	2	133	GLU	CB-CG-CD	-5.90	102.57	112.60
1	F	91	ARG	CA-C-N	5.89	128.17	120.28
1	F	91	ARG	C-N-CA	5.89	128.17	120.28
1	B	29	GLU	N-CA-CB	5.88	119.28	110.22
1	F	27	ALA	N-CA-C	5.88	117.69	111.28
2	3	167	LEU	CA-C-N	5.88	128.16	120.28
2	3	167	LEU	C-N-CA	5.88	128.16	120.28
2	5	181	ALA	CA-C-O	-5.88	112.56	120.15
2	4	158	GLU	N-CA-C	-5.88	104.77	112.41
2	7	160	GLY	N-CA-C	-5.88	103.60	112.60
1	G	158	GLU	O-C-N	-5.88	116.63	123.27
1	C	130	ARG	CA-C-N	5.88	125.85	120.21
1	C	130	ARG	C-N-CA	5.88	125.85	120.21
2	6	202	GLU	CA-C-N	5.88	128.63	120.29
2	6	202	GLU	C-N-CA	5.88	128.63	120.29
2	7	99	ASN	OD1-CG-ND2	5.88	128.48	122.60
2	5	157	PRO	N-CD-CG	5.88	112.01	103.20
1	F	115	LYS	N-CA-CB	5.87	118.59	110.07
1	D	69	LYS	N-CA-C	-5.87	99.16	108.73
2	1	169	VAL	N-CA-C	-5.87	104.63	110.62
2	7	42	ALA	CA-C-N	5.87	132.75	121.54
2	7	42	ALA	C-N-CA	5.87	132.75	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	GLU	O-C-N	-5.87	116.03	122.07
1	E	43	LYS	CA-C-O	5.86	126.13	119.27
1	E	200	ILE	N-CA-C	-5.86	106.01	113.22
2	3	66	LEU	CA-C-O	-5.86	114.20	120.42
2	2	102	ARG	CA-C-O	5.86	127.66	119.80
1	F	196	MET	CA-C-O	-5.86	114.67	120.82
2	4	38	ALA	O-C-N	5.86	128.83	122.15
1	B	239	ARG	CA-C-N	5.86	127.94	120.56
1	B	239	ARG	C-N-CA	5.86	127.94	120.56
1	B	67	ILE	N-CA-CB	5.86	119.28	111.90
1	G	38	ILE	N-CA-CB	5.85	120.89	111.23
2	4	103	TYR	N-CA-C	-5.85	105.03	111.82
1	C	120	LYS	N-CA-CB	5.85	119.23	110.22
2	1	30	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	B	174	PHE	CA-CB-CG	5.85	119.65	113.80
2	6	95	SER	CB-CA-C	-5.85	101.70	110.88
2	1	170	ARG	CA-C-N	5.84	128.11	120.28
2	1	170	ARG	C-N-CA	5.84	128.11	120.28
1	E	68	TYR	N-CA-C	-5.84	100.19	109.59
1	F	188	ALA	CA-C-N	5.84	128.03	120.44
1	F	188	ALA	C-N-CA	5.84	128.03	120.44
2	6	173	TYR	CA-C-O	-5.84	114.36	120.55
1	A	222	LYS	N-CA-C	-5.84	100.44	109.14
1	F	118	ASP	CA-C-N	5.84	128.38	120.44
1	F	118	ASP	C-N-CA	5.84	128.38	120.44
1	A	205	VAL	CA-C-N	5.84	125.54	119.82
1	A	205	VAL	C-N-CA	5.84	125.54	119.82
2	2	68	ARG	N-CA-CB	5.84	118.70	110.12
2	2	160	GLY	N-CA-C	-5.84	103.74	113.02
2	2	212	ARG	N-CA-CB	5.83	120.35	110.49
2	2	140	THR	CA-C-O	-5.83	115.21	121.56
1	F	16	SER	O-C-N	-5.83	116.94	121.14
2	1	166	GLU	N-CA-C	-5.83	104.85	111.14
1	D	55	GLY	CA-C-N	5.82	131.42	121.87
1	D	55	GLY	C-N-CA	5.82	131.42	121.87
2	7	69	ILE	O-C-N	-5.82	116.21	121.91
2	5	204	VAL	CA-C-N	5.82	128.65	120.28
2	5	204	VAL	C-N-CA	5.82	128.65	120.28
2	6	48	ILE	O-C-N	-5.82	116.53	122.23
2	6	125	ILE	N-CA-C	-5.82	100.03	108.17
2	6	90	ILE	N-CA-C	-5.81	105.06	110.53
2	2	100	SER	N-CA-C	-5.81	105.08	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	GLN	CB-CA-C	-5.81	101.15	110.79
2	4	16	GLY	N-CA-C	-5.81	99.42	113.18
1	C	104	ASP	CA-CB-CG	5.80	118.41	112.60
1	E	95	GLU	N-CA-CB	5.80	118.65	110.12
2	5	136	ASP	CA-CB-CG	5.80	118.41	112.60
2	5	204	VAL	CA-C-O	-5.80	114.70	120.85
1	D	73	HIS	CA-CB-CG	5.80	119.60	113.80
1	A	221	PHE	N-CA-CB	5.80	118.22	109.34
1	D	180	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	6	140	THR	CB-CA-C	5.80	121.86	109.10
1	A	177	LYS	CB-CA-C	-5.80	100.56	110.24
2	4	194	ASP	CA-CB-CG	-5.79	106.81	112.60
1	A	61	ALA	CA-C-N	5.79	131.47	122.26
1	A	61	ALA	C-N-CA	5.79	131.47	122.26
2	6	27	THR	N-CA-C	-5.79	100.49	109.24
1	C	42	CYS	N-CA-C	-5.79	100.70	108.86
1	G	124	THR	N-CA-C	-5.79	106.14	113.43
2	4	29	LYS	N-CA-CB	5.79	119.70	110.73
2	7	78	GLU	O-C-N	5.79	128.03	122.07
2	4	102	ARG	N-CA-C	-5.78	106.20	113.20
2	4	29	LYS	CB-CA-C	-5.78	100.95	110.72
2	4	99	ASN	CA-CB-CG	-5.78	106.82	112.60
1	A	232	TYR	N-CA-CB	5.78	118.71	110.16
1	C	12	ILE	CA-CB-CG2	-5.78	100.68	110.50
1	B	112	LEU	N-CA-CB	5.77	118.38	110.01
1	E	31	VAL	N-CA-C	5.77	115.96	110.42
1	F	160	LYS	O-C-N	-5.77	115.57	122.15
2	7	166	GLU	N-CA-C	5.77	117.57	111.28
2	1	67	ALA	CA-C-N	5.77	128.32	120.54
2	1	67	ALA	C-N-CA	5.77	128.32	120.54
1	G	132	PHE	N-CA-CB	5.77	119.27	109.87
2	6	196	PHE	N-CA-C	-5.77	97.81	107.32
2	4	116	ASP	CA-C-N	5.76	128.58	120.28
2	4	116	ASP	C-N-CA	5.76	128.58	120.28
1	A	117	CYS	CA-CB-SG	-5.76	101.16	114.40
1	E	173	GLU	CB-CA-C	-5.76	101.23	110.79
1	F	56	SER	CA-C-N	5.76	128.27	120.44
1	F	56	SER	C-N-CA	5.76	128.27	120.44
2	5	87	VAL	CA-CB-CG1	-5.75	100.62	110.40
2	3	163	GLU	CA-C-N	5.75	127.99	120.28
2	3	163	GLU	C-N-CA	5.75	127.99	120.28
2	6	16	GLY	N-CA-C	-5.75	99.55	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	168	ALA	CA-C-N	5.75	128.34	120.46
2	1	168	ALA	C-N-CA	5.75	128.34	120.46
2	5	191	ILE	CB-CA-C	5.75	118.18	110.42
1	D	97	GLN	CA-C-N	5.75	128.34	120.46
1	D	97	GLN	C-N-CA	5.75	128.34	120.46
1	F	221	PHE	CA-CB-CG	-5.75	108.05	113.80
2	7	51	ARG	NE-CZ-NH1	-5.75	115.75	121.50
2	3	168	ALA	CA-C-N	5.75	127.80	120.56
2	3	168	ALA	C-N-CA	5.75	127.80	120.56
1	A	157	LEU	CA-C-N	5.74	129.96	120.94
1	A	157	LEU	C-N-CA	5.74	129.96	120.94
2	5	178	ARG	CA-C-O	-5.74	114.43	120.63
2	7	36	PHE	CA-C-O	5.74	126.86	120.43
2	7	104	PHE	CA-C-O	-5.74	112.30	120.16
2	3	139	ALA	N-CA-CB	5.74	120.18	110.49
1	A	36	THR	N-CA-C	5.73	118.15	110.35
1	E	237	ASN	CA-C-N	5.73	127.89	120.44
1	E	237	ASN	C-N-CA	5.73	127.89	120.44
1	E	187	ASP	N-CA-CB	5.73	118.54	110.12
1	F	57	LYS	N-CA-C	-5.73	104.95	111.14
2	4	192	THR	CA-CB-CG2	5.73	120.24	110.50
1	C	225	SER	CA-C-O	-5.73	112.31	120.16
2	4	87	VAL	CA-C-O	5.72	126.90	120.95
1	C	22	PHE	N-CA-C	5.72	118.73	111.69
1	F	107	ILE	O-C-N	-5.72	116.73	122.62
2	2	188	VAL	O-C-N	-5.72	116.71	123.00
1	F	51	ASP	CA-CB-CG	5.72	118.32	112.60
1	F	113	ALA	N-CA-C	-5.72	105.13	111.36
2	2	159	ILE	CA-CB-CG1	5.72	120.12	110.40
2	2	127	PRO	N-CA-C	-5.72	108.12	114.92
2	7	95	SER	CA-C-N	5.72	127.94	120.28
2	7	95	SER	C-N-CA	5.72	127.94	120.28
1	A	125	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	D	87	VAL	CA-C-N	5.71	127.94	120.28
1	D	87	VAL	C-N-CA	5.71	127.94	120.28
1	A	45	GLY	O-C-N	-5.71	118.30	123.96
1	F	40	ILE	N-CA-C	-5.71	99.95	108.46
1	F	92	ALA	N-CA-CB	5.71	118.52	110.12
1	A	27	ALA	N-CA-C	-5.71	105.06	111.28
1	C	237	ASN	N-CA-C	-5.71	105.19	111.82
2	1	162	ASP	CA-CB-CG	-5.71	106.89	112.60
2	4	182	SER	O-C-N	-5.71	116.73	123.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	38	ALA	N-CA-CB	5.71	118.70	110.20
2	3	104	PHE	N-CA-C	-5.71	103.09	108.22
1	E	243	LEU	CA-C-N	5.70	131.91	122.73
1	E	243	LEU	C-N-CA	5.70	131.91	122.73
2	3	18	VAL	N-CA-CB	5.70	117.50	111.00
1	C	124	THR	N-CA-C	-5.70	106.12	114.39
1	D	14	VAL	N-CA-CB	5.70	121.18	112.06
1	D	174	PHE	CA-C-O	-5.70	113.66	120.10
1	C	130	ARG	N-CA-CB	-5.70	103.13	109.74
1	B	112	LEU	CB-CA-C	-5.70	101.93	110.88
1	B	96	ALA	N-CA-C	5.70	117.17	111.07
2	2	179	ASP	N-CA-C	-5.69	100.29	108.60
2	1	94	THR	N-CA-C	5.69	117.48	111.28
1	G	98	ILE	CA-C-N	5.69	127.84	120.44
1	G	98	ILE	C-N-CA	5.69	127.84	120.44
2	5	74	ALA	N-CA-CB	5.69	118.26	110.01
2	2	126	ASP	CA-C-O	-5.69	114.51	120.88
2	4	185	GLY	CA-C-O	-5.69	116.67	122.59
1	B	36	THR	CA-C-O	5.68	127.40	121.15
1	B	171	VAL	CA-C-N	5.68	128.36	120.29
1	B	171	VAL	C-N-CA	5.68	128.36	120.29
1	B	240	ILE	CA-C-O	-5.68	115.15	121.17
1	A	126	TYR	N-CA-CB	5.68	118.64	110.06
1	E	130	ARG	CA-C-O	-5.68	114.79	120.64
2	2	190	LYS	N-CA-C	-5.68	100.14	109.40
2	4	30	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	D	109	VAL	CA-C-O	-5.68	114.83	120.85
1	G	131	PRO	O-C-N	5.68	129.52	122.71
2	7	115	ILE	N-CA-C	-5.68	100.05	108.45
1	B	124	THR	N-CA-C	-5.67	106.03	113.12
1	C	86	ARG	N-CA-C	5.67	117.14	111.07
1	B	142	ASP	CA-C-O	5.67	126.62	120.55
1	E	95	GLU	O-C-N	-5.67	116.11	122.12
1	F	37	ALA	CA-C-N	5.67	129.56	121.96
1	F	37	ALA	C-N-CA	5.67	129.56	121.96
1	E	70	ILE	CA-C-O	5.67	125.63	120.30
1	F	182	ASP	N-CA-C	-5.67	100.55	109.50
2	2	109	GLN	N-CA-C	-5.67	99.17	108.41
1	A	26	TYR	CA-C-N	5.67	127.87	120.28
1	A	26	TYR	C-N-CA	5.67	127.87	120.28
1	G	134	VAL	CA-C-O	5.67	125.72	120.96
1	B	207	GLU	N-CA-C	-5.66	106.14	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	112	ILE	N-CA-C	-5.66	100.18	108.11
1	B	64	ILE	CA-C-N	5.66	131.90	122.73
1	B	64	ILE	C-N-CA	5.66	131.90	122.73
1	E	94	ILE	CA-C-O	-5.66	114.77	121.05
2	2	208	LEU	CA-C-O	5.66	125.97	119.35
1	D	93	ARG	O-C-N	-5.66	116.12	122.12
1	E	228	GLU	CA-C-N	5.66	128.32	120.29
1	E	228	GLU	C-N-CA	5.66	128.32	120.29
1	C	119	PHE	CA-C-N	5.65	128.42	120.28
1	C	119	PHE	C-N-CA	5.65	128.42	120.28
1	G	61	ALA	CB-CA-C	-5.65	104.00	111.74
2	4	196	PHE	N-CA-C	-5.65	95.28	107.49
1	B	139	ALA	N-CA-CB	5.65	120.66	110.83
2	4	36	PHE	CA-CB-CG	-5.65	108.15	113.80
2	5	30	ARG	N-CA-C	-5.65	100.76	109.52
2	7	162	ASP	N-CA-C	-5.65	105.20	111.36
1	F	148	TYR	CA-C-O	5.64	127.71	121.11
1	G	14	VAL	O-C-N	-5.64	116.64	123.02
1	C	73	HIS	ND1-CE1-NE2	5.64	114.04	108.40
1	E	67	ILE	CA-C-N	5.64	131.11	122.93
1	E	67	ILE	C-N-CA	5.64	131.11	122.93
1	B	113	ALA	O-C-N	5.64	128.09	122.12
1	E	178	GLU	CA-C-N	5.64	129.11	121.05
1	E	178	GLU	C-N-CA	5.64	129.11	121.05
1	F	131	PRO	CB-CA-C	-5.63	104.19	111.46
1	F	81	LEU	CA-C-N	5.63	128.18	120.46
1	F	81	LEU	C-N-CA	5.63	128.18	120.46
1	F	131	PRO	CA-C-O	-5.63	114.92	121.34
2	7	19	CYS	CA-C-O	-5.63	115.05	121.58
1	B	215	LYS	CB-CG-CD	5.63	124.24	111.30
1	E	100	ARG	N-CA-CB	5.63	118.39	110.12
1	F	193	LEU	N-CA-CB	5.63	118.89	110.22
2	7	115	ILE	CA-C-N	5.63	131.88	122.20
2	7	115	ILE	C-N-CA	5.63	131.88	122.20
1	F	110	LYS	O-C-N	5.62	128.08	122.12
2	3	62	ASP	CA-C-N	5.62	127.75	120.44
2	3	62	ASP	C-N-CA	5.62	127.75	120.44
1	E	241	ARG	N-CA-C	-5.62	105.06	111.07
2	3	51	ARG	NE-CZ-NH1	-5.62	115.88	121.50
2	5	107	LEU	N-CA-C	-5.61	105.64	112.88
1	E	90	ASP	CA-C-N	5.61	127.80	120.28
1	E	90	ASP	C-N-CA	5.61	127.80	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	LEU	CB-CA-C	-5.61	100.55	109.80
1	F	218	ASP	N-CA-C	-5.60	104.80	111.69
2	2	43	LYS	N-CA-CB	5.60	119.31	110.23
2	6	198	GLN	N-CA-C	-5.60	98.22	108.02
1	B	196	MET	CA-C-N	5.60	126.20	119.98
1	B	196	MET	C-N-CA	5.60	126.20	119.98
1	C	41	LYS	N-CA-C	-5.60	100.76	109.72
2	6	108	VAL	CA-CB-CG2	5.59	119.91	110.40
2	6	122	ILE	N-CA-C	-5.59	100.12	108.46
1	E	125	GLN	CA-C-O	5.59	126.82	120.00
2	6	31	ALA	N-CA-C	-5.59	105.22	113.61
1	G	31	VAL	N-CA-C	-5.59	105.06	110.42
1	C	53	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	E	136	LEU	N-CA-C	-5.59	100.86	109.52
2	6	112	ILE	N-CA-CB	5.59	117.69	110.99
2	6	148	TYR	CB-CG-CD1	-5.59	112.42	120.80
2	6	124	SER	CA-C-N	5.58	130.12	123.19
2	6	124	SER	C-N-CA	5.58	130.12	123.19
1	E	65	GLU	CB-CG-CD	-5.58	103.11	112.60
2	4	67	ALA	N-CA-CB	5.58	118.33	110.12
2	7	191	ILE	N-CA-C	-5.58	99.60	107.75
2	3	147	ALA	N-CA-CB	5.58	118.32	110.12
1	B	30	ALA	CA-C-O	-5.58	114.64	120.55
1	C	238	GLU	CA-C-O	-5.58	114.96	120.82
2	4	158	GLU	CA-C-N	5.58	128.57	120.98
2	4	158	GLU	C-N-CA	5.58	128.57	120.98
2	2	119	GLY	N-CA-C	-5.58	99.96	113.18
2	5	62	ASP	CB-CA-C	-5.58	101.37	110.85
1	F	192	GLY	CA-C-N	5.57	128.30	120.28
1	F	192	GLY	C-N-CA	5.57	128.30	120.28
1	F	233	VAL	O-C-N	5.57	127.56	121.83
1	B	175	PHE	CB-CG-CD1	5.57	130.16	120.70
2	2	198	GLN	CA-C-O	5.57	126.25	120.30
1	A	184	SER	N-CA-C	-5.56	100.61	109.96
1	D	232	TYR	N-CA-C	-5.56	105.61	112.90
1	B	83	ALA	CA-C-N	5.56	128.19	120.29
1	B	83	ALA	C-N-CA	5.56	128.19	120.29
1	C	208	ASN	N-CA-C	-5.56	104.74	112.30
1	D	125	GLN	OE1-CD-NE2	5.56	128.16	122.60
2	5	87	VAL	CB-CA-C	-5.56	103.55	112.16
1	G	40	ILE	CB-CA-C	5.55	117.67	110.12
2	2	87	VAL	O-C-N	5.55	127.26	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	28	GLU	CA-C-N	5.55	128.99	120.82
2	3	28	GLU	C-N-CA	5.55	128.99	120.82
2	5	45	ILE	CB-CA-C	5.55	118.44	110.33
2	2	108	VAL	CA-C-N	5.55	130.83	123.00
2	2	108	VAL	C-N-CA	5.55	130.83	123.00
1	F	210	GLU	CA-C-O	-5.55	114.70	120.70
1	C	76	ALA	O-C-N	5.55	130.04	123.33
1	E	85	ALA	O-C-N	5.55	127.80	122.03
2	1	131	ALA	CA-C-O	5.55	126.24	120.30
1	D	59	LEU	N-CA-CB	5.55	119.31	110.16
1	G	226	PRO	CA-C-N	5.55	127.98	120.44
1	G	226	PRO	C-N-CA	5.55	127.98	120.44
2	5	62	ASP	CA-C-N	5.54	127.71	120.28
2	5	62	ASP	C-N-CA	5.54	127.71	120.28
1	C	233	VAL	CA-C-N	5.54	128.16	120.29
