



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:37 PM UTC

PDB ID : 8Q4G / pdb_00008q4g
EMDB ID : EMD-18147
Title : Thin filament from FIB milled relaxed left ventricular mouse myofibrils
Authors : Tamborrini, D.; Wang, Z.; Wagner, T.; Tacke, S.; Stabrin, M.; Grange, M.; Kho, A.L.; Bennet, P.; Rees, M.; Gautel, M.; Raunser, S.
Deposited on : 2023-08-06
Resolution : 8.00 Å(reported)
Based on initial model : .

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:

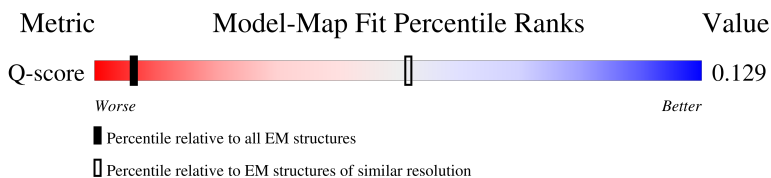
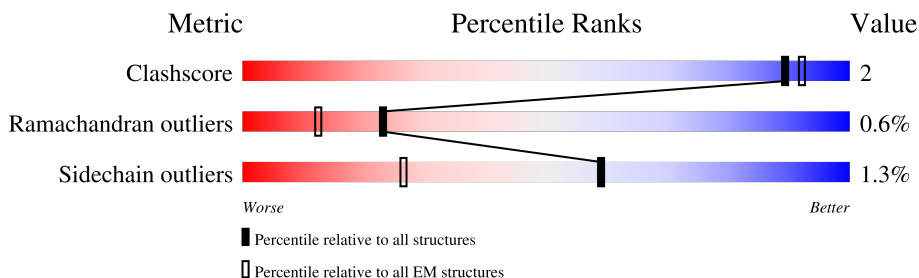
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 8.00 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	361 (7.50 - 8.50)

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	372	
1	B	372	
1	C	372	
1	D	372	

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Mol	Chain	Length	Quality of chain
1	E	372	35% 57% 41%
1	F	372	28% 70% 28%
1	I	372	31% 70% 28%
2	G	179	15% 54% 44%
2	H	179	13% 46% 51%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23265 atoms, of which 0 are hydrogens and 0 are deuteriums.

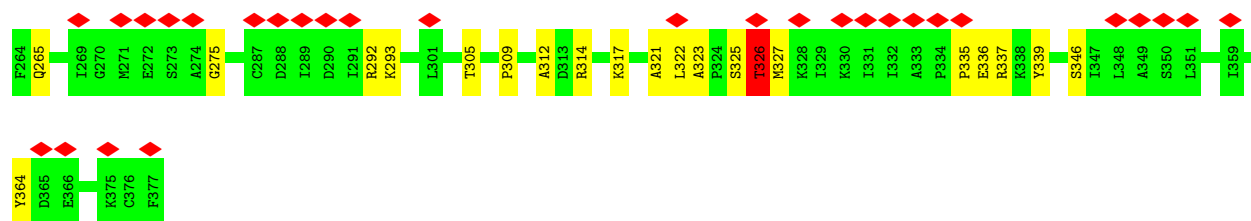
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Actin, alpha cardiac muscle 1.

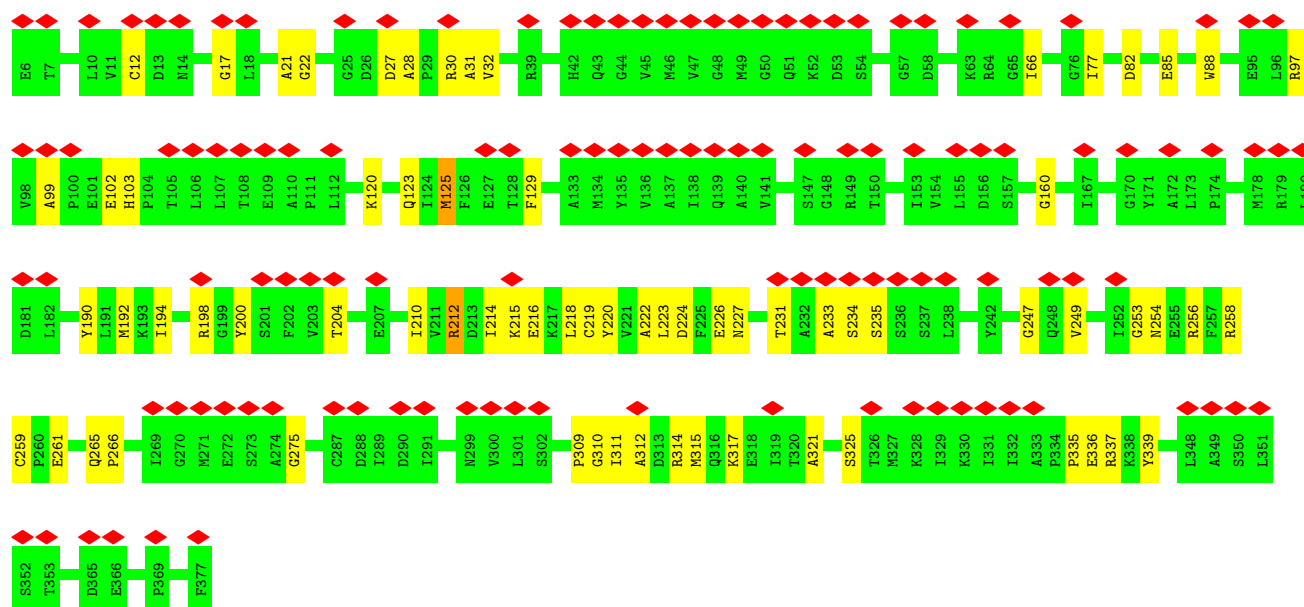
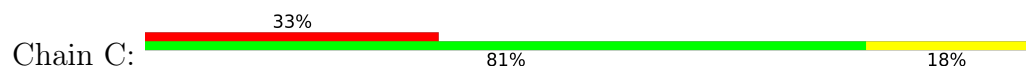
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	372	Total	C	N	O	S	0	0
			2907	1841	490	556	20		
1	B	372	Total	C	N	O	S	0	0
			2907	1841	490	556	20		
1	C	372	Total	C	N	O	S	0	0
			2907	1841	490	556	20		
1	D	372	Total	C	N	O	S	0	0
			2907	1841	490	556	20		
1	E	372	Total	C	N	O	S	0	0
			2907	1841	490	556	20		
1	F	372	Total	C	N	O	S	0	0
			2907	1841	490	556	20		
1	I	372	Total	C	N	O	S	0	0
			2907	1841	490	556	20		

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

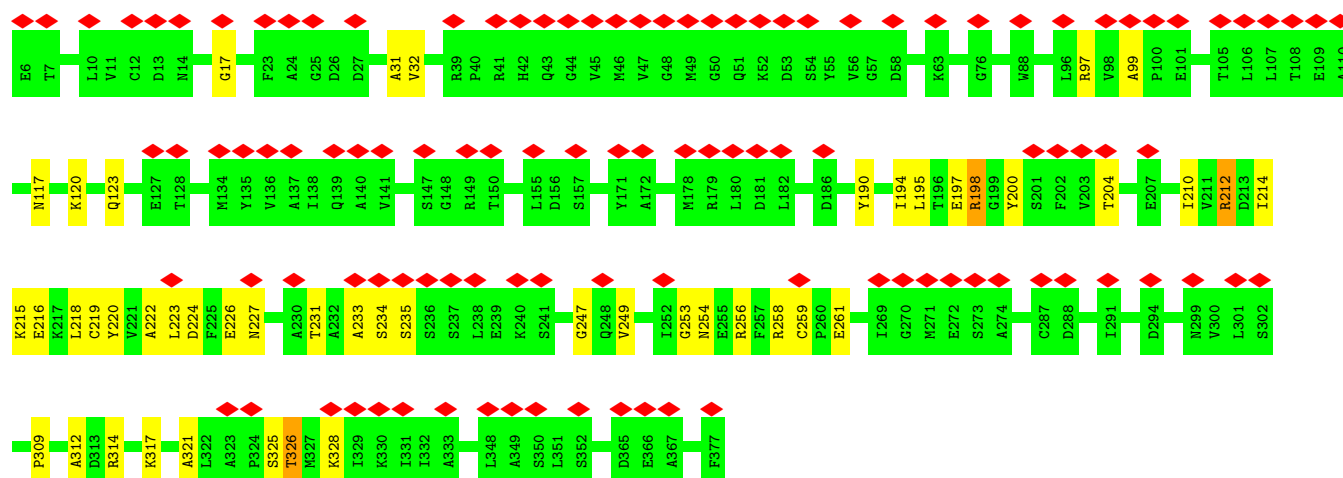
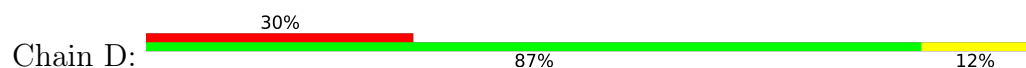
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	179	Total	C	N	O	S	0	0
			1458	896	245	314	3		
2	H	179	Total	C	N	O	S	0	0
			1458	896	245	314	3		



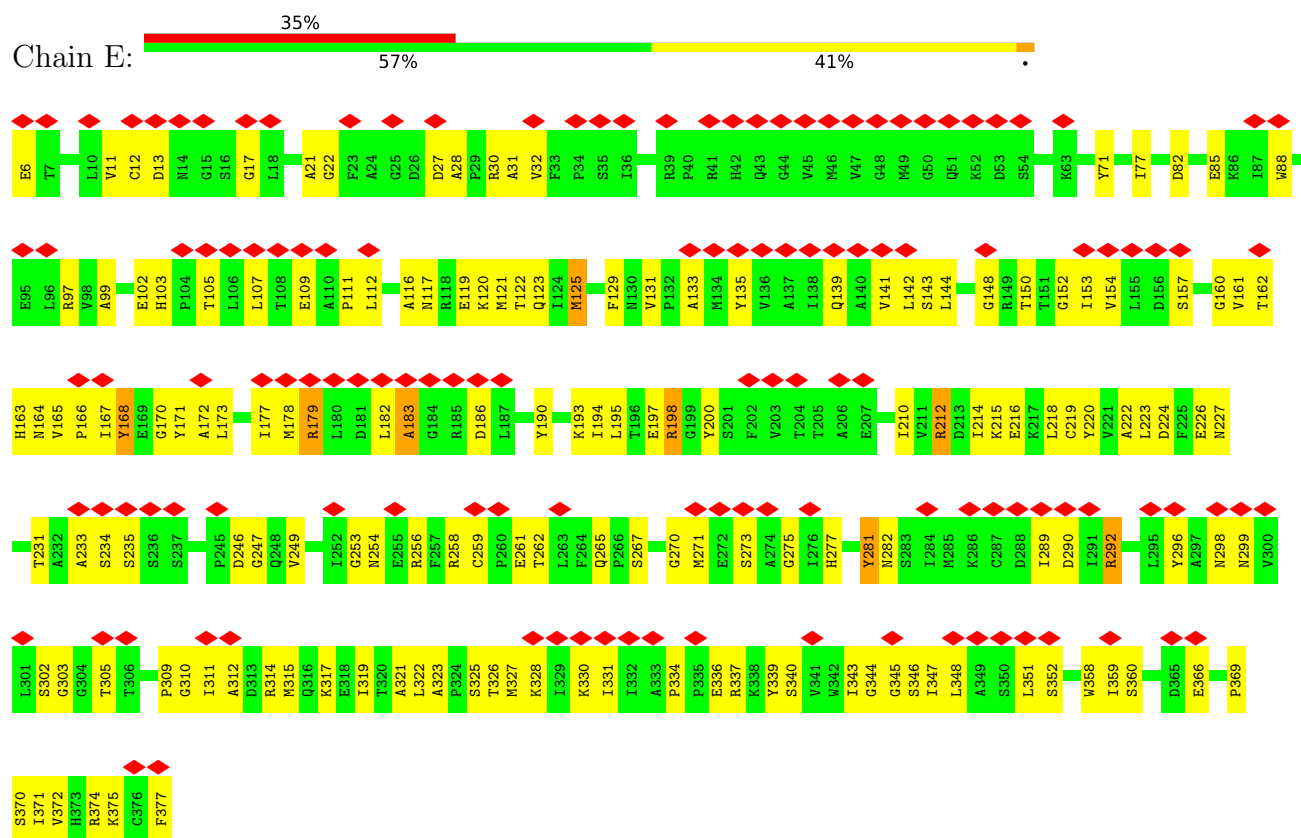
- Molecule 1: Actin, alpha cardiac muscle 1



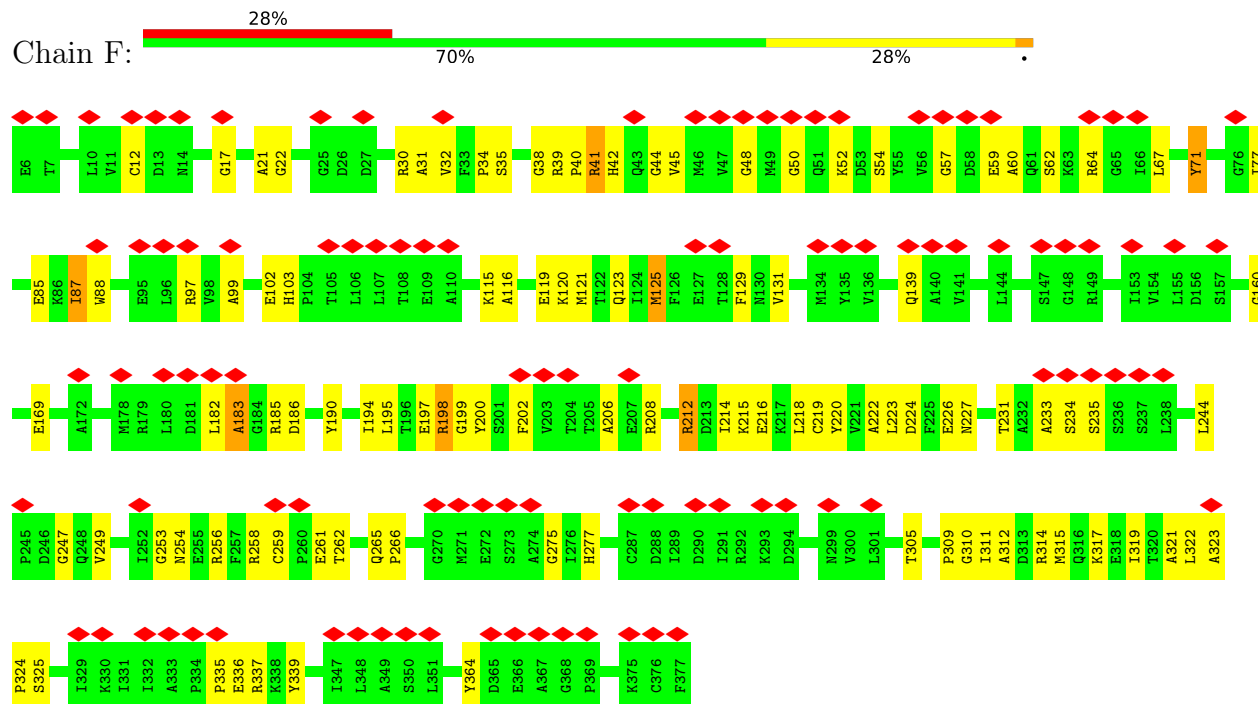
- Molecule 1: Actin, alpha cardiac muscle 1