1	C	233	VAL	C-N-CA	5.54	128.16	120.29
1	D	28	ARG	N-CA-CB	5.54	118.26	110.12
1	D	212	GLY	CA-C-O	-5.54	116.75	121.57
1	F	224	VAL	CA-C-N	5.54	129.07	120.60
1	F	224	VAL	C-N-CA	5.54	129.07	120.60
2	5	189	VAL	N-CA-CB	5.53	122.13	111.62
2	3	18	VAL	CB-CA-C	-5.53	104.27	110.96
1	F	172	THR	O-C-N	5.53	127.76	122.07
2	5	78	GLU	CA-C-N	5.53	127.52	120.56
2	5	78	GLU	C-N-CA	5.53	127.52	120.56
1	B	148	TYR	CA-CB-CG	-5.52	103.96	113.90
1	F	144	VAL	CA-C-N	5.52	125.45	119.76
1	F	144	VAL	C-N-CA	5.52	125.45	119.76
1	F	221	PHE	O-C-N	5.52	129.94	122.59
2	7	181	ALA	N-CA-C	-5.52	106.67	113.41
2	1	134	GLU	CA-C-O	5.52	126.32	120.36
2	7	28	GLU	N-CA-C	-5.52	99.90	108.90
2	7	29	LYS	CA-C-O	5.52	126.45	120.55
1	C	41	LYS	CA-C-O	5.51	127.34	121.11
1	E	38	ILE	CB-CA-C	5.51	120.33	111.29
2	2	70	ILE	CA-C-N	5.51	127.61	120.44
2	2	70	ILE	C-N-CA	5.51	127.61	120.44
1	B	163	ALA	O-C-N	5.51	129.32	123.42
2	6	164	ALA	CA-C-N	5.51	127.51	120.56
2	6	164	ALA	C-N-CA	5.51	127.51	120.56
2	7	144	SER	CA-C-N	5.51	128.12	120.29
2	7	144	SER	C-N-CA	5.51	128.12	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	194	ASP	N-CA-C	-5.51	107.81	114.75
2	3	126	ASP	CA-CB-CG	-5.51	107.09	112.60
2	6	85	PRO	CA-C-O	-5.51	114.70	121.31
1	A	241	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	D	121	GLN	N-CA-CB	5.50	118.21	110.12
1	C	114	LYS	CB-CA-C	-5.50	102.24	110.88
1	F	17	PRO	N-CA-CB	5.50	108.58	103.41
1	A	169	ASN	CA-CB-CG	-5.50	107.10	112.60
2	7	212	ARG	CG-CD-NE	-5.50	99.91	112.00
1	B	229	LEU	CA-C-N	5.50	129.10	120.97
1	B	229	LEU	C-N-CA	5.50	129.10	120.97
1	G	111	GLU	CA-C-N	5.50	127.92	120.44
1	G	111	GLU	C-N-CA	5.50	127.92	120.44
1	G	144	VAL	CA-C-N	5.49	125.81	119.93
1	G	144	VAL	C-N-CA	5.49	125.81	119.93
2	6	55	THR	N-CA-C	-5.49	101.21	109.95
2	3	128	ILE	CB-CG1-CD1	-5.49	102.27	113.80
2	5	70	ILE	N-CA-CB	5.49	116.97	110.55
1	C	36	THR	CA-C-O	5.49	127.18	120.92
1	E	175	PHE	CA-CB-CG	5.49	119.29	113.80
1	G	46	VAL	CA-C-O	5.49	126.80	120.76
1	G	30	ALA	CA-C-N	5.49	127.48	120.56
1	G	30	ALA	C-N-CA	5.49	127.48	120.56
1	G	28	ARG	CA-C-N	5.48	128.07	120.29
1	G	28	ARG	C-N-CA	5.48	128.07	120.29
1	F	187	ASP	CA-C-N	5.48	127.62	120.28
1	F	187	ASP	C-N-CA	5.48	127.62	120.28
2	1	151	LEU	N-CA-CB	-5.48	102.06	110.01
2	3	192	THR	CA-C-O	-5.48	113.37	119.34
1	F	241	ARG	CA-C-N	5.48	127.62	120.28
1	F	241	ARG	C-N-CA	5.48	127.62	120.28
2	6	200	SER	CA-C-N	5.48	126.69	119.84
2	6	200	SER	C-N-CA	5.48	126.69	119.84
2	3	175	ALA	N-CA-CB	5.47	118.17	110.12
2	5	200	SER	N-CA-CB	5.47	120.11	110.37
1	C	153	SER	CA-C-N	5.47	132.13	121.41
1	C	153	SER	C-N-CA	5.47	132.13	121.41
1	D	98	ILE	CA-CB-CG2	5.47	119.79	110.50
1	G	59	LEU	N-CA-C	-5.46	101.77	109.96
2	7	153	ASP	CA-CB-CG	-5.46	107.14	112.60
1	F	236	ALA	CA-C-N	5.46	127.86	120.38
1	F	236	ALA	C-N-CA	5.46	127.86	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	ASP	CA-C-N	5.46	125.15	119.64
1	C	151	ASP	C-N-CA	5.46	125.15	119.64
1	D	245	LYS	N-CA-CB	5.46	118.70	110.30
1	B	27	ALA	CA-C-O	5.45	126.24	119.97
1	E	209	ILE	O-C-N	5.45	129.10	123.05
2	3	88	ARG	N-CA-C	5.45	117.22	111.28
2	7	39	SER	CA-C-N	5.45	127.59	120.28
2	7	39	SER	C-N-CA	5.45	127.59	120.28
1	A	182	ASP	CA-CB-CG	5.45	118.05	112.60
2	3	67	ALA	N-CA-C	-5.45	105.34	111.28
2	6	32	THR	N-CA-CB	5.45	118.11	109.71
2	7	57	ALA	N-CA-C	-5.45	101.00	109.72
1	A	177	LYS	N-CA-CB	5.45	119.48	110.33
2	2	150	VAL	CA-C-N	5.45	127.52	120.44
2	2	150	VAL	C-N-CA	5.45	127.52	120.44
2	4	92	THR	N-CA-CB	5.45	118.13	110.12
2	6	205	GLU	N-CA-CB	5.45	118.61	110.22
2	7	44	LYS	CA-C-N	5.45	130.51	122.94
2	7	44	LYS	C-N-CA	5.45	130.51	122.94
1	B	104	ASP	CA-C-O	-5.45	114.27	121.08
1	A	36	THR	CA-C-N	5.44	131.07	122.36
1	A	36	THR	C-N-CA	5.44	131.07	122.36
2	3	153	ASP	O-C-N	-5.44	115.94	122.15
1	B	40	ILE	N-CA-C	-5.44	100.28	108.12
1	F	69	LYS	O-C-N	-5.44	116.67	123.04
2	1	88	ARG	NE-CZ-NH1	-5.44	116.06	121.50
2	2	185	GLY	N-CA-C	-5.44	95.45	110.68
1	C	134	VAL	CA-C-O	5.44	126.46	120.64
1	A	207	GLU	CB-CG-CD	-5.43	103.36	112.60
1	E	71	ASP	N-CA-C	-5.43	101.22	108.34
2	5	27	THR	N-CA-C	-5.43	100.67	108.60
2	5	152	GLU	CA-C-N	5.43	128.97	120.82
2	5	152	GLU	C-N-CA	5.43	128.97	120.82
1	D	116	ILE	CA-C-N	5.43	131.22	121.66
1	D	116	ILE	C-N-CA	5.43	131.22	121.66
2	2	29	LYS	N-CA-CB	5.43	118.21	110.67
2	6	174	SER	N-CA-CB	5.43	118.10	110.12
1	B	45	GLY	N-CA-C	-5.42	103.47	110.69
1	G	144	VAL	N-CA-C	-5.42	97.16	108.88
2	2	23	VAL	CB-CA-C	-5.42	101.26	111.30
2	3	87	VAL	CA-C-N	5.42	127.55	120.28
2	3	87	VAL	C-N-CA	5.42	127.55	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	77	TYR	CA-CB-CG	5.42	123.66	113.90
1	F	99	ASN	CA-CB-CG	-5.42	107.18	112.60
1	B	203	GLU	CB-CG-CD	-5.42	103.39	112.60
2	3	97	LEU	O-C-N	-5.42	115.61	122.27
2	4	106	TYR	N-CA-C	-5.42	100.41	109.24
1	C	232	TYR	CA-C-N	5.41	127.87	120.46
1	C	232	TYR	C-N-CA	5.41	127.87	120.46
2	5	77	TYR	O-C-N	5.41	127.72	122.09
2	1	82	GLU	N-CA-CB	5.41	119.90	111.84
2	3	46	TYR	CA-C-O	-5.41	114.86	120.70
1	A	228	GLU	CA-C-O	5.41	126.21	120.10
2	3	187	ASP	N-CA-C	-5.41	100.88	109.59
1	E	212	GLY	N-CA-C	-5.41	103.25	111.14
1	B	151	ASP	CA-CB-CG	-5.40	107.20	112.60
1	F	110	LYS	CA-C-O	-5.40	114.83	120.55
2	1	36	PHE	CA-C-N	5.40	129.23	122.48
2	1	36	PHE	C-N-CA	5.40	129.23	122.48
2	4	96	ASN	N-CA-C	-5.40	105.47	111.36
2	7	81	ARG	NE-CZ-NH1	5.40	126.90	121.50
2	4	160	GLY	N-CA-C	-5.40	104.36	112.89
1	F	145	PRO	CB-CA-C	5.39	118.42	111.46
2	6	40	LYS	N-CA-C	-5.39	99.31	110.80
1	G	51	ASP	CA-CB-CG	5.39	117.99	112.60
1	F	229	LEU	O-C-N	5.39	128.69	122.17
2	3	209	ALA	CA-C-O	-5.39	112.96	119.27
1	F	112	LEU	CA-C-N	5.39	127.94	120.29
1	F	112	LEU	C-N-CA	5.39	127.94	120.29
2	2	82	GLU	N-CA-CB	5.38	120.87	112.25
2	2	122	ILE	N-CA-C	-5.38	100.48	108.45
1	F	135	SER	N-CA-C	-5.38	99.66	108.76
1	C	184	SER	CA-C-N	5.38	127.49	120.28
1	C	184	SER	C-N-CA	5.38	127.49	120.28
1	E	193	LEU	O-C-N	-5.38	116.02	122.15
1	G	56	SER	N-CA-C	-5.38	101.46	109.96
2	6	83	ARG	N-CA-C	-5.38	98.80	108.48
1	G	26	TYR	CB-CG-CD1	5.38	128.87	120.80
1	A	81	LEU	CA-C-N	5.38	129.43	120.62
1	A	81	LEU	C-N-CA	5.38	129.43	120.62
1	G	131	PRO	N-CA-C	5.38	119.02	111.33
2	3	91	ALA	CA-C-N	5.38	127.43	120.44
2	3	91	ALA	C-N-CA	5.38	127.43	120.44
1	A	125	GLN	CG-CD-OE1	5.37	131.55	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	144	VAL	CA-C-N	5.37	125.37	119.89
1	E	144	VAL	C-N-CA	5.37	125.37	119.89
2	6	121	SER	O-C-N	-5.37	117.12	123.25
1	C	19	GLY	CA-C-O	5.37	126.13	119.25
2	5	158	GLU	CA-C-N	5.37	127.77	120.63
2	5	158	GLU	C-N-CA	5.37	127.77	120.63
1	E	95	GLU	CA-C-N	5.37	127.47	120.28
1	E	95	GLU	C-N-CA	5.37	127.47	120.28
2	3	162	ASP	CA-C-O	-5.37	114.73	120.42
1	C	223	GLU	CA-C-O	5.37	126.23	120.38
1	F	182	ASP	CA-CB-CG	5.37	117.97	112.60
1	F	217	ASP	N-CA-CB	5.37	118.01	110.12
2	7	132	ILE	CA-C-O	5.36	125.56	120.25
2	2	28	GLU	N-CA-CB	5.36	118.57	110.42
1	A	243	LEU	CB-CA-C	-5.36	101.89	110.79
1	C	187	ASP	CB-CA-C	-5.36	102.43	110.90
2	4	209	ALA	N-CA-C	-5.36	106.33	112.92
2	2	38	ALA	O-C-N	-5.36	115.68	122.27
2	2	154	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	6	82	GLU	N-CA-CB	5.36	120.22	112.13
2	5	57	ALA	N-CA-C	-5.35	100.45	109.07
1	A	95	GLU	N-CA-CB	5.35	118.08	110.16
1	B	87	VAL	CA-CB-CG1	5.35	119.50	110.40
2	7	27	THR	CA-CB-OG1	5.35	117.63	109.60
1	C	220	THR	N-CA-C	-5.35	98.55	107.80
1	D	24	VAL	N-CA-C	5.35	116.12	110.72
2	3	52	MET	N-CA-CB	5.35	121.48	111.53
2	4	89	ALA	CA-C-N	5.35	128.01	120.42
2	4	89	ALA	C-N-CA	5.35	128.01	120.42
1	E	118	ASP	CA-C-N	5.35	127.39	120.44
1	E	118	ASP	C-N-CA	5.35	127.39	120.44
2	7	65	PHE	CA-CB-CG	5.35	119.15	113.80
1	G	53	ARG	CA-C-N	5.35	131.59	121.97
1	G	53	ARG	C-N-CA	5.35	131.59	121.97
1	G	104	ASP	CA-CB-CG	5.35	117.95	112.60
2	3	91	ALA	CB-CA-C	-5.35	101.76	110.85
1	B	75	CYS	N-CA-CB	5.34	121.09	111.37
1	B	172	THR	N-CA-C	-5.34	105.54	111.36
2	1	146	THR	CA-C-N	5.34	127.44	120.28
2	1	146	THR	C-N-CA	5.34	127.44	120.28
2	2	33	MET	CG-SD-CE	-5.34	89.15	100.90
2	6	206	GLN	CB-CG-CD	-5.34	103.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	30	ARG	N-CA-CB	5.34	117.95	109.51
1	D	229	LEU	CA-C-O	-5.34	114.89	120.55
1	E	79	SER	N-CA-C	-5.34	99.90	108.55
1	E	190	VAL	O-C-N	5.34	127.05	121.87
1	D	68	TYR	N-CA-CB	5.33	119.28	110.69
1	E	228	GLU	N-CA-C	-5.33	105.55	111.36
1	C	144	VAL	N-CA-C	-5.33	97.36	108.88
1	C	178	GLU	CA-C-N	5.33	128.67	121.05
1	C	178	GLU	C-N-CA	5.33	128.67	121.05
2	1	77	TYR	O-C-N	5.33	127.63	122.09
2	6	123	TYR	O-C-N	-5.33	116.86	123.36
2	4	71	LYS	N-CA-C	5.33	116.77	111.07
1	C	53	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	C	188	ALA	CA-C-N	5.33	127.36	120.44
1	C	188	ALA	C-N-CA	5.33	127.36	120.44
1	G	199	SER	N-CA-CB	5.33	117.73	110.01
2	1	65	PHE	CA-C-N	5.33	127.42	120.28
2	1	65	PHE	C-N-CA	5.33	127.42	120.28
2	2	182	SER	N-CA-C	-5.33	101.02	109.59
1	D	200	ILE	N-CA-C	-5.32	106.68	112.80
1	G	195	ALA	CA-C-N	5.32	127.41	120.28
1	G	195	ALA	C-N-CA	5.32	127.41	120.28
1	G	180	ARG	N-CA-C	-5.32	101.49	109.95
2	1	175	ALA	N-CA-C	5.32	117.16	111.36
2	6	186	ILE	N-CA-CB	5.31	120.07	111.36
1	A	241	ARG	N-CA-C	5.31	117.07	111.28
2	5	102	ARG	CB-CG-CD	5.31	123.50	111.30
1	E	88	LEU	CA-C-N	5.31	127.25	120.56
1	E	88	LEU	C-N-CA	5.31	127.25	120.56
2	1	170	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	D	175	PHE	N-CA-C	-5.30	106.32	112.89
1	E	15	PHE	CB-CA-C	-5.30	100.44	109.51
2	1	150	VAL	CB-CA-C	-5.30	104.90	112.22
1	B	46	VAL	CA-C-O	-5.30	114.93	120.76
1	C	206	PRO	O-C-N	5.30	129.63	122.37
1	D	83	ALA	CA-C-N	5.30	127.81	120.29
1	D	83	ALA	C-N-CA	5.30	127.81	120.29
1	E	49	ILE	CA-C-O	5.30	126.59	120.76
2	3	199	TYR	CB-CA-C	-5.29	101.21	109.84
2	6	153	ASP	CA-C-N	-5.29	113.80	122.54
2	6	153	ASP	C-N-CA	-5.29	113.80	122.54
2	4	98	LEU	N-CA-CB	5.29	117.68	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	37	ILE	N-CA-C	-5.29	100.50	108.12
1	B	132	PHE	CB-CA-C	-5.29	101.62	110.29
2	6	187	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	217	ASP	N-CA-CB	5.29	118.47	110.28
1	C	239	ARG	NE-CZ-NH1	-5.28	116.22	121.50
2	7	36	PHE	CA-C-N	5.28	128.17	120.98
2	7	36	PHE	C-N-CA	5.28	128.17	120.98
1	B	142	ASP	N-CA-CB	5.28	117.95	110.13
2	7	208	LEU	N-CA-C	-5.28	106.84	113.28
1	E	127	GLY	O-C-N	-5.28	114.39	122.26
2	1	73	GLU	CA-C-O	-5.28	113.90	119.97
2	2	175	ALA	CA-C-N	5.28	127.88	120.28
2	2	175	ALA	C-N-CA	5.28	127.88	120.28
2	1	59	SER	CA-C-N	5.28	128.29	120.74
2	1	59	SER	C-N-CA	5.28	128.29	120.74
1	D	196	MET	N-CA-C	5.27	117.71	111.33
2	1	104	PHE	CG-CD2-CE2	5.27	129.66	120.70
2	4	114	GLY	CA-C-O	-5.27	117.27	120.91
1	C	47	ILE	N-CA-CB	5.27	122.46	112.24
2	2	28	GLU	CA-C-N	5.27	130.75	122.11
2	2	28	GLU	C-N-CA	5.27	130.75	122.11
2	3	124	SER	CA-C-O	-5.26	115.13	120.71
1	B	99	ASN	CA-C-N	5.26	127.33	120.28
1	B	99	ASN	C-N-CA	5.26	127.33	120.28
1	G	235	ARG	NE-CZ-NH2	5.26	123.94	119.20
2	1	168	ALA	N-CA-CB	5.26	117.63	110.01
2	3	65	PHE	CA-C-N	5.26	127.76	120.29
2	3	65	PHE	C-N-CA	5.26	127.76	120.29
2	5	81	ARG	CB-CA-C	-5.26	101.83	110.72
1	G	219	ARG	N-CA-CB	5.26	120.29	112.30
2	6	203	GLU	CA-C-O	-5.26	114.85	120.42
1	E	105	GLU	N-CA-CB	5.25	119.72	110.37
2	7	201	PRO	CA-C-N	5.25	127.63	120.54
2	7	201	PRO	C-N-CA	5.25	127.63	120.54
1	A	85	ALA	CA-C-O	-5.25	115.30	120.82
1	F	178	GLU	N-CA-C	5.25	118.85	112.23
1	G	94	ILE	CB-CA-C	5.25	119.23	112.14
1	D	163	ALA	CA-C-N	5.25	131.03	122.69
1	D	163	ALA	C-N-CA	5.25	131.03	122.69
1	G	132	PHE	N-CA-C	-5.25	101.22	109.25
2	3	180	SER	N-CA-C	-5.25	106.47	112.92
1	B	169	ASN	CA-CB-CG	-5.25	107.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	182	SER	CA-C-O	-5.25	115.82	121.38
1	B	108	THR	CA-C-O	-5.24	115.62	121.81
1	C	127	GLY	N-CA-C	-5.24	106.65	115.62
2	5	28	GLU	N-CA-C	-5.24	101.73	110.17
2	6	207	ILE	CA-C-O	5.24	126.32	120.71
1	E	14	VAL	N-CA-CB	5.24	120.16	112.35
1	F	37	ALA	N-CA-C	-5.24	101.33	109.14
2	5	192	THR	N-CA-C	-5.24	104.91	113.19
1	B	30	ALA	O-C-N	5.24	127.67	122.12
1	A	222	LYS	O-C-N	-5.24	116.36	122.96
1	E	82	VAL	CA-C-N	5.24	127.56	120.44
1	E	82	VAL	C-N-CA	5.24	127.56	120.44
2	7	188	VAL	N-CA-C	-5.24	100.33	108.81
1	D	48	LEU	CB-CA-C	-5.23	100.23	109.70
2	6	18	VAL	CA-CB-CG2	-5.23	101.50	110.40
1	C	219	ARG	N-CA-CB	5.23	120.67	112.46
2	2	126	ASP	N-CA-CB	5.23	117.00	109.78
2	3	172	ILE	N-CA-CB	5.23	117.65	110.54
2	6	26	ALA	N-CA-C	-5.23	100.78	108.99
1	C	241	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	B	15	PHE	N-CA-CB	5.23	117.73	110.26
1	C	84	ASP	CB-CA-C	-5.23	102.11	110.79
1	E	203	GLU	CA-C-O	5.23	127.26	121.56
1	G	84	ASP	CA-CB-CG	-5.23	107.37	112.60
1	F	84	ASP	N-CA-C	-5.22	105.50	111.14
1	E	168	ARG	N-CA-CB	5.22	117.58	110.01
1	D	47	ILE	N-CA-C	-5.22	100.97	108.53
1	D	156	LEU	O-C-N	5.22	129.63	123.27
1	E	217	ASP	N-CA-C	-5.22	106.76	113.02
1	D	222	LYS	N-CA-C	-5.21	101.15	109.23
2	5	196	PHE	CA-CB-CG	-5.21	108.58	113.80
1	F	239	ARG	CA-C-N	5.21	127.82	120.42
1	F	239	ARG	C-N-CA	5.21	127.82	120.42
1	B	166	MET	N-CA-C	5.21	117.64	111.33
2	4	129	GLY	CA-C-N	5.21	127.83	121.06
2	4	129	GLY	C-N-CA	5.21	127.83	121.06
2	5	65	PHE	N-CA-C	5.21	116.64	111.07
1	G	93	ARG	CG-CD-NE	-5.21	100.54	112.00
1	A	160	LYS	N-CA-C	-5.21	106.88	114.12
1	E	179	TYR	CA-C-N	5.21	131.49	122.64
1	E	179	TYR	C-N-CA	5.21	131.49	122.64
2	3	96	ASN	N-CA-CB	5.21	117.77	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	PRO	N-CD-CG	5.21	111.01	103.20
1	F	126	TYR	CB-CA-C	5.20	119.11	109.70
2	5	164	ALA	CA-C-N	5.20	127.81	120.42
2	5	164	ALA	C-N-CA	5.20	127.81	120.42
1	G	108	THR	CA-C-N	5.20	127.81	120.42
1	G	108	THR	C-N-CA	5.20	127.81	120.42
1	A	149	GLU	N-CA-C	-5.20	99.49	108.69
1	B	215	LYS	CA-C-O	-5.20	115.68	121.81
2	1	211	PHE	N-CA-C	-5.20	106.34	113.30
2	2	89	ALA	O-C-N	5.19	127.62	122.12
2	2	137	ILE	O-C-N	-5.19	117.58	123.03
2	4	93	LEU	O-C-N	5.19	127.42	122.07
2	4	173	TYR	N-CA-C	5.19	117.34	111.11
1	B	56	SER	N-CA-C	-5.19	101.40	109.14
2	1	161	VAL	CA-C-N	5.19	127.23	120.28
2	1	161	VAL	C-N-CA	5.19	127.23	120.28
1	B	164	ILE	N-CA-C	-5.19	100.39	108.95
2	5	196	PHE	N-CA-C	-5.19	98.10	107.75
1	B	229	LEU	N-CA-C	-5.19	105.54	111.14
1	D	245	LYS	CB-CG-CD	5.18	123.23	111.30
2	1	144	SER	N-CA-C	5.18	117.67	111.71
1	A	96	ALA	CA-C-N	5.18	128.19	120.31
1	A	96	ALA	C-N-CA	5.18	128.19	120.31
1	C	107	ILE	N-CA-C	-5.18	102.91	109.80
2	6	196	PHE	CB-CG-CD1	5.18	129.51	120.70
1	C	15	PHE	CA-CB-CG	-5.18	108.62	113.80
1	E	113	ALA	CA-C-N	5.18	127.22	120.28
1	E	113	ALA	C-N-CA	5.18	127.22	120.28
1	G	246	LYS	CG-CD-CE	5.18	123.22	111.30
1	F	238	GLU	CA-C-O	-5.18	115.38	120.82
2	7	46	TYR	CG-CD1-CE1	-5.18	113.43	121.20
1	C	50	ALA	CA-C-N	5.18	129.23	121.72
1	C	50	ALA	C-N-CA	5.18	129.23	121.72
2	1	49	ALA	CA-C-N	5.18	127.94	120.38
2	1	49	ALA	C-N-CA	5.18	127.94	120.38
1	C	174	PHE	CA-C-O	5.17	126.25	120.82
2	5	154	ARG	CA-C-N	-5.17	112.82	120.94
2	5	154	ARG	C-N-CA	-5.17	112.82	120.94
2	6	188	VAL	N-CA-C	-5.17	100.61	108.17
2	7	103	TYR	N-CA-C	-5.17	106.37	113.30
2	7	117	SER	N-CA-C	5.17	117.66	111.71
1	B	66	LYS	CA-C-O	5.17	124.21	118.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	TYR	CB-CA-C	-5.17	100.76	109.50
1	E	22	PHE	N-CA-CB	5.17	118.97	110.39
1	G	191	LEU	N-CA-C	5.17	116.92	111.28
2	1	195	GLU	N-CA-C	-5.17	100.88	108.79
2	5	156	THR	O-C-N	-5.17	118.40	121.71
1	D	199	SER	O-C-N	5.17	127.47	122.09
2	6	93	LEU	CA-C-N	5.17	127.21	120.28
2	6	93	LEU	C-N-CA	5.17	127.21	120.28
1	C	108	THR	N-CA-CB	5.17	118.30	110.45
1	E	51	ASP	CA-CB-CG	5.17	117.77	112.60
2	2	57	ALA	N-CA-C	-5.17	100.75	109.07
2	6	139	ALA	CA-C-O	-5.17	113.12	120.51
2	1	14	THR	CA-CB-OG1	-5.17	101.85	109.60
1	C	58	LEU	CB-CA-C	-5.16	102.42	110.94
1	B	17	PRO	N-CA-C	-5.16	107.90	114.35
2	2	199	TYR	CA-CB-CG	-5.16	104.61	113.90
2	4	104	PHE	N-CA-C	-5.16	99.86	108.94
2	5	190	LYS	N-CA-C	-5.16	101.28	109.59
1	D	215	LYS	N-CA-CB	5.16	119.04	110.63
1	E	205	VAL	O-C-N	-5.16	115.22	121.10
1	C	177	LYS	N-CA-C	-5.16	105.82	112.68
2	5	49	ALA	N-CA-C	-5.16	101.59	108.86
2	5	174	SER	O-C-N	-5.16	116.73	122.09
2	7	141	GLY	O-C-N	-5.16	116.55	123.67
1	D	186	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	137	LEU	CB-CA-C	-5.15	101.61	110.16
2	2	165	VAL	N-CA-CB	5.15	118.31	110.58
1	A	201	GLU	CA-C-O	5.15	127.41	121.28
1	A	220	THR	N-CA-C	-5.15	99.72	108.26
2	4	104	PHE	N-CA-CB	5.15	119.12	110.99
1	C	73	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
1	D	22	PHE	N-CA-CB	5.14	119.06	110.32
1	F	209	ILE	O-C-N	-5.14	117.33	123.04
1	B	132	PHE	CA-CB-CG	-5.14	108.66	113.80
1	B	229	LEU	N-CA-CB	5.14	117.52	110.07
2	2	102	ARG	CD-NE-CZ	-5.14	117.20	124.40
2	2	181	ALA	N-CA-C	5.14	118.33	111.75
1	B	93	ARG	CB-CA-C	-5.14	102.81	110.88
2	6	178	ARG	O-C-N	5.14	128.36	122.25
2	5	177	LYS	CA-C-N	5.14	127.42	120.38
2	5	177	LYS	C-N-CA	5.14	127.42	120.38
1	B	28	ARG	CA-C-N	5.13	127.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ARG	C-N-CA	5.13	127.67	120.28
2	3	211	PHE	CA-CB-CG	-5.13	108.67	113.80
2	7	196	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	155	ALA	O-C-N	-5.13	117.20	123.16
1	G	170	ALA	CA-C-N	5.13	127.71	120.42
1	G	170	ALA	C-N-CA	5.13	127.71	120.42
2	3	188	VAL	N-CA-C	-5.13	100.50	108.81
2	5	132	ILE	CA-CB-CG2	5.13	119.22	110.50
1	G	110	LYS	CA-C-O	-5.13	115.43	120.82
1	G	237	ASN	CA-C-N	5.13	127.92	120.79
1	G	237	ASN	C-N-CA	5.13	127.92	120.79
1	D	197	GLY	CA-C-O	5.13	125.83	120.80
1	F	177	LYS	CA-C-O	-5.13	114.35	120.56
2	5	117	SER	N-CA-C	5.13	116.87	111.28
1	F	95	GLU	N-CA-CB	5.13	117.75	110.16
1	E	120	LYS	O-C-N	5.12	127.55	122.12
1	F	147	LEU	N-CA-C	-5.12	100.35	109.06
2	2	62	ASP	N-CA-C	-5.12	105.77	112.23
1	E	182	ASP	O-C-N	-5.12	117.23	123.27
2	5	188	VAL	CA-CB-CG2	5.12	119.11	110.40
1	B	173	GLU	CA-C-N	5.12	127.10	120.44
1	B	173	GLU	C-N-CA	5.12	127.10	120.44
2	5	165	VAL	CA-C-N	5.12	127.56	120.29
2	5	165	VAL	C-N-CA	5.12	127.56	120.29
1	F	119	PHE	CA-C-N	5.12	127.56	120.29
1	F	119	PHE	C-N-CA	5.12	127.56	120.29
1	A	124	THR	CA-C-O	-5.12	115.00	120.42
1	A	197	GLY	CA-C-N	5.12	127.09	120.44
1	A	197	GLY	C-N-CA	5.12	127.09	120.44
1	D	131	PRO	CA-C-O	-5.12	115.56	121.95
2	5	172	ILE	CA-C-N	5.12	127.55	120.29
2	5	172	ILE	C-N-CA	5.12	127.55	120.29
2	6	68	ARG	NH1-CZ-NH2	5.12	125.95	119.30
2	7	33	MET	CB-CA-C	-5.12	100.70	109.65
1	D	16	SER	CA-C-N	5.11	126.23	119.84
1	D	16	SER	C-N-CA	5.11	126.23	119.84
1	G	202	SER	CA-C-N	5.11	128.47	120.75
1	G	202	SER	C-N-CA	5.11	128.47	120.75
2	4	49	ALA	N-CA-C	-5.11	101.64	108.34
2	6	78	GLU	CB-CA-C	-5.11	102.85	110.88
1	A	241	ARG	CA-C-N	5.11	127.13	120.28
1	A	241	ARG	C-N-CA	5.11	127.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	ARG	N-CA-CB	5.11	117.72	110.16
2	7	201	PRO	N-CA-CB	5.11	108.61	103.25
1	E	233	VAL	CA-C-N	5.11	127.08	120.44
1	E	233	VAL	C-N-CA	5.11	127.08	120.44
1	F	16	SER	CA-C-N	5.11	125.18	119.87
1	F	16	SER	C-N-CA	5.11	125.18	119.87
2	6	210	LYS	O-C-N	-5.11	115.46	122.46
1	A	21	LEU	CA-C-O	-5.10	114.90	120.36
1	E	244	LEU	N-CA-C	-5.10	106.90	112.72
1	B	19	GLY	N-CA-C	5.10	122.94	113.76
1	E	82	VAL	N-CA-CB	5.10	117.48	110.54
1	G	82	VAL	CA-C-N	5.10	127.11	120.28
1	G	82	VAL	C-N-CA	5.10	127.11	120.28
2	2	50	ASP	CA-C-O	-5.10	115.44	120.90
2	3	80	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	D	41	LYS	O-C-N	-5.10	117.23	123.30
1	G	218	ASP	N-CA-C	-5.10	105.18	111.40
2	5	156	THR	N-CA-C	-5.10	100.60	108.55
1	A	160	LYS	CB-CA-C	-5.09	100.82	109.38
1	G	121	GLN	CG-CD-NE2	5.09	124.04	116.40
1	E	53	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	165	GLY	CA-C-N	5.09	127.35	120.38
1	B	165	GLY	C-N-CA	5.09	127.35	120.38
1	F	21	LEU	N-CA-CB	5.09	118.08	109.94
2	4	95	SER	CA-C-N	5.08	127.51	120.29
2	4	95	SER	C-N-CA	5.08	127.51	120.29
1	E	191	LEU	CA-C-O	5.08	126.34	120.90
2	4	178	ARG	CB-CA-C	-5.08	102.21	110.85
2	2	135	LYS	CA-C-N	5.08	134.95	123.16
2	2	135	LYS	C-N-CA	5.08	134.95	123.16
2	2	153	ASP	CB-CA-C	-5.08	101.40	110.70
2	7	38	ALA	N-CA-C	5.08	117.94	111.69
1	E	169	ASN	CA-C-N	5.08	127.04	120.44
1	E	169	ASN	C-N-CA	5.08	127.04	120.44
2	3	167	LEU	CB-CA-C	-5.08	102.90	110.88
1	C	103	TYR	CA-C-N	5.08	129.40	122.34
1	C	103	TYR	C-N-CA	5.08	129.40	122.34
1	D	236	ALA	O-C-N	5.08	127.30	122.07
1	E	152	PRO	N-CA-CB	5.08	108.56	103.48
1	E	29	GLU	CA-C-N	5.08	127.08	120.28
1	E	29	GLU	C-N-CA	5.08	127.08	120.28
1	A	204	LEU	CA-C-N	5.08	131.52	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	LEU	C-N-CA	5.08	131.52	122.13
1	A	23	GLN	OE1-CD-NE2	5.07	127.67	122.60
1	B	221	PHE	CA-CB-CG	-5.07	108.73	113.80
2	1	206	GLN	CA-C-O	5.07	125.60	119.11
2	3	15	VAL	CA-CB-CG1	-5.07	101.78	110.40
2	5	196	PHE	N-CA-CB	5.07	118.76	110.39
2	7	114	GLY	CA-C-O	-5.07	116.43	120.79
1	D	26	TYR	CB-CG-CD2	5.07	128.40	120.80
1	C	121	GLN	CA-C-O	-5.07	115.05	120.42
1	F	28	ARG	NH1-CZ-NH2	5.07	125.89	119.30
1	F	224	VAL	CA-CB-CG2	-5.07	101.79	110.40
2	7	204	VAL	CB-CA-C	-5.07	105.23	112.22
2	5	67	ALA	N-CA-CB	5.06	117.56	110.12
2	7	50	ASP	CA-CB-CG	-5.06	107.54	112.60
1	A	46	VAL	CA-CB-CG2	-5.06	101.79	110.40
2	1	164	ALA	CA-C-O	5.06	125.59	119.31
1	C	172	THR	N-CA-C	5.06	116.48	111.07
2	4	96	ASN	CA-C-N	5.06	127.06	120.28
2	4	96	ASN	C-N-CA	5.06	127.06	120.28
1	A	224	VAL	N-CA-C	-5.06	101.05	108.54
2	1	194	ASP	CA-CB-CG	5.06	117.66	112.60
2	7	167	LEU	O-C-N	-5.06	116.63	122.09
1	D	77	ALA	CB-CA-C	-5.06	101.36	110.36
1	D	235	ARG	O-C-N	5.06	127.92	122.15
2	1	78	GLU	N-CA-CB	5.06	117.34	110.01
1	E	170	ALA	CA-C-N	5.05	127.60	120.42
1	E	170	ALA	C-N-CA	5.05	127.60	120.42
1	G	63	THR	CB-CA-C	-5.05	102.64	109.16
1	C	170	ALA	CA-C-N	5.05	127.02	120.56
1	C	170	ALA	C-N-CA	5.05	127.02	120.56
1	F	187	ASP	CB-CA-C	-5.05	102.27	110.85
2	3	185	GLY	CA-C-N	5.05	130.07	122.75
2	3	185	GLY	C-N-CA	5.05	130.07	122.75
2	7	168	ALA	CA-C-N	5.05	126.92	120.56
2	7	168	ALA	C-N-CA	5.05	126.92	120.56
2	1	192	THR	N-CA-C	-5.04	107.16	113.72
2	3	166	GLU	CA-C-N	5.04	127.00	120.44
2	3	166	GLU	C-N-CA	5.04	127.00	120.44
2	5	169	VAL	CG1-CB-CG2	5.04	121.90	110.80
1	A	42	CYS	N-CA-C	-5.04	101.45	108.96
1	F	64	ILE	N-CA-C	-5.04	98.85	109.34
2	2	104	PHE	N-CA-C	-5.04	100.06	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	LEU	N-CA-C	5.04	116.85	111.36
2	4	67	ALA	CB-CA-C	-5.04	102.42	110.79
1	D	241	ARG	CG-CD-NE	-5.04	100.92	112.00
2	2	97	LEU	N-CA-C	5.04	116.77	111.28
1	C	231	PRO	CA-C-N	5.04	127.03	120.28
1	C	231	PRO	C-N-CA	5.04	127.03	120.28
1	F	137	LEU	CB-CA-C	-5.04	102.63	110.74
2	2	151	LEU	CA-C-N	5.04	129.13	120.72
2	2	151	LEU	C-N-CA	5.04	129.13	120.72
2	4	57	ALA	CA-C-N	5.04	129.27	122.42
2	4	57	ALA	C-N-CA	5.04	129.27	122.42
1	B	84	ASP	CA-C-N	5.04	126.99	120.44
1	B	84	ASP	C-N-CA	5.04	126.99	120.44
2	5	46	TYR	CB-CG-CD1	-5.04	113.25	120.80
1	G	153	SER	N-CA-CB	5.03	117.52	110.12
1	D	99	ASN	N-CA-C	5.03	116.76	111.28
1	E	37	ALA	N-CA-C	-5.03	102.45	109.69
2	2	41	ALA	O-C-N	-5.03	116.10	122.19
1	C	95	GLU	CA-C-N	5.03	126.98	120.44
1	C	95	GLU	C-N-CA	5.03	126.98	120.44
1	D	142	ASP	N-CA-C	-5.03	105.99	112.68
2	7	158	GLU	CB-CG-CD	-5.03	104.05	112.60
1	E	86	ARG	O-C-N	5.03	127.25	122.07
2	1	168	ALA	CB-CA-C	-5.03	102.99	110.88
2	1	191	ILE	CA-C-O	-5.03	115.39	120.31
2	3	145	LEU	CA-C-N	5.02	127.46	120.63
2	3	145	LEU	C-N-CA	5.02	127.46	120.63
2	3	100	SER	CA-C-N	5.02	131.13	121.54
2	3	100	SER	C-N-CA	5.02	131.13	121.54
2	6	55	THR	CA-C-O	-5.02	115.48	121.16
2	3	122	ILE	CA-C-N	5.02	129.52	122.09
2	3	122	ILE	C-N-CA	5.02	129.52	122.09
2	5	78	GLU	CB-CA-C	-5.02	103.00	110.88
1	A	85	ALA	CB-CA-C	-5.02	103.00	110.88
1	F	72	GLU	CB-CG-CD	-5.02	104.07	112.60
2	1	63	ALA	CB-CA-C	-5.02	102.46	110.79
1	A	104	ASP	N-CA-CB	5.02	119.31	111.84
1	C	143	GLU	O-C-N	-5.01	115.92	122.59
2	7	62	ASP	CA-CB-CG	-5.01	107.59	112.60
2	2	56	THR	O-C-N	-5.01	117.45	123.31
2	3	52	MET	N-CA-C	-5.01	101.47	109.23
1	B	202	SER	CA-C-N	5.01	128.80	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	SER	C-N-CA	5.01	128.80	120.94
1	D	219	ARG	N-CA-CB	5.01	120.32	112.46
2	6	32	THR	CB-CA-C	-5.01	102.75	110.26
1	D	78	THR	O-C-N	-5.00	117.47	123.27
2	5	150	VAL	N-CA-CB	5.00	117.34	110.54