- Molecule 1: Actin, alpha cardiac muscle 1

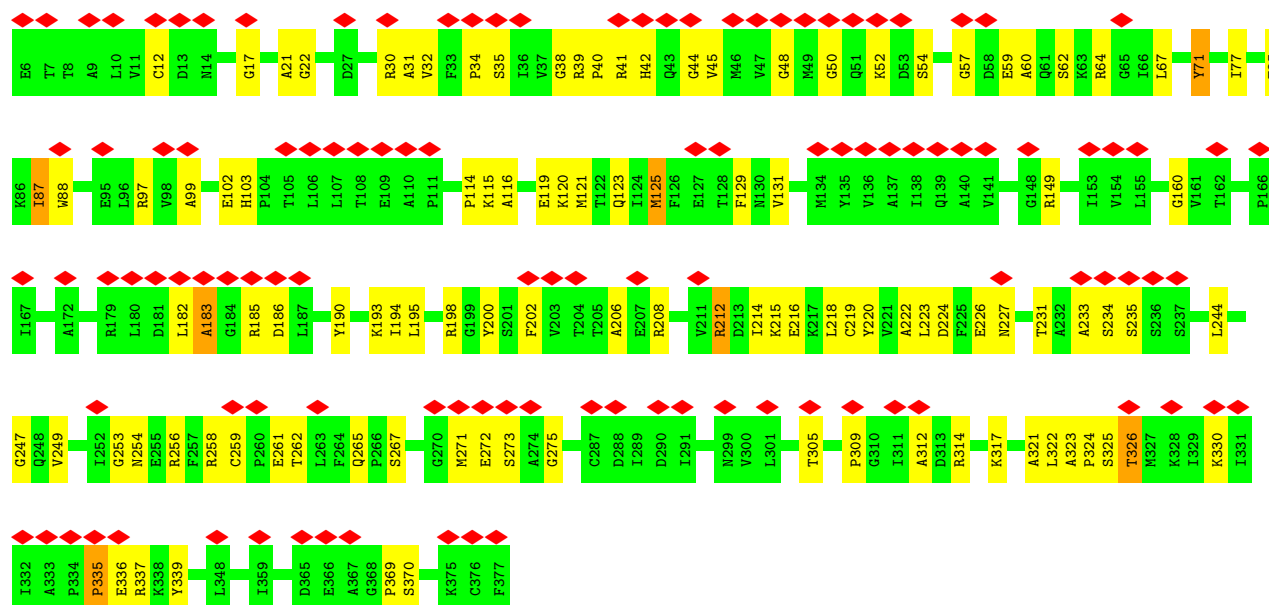


• Molecule 1: Actin, alpha cardiac muscle 1

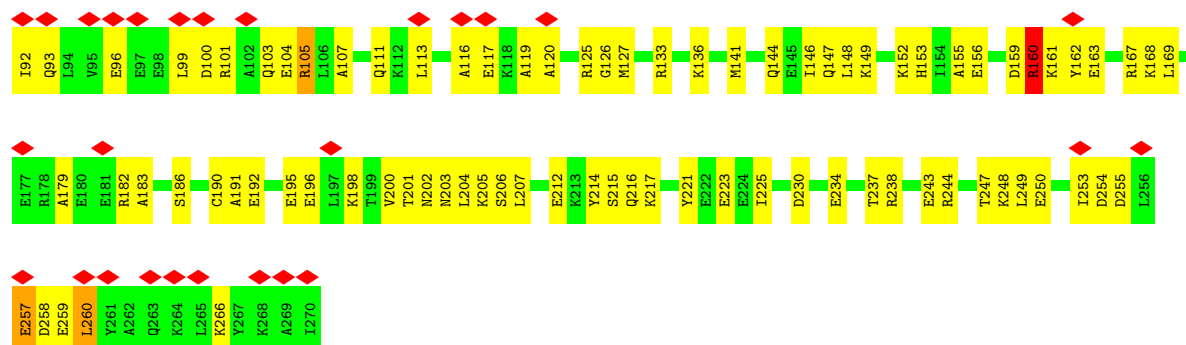


• Molecule 1: Actin, alpha cardiac muscle 1

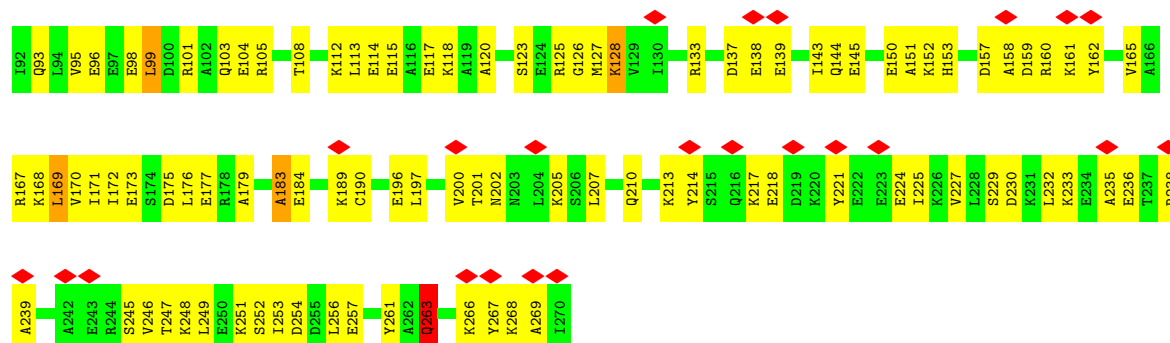




• Molecule 2: Tropomyosin alpha-1 chain



• Molecule 2: Tropomyosin alpha-1 chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	100447	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 ($e^-/\text{\AA}^2$)	140	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.953	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	293.504, 293.504, 293.504	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.293, 2.293, 2.293	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	2.00	75/2970 (2.5%)	2.18	131/4023 (3.3%)
1	B	1.51	35/2970 (1.2%)	1.83	69/4023 (1.7%)
1	C	1.48	36/2970 (1.2%)	1.78	59/4023 (1.5%)
1	D	1.36	26/2970 (0.9%)	1.68	43/4023 (1.1%)
1	E	2.07	82/2970 (2.8%)	2.25	144/4023 (3.6%)
1	F	1.80	57/2970 (1.9%)	2.06	100/4023 (2.5%)
1	I	1.80	55/2970 (1.9%)	2.07	108/4023 (2.7%)
2	G	2.22	51/1464 (3.5%)	2.44	82/1950 (4.2%)
2	H	2.21	51/1464 (3.5%)	2.62	132/1950 (6.8%)
All	All	1.80	468/23718 (2.0%)	2.06	868/32061 (2.7%)

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	6
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	7
1	F	0	3
1	I	0	2
2	G	0	2
2	H	0	2
All	All	0	26

All (468) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	13	ASP	CA-CB	12.06	1.68	1.52
1	A	13	ASP	CA-CB	12.00	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	38	GLY	CA-C	-9.84	1.45	1.52
1	I	38	GLY	CA-C	-9.80	1.45	1.52
2	H	157	ASP	CA-C	-9.16	1.40	1.52
2	H	253	ILE	CA-C	-8.97	1.41	1.52
1	D	97	ARG	CZ-NH2	8.65	1.44	1.33
1	F	97	ARG	CZ-NH2	8.63	1.44	1.33
1	I	97	ARG	CZ-NH2	8.63	1.44	1.33
1	A	97	ARG	CZ-NH2	8.62	1.44	1.33
1	C	97	ARG	CZ-NH2	8.61	1.44	1.33
1	B	97	ARG	CZ-NH2	8.60	1.44	1.33
1	E	97	ARG	CZ-NH2	8.60	1.44	1.33
1	E	345	GLY	CA-C	-8.31	1.42	1.52
1	A	345	GLY	CA-C	-8.26	1.42	1.52
2	G	127	MET	N-CA	-8.21	1.36	1.46
1	E	167	ILE	CA-C	-8.07	1.42	1.52
2	G	155	ALA	CA-C	-8.06	1.42	1.52
1	A	167	ILE	CA-C	-8.03	1.42	1.52
2	G	101	ARG	CA-C	-8.01	1.42	1.52
1	A	327	MET	CA-C	-7.99	1.43	1.52
1	E	327	MET	CA-C	-7.96	1.43	1.52
2	H	105	ARG	N-CA	-7.91	1.36	1.46
1	A	360	SER	CA-C	-7.59	1.42	1.53
1	E	360	SER	CA-C	-7.55	1.42	1.53
1	D	325	SER	N-CA	-7.39	1.38	1.46
2	G	198	LYS	N-CA	-7.15	1.37	1.46
1	F	214	ILE	CA-C	-7.00	1.44	1.52
1	B	214	ILE	CA-C	-6.99	1.44	1.52
1	D	214	ILE	CA-C	-6.99	1.44	1.52
1	B	220	TYR	N-CA	-6.97	1.37	1.45
1	E	220	TYR	N-CA	-6.97	1.37	1.45
1	I	220	TYR	N-CA	-6.94	1.37	1.45
2	H	245	SER	CA-CB	6.94	1.64	1.53
1	C	220	TYR	C-N	6.93	1.42	1.33
1	D	220	TYR	N-CA	-6.93	1.37	1.45
1	I	214	ILE	CA-C	-6.93	1.44	1.52
1	B	22	GLY	CA-C	-6.93	1.45	1.52
1	C	22	GLY	CA-C	-6.93	1.45	1.52
1	I	220	TYR	C-N	6.93	1.42	1.33
1	I	206	ALA	CA-C	-6.92	1.43	1.52
1	E	220	TYR	C-N	6.92	1.42	1.33
1	A	220	TYR	C-N	6.92	1.42	1.33
1	A	220	TYR	N-CA	-6.92	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	220	TYR	N-CA	-6.91	1.37	1.45
1	F	206	ALA	CA-C	-6.91	1.43	1.52
1	F	220	TYR	C-N	6.91	1.42	1.33
1	D	220	TYR	C-N	6.91	1.42	1.33
1	B	220	TYR	C-N	6.90	1.42	1.33
1	A	214	ILE	CA-C	-6.89	1.44	1.52
1	E	22	GLY	CA-C	-6.89	1.45	1.52
1	F	41	ARG	C-N	6.89	1.43	1.33
1	E	214	ILE	CA-C	-6.88	1.44	1.52
1	E	12	CYS	C-N	6.87	1.43	1.33
1	C	214	ILE	CA-C	-6.87	1.44	1.52
2	H	263	GLN	CA-CB	6.86	1.64	1.53
2	G	182	ARG	NE-CZ	6.85	1.40	1.33
1	A	22	GLY	CA-C	-6.84	1.45	1.52
1	C	220	TYR	N-CA	-6.84	1.37	1.45
1	A	12	CYS	C-N	6.81	1.43	1.33
1	D	219	CYS	CA-CB	6.80	1.64	1.53
1	E	219	CYS	CA-CB	6.78	1.64	1.53
1	B	131	VAL	N-CA	-6.78	1.39	1.47
1	A	219	CYS	CA-CB	6.76	1.64	1.53
1	C	219	CYS	CA-CB	6.76	1.64	1.53
1	I	131	VAL	N-CA	-6.76	1.39	1.47
2	H	128	LYS	CA-CB	6.75	1.63	1.53
2	H	227	VAL	N-CA	-6.75	1.38	1.46
1	I	219	CYS	CA-CB	6.75	1.64	1.53
1	B	219	CYS	CA-CB	6.74	1.64	1.53
1	F	219	CYS	CA-CB	6.73	1.64	1.53
2	G	133	ARG	CD-NE	6.69	1.55	1.46
2	G	190	CYS	C-N	6.67	1.42	1.33
2	H	128	LYS	C-N	6.65	1.42	1.33
1	E	337	ARG	NE-CZ	6.65	1.40	1.33
2	G	215	SER	CA-CB	6.62	1.63	1.53
1	E	85	GLU	N-CA	-6.60	1.38	1.46
2	H	221	TYR	N-CA	-6.59	1.38	1.46
1	C	337	ARG	NE-CZ	6.59	1.40	1.33
2	G	204	LEU	N-CA	-6.58	1.38	1.46
2	G	100	ASP	N-CA	6.57	1.54	1.46
1	I	85	GLU	N-CA	-6.56	1.38	1.46
1	F	85	GLU	N-CA	-6.54	1.38	1.46
1	I	337	ARG	NE-CZ	6.54	1.40	1.33
1	A	337	ARG	NE-CZ	6.54	1.40	1.33
1	F	337	ARG	NE-CZ	6.53	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	ARG	NE-CZ	6.52	1.40	1.33
2	G	133	ARG	NE-CZ	6.49	1.40	1.33
1	E	358	TRP	CA-CB	6.47	1.63	1.53
2	G	103	GLN	CA-CB	6.47	1.63	1.53
1	C	85	GLU	N-CA	-6.46	1.38	1.46
1	A	358	TRP	CA-CB	6.45	1.63	1.53
1	F	305	THR	N-CA	6.45	1.54	1.46
2	H	114	GLU	CA-CB	6.44	1.63	1.53
1	A	85	GLU	N-CA	-6.44	1.38	1.46
2	G	237	THR	CA-C	-6.43	1.44	1.52
1	I	305	THR	N-CA	6.43	1.54	1.46
2	G	223	GLU	CA-C	-6.42	1.44	1.52
1	B	85	GLU	N-CA	-6.42	1.38	1.46
1	C	325	SER	N-CA	-6.42	1.38	1.46
1	B	305	THR	N-CA	6.42	1.54	1.46
1	E	133	ALA	N-CA	-6.39	1.38	1.46
1	E	305	THR	N-CA	6.39	1.54	1.46
1	I	259	CYS	CA-CB	6.39	1.61	1.53
1	A	133	ALA	N-CA	-6.39	1.38	1.46
2	G	146	ILE	C-N	6.39	1.42	1.33
1	A	305	THR	N-CA	6.39	1.54	1.46
2	H	153	HIS	CA-CB	6.38	1.63	1.53
1	C	259	CYS	CA-CB	6.38	1.61	1.53
1	E	259	CYS	CA-CB	6.37	1.61	1.53
1	D	200	TYR	C-N	6.37	1.41	1.33
1	F	259	CYS	CA-CB	6.37	1.61	1.53
2	G	200	VAL	CA-CB	6.36	1.62	1.54
1	E	152	GLY	N-CA	-6.36	1.39	1.45
1	E	200	TYR	C-N	6.36	1.41	1.33
2	G	248	LYS	N-CA	-6.35	1.38	1.46
1	D	259	CYS	CA-CB	6.35	1.61	1.53
1	B	259	CYS	CA-CB	6.34	1.61	1.53
1	E	120	LYS	CA-C	-6.33	1.44	1.52
1	E	358	TRP	C-N	6.32	1.39	1.33
2	H	268	LYS	C-N	6.31	1.42	1.33
1	A	179	ARG	CA-C	-6.31	1.45	1.52
1	B	120	LYS	CA-C	-6.30	1.44	1.52
2	H	158	ALA	CA-C	-6.30	1.44	1.52
1	A	259	CYS	CA-CB	6.29	1.61	1.53
2	H	120	ALA	C-O	-6.29	1.16	1.24
1	A	120	LYS	CA-C	-6.29	1.44	1.52
1	I	120	LYS	CA-C	-6.28	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	176	LEU	CA-C	-6.26	1.44	1.52
1	I	41	ARG	C-N	6.26	1.43	1.33
2	H	189	LYS	CA-CB	6.25	1.63	1.53
2	H	197	LEU	CA-C	-6.25	1.44	1.52
1	A	152	GLY	N-CA	-6.25	1.39	1.45
1	F	120	LYS	CA-C	-6.23	1.44	1.52
1	A	358	TRP	C-N	6.21	1.39	1.33
1	C	120	LYS	CA-C	-6.21	1.44	1.52
1	E	178	MET	CA-C	-6.20	1.45	1.52
1	A	135	TYR	C-N	6.19	1.41	1.33
1	E	179	ARG	CA-C	-6.18	1.45	1.52
1	A	178	MET	CA-C	-6.18	1.45	1.52
1	D	120	LYS	CA-C	-6.17	1.44	1.52
1	F	200	TYR	C-N	6.16	1.42	1.33
1	I	200	TYR	C-N	6.15	1.42	1.33
1	A	200	TYR	C-N	6.14	1.42	1.33
1	B	200	TYR	C-N	6.14	1.42	1.33
1	C	21	ALA	C-N	6.14	1.39	1.33
1	E	21	ALA	C-N	6.11	1.39	1.33
1	E	135	TYR	C-N	6.11	1.41	1.33
1	D	249	VAL	CA-CB	-6.10	1.47	1.54
1	I	249	VAL	CA-CB	-6.10	1.47	1.54
2	G	167	ARG	CD-NE	6.10	1.54	1.46
2	H	238	ARG	NE-CZ	6.10	1.39	1.33
1	B	322	LEU	N-CA	6.09	1.53	1.46
1	B	249	VAL	CA-CB	-6.09	1.47	1.54