There are no chirality outliers.

All (115) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	106	TYR	Sidechain
2	1	148	TYR	Sidechain
2	1	178	ARG	Sidechain
2	1	197	TYR	Sidechain
2	1	80	ARG	Sidechain
2	2	101	TYR	Sidechain
2	2	139	ALA	Mainchain,Peptide
2	2	140	THR	Mainchain
2	2	170	ARG	Sidechain
2	2	199	TYR	Sidechain
2	2	68	ARG	Sidechain
2	2	80	ARG	Sidechain
2	3	123	TYR	Sidechain
2	3	195	GLU	Peptide
2	3	30	ARG	Sidechain
2	3	68	ARG	Sidechain
2	4	101	TYR	Sidechain
2	4	103	TYR	Sidechain
2	4	106	TYR	Sidechain
2	4	139	ALA	Mainchain,Peptide
2	4	140	THR	Mainchain
2	4	173	TYR	Sidechain
2	4	51	ARG	Sidechain
2	4	83	ARG	Sidechain
2	5	101	TYR	Sidechain
2	5	102	ARG	Sidechain
2	5	140	THR	Mainchain
2	5	148	TYR	Sidechain
2	5	170	ARG	Sidechain
2	5	178	ARG	Sidechain
2	5	195	GLU	Peptide
2	5	211	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	5	36	PHE	Sidechain
2	5	80	ARG	Sidechain
2	6	123	TYR	Sidechain
2	6	139	ALA	Peptide
2	6	140	THR	Mainchain
2	6	148	TYR	Sidechain
2	6	170	ARG	Sidechain
2	6	178	ARG	Sidechain
2	6	65	PHE	Sidechain
2	6	83	ARG	Sidechain
2	7	103	TYR	Sidechain
2	7	106	TYR	Sidechain
2	7	132	ILE	Peptide
2	7	140	THR	Mainchain
2	7	212	ARG	Sidechain
2	7	81	ARG	Sidechain
1	A	103	TYR	Sidechain
1	A	148	TYR	Sidechain
1	A	175	PHE	Sidechain
1	A	221	PHE	Sidechain
1	A	26	TYR	Sidechain
1	A	28	ARG	Sidechain
1	A	86	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	179	TYR	Sidechain
1	B	220	THR	Peptide
1	B	239	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	68	TYR	Sidechain
1	C	119	PHE	Sidechain
1	C	130	ARG	Sidechain
1	C	132	PHE	Sidechain
1	C	175	PHE	Sidechain
1	C	181	ASP	Peptide
1	C	213	TYR	Sidechain
1	C	220	THR	Peptide
1	C	221	PHE	Sidechain
1	C	232	TYR	Sidechain
1	C	33	ARG	Sidechain
1	D	123	TYR	Sidechain
1	D	179	TYR	Sidechain
1	D	182	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	D	20	ARG	Sidechain
1	D	22	PHE	Sidechain
1	D	220	THR	Mainchain,Peptide
1	D	224	VAL	Peptide
1	D	37	ALA	Peptide
1	D	86	ARG	Sidechain
1	E	103	TYR	Sidechain
1	E	148	TYR	Sidechain
1	E	179	TYR	Sidechain
1	E	185	PHE	Sidechain
1	E	213	TYR	Sidechain
1	E	215	LYS	Mainchain
1	E	220	THR	Peptide
1	E	224	VAL	Peptide
1	E	239	ARG	Sidechain
1	E	241	ARG	Sidechain
1	E	53	ARG	Sidechain
1	F	103	TYR	Sidechain
1	F	148	TYR	Sidechain
1	F	20	ARG	Sidechain
1	F	213	TYR	Sidechain
1	F	220	THR	Peptide
1	F	224	VAL	Mainchain
1	F	28	ARG	Sidechain
1	F	86	ARG	Sidechain
1	F	93	ARG	Sidechain
1	G	100	ARG	Sidechain
1	G	126	TYR	Sidechain
1	G	130	ARG	Sidechain
1	G	182	ASP	Peptide
1	G	213	TYR	Sidechain
1	G	220	THR	Peptide
1	G	26	TYR	Sidechain
1	G	37	ALA	Peptide
1	G	52	LYS	Peptide
1	G	53	ARG	Mainchain,Peptide
1	G	54	VAL	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	1850	0	1890	13	0
1	B	1850	0	1890	9	0
1	C	1850	0	1890	9	0
1	D	1850	0	1890	10	0
1	E	1850	0	1890	6	0
1	F	1850	0	1890	4	0
1	G	1850	0	1890	11	0
2	1	1553	0	1580	6	0
2	2	1553	0	1580	7	0
2	3	1553	0	1580	11	0
2	4	1553	0	1580	7	0
2	5	1553	0	1580	47	0
2	6	1553	0	1580	8	0
2	7	1553	0	1580	9	0
All	All	23821	0	24290	145	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 3.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:211:PHE:CD2	2:5:211:PHE:CG	2.18	1.31
2:5:170:ARG:HD3	2:5:211:PHE:CD1	1.66	1.29
2:5:211:PHE:CD2	2:5:211:PHE:CE2	2.19	1.29
2:5:211:PHE:CE1	2:5:211:PHE:CZ	2.20	1.27
2:5:211:PHE:CD1	2:5:211:PHE:CE1	2.22	1.27
2:5:170:ARG:CZ	2:5:211:PHE:CE1	2.19	1.24
2:5:211:PHE:CE2	2:5:211:PHE:CZ	2.26	1.22
2:5:170:ARG:NH1	2:5:211:PHE:CD1	2.08	1.21
2:5:170:ARG:HG2	2:5:211:PHE:CE1	1.79	1.18
2:5:170:ARG:CD	2:5:211:PHE:CD1	2.27	1.18
2:5:170:ARG:NE	2:5:211:PHE:CD2	2.16	1.13
2:5:170:ARG:NH1	2:5:211:PHE:CG	2.21	1.08
2:5:170:ARG:NE	2:5:211:PHE:CE2	2.22	1.08
2:5:170:ARG:NE	2:5:211:PHE:CZ	2.22	1.06
2:5:170:ARG:CD	2:5:211:PHE:CG	2.41	1.04
2:5:170:ARG:CZ	2:5:211:PHE:CZ	2.42	1.02
2:5:170:ARG:CZ	2:5:211:PHE:CG	2.42	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:170:ARG:NE	2:5:211:PHE:CG	2.30	1.00
2:5:170:ARG:CZ	2:5:211:PHE:CD2	2.45	0.98
2:5:170:ARG:HD3	2:5:211:PHE:CG	2.00	0.96
2:5:170:ARG:CG	2:5:211:PHE:CD1	2.48	0.96
2:5:170:ARG:NH2	2:5:211:PHE:CE2	2.33	0.96
2:5:166:GLU:OE1	2:5:211:PHE:CE1	2.18	0.95
2:1:40:LYS:HE2	2:2:137:ILE:HD11	1.51	0.92
2:5:170:ARG:HG2	2:5:211:PHE:CD1	2.05	0.91
2:5:170:ARG:CG	2:5:211:PHE:CE1	2.53	0.91
2:5:170:ARG:NH2	2:5:211:PHE:CZ	2.38	0.91
2:5:137:ILE:HD11	2:5:155:PHE:CD1	2.06	0.90
2:5:166:GLU:OE1	2:5:211:PHE:HE1	1.54	0.90
2:5:170:ARG:CZ	2:5:211:PHE:CE2	2.63	0.80
2:2:137:ILE:HD12	2:2:137:ILE:H	1.46	0.79
2:5:170:ARG:NH1	2:5:211:PHE:CE1	2.52	0.76
2:5:170:ARG:NE	2:5:211:PHE:CE1	2.54	0.76
2:5:170:ARG:CZ	2:5:211:PHE:CD1	2.69	0.75
2:5:115:ILE:HG21	2:5:193:GLU:HG2	1.70	0.74
1:E:70:ILE:HG21	1:E:112:LEU:HD21	1.73	0.71
1:F:125:GLN:O	1:G:129:VAL:HG23	1.91	0.70
2:1:45:ILE:HD11	2:1:189:VAL:HG22	1.75	0.69
2:5:170:ARG:CD	2:5:211:PHE:CE1	2.83	0.61
1:A:124:THR:HG23	1:B:130:ARG:HH21	1.65	0.61
2:2:17:LEU:HA	2:2:137:ILE:HG22	1.83	0.60
2:5:54:MET:HE2	2:5:67:ALA:HB2	1.84	0.60
2:5:137:ILE:HD11	2:5:155:PHE:CG	2.37	0.59
1:C:163:ALA:HB2	1:C:171:VAL:HG11	1.84	0.58
2:7:29:LYS:HE3	2:7:201:PRO:HD3	1.85	0.58
1:B:121:GLN:CG	1:C:83:ALA:HB1	2.34	0.58
1:B:38:ILE:HG23	1:B:49:ILE:HG23	1.86	0.57
2:6:43:LYS:HE2	2:6:198:GLN:HE22	1.69	0.57
1:D:163:ALA:HB2	1:D:171:VAL:HG11	1.87	0.56
2:2:137:ILE:HD12	2:2:137:ILE:N	2.18	0.56
2:3:21:ASP:HB2	2:3:161:VAL:HG13	1.89	0.55
1:A:38:ILE:HG23	1:A:49:ILE:HB	1.87	0.55
1:A:70:ILE:HG21	1:A:112:LEU:HD21	1.87	0.54
2:4:65:PHE:CE2	2:4:69:ILE:HD11	2.42	0.54
2:5:166:GLU:CD	2:5:211:PHE:CZ	2.85	0.54
1:B:121:GLN:HG3	1:C:83:ALA:HB1	1.88	0.54
2:5:115:ILE:HG21	2:5:193:GLU:CG	2.38	0.53
1:C:49:ILE:HG23	1:C:211:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:211:PHE:CG	2:5:211:PHE:CD1	2.97	0.53
1:D:196:MET:HA	1:D:196:MET:HE3	1.91	0.52
2:1:137:ILE:HD12	2:1:151:LEU:HG	1.90	0.52
1:G:171:VAL:HG13	1:G:195:ALA:HB1	1.91	0.52
1:E:211:VAL:HG21	1:E:229:LEU:HD11	1.92	0.52
1:F:88:LEU:HD21	1:F:120:LYS:HE2	1.92	0.51
2:5:170:ARG:NH2	2:5:211:PHE:CD2	2.77	0.51
2:7:60:VAL:O	2:7:63:ALA:HB3	2.10	0.51
2:1:40:LYS:HE2	2:2:137:ILE:CD1	2.31	0.50
2:4:155:PHE:CE1	2:4:159:ILE:HG21	2.47	0.50
1:C:47:ILE:HD13	1:C:189:MET:HA	1.94	0.50
1:C:108:THR:HG21	2:4:83:ARG:HH22	1.77	0.50
2:2:66:LEU:HD23	2:2:110:LEU:HD21	1.95	0.49
2:3:137:ILE:HG23	2:3:151:LEU:HD23	1.94	0.48
2:1:112:ILE:HD12	2:1:125:ILE:HD13	1.95	0.48
1:G:151:ASP:HB2	1:G:155:ALA:HB3	1.96	0.48
2:5:23:VAL:HG23	2:5:115:ILE:HD11	1.96	0.48
2:7:154:ARG:HB2	2:7:167:LEU:HD13	1.96	0.48
2:7:137:ILE:HD11	2:7:155:PHE:CD1	2.49	0.48
1:E:54:VAL:HG23	1:E:59:LEU:HB3	1.96	0.48
1:B:92:ALA:HB2	1:B:116:ILE:HG21	1.96	0.48
1:C:70:ILE:HG21	1:C:112:LEU:HD21	1.94	0.48
1:D:47:ILE:HD11	1:D:185:PHE:CE1	2.49	0.47
1:D:233:VAL:HG12	1:D:237:ASN:ND2	2.30	0.47
1:A:40:ILE:CD1	1:A:192:GLY:HA3	2.45	0.47
2:5:170:ARG:HA	2:5:211:PHE:CD1	2.49	0.47
1:A:49:ILE:HG12	1:A:211:VAL:HG13	1.96	0.47
2:6:186:ILE:HD11	2:6:204:VAL:HG11	1.96	0.47
1:G:190:VAL:O	1:G:194:VAL:HG23	2.15	0.47
2:3:111:LEU:HD13	2:3:138:VAL:HG13	1.97	0.47
1:G:117:CYS:SG	1:G:150:THR:HG23	2.55	0.46
2:7:49:ALA:HB3	2:7:52:MET:SD	2.55	0.46
1:E:174:PHE:CD1	1:E:195:ALA:HB2	2.51	0.46
1:G:204:LEU:H	1:G:237:ASN:HD21	1.63	0.46
1:B:189:MET:HE1	1:B:211:VAL:HG11	1.97	0.46
2:4:137:ILE:HG23	2:4:151:LEU:HD12	1.98	0.46
1:A:27:ALA:O	1:A:30:ALA:HB3	2.16	0.46
2:4:80:ARG:HD2	2:4:81:ARG:HH12	1.81	0.46
1:A:113:ALA:HB1	1:A:156:LEU:CD1	2.46	0.45
1:C:121:GLN:HE21	1:D:87:VAL:HG21	1.80	0.45
1:D:47:ILE:HD12	1:D:47:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:HB3	1:A:134:VAL:HG12	1.98	0.45
2:5:186:ILE:HG21	2:5:204:VAL:HG11	1.99	0.45
2:6:64:GLN:HG3	2:7:130:GLY:HA2	1.98	0.45
2:3:54:MET:HE2	2:3:112:ILE:HD11	1.99	0.44
2:7:172:ILE:HB	2:7:186:ILE:HD11	1.99	0.44
1:E:72:GLU:O	1:E:220:THR:HG23	2.16	0.44
1:A:91:ARG:HA	1:A:94:ILE:HD12	1.99	0.44
1:A:113:ALA:HB1	1:A:156:LEU:HD11	1.99	0.43
2:6:125:ILE:HD12	2:6:125:ILE:N	2.33	0.43
1:B:195:ALA:HA	1:B:198:LEU:HD12	1.99	0.43
2:4:18:VAL:HB	2:4:136:ASP:HA	2.00	0.43
1:E:72:GLU:HB2	1:E:100:ARG:HH22	1.82	0.43
1:G:145:PRO:HG3	1:G:216:VAL:HG23	2.00	0.43
2:5:137:ILE:HD11	2:5:155:PHE:CE1	2.52	0.43
2:5:115:ILE:CG2	2:5:193:GLU:HG2	2.42	0.43
2:6:18:VAL:HB	2:6:136:ASP:HA	2.01	0.43
1:D:224:VAL:HG12	1:D:225:SER:H	1.82	0.43
2:3:137:ILE:HG23	2:3:151:LEU:CD2	2.49	0.43
1:A:36:THR:HB	1:A:167:GLY:H	1.84	0.43
1:B:121:GLN:HG2	1:C:83:ALA:HB1	2.00	0.42
1:G:145:PRO:HG3	1:G:216:VAL:CG2	2.49	0.42
2:3:45:ILE:HG12	2:3:55:THR:HG22	2.01	0.42
2:5:132:ILE:HG21	2:5:132:ILE:HD13	1.80	0.42
1:F:163:ALA:HB3	1:F:168:ARG:HA	2.01	0.42
2:7:12:THR:HG21	2:7:58:GLY:H	1.84	0.42
1:D:213:TYR:CE2	1:D:224:VAL:HG22	2.55	0.41
2:3:169:VAL:CG2	2:3:188:VAL:HG21	2.50	0.41
2:4:80:ARG:HD2	2:4:81:ARG:NH1	2.35	0.41
2:6:41:ALA:HB3	2:7:133:GLU:O	2.19	0.41
1:D:204:LEU:HD13	1:D:209:ILE:HD13	2.03	0.41
1:B:73:HIS:O	1:B:214:VAL:HG21	2.19	0.41
2:3:109:GLN:HG2	2:3:126:ASP:HA	2.02	0.41
2:6:84:LYS:HB3	2:6:84:LYS:HE3	1.92	0.41
1:A:12:ILE:HG23	1:G:14:VAL:CG1	2.49	0.41
1:A:121:GLN:O	1:A:124:THR:HG22	2.21	0.41
1:G:121:GLN:HE22	1:G:125:GLN:NE2	2.19	0.41
2:3:169:VAL:HG22	2:3:188:VAL:HG21	2.03	0.41
1:F:183:LEU:HD13	1:F:188:ALA:HA	2.02	0.41
1:G:156:LEU:HD12	1:G:156:LEU:HA	1.94	0.41
2:2:137:ILE:HD13	2:2:148:TYR:CE1	2.56	0.41
2:3:54:MET:CE	2:3:112:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:188:VAL:HG12	2:3:189:VAL:N	2.36	0.41
2:5:154:ARG:HB2	2:5:167:LEU:HD13	2.03	0.41
1:D:40:ILE:HD12	1:D:40:ILE:N	2.36	0.41
2:6:56:THR:HG21	2:6:63:ALA:HB1	2.03	0.40
2:1:48:ILE:HG21	2:1:90:ILE:HG21	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	233/235 (99%)	220 (94%)	11 (5%)	2 (1%)	14	45
1	B	233/235 (99%)	219 (94%)	10 (4%)	4 (2%)	7	34
1	C	233/235 (99%)	217 (93%)	12 (5%)	4 (2%)	7	34
1	D	233/235 (99%)	219 (94%)	9 (4%)	5 (2%)	5	31
1	E	233/235 (99%)	212 (91%)	16 (7%)	5 (2%)	5	31
1	F	233/235 (99%)	221 (95%)	9 (4%)	3 (1%)	9	38
1	G	233/235 (99%)	215 (92%)	11 (5%)	7 (3%)	3	26
2	1	200/202 (99%)	186 (93%)	12 (6%)	2 (1%)	12	43
2	2	200/202 (99%)	185 (92%)	13 (6%)	2 (1%)	12	43
2	3	200/202 (99%)	183 (92%)	16 (8%)	1 (0%)	24	56
2	4	200/202 (99%)	188 (94%)	10 (5%)	2 (1%)	12	43
2	5	200/202 (99%)	183 (92%)	15 (8%)	2 (1%)	12	43
2	6	200/202 (99%)	184 (92%)	12 (6%)	4 (2%)	6	32
2	7	200/202 (99%)	183 (92%)	13 (6%)	4 (2%)	6	32
All	All	3031/3059 (99%)	2815 (93%)	169 (6%)	47 (2%)	10	35

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	38	ILE
1	C	181	ASP
1	D	62	ASP
1	E	221	PHE
1	G	38	ILE
1	G	53	ARG
1	G	54	VAL
2	3	139	ALA
2	6	38	ALA
2	6	106	TYR
2	6	139	ALA
2	6	140	THR
2	7	41	ALA
1	B	73	HIS
1	C	221	PHE
1	D	38	ILE
1	D	183	LEU
1	E	34	GLY
1	F	125	GLN
1	F	221	PHE
1	G	55	GLY
1	G	221	PHE
2	2	83	ARG
1	A	143	GLU
1	B	221	PHE
1	C	143	GLU
2	2	40	LYS
2	4	35	ASN
2	7	133	GLU
2	7	136	ASP
1	B	178	GLU
1	D	73	HIS
1	D	143	GLU
1	E	143	GLU
1	G	143	GLU
2	4	154	ARG
2	5	133	GLU
1	B	38	ILE
1	E	62	ASP
1	F	64	ILE
2	1	21	ASP
2	7	43	LYS

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Mol	Chain	Res	Type
2	1	136	ASP
2	5	200	SER
1	A	34	GLY
1	G	225	SER
1	E	38	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/198 (100%)	189 (96%)	9 (4%)	24	49
1	B	198/198 (100%)	193 (98%)	5 (2%)	42	61
1	C	198/198 (100%)	187 (94%)	11 (6%)	19	46
1	D	198/198 (100%)	190 (96%)	8 (4%)	28	52
1	E	198/198 (100%)	188 (95%)	10 (5%)	21	47
1	F	198/198 (100%)	187 (94%)	11 (6%)	19	46
1	G	198/198 (100%)	189 (96%)	9 (4%)	24	49
2	1	164/164 (100%)	156 (95%)	8 (5%)	22	48
2	2	164/164 (100%)	154 (94%)	10 (6%)	17	44
2	3	164/164 (100%)	156 (95%)	8 (5%)	22	48
2	4	164/164 (100%)	159 (97%)	5 (3%)	36	57
2	5	164/164 (100%)	157 (96%)	7 (4%)	26	50
2	6	164/164 (100%)	153 (93%)	11 (7%)	15	42
2	7	164/164 (100%)	153 (93%)	11 (7%)	15	42
All	All	2534/2534 (100%)	2411 (95%)	123 (5%)	24	48