1	F	249	VAL	CA-CB	-6.08	1.47	1.54
1	A	249	VAL	CA-CB	-6.08	1.47	1.54
1	F	322	LEU	N-CA	6.06	1.53	1.46
1	C	249	VAL	CA-CB	-6.05	1.47	1.54
1	A	322	LEU	N-CA	6.04	1.53	1.46
1	E	328	LYS	N-CA	-6.04	1.38	1.46
2	G	104	GLU	CA-C	6.04	1.60	1.52
1	E	249	VAL	CA-CB	-6.03	1.47	1.54
1	B	160	GLY	CA-C	6.03	1.60	1.51
1	I	160	GLY	CA-C	6.03	1.60	1.51
1	I	271	MET	CA-C	-6.02	1.45	1.52
1	I	322	LEU	N-CA	6.02	1.53	1.46
2	H	173	GLU	CA-CB	6.01	1.62	1.53
1	A	160	GLY	CA-C	6.01	1.60	1.51
2	H	112	LYS	C-N	6.00	1.41	1.33
1	A	328	LYS	N-CA	-6.00	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ALA	CA-C	-6.00	1.45	1.52
2	H	125	ARG	CZ-NH2	6.00	1.41	1.33
2	H	160	ARG	CD-NE	6.00	1.54	1.46
1	E	322	LEU	N-CA	5.99	1.53	1.46
1	E	160	GLY	CA-C	5.99	1.60	1.51
2	H	268	LYS	CA-C	-5.99	1.45	1.52
1	E	133	ALA	CA-C	-5.98	1.45	1.52
1	F	103	HIS	CE1-NE2	5.98	1.38	1.32
2	G	133	ARG	C-N	-5.98	1.26	1.33
2	H	248	LYS	N-CA	-5.98	1.39	1.46
1	E	271	MET	CA-C	-5.97	1.45	1.52
1	I	21	ALA	C-N	5.97	1.39	1.33
1	C	310	GLY	C-N	5.96	1.41	1.33
1	F	160	GLY	CA-C	5.95	1.60	1.51
1	A	310	GLY	C-N	5.94	1.41	1.33
2	H	98	GLU	C-N	5.94	1.41	1.33
2	G	120	ALA	C-N	5.93	1.41	1.33
1	F	310	GLY	C-N	5.92	1.41	1.33
1	F	21	ALA	C-N	5.92	1.39	1.33
1	E	249	VAL	C-N	5.92	1.41	1.33
1	E	310	GLY	C-N	5.92	1.41	1.33
1	A	340	SER	CA-CB	5.91	1.62	1.53
1	B	249	VAL	C-N	5.90	1.41	1.33
2	H	205	LYS	CA-C	-5.90	1.45	1.52
1	A	325	SER	N-CA	-5.90	1.37	1.46
2	H	183	ALA	C-N	5.89	1.41	1.33
1	C	103	HIS	CE1-NE2	5.89	1.38	1.32
1	C	249	VAL	C-N	5.89	1.41	1.33
1	I	103	HIS	CE1-NE2	5.89	1.38	1.32
1	D	249	VAL	C-N	5.88	1.41	1.33
2	G	257	GLU	CA-C	-5.88	1.45	1.52
1	A	103	HIS	CE1-NE2	5.88	1.38	1.32
1	B	103	HIS	CE1-NE2	5.88	1.38	1.32
1	F	249	VAL	C-N	5.87	1.41	1.33
2	G	179	ALA	CA-C	5.87	1.60	1.52
1	A	249	VAL	C-N	5.87	1.41	1.33
1	E	325	SER	N-CA	-5.86	1.38	1.46
2	H	175	ASP	N-CA	-5.86	1.39	1.46
2	H	268	LYS	N-CA	-5.86	1.39	1.46
1	E	139	GLN	CA-C	5.85	1.60	1.52
1	A	139	GLN	CA-C	5.85	1.60	1.52
1	I	249	VAL	C-N	5.85	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	ASN	CA-C	-5.85	1.45	1.52
1	E	152	GLY	CA-C	-5.85	1.46	1.52
1	E	103	HIS	CE1-NE2	5.84	1.38	1.32
1	E	340	SER	CA-CB	5.84	1.62	1.53
1	E	88	TRP	CA-C	-5.84	1.45	1.52
1	I	88	TRP	CA-C	-5.83	1.45	1.52
1	F	227	ASN	CA-C	-5.83	1.45	1.52
1	A	152	GLY	CA-C	-5.82	1.46	1.52
1	E	299	ASN	CA-CB	5.82	1.60	1.52
1	F	22	GLY	CA-C	-5.81	1.45	1.52
1	E	334	PRO	C-N	5.81	1.41	1.34
1	E	227	ASN	CA-C	-5.80	1.45	1.52
1	C	88	TRP	CA-C	-5.80	1.45	1.52
1	C	227	ASN	CA-C	-5.79	1.45	1.52
1	A	334	PRO	C-N	5.79	1.41	1.34
1	A	299	ASN	CA-CB	5.79	1.60	1.52
1	D	227	ASN	CA-C	-5.78	1.45	1.52
1	I	22	GLY	CA-C	-5.78	1.45	1.52
2	G	196	GLU	C-N	-5.77	1.26	1.33
1	I	227	ASN	CA-C	-5.77	1.45	1.52
1	B	88	TRP	CA-C	-5.77	1.45	1.52
2	G	207	LEU	N-CA	5.77	1.53	1.46
1	B	227	ASN	CA-C	-5.75	1.45	1.52
2	H	101	ARG	CA-CB	5.75	1.62	1.53
1	A	88	TRP	CA-C	-5.75	1.45	1.52
1	F	88	TRP	CA-C	-5.75	1.45	1.52
2	G	248	LYS	CA-CB	-5.75	1.44	1.53
1	E	166	PRO	CA-C	-5.73	1.46	1.52
1	I	35	SER	C-N	5.72	1.40	1.33
1	A	309	PRO	N-CD	-5.72	1.39	1.47
1	E	309	PRO	N-CD	-5.72	1.39	1.47
2	G	186	SER	N-CA	-5.72	1.39	1.46
1	F	35	SER	C-N	5.72	1.40	1.33
1	A	166	PRO	CA-C	-5.71	1.46	1.52
1	F	208	ARG	CA-CB	5.70	1.62	1.53
2	H	249	LEU	C-N	5.70	1.41	1.34
1	F	309	PRO	N-CD	-5.70	1.39	1.47
2	G	113	LEU	CA-CB	5.70	1.62	1.53
1	F	64	ARG	NE-CZ	5.69	1.39	1.33
2	H	252	SER	CA-C	-5.69	1.45	1.52
2	G	206	SER	CA-C	5.69	1.60	1.52
1	I	17	GLY	CA-C	5.69	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	170	VAL	CA-C	5.68	1.59	1.52
2	G	111	GLN	CA-CB	5.68	1.62	1.53
1	D	309	PRO	N-CD	-5.67	1.39	1.47
1	I	64	ARG	NE-CZ	5.67	1.39	1.33
1	B	198	ARG	CZ-NH2	5.67	1.40	1.33
1	B	231	THR	N-CA	-5.67	1.39	1.46
1	I	67	LEU	CA-C	-5.67	1.46	1.52
1	I	309	PRO	N-CD	-5.67	1.39	1.47
2	G	238	ARG	CZ-NH2	5.67	1.40	1.33
1	B	309	PRO	N-CD	-5.67	1.39	1.47
1	I	325	SER	N-CA	-5.67	1.38	1.46
1	E	144	LEU	C-O	-5.66	1.17	1.24
1	F	41	ARG	NE-CZ	5.66	1.39	1.33
1	C	309	PRO	N-CD	-5.66	1.39	1.47
1	I	231	THR	N-CA	-5.66	1.39	1.46
1	F	67	LEU	CA-C	-5.65	1.46	1.52
1	D	198	ARG	CZ-NH2	5.65	1.40	1.33
1	A	144	LEU	C-O	-5.65	1.17	1.24
1	A	161	VAL	CA-C	-5.64	1.45	1.52
1	B	325	SER	N-CA	-5.64	1.38	1.46
1	E	198	ARG	CZ-NH2	5.64	1.40	1.33
1	F	325	SER	N-CA	-5.64	1.38	1.46
1	I	208	ARG	CA-CB	5.64	1.62	1.53
2	H	269	ALA	N-CA	-5.63	1.39	1.46
1	A	231	THR	N-CA	-5.63	1.39	1.46
1	E	347	ILE	CA-CB	5.63	1.60	1.54
1	C	317	LYS	CA-C	-5.63	1.45	1.52
1	A	198	ARG	CZ-NH2	5.62	1.40	1.33
1	F	17	GLY	CA-C	5.62	1.59	1.51
1	I	41	ARG	NE-CZ	5.62	1.39	1.33
1	D	231	THR	N-CA	-5.62	1.39	1.46
1	D	326	THR	N-CA	5.61	1.52	1.46
1	I	57	GLY	C-N	5.61	1.41	1.34
2	H	179	ALA	CA-C	-5.61	1.45	1.52
2	H	101	ARG	N-CA	-5.61	1.39	1.46
1	A	347	ILE	CA-CB	5.61	1.60	1.54
1	C	231	THR	N-CA	-5.61	1.39	1.46
1	C	198	ARG	CZ-NH2	5.61	1.40	1.33
1	F	57	GLY	C-N	5.60	1.41	1.34
1	F	231	THR	N-CA	-5.60	1.39	1.46
1	F	198	ARG	CZ-NH2	5.59	1.40	1.33
1	I	198	ARG	CZ-NH2	5.59	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	161	VAL	CA-C	-5.59	1.45	1.52
1	F	216	GLU	C-O	-5.59	1.17	1.24
1	E	231	THR	N-CA	-5.58	1.39	1.46
2	G	234	GLU	CA-CB	5.58	1.62	1.53
1	A	131	VAL	N-CA	-5.58	1.39	1.46
1	E	177	ILE	CB-CG1	5.57	1.64	1.53
1	B	216	GLU	C-O	-5.56	1.17	1.24
1	E	200	TYR	CA-C	-5.56	1.47	1.53
2	G	117	GLU	CA-C	-5.56	1.45	1.52
1	E	317	LYS	CA-C	-5.56	1.45	1.52
1	C	216	GLU	C-O	-5.56	1.17	1.24
1	A	216	GLU	C-O	-5.56	1.17	1.24
2	G	92	ILE	N-CA	5.56	1.56	1.46
2	G	147	GLN	CA-C	5.55	1.59	1.52
1	B	317	LYS	CA-C	-5.55	1.45	1.52
1	F	317	LYS	CA-C	-5.55	1.45	1.52
1	I	216	GLU	C-O	-5.54	1.17	1.24
1	I	317	LYS	CA-C	-5.54	1.45	1.52
1	I	200	TYR	CA-C	-5.54	1.47	1.53
1	C	200	TYR	CA-C	-5.53	1.47	1.53
1	B	200	TYR	CA-C	-5.53	1.47	1.53
1	E	339	TYR	C-N	5.53	1.41	1.33
1	E	131	VAL	N-CA	-5.53	1.39	1.46
1	A	317	LYS	CA-C	-5.53	1.45	1.52
1	D	317	LYS	CA-C	-5.53	1.45	1.52
1	D	200	TYR	CA-C	-5.52	1.47	1.53
1	A	177	ILE	CB-CG1	5.51	1.64	1.53
1	D	216	GLU	C-O	-5.51	1.17	1.24
1	E	216	GLU	C-O	-5.51	1.17	1.24
2	G	148	LEU	CA-CB	5.51	1.62	1.53
1	A	200	TYR	CA-C	-5.50	1.47	1.53
1	F	200	TYR	CA-C	-5.50	1.47	1.53
2	G	160	ARG	CD-NE	5.49	1.53	1.46
1	F	206	ALA	N-CA	-5.48	1.39	1.46
1	I	206	ALA	N-CA	-5.47	1.39	1.46
2	G	148	LEU	N-CA	-5.46	1.39	1.46
1	F	131	VAL	N-CA	-5.46	1.39	1.46
1	F	212	ARG	C-N	5.45	1.41	1.33
1	A	212	ARG	C-N	5.43	1.41	1.33
2	G	105	ARG	N-CA	-5.43	1.39	1.46
1	E	148	GLY	C-N	5.42	1.41	1.33
2	G	254	ASP	CA-CB	5.42	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	212	ARG	C-N	5.42	1.41	1.33
1	D	212	ARG	C-N	5.41	1.41	1.33
1	E	179	ARG	CD-NE	5.41	1.53	1.46
1	I	259	CYS	C-N	-5.41	1.28	1.34
1	A	179	ARG	CD-NE	5.41	1.53	1.46
1	A	171	TYR	C-N	5.40	1.40	1.33
2	G	161	LYS	C-N	5.39	1.41	1.33
2	G	221	TYR	C-N	5.39	1.41	1.33
1	C	259	CYS	C-N	-5.39	1.28	1.34
1	E	212	ARG	C-N	5.39	1.41	1.33
2	G	116	ALA	C-N	5.38	1.40	1.33
2	G	258	ASP	CA-C	-5.38	1.46	1.52
1	I	212	ARG	C-N	5.38	1.41	1.33
2	H	105	ARG	CD-NE	5.37	1.53	1.46
1	B	259	CYS	C-N	-5.37	1.28	1.34
1	F	41	ARG	N-CA	-5.36	1.39	1.46
1	A	259	CYS	C-N	-5.36	1.28	1.34
1	E	259	CYS	C-N	-5.36	1.28	1.34
1	A	105	THR	CA-C	-5.35	1.46	1.52
1	A	148	GLY	C-N	5.35	1.40	1.33
2	G	186	SER	CA-C	-5.35	1.46	1.52
1	E	105	THR	CA-C	-5.34	1.46	1.52
1	E	275	GLY	C-N	5.33	1.40	1.33
2	H	153	HIS	N-CA	5.32	1.52	1.46
1	A	275	GLY	C-N	5.32	1.40	1.33
1	E	171	TYR	C-N	5.32	1.40	1.33
2	H	118	LYS	CA-C	-5.32	1.46	1.52
1	F	259	CYS	C-N	-5.31	1.28	1.34
2	H	113	LEU	CA-CB	5.31	1.61	1.53
2	H	184	GLU	C-N	5.30	1.40	1.33
1	F	311	ILE	CA-C	-5.30	1.46	1.52
1	D	259	CYS	C-N	-5.29	1.28	1.34
1	I	34	PRO	C-O	-5.28	1.17	1.23
1	I	41	ARG	N-CA	-5.28	1.39	1.46
1	C	311	ILE	CA-C	-5.28	1.46	1.52
1	A	311	ILE	CA-C	-5.27	1.46	1.52
1	E	267	SER	C-N	5.27	1.41	1.34
1	I	77	ILE	N-CA	-5.27	1.40	1.46
1	I	267	SER	C-N	5.27	1.41	1.34
1	E	226	GLU	C-N	5.26	1.41	1.33
1	C	226	GLU	C-N	5.26	1.41	1.33
1	A	226	GLU	C-N	5.26	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	226	GLU	C-N	5.26	1.41	1.33
1	A	112	LEU	C-N	5.25	1.41	1.33
1	E	77	ILE	N-CA	-5.25	1.40	1.46
1	D	226	GLU	C-N	5.25	1.41	1.33
1	E	311	ILE	CA-C	-5.25	1.46	1.52
1	E	112	LEU	C-N	5.24	1.41	1.33
2	H	104	GLU	CA-C	-5.24	1.46	1.52
1	F	226	GLU	C-N	5.24	1.41	1.33
1	F	34	PRO	C-O	-5.24	1.17	1.23
1	C	77	ILE	N-CA	-5.24	1.40	1.46
1	B	226	GLU	C-N	5.22	1.41	1.33
2	H	144	GLN	C-N	5.22	1.40	1.33
1	I	60	ALA	CA-C	-5.22	1.46	1.52
1	F	247	GLY	N-CA	-5.20	1.37	1.45
1	A	303	GLY	CA-C	-5.18	1.45	1.52
1	F	223	LEU	C-N	5.17	1.40	1.33
1	F	60	ALA	CA-C	-5.17	1.46	1.52
1	F	77	ILE	N-CA	-5.17	1.40	1.46
2	H	177	GLU	CA-C	-5.17	1.46	1.52
1	I	222	ALA	CA-C	-5.17	1.46	1.52
1	I	247	GLY	N-CA	-5.17	1.37	1.45
1	E	303	GLY	CA-C	-5.16	1.45	1.52
1	B	222	ALA	CA-C	-5.16	1.46	1.52
2	G	163	GLU	C-N	5.16	1.40	1.33
1	E	223	LEU	C-N	5.15	1.40	1.33
1	C	222	ALA	CA-C	-5.15	1.46	1.52
1	A	223	LEU	C-N	5.14	1.40	1.33
1	F	266	PRO	C-O	-5.14	1.17	1.24
1	B	223	LEU	C-N	5.14	1.40	1.33
2	H	217	LYS	N-CA	-5.14	1.39	1.46
1	C	223	LEU	C-N	5.13	1.40	1.33
1	D	223	LEU	C-N	5.13	1.40	1.33
1	E	222	ALA	CA-C	-5.13	1.46	1.52
1	A	222	ALA	CA-C	-5.13	1.46	1.52
1	E	351	LEU	C-N	5.13	1.41	1.34
1	A	102	GLU	C-N	5.13	1.38	1.33
2	H	233	LYS	N-CA	-5.12	1.40	1.46
1	F	102	GLU	C-N	5.12	1.38	1.33
2	G	250	GLU	CA-CB	5.12	1.61	1.53
1	D	32	VAL	CA-C	-5.12	1.46	1.52
2	G	243	GLU	C-N	5.12	1.40	1.34
1	C	102	GLU	C-N	5.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	PRO	C-O	-5.11	1.17	1.24
1	B	102	GLU	C-N	5.11	1.38	1.33
1	C	32	VAL	CA-C	-5.11	1.46	1.52
1	F	222	ALA	CA-C	-5.11	1.46	1.52
2	H	118	LYS	CA-CB	5.11	1.61	1.53
2	H	213	LYS	C-N	5.11	1.40	1.33
1	E	170	GLY	C-N	5.10	1.40	1.33
1	I	32	VAL	CA-C	-5.09	1.46	1.52
1	E	32	VAL	CA-C	-5.09	1.46	1.52
1	F	32	VAL	CA-C	-5.09	1.46	1.52
2	H	151	ALA	CA-CB	5.09	1.61	1.53
1	B	12	CYS	CA-CB	5.08	1.60	1.53
2	H	224	GLU	N-CA	5.08	1.52	1.46
1	I	223	LEU	C-N	5.08	1.40	1.33
1	A	351	LEU	C-N	5.08	1.41	1.34
1	D	222	ALA	CA-C	-5.08	1.46	1.52
1	E	281	TYR	N-CA	-5.07	1.40	1.46
1	A	170	GLY	C-N	5.06	1.40	1.33
2	H	239	ALA	CA-C	-5.06	1.46	1.52
1	I	102	GLU	C-N	5.05	1.38	1.33
1	F	335	PRO	N-CA	-5.05	1.40	1.47
2	G	250	GLU	CA-C	-5.05	1.46	1.52
2	G	153	HIS	CG-ND1	-5.05	1.32	1.38
1	A	322	LEU	CA-CB	5.04	1.61	1.53
1	E	117	ASN	C-N	5.04	1.40	1.33
1	A	335	PRO	N-CA	-5.04	1.40	1.47
1	C	335	PRO	N-CA	-5.03	1.40	1.47
1	E	102	GLU	C-N	5.03	1.38	1.33
1	E	117	ASN	CA-C	-5.03	1.46	1.52
2	G	168	LYS	CA-C	-5.03	1.46	1.52
1	E	366	GLU	C-N	5.03	1.40	1.33
1	B	117	ASN	CA-C	-5.03	1.46	1.52
1	B	335	PRO	N-CA	-5.03	1.40	1.47
1	C	12	CYS	CA-CB	5.02	1.60	1.53
1	I	12	CYS	CA-CB	5.02	1.60	1.53
1	A	366	GLU	C-N	5.02	1.40	1.33
1	I	335	PRO	N-CA	-5.02	1.40	1.47
1	A	143	SER	C-N	5.02	1.40	1.33
1	E	143	SER	C-N	5.01	1.40	1.33
1	F	208	ARG	N-CA	5.01	1.52	1.46
1	E	331	ILE	N-CA	5.01	1.52	1.46
1	F	12	CYS	CA-CB	5.01	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	ILE	N-CA	5.01	1.52	1.46
1	A	122	THR	N-CA	5.00	1.52	1.46
1	D	117	ASN	CA-C	-5.00	1.46	1.52
1	E	122	THR	N-CA	5.00	1.52	1.46