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	89	ILE
1	A	104	ASP
1	A	109	VAL
1	A	182	ASP
1	A	196	MET
1	A	226	PRO
1	A	229	LEU
1	B	49	ILE
1	B	59	LEU
1	B	63	THR
1	B	124	THR
1	B	213	TYR
1	C	40	ILE
1	C	60	GLU
1	C	67	ILE
1	C	81	LEU
1	C	98	ILE
1	C	180	ARG
1	C	182	ASP
1	C	203	GLU
1	C	209	ILE
1	C	226	PRO
1	C	229	LEU
1	D	169	ASN
1	D	174	PHE
1	D	183	LEU
1	D	196	MET
1	D	198	LEU
1	D	209	ILE
1	D	217	ASP
1	D	224	VAL
1	E	14	VAL
1	E	54	VAL
1	E	63	THR
1	E	89	ILE
1	E	108	THR
1	E	129	VAL
1	E	151	ASP
1	E	169	ASN
1	E	198	LEU
1	E	224	VAL
1	F	21	LEU

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Mol	Chain	Res	Type
1	F	22	PHE
1	F	58	LEU
1	F	68	TYR
1	F	78	THR
1	F	81	LEU
1	F	129	VAL
1	F	144	VAL
1	F	162	THR
1	F	186	ASP
1	F	229	LEU
1	G	14	VAL
1	G	20	ARG
1	G	38	ILE
1	G	40	ILE
1	G	57	LYS
1	G	59	LEU
1	G	65	GLU
1	G	105	GLU
1	G	216	VAL
2	1	27	THR
2	1	72	ILE
2	1	120	LYS
2	1	128	ILE
2	1	132	ILE
2	1	137	ILE
2	1	170	ARG
2	1	202	GLU
2	2	14	THR
2	2	28	GLU
2	2	56	THR
2	2	60	VAL
2	2	72	ILE
2	2	75	ASN
2	2	132	ILE
2	2	137	ILE
2	2	179	ASP
2	2	194	ASP
2	3	39	SER
2	3	40	LYS
2	3	108	VAL
2	3	109	GLN
2	3	125	ILE

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Mol	Chain	Res	Type
2	3	137	ILE
2	3	148	TYR
2	3	208	LEU
2	4	28	GLU
2	4	72	ILE
2	4	110	LEU
2	4	121	SER
2	4	161	VAL
2	5	17	LEU
2	5	27	THR
2	5	72	ILE
2	5	150	VAL
2	5	161	VAL
2	5	189	VAL
2	5	205	GLU
2	6	14	THR
2	6	28	GLU
2	6	69	ILE
2	6	80	ARG
2	6	87	VAL
2	6	105	PRO
2	6	134	GLU
2	6	137	ILE
2	6	148	TYR
2	6	156	THR
2	6	201	PRO
2	7	17	LEU
2	7	28	GLU
2	7	72	ILE
2	7	96	ASN
2	7	109	GLN
2	7	112	ILE
2	7	128	ILE
2	7	132	ILE
2	7	161	VAL
2	7	178	ARG
2	7	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN

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Mol	Chain	Res	Type
1	A	73	HIS
1	A	125	GLN
1	A	169	ASN
1	B	73	HIS
1	B	97	GLN
1	B	169	ASN
1	D	73	HIS
1	D	122	GLN
1	D	169	ASN
1	D	237	ASN
1	E	23	GLN
1	E	237	ASN
1	F	73	HIS
1	G	121	GLN
1	G	237	ASN
2	2	99	ASN
2	3	64	GLN
2	3	75	ASN
2	3	99	ASN
2	4	75	ASN
2	6	47	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](#)

There are no chain breaks in this entry.

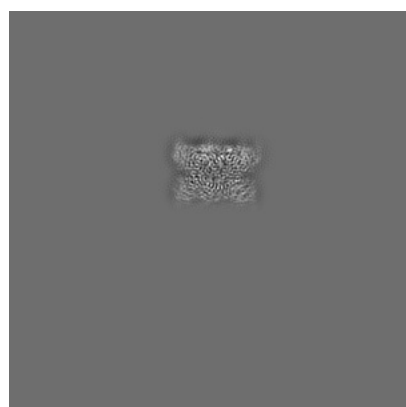
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0211. These allow visual inspection of the internal detail of the map and identification of artifacts.