All (868) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	VAL	N-CA-C	-12.07	102.25	113.71
1	B	203	VAL	N-CA-C	-12.04	102.27	113.71
2	G	125	ARG	NE-CZ-NH2	11.07	129.17	119.20
1	A	254	ASN	CA-CB-CG	10.99	123.59	112.60
1	C	254	ASN	CA-CB-CG	10.94	123.54	112.60
1	D	254	ASN	CA-CB-CG	10.94	123.54	112.60
1	B	254	ASN	CA-CB-CG	10.93	123.53	112.60
1	I	254	ASN	CA-CB-CG	10.93	123.53	112.60
1	E	254	ASN	CA-CB-CG	10.92	123.52	112.60
1	F	254	ASN	CA-CB-CG	10.89	123.49	112.60
2	H	232	LEU	O-C-N	10.13	132.86	122.12
2	H	205	LYS	N-CA-C	9.81	121.98	111.28
1	C	129	PHE	CA-CB-CG	-9.71	104.09	113.80
1	F	129	PHE	CA-CB-CG	-9.71	104.09	113.80
1	A	129	PHE	CA-CB-CG	-9.71	104.09	113.80
1	I	129	PHE	CA-CB-CG	-9.71	104.09	113.80
2	H	133	ARG	NE-CZ-NH2	9.70	127.93	119.20
1	B	129	PHE	CA-CB-CG	-9.69	104.11	113.80
1	E	129	PHE	CA-CB-CG	-9.67	104.13	113.80
2	G	103	GLN	N-CA-C	9.18	121.29	111.28
2	G	238	ARG	NE-CZ-NH2	8.94	127.24	119.20
2	H	160	ARG	NE-CZ-NH2	8.89	127.20	119.20
2	H	247	THR	CA-C-N	8.88	132.90	120.29
2	H	247	THR	C-N-CA	8.88	132.90	120.29
1	F	71	TYR	CA-C-N	8.82	128.46	118.85
1	F	71	TYR	C-N-CA	8.82	128.46	118.85
1	I	71	TYR	CA-C-N	8.79	128.43	118.85
1	I	71	TYR	C-N-CA	8.79	128.43	118.85
1	E	267	SER	N-CA-C	8.76	123.07	112.38
1	I	267	SER	N-CA-C	8.74	123.04	112.38
2	G	254	ASP	CA-CB-CG	8.72	121.32	112.60
1	D	325	SER	O-C-N	-8.66	110.46	122.06
1	A	277	HIS	CE1-NE2-CD2	-8.51	100.49	109.00
1	E	277	HIS	CE1-NE2-CD2	-8.49	100.50	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	167	ARG	NE-CZ-NH1	-8.49	113.01	121.50
1	F	277	HIS	CE1-NE2-CD2	-8.49	100.51	109.00
1	F	244	LEU	CA-C-N	8.44	129.82	120.45
1	F	244	LEU	C-N-CA	8.44	129.82	120.45
1	I	244	LEU	CA-C-N	8.44	129.81	120.45
1	I	244	LEU	C-N-CA	8.44	129.81	120.45
1	E	99	ALA	CA-C-N	8.26	128.36	119.28
1	E	99	ALA	C-N-CA	8.26	128.36	119.28
2	G	101	ARG	NE-CZ-NH2	8.25	126.62	119.20
1	A	99	ALA	CA-C-N	8.24	128.35	119.28
1	A	99	ALA	C-N-CA	8.24	128.35	119.28
1	C	99	ALA	CA-C-N	8.24	128.35	119.28
1	C	99	ALA	C-N-CA	8.24	128.35	119.28
1	B	99	ALA	CA-C-N	8.22	128.33	119.28
1	B	99	ALA	C-N-CA	8.22	128.33	119.28
1	I	99	ALA	CA-C-N	8.22	128.32	119.28
1	I	99	ALA	C-N-CA	8.22	128.32	119.28
1	E	164	ASN	CA-CB-CG	-8.21	104.39	112.60
1	A	164	ASN	CA-CB-CG	-8.20	104.41	112.60
1	F	99	ALA	CA-C-N	8.19	128.28	119.28
1	F	99	ALA	C-N-CA	8.19	128.28	119.28
1	A	103	HIS	CA-CB-CG	-8.15	105.64	113.80
1	F	103	HIS	CA-CB-CG	-8.14	105.66	113.80
1	I	103	HIS	CA-CB-CG	-8.13	105.67	113.80
1	C	103	HIS	CA-CB-CG	-8.12	105.68	113.80
1	E	103	HIS	CA-CB-CG	-8.11	105.69	113.80
1	B	103	HIS	CA-CB-CG	-8.10	105.70	113.80
1	I	52	LYS	N-CA-CB	8.10	123.20	111.05
1	F	52	LYS	N-CA-CB	8.09	123.19	111.05
1	F	52	LYS	N-CA-C	-8.08	97.45	109.81
1	I	52	LYS	N-CA-C	-8.07	97.46	109.81
1	F	277	HIS	CG-CD2-NE2	7.94	115.14	107.20
1	E	277	HIS	CG-CD2-NE2	7.93	115.13	107.20
2	H	239	ALA	CA-C-N	7.92	130.89	120.28
2	H	239	ALA	C-N-CA	7.92	130.89	120.28
1	A	277	HIS	CG-CD2-NE2	7.91	115.11	107.20
1	E	30	ARG	NE-CZ-NH2	7.90	126.31	119.20
1	B	30	ARG	NE-CZ-NH2	7.88	126.29	119.20
1	F	30	ARG	NE-CZ-NH2	7.87	126.28	119.20
1	C	30	ARG	NE-CZ-NH2	7.85	126.27	119.20
1	F	42	HIS	CE1-NE2-CD2	-7.84	101.16	109.00
1	I	30	ARG	NE-CZ-NH2	7.83	126.25	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	42	HIS	CE1-NE2-CD2	-7.83	101.17	109.00
2	H	217	LYS	CA-C-N	7.82	130.61	120.44
2	H	217	LYS	C-N-CA	7.82	130.61	120.44
2	H	269	ALA	N-CA-C	7.79	119.77	111.28
1	I	64	ARG	NE-CZ-NH2	7.76	126.19	119.20
1	I	254	ASN	CA-C-N	7.75	131.44	120.28
1	I	254	ASN	C-N-CA	7.75	131.44	120.28
1	F	64	ARG	NE-CZ-NH2	7.74	126.17	119.20
1	A	254	ASN	CA-C-N	7.74	131.42	120.28
1	A	254	ASN	C-N-CA	7.74	131.42	120.28
1	B	254	ASN	CA-C-N	7.72	131.40	120.28
1	B	254	ASN	C-N-CA	7.72	131.40	120.28
1	E	254	ASN	CA-C-N	7.72	131.39	120.28
1	E	254	ASN	C-N-CA	7.72	131.39	120.28
1	F	254	ASN	CA-C-N	7.72	131.39	120.28
1	F	254	ASN	C-N-CA	7.72	131.39	120.28
1	C	254	ASN	CA-C-N	7.71	131.39	120.28
1	C	254	ASN	C-N-CA	7.71	131.39	120.28
1	D	254	ASN	CA-C-N	7.71	131.39	120.28
1	D	254	ASN	C-N-CA	7.71	131.39	120.28
2	G	249	LEU	CA-C-N	7.70	130.45	120.44
2	G	249	LEU	C-N-CA	7.70	130.45	120.44
1	A	265	GLN	CA-C-N	7.68	127.39	119.56
1	A	265	GLN	C-N-CA	7.68	127.39	119.56
1	I	39	ARG	CA-C-N	7.68	128.15	119.93
1	I	39	ARG	C-N-CA	7.68	128.15	119.93
1	E	265	GLN	CA-C-N	7.68	127.39	119.56
1	E	265	GLN	C-N-CA	7.68	127.39	119.56
1	I	265	GLN	CA-C-N	7.68	127.39	119.56
1	I	265	GLN	C-N-CA	7.68	127.39	119.56
1	F	39	ARG	CA-C-N	7.67	128.14	119.93
1	F	39	ARG	C-N-CA	7.67	128.14	119.93
1	B	265	GLN	CA-C-N	7.65	127.37	119.56
1	B	265	GLN	C-N-CA	7.65	127.37	119.56
2	H	169	LEU	N-CA-C	-7.62	102.91	111.07
2	G	247	THR	CA-C-N	7.62	131.10	120.29
2	G	247	THR	C-N-CA	7.62	131.10	120.29
1	E	142	LEU	CA-C-O	-7.58	112.52	120.55
2	H	238	ARG	NE-CZ-NH2	7.55	126.00	119.20
1	E	292	ARG	NE-CZ-NH1	-7.52	113.98	121.50
1	A	142	LEU	CA-C-O	-7.52	112.58	120.55
1	A	292	ARG	NE-CZ-NH1	-7.50	114.00	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	105	ARG	NE-CZ-NH1	-7.46	114.04	121.50
2	H	268	LYS	O-C-N	7.44	130.01	122.12
2	H	145	GLU	O-C-N	7.43	129.99	122.12
2	H	167	ARG	NE-CZ-NH2	7.42	125.88	119.20
2	H	251	LYS	N-CA-C	-7.41	102.15	112.45
1	A	369	PRO	CA-C-N	7.40	133.08	120.72
1	A	369	PRO	C-N-CA	7.40	133.08	120.72
1	E	369	PRO	CA-C-N	7.39	133.07	120.72
1	E	369	PRO	C-N-CA	7.39	133.07	120.72
1	E	314	ARG	NE-CZ-NH2	7.38	125.84	119.20
2	H	232	LEU	CA-C-O	-7.38	112.73	120.55
1	I	85	GLU	N-CA-C	7.38	119.32	111.28
1	F	85	GLU	N-CA-C	7.37	119.31	111.28
1	F	265	GLN	CA-C-N	7.37	127.38	119.28
1	F	265	GLN	C-N-CA	7.37	127.38	119.28
1	C	265	GLN	CA-C-N	7.35	127.37	119.28
1	C	265	GLN	C-N-CA	7.35	127.37	119.28
2	G	255	ASP	N-CA-C	7.34	119.28	111.28
1	B	314	ARG	NE-CZ-NH2	7.34	125.81	119.20
1	A	314	ARG	NE-CZ-NH2	7.33	125.80	119.20
1	A	292	ARG	CA-C-N	7.33	129.97	120.44
1	A	292	ARG	C-N-CA	7.33	129.97	120.44
1	D	314	ARG	NE-CZ-NH2	7.33	125.80	119.20
1	F	314	ARG	NE-CZ-NH2	7.33	125.80	119.20
1	I	314	ARG	NE-CZ-NH2	7.33	125.79	119.20
1	C	314	ARG	NE-CZ-NH2	7.32	125.78	119.20
1	E	292	ARG	CA-C-N	7.31	129.94	120.44
1	E	292	ARG	C-N-CA	7.31	129.94	120.44
1	E	85	GLU	N-CA-C	7.30	119.24	111.28
1	A	173	LEU	O-C-N	7.27	128.03	121.19
1	E	173	LEU	O-C-N	7.26	128.02	121.19
1	C	28	ALA	O-C-N	-7.25	116.77	121.85
1	C	325	SER	O-C-N	-7.25	113.09	122.37
2	G	230	ASP	N-CA-C	-7.25	103.46	111.36
1	B	28	ALA	O-C-N	-7.22	116.79	121.85
1	E	348	LEU	N-CA-C	7.22	118.79	111.07
2	H	145	GLU	CA-C-N	7.22	129.80	120.56
2	H	145	GLU	C-N-CA	7.22	129.80	120.56
1	E	28	ALA	O-C-N	-7.21	116.81	121.85