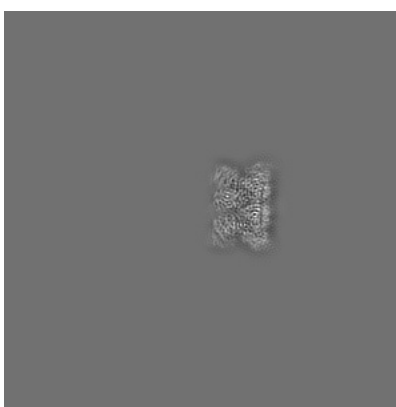
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

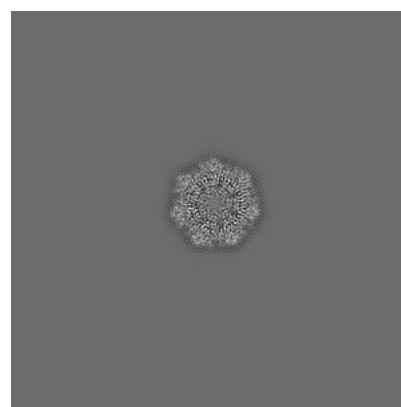
6.1.1 Primary map



X



Y

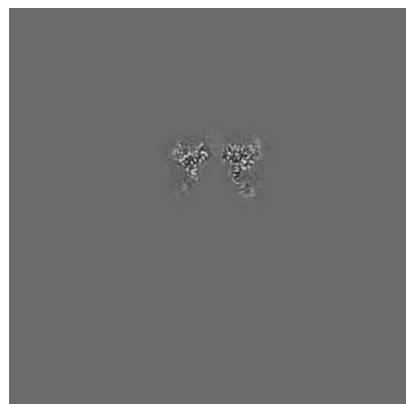


Z

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

6.2 Central slices [i](#)

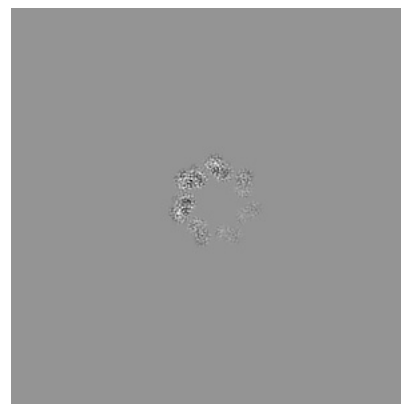
6.2.1 Primary map



X Index: 192



Y Index: 192

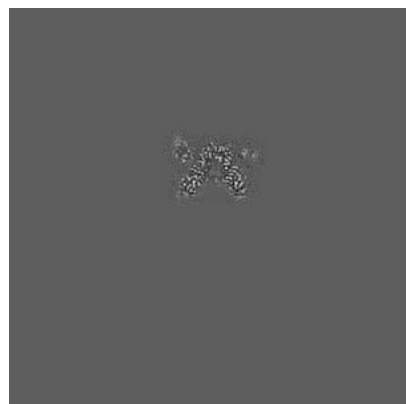


Z Index: 192

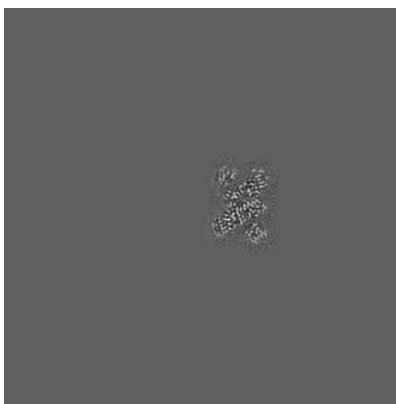
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

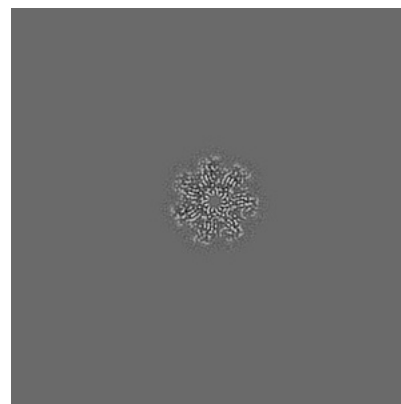
6.3.1 Primary map



X Index: 180



Y Index: 217

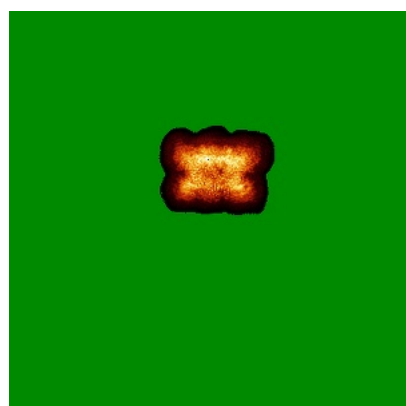


Z Index: 242

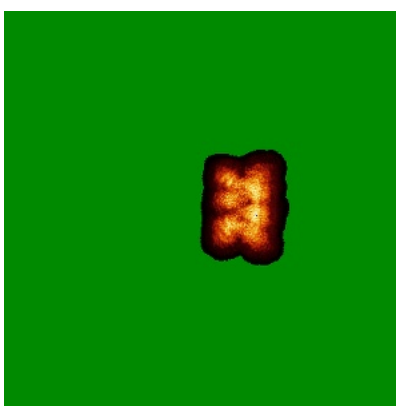
The images above show the largest variance slices of the map in three orthogonal directions.

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

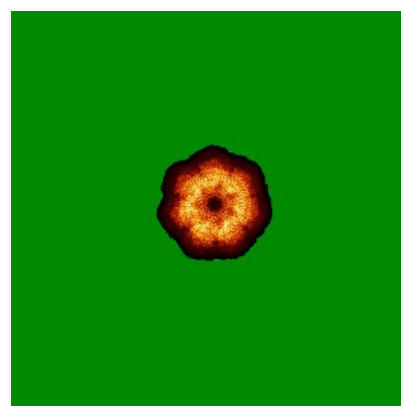
6.4.1 Primary map



X



Y

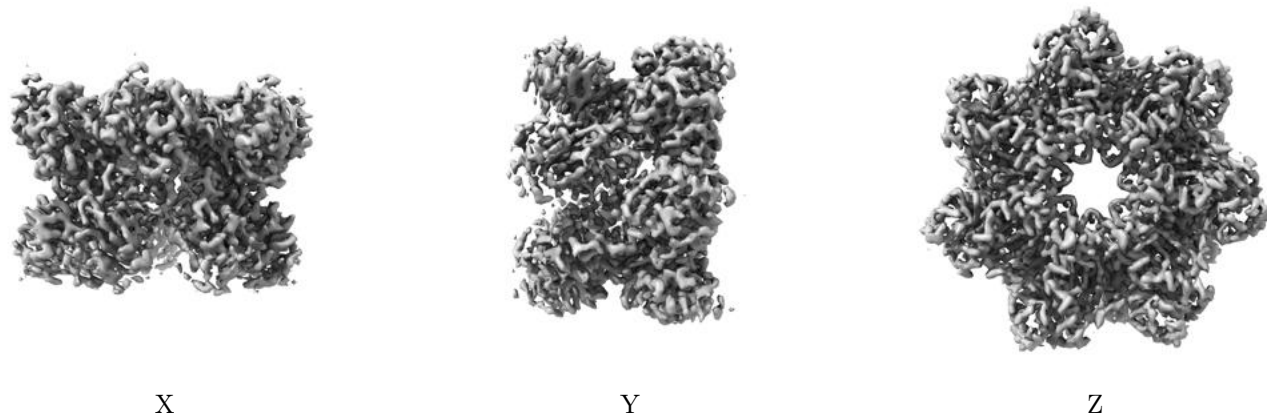


Z

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 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

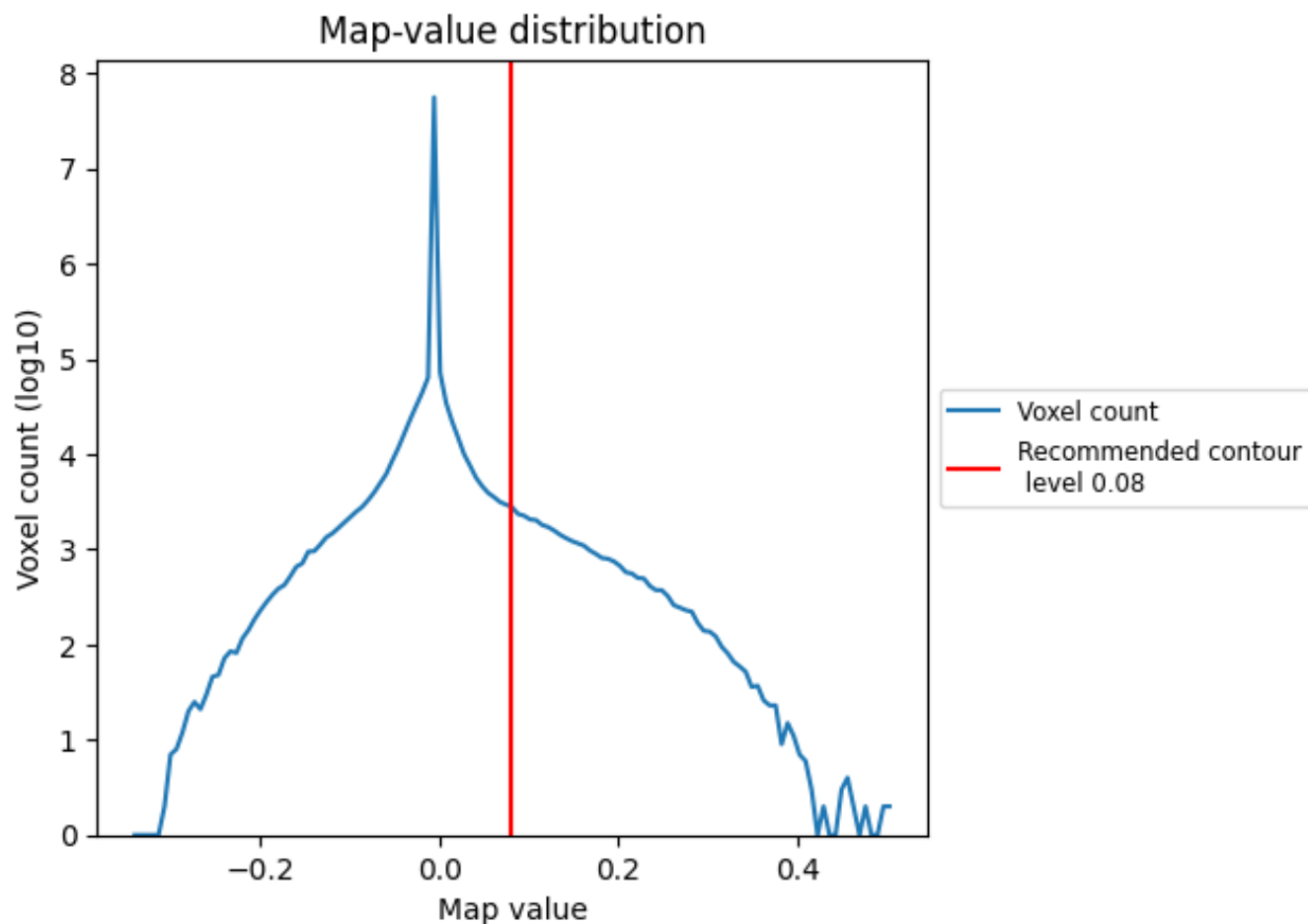
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

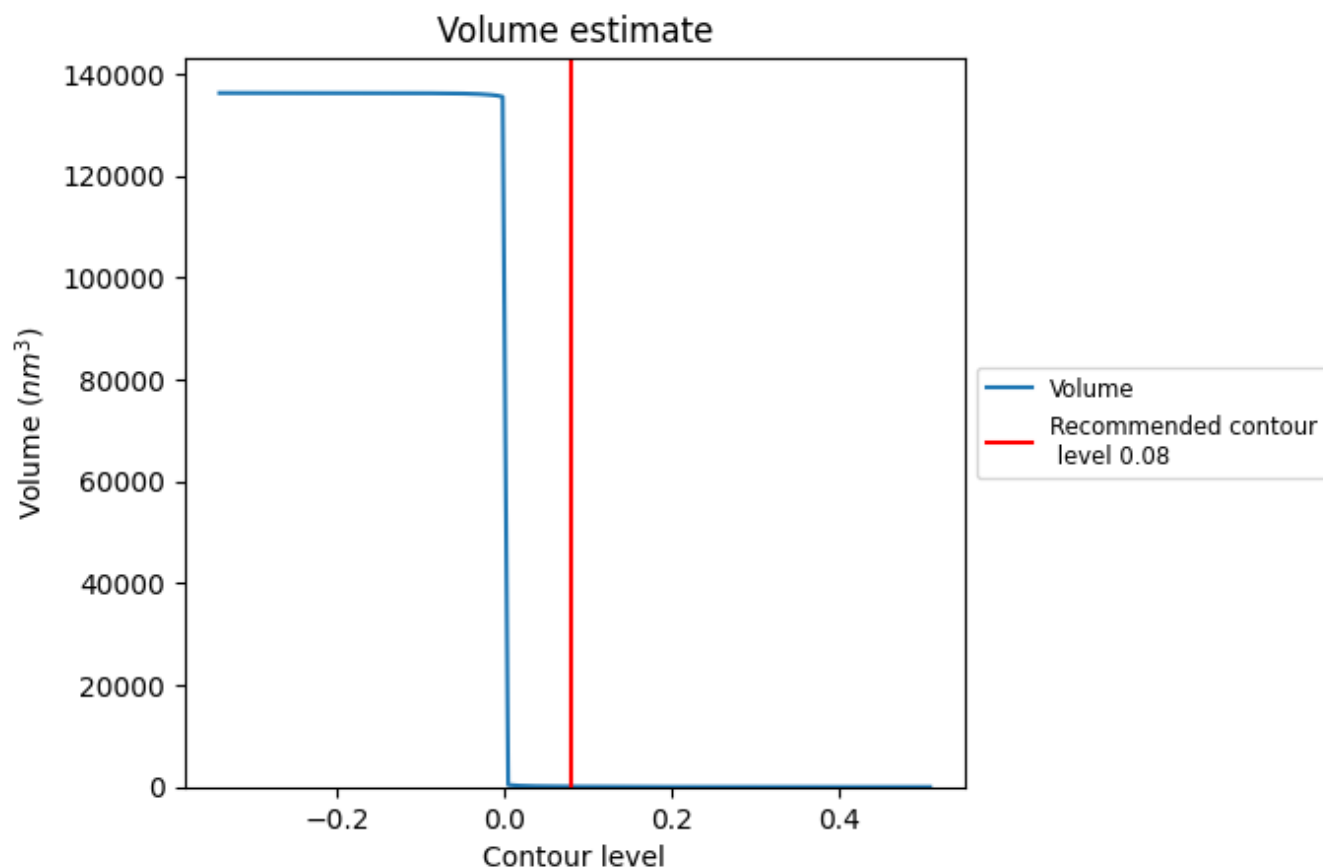
This section contains the results of statistical analysis of the map.

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.

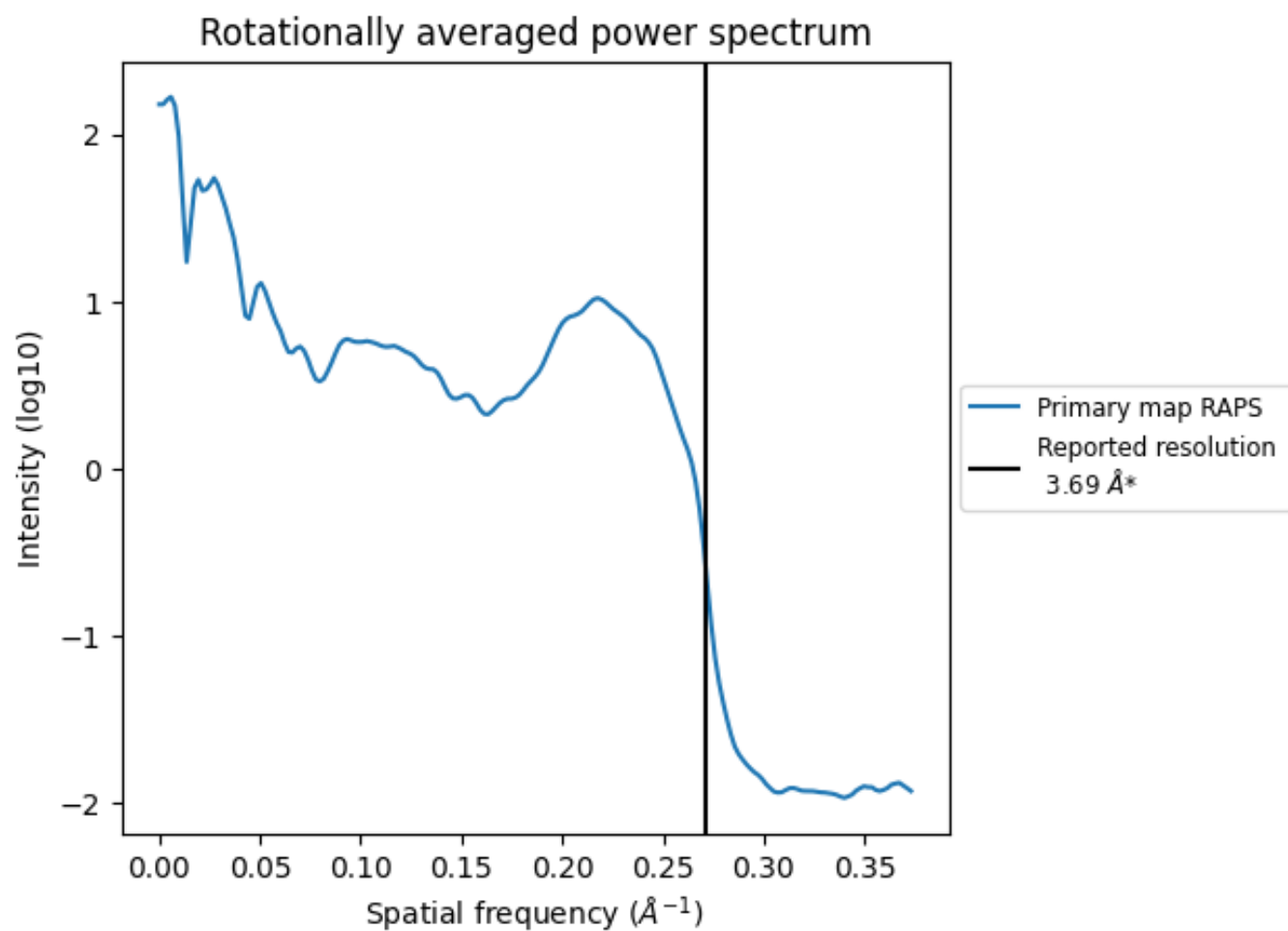
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm^3 ; this corresponds to an approximate mass of 74 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 0.271 Å⁻¹

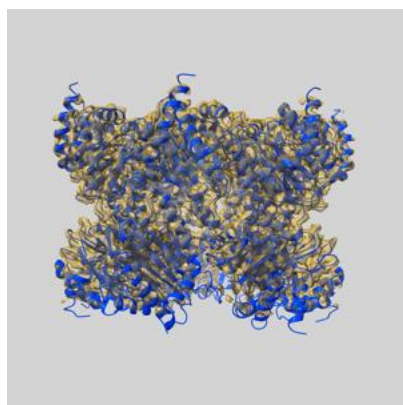
8 Fourier-Shell correlation

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

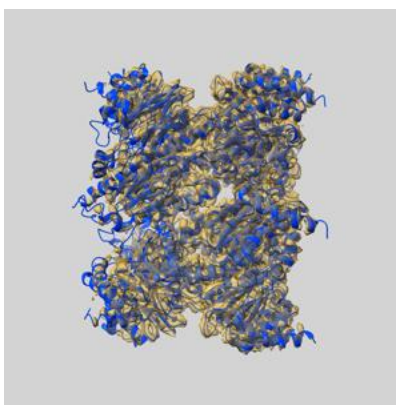
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0211 and PDB model 6HE7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

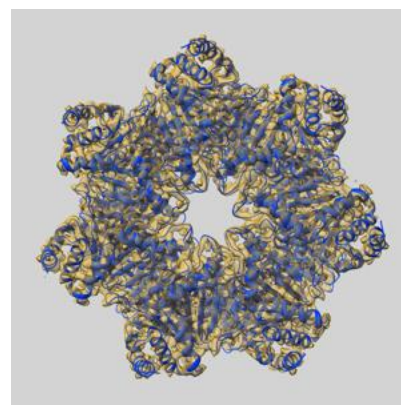
9.1 Map-model overlay [i](#)



X



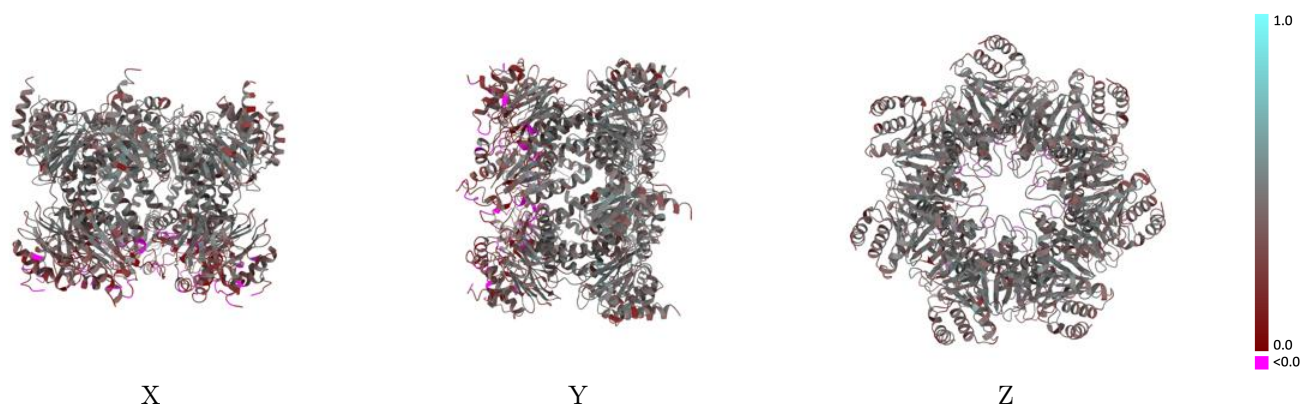
Y



Z

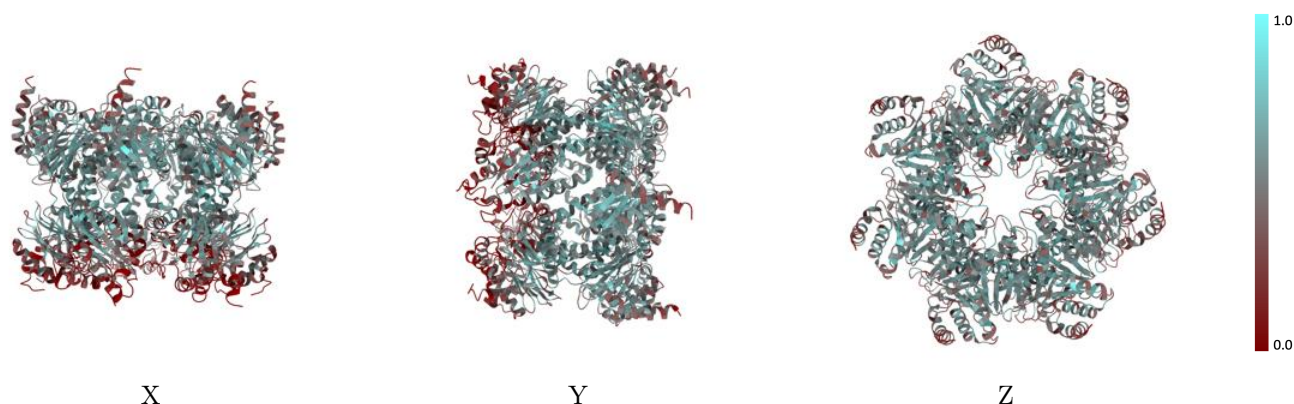
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



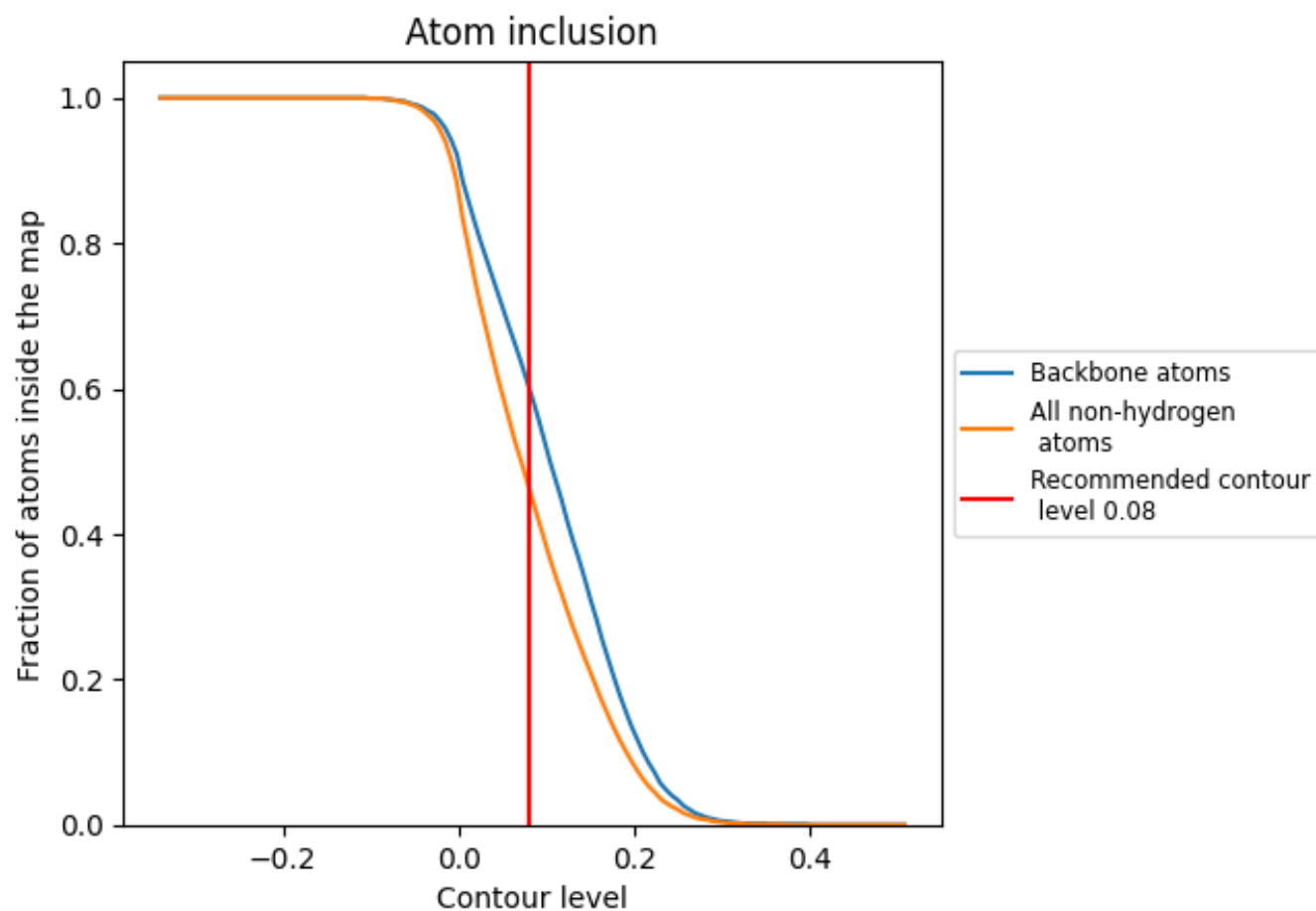
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 47% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4660	0.3830
1	0.3630	0.3250
2	0.3540	0.3070
3	0.3750	0.3410
4	0.3710	0.3320
5	0.3670	0.3160
6	0.3600	0.3270
7	0.3510	0.3140
A	0.5540	0.4330
B	0.5540	0.4340
C	0.5610	0.4340
D	0.5450	0.4350
E	0.5520	0.4380
F	0.5490	0.4250
G	0.5550	0.4350