1	A	348	LEU	N-CA-C	7.20	118.78	111.07
2	H	225	ILE	CA-C-O	-7.17	113.50	120.95
1	E	123	GLN	N-CA-C	7.16	118.73	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	123	GLN	N-CA-C	7.15	118.72	111.07
1	A	123	GLN	N-CA-C	7.14	118.71	111.07
1	E	344	GLY	O-C-N	7.14	129.05	122.19
2	H	103	GLN	N-CA-CB	7.14	120.73	110.16
1	A	344	GLY	O-C-N	7.14	129.04	122.19
1	D	123	GLN	N-CA-C	7.12	118.68	111.07
1	F	123	GLN	N-CA-C	7.12	118.68	111.07
1	B	123	GLN	N-CA-C	7.11	118.68	111.07
1	I	271	MET	CA-C-N	7.06	134.18	122.54
1	I	271	MET	C-N-CA	7.06	134.18	122.54
1	I	312	ALA	N-CA-C	7.03	118.94	111.28
1	E	271	MET	CA-C-N	7.03	134.13	122.54
1	E	271	MET	C-N-CA	7.03	134.13	122.54
1	C	99	ALA	CA-C-O	-7.01	114.06	119.46
2	H	165	VAL	CA-C-N	7.01	129.56	120.44
2	H	165	VAL	C-N-CA	7.01	129.56	120.44
1	B	312	ALA	N-CA-C	6.99	118.90	111.28
2	H	150	GLU	CB-CA-C	-6.99	99.18	110.79
1	D	99	ALA	CA-C-O	-6.99	114.08	119.46
1	D	312	ALA	N-CA-C	6.97	118.88	111.28
2	H	118	LYS	CA-C-N	6.96	130.16	120.29
2	H	118	LYS	C-N-CA	6.96	130.16	120.29
1	A	99	ALA	CA-C-O	-6.95	114.11	119.46
1	B	99	ALA	CA-C-O	-6.95	114.11	119.46
1	F	312	ALA	N-CA-C	6.95	118.94	111.36
2	H	200	VAL	CA-C-N	6.95	129.59	120.28
2	H	200	VAL	C-N-CA	6.95	129.59	120.28
1	E	312	ALA	N-CA-C	6.94	118.92	111.36
2	G	133	ARG	N-CA-CB	6.93	120.42	110.16
2	H	112	LYS	CA-C-N	6.93	129.57	120.28
2	H	112	LYS	C-N-CA	6.93	129.57	120.28
1	F	99	ALA	CA-C-O	-6.92	114.13	119.46
1	I	99	ALA	CA-C-O	-6.92	114.13	119.46
1	E	99	ALA	CA-C-O	-6.92	114.13	119.46
1	A	312	ALA	N-CA-C	6.92	118.90	111.36
1	C	312	ALA	N-CA-C	6.91	118.89	111.36
1	I	185	ARG	NE-CZ-NH2	6.89	125.41	119.20
2	H	207	LEU	CA-C-N	6.87	129.49	120.28
2	H	207	LEU	C-N-CA	6.87	129.49	120.28
2	G	133	ARG	NE-CZ-NH2	6.87	125.38	119.20
2	G	266	LYS	CA-C-N	6.87	130.04	120.29
2	G	266	LYS	C-N-CA	6.87	130.04	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	GLY	N-CA-C	6.86	119.88	112.33
1	F	185	ARG	NE-CZ-NH2	6.86	125.37	119.20
2	H	227	VAL	CA-CB-CG2	-6.85	98.75	110.40
1	D	212	ARG	NE-CZ-NH1	-6.83	114.67	121.50
1	I	212	ARG	NE-CZ-NH1	-6.83	114.67	121.50
1	A	212	ARG	NE-CZ-NH1	-6.81	114.69	121.50
1	F	212	ARG	NE-CZ-NH1	-6.81	114.69	121.50
2	G	105	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	E	152	GLY	CA-C-O	-6.80	114.75	121.48
1	A	152	GLY	CA-C-O	-6.80	114.75	121.48
1	E	212	ARG	NE-CZ-NH1	-6.80	114.70	121.50
1	E	374	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	C	212	ARG	NE-CZ-NH1	-6.78	114.72	121.50
2	G	101	ARG	NE-CZ-NH1	-6.77	114.73	121.50
1	F	256	ARG	N-CA-C	6.77	118.65	111.28
2	H	254	ASP	N-CA-CB	6.76	120.02	109.94
1	A	374	ARG	NE-CZ-NH1	-6.76	114.74	121.50
1	A	321	ALA	N-CA-CB	6.74	120.14	110.16
1	B	321	ALA	N-CA-CB	6.74	120.13	110.16
1	D	321	ALA	N-CA-CB	6.74	120.13	110.16
1	F	321	ALA	N-CA-CB	6.73	120.12	110.16
1	E	107	LEU	N-CA-CB	6.73	121.60	110.63
1	I	321	ALA	N-CA-CB	6.73	120.12	110.16
1	I	256	ARG	N-CA-C	6.73	118.61	111.28
1	A	107	LEU	N-CA-CB	6.72	121.59	110.63
1	E	256	ARG	N-CA-C	6.72	118.61	111.28
1	E	321	ALA	N-CA-CB	6.72	120.11	110.16
1	D	256	ARG	N-CA-C	6.72	118.60	111.28
1	A	256	ARG	N-CA-C	6.71	118.60	111.28
1	B	256	ARG	N-CA-C	6.71	118.59	111.28
1	C	256	ARG	N-CA-C	6.71	118.59	111.28
1	C	321	ALA	N-CA-CB	6.70	120.08	110.16
1	F	34	PRO	N-CA-C	6.70	121.59	111.14
1	I	34	PRO	N-CA-C	6.70	121.59	111.14
2	H	210	GLN	OE1-CD-NE2	6.70	129.29	122.60
2	H	168	LYS	CA-C-N	6.68	129.12	120.44
2	H	168	LYS	C-N-CA	6.68	129.12	120.44
2	H	114	GLU	CA-C-N	6.64	129.08	120.44
2	H	114	GLU	C-N-CA	6.64	129.08	120.44
2	H	230	ASP	CA-C-N	6.64	129.71	120.29
2	H	230	ASP	C-N-CA	6.64	129.71	120.29
1	A	359	ILE	CB-CA-C	-6.63	104.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	107	ALA	O-C-N	6.62	128.89	122.07
1	I	323	ALA	CB-CA-C	-6.61	99.56	108.87
1	B	218	LEU	CA-C-O	-6.59	111.92	118.97
2	H	137	ASP	CB-CA-C	-6.59	99.65	110.85
1	B	323	ALA	CB-CA-C	-6.59	99.58	108.87
1	A	323	ALA	CB-CA-C	-6.58	99.59	108.87
1	E	359	ILE	CB-CA-C	-6.58	104.12	111.23
1	E	323	ALA	CB-CA-C	-6.58	99.60	108.87
1	F	323	ALA	CB-CA-C	-6.57	99.60	108.87
1	B	131	VAL	CA-C-O	-6.56	113.99	119.76
1	A	150	THR	CA-CB-OG1	6.56	119.44	109.60
2	H	190	CYS	CA-C-N	6.55	129.06	120.28
2	H	190	CYS	C-N-CA	6.55	129.06	120.28
1	E	150	THR	CA-CB-OG1	6.55	119.43	109.60
2	G	207	LEU	N-CA-CB	6.55	119.75	110.12
1	F	218	LEU	CA-C-O	-6.54	111.97	118.97
1	E	218	LEU	CA-C-O	-6.54	111.97	118.97
1	C	85	GLU	N-CA-C	6.54	119.24	111.33
1	A	85	GLU	N-CA-C	6.54	119.24	111.33
1	I	131	VAL	CA-C-O	-6.54	114.01	119.76
1	B	85	GLU	N-CA-C	6.53	119.23	111.33
2	G	204	LEU	N-CA-CB	6.53	119.47	110.01
1	D	218	LEU	CA-C-O	-6.52	111.99	118.97
1	A	302	SER	N-CA-C	6.52	119.34	109.23
1	I	218	LEU	CA-C-O	-6.51	112.00	118.97
1	C	218	LEU	CA-C-O	-6.51	112.00	118.97
2	G	191	ALA	CA-C-N	6.51	128.90	120.44
2	G	191	ALA	C-N-CA	6.51	128.90	120.44
1	A	218	LEU	CA-C-O	-6.51	112.01	118.97
1	E	289	ILE	CA-C-N	6.50	129.65	120.28
1	E	289	ILE	C-N-CA	6.50	129.65	120.28
1	E	371	ILE	CA-CB-CG1	6.49	121.44	110.40
1	E	302	SER	N-CA-C	6.49	119.28	109.23
1	A	289	ILE	CA-C-N	6.48	129.62	120.28
1	A	289	ILE	C-N-CA	6.48	129.62	120.28
2	G	152	LYS	N-CA-C	-6.48	104.14	111.14
1	E	343	ILE	CA-C-N	6.48	127.17	119.98
1	E	343	ILE	C-N-CA	6.48	127.17	119.98
1	F	123	GLN	OE1-CD-NE2	6.47	129.07	122.60
1	I	42	HIS	CG-CD2-NE2	6.46	113.66	107.20
1	A	371	ILE	CA-CB-CG1	6.46	121.38	110.40
1	F	42	HIS	CG-CD2-NE2	6.46	113.66	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ILE	CA-C-N	6.45	127.14	119.98
1	A	343	ILE	C-N-CA	6.45	127.14	119.98
1	D	123	GLN	OE1-CD-NE2	6.45	129.05	122.60
2	H	248	LYS	N-CA-CB	6.45	119.70	110.16
1	A	123	GLN	OE1-CD-NE2	6.44	129.04	122.60
1	B	123	GLN	OE1-CD-NE2	6.44	129.04	122.60
1	F	50	GLY	CA-C-O	-6.43	114.96	121.90
1	I	50	GLY	CA-C-O	-6.42	114.96	121.90
1	E	123	GLN	OE1-CD-NE2	6.41	129.01	122.60
1	C	123	GLN	OE1-CD-NE2	6.41	129.01	122.60
1	E	344	GLY	CA-C-O	-6.41	114.15	120.75
1	I	123	GLN	OE1-CD-NE2	6.41	129.00	122.60
1	B	131	VAL	N-CA-CB	6.40	118.21	110.33
2	G	125	ARG	N-CA-C	6.40	118.25	111.28
2	H	133	ARG	CA-C-N	6.39	128.75	120.44
2	H	133	ARG	C-N-CA	6.39	128.75	120.44
2	H	168	LYS	N-CA-C	6.39	118.24	111.28
1	I	131	VAL	N-CA-CB	6.39	118.19	110.33
1	I	34	PRO	N-CA-CB	6.38	108.99	103.31
1	F	34	PRO	N-CA-CB	6.37	108.98	103.31
2	H	225	ILE	O-C-N	6.37	128.05	121.87
1	C	123	GLN	N-CA-C	6.35	118.73	111.11
1	A	344	GLY	CA-C-O	-6.35	114.21	120.75
2	G	125	ARG	NH1-CZ-NH2	-6.33	111.07	119.30
1	E	183	ALA	N-CA-CB	6.33	121.18	110.49
2	H	159	ASP	N-CA-CB	6.33	119.42	110.12
1	B	183	ALA	N-CA-CB	6.31	121.16	110.49
1	F	183	ALA	N-CA-CB	6.31	121.15	110.49
1	I	183	ALA	N-CA-CB	6.30	121.14	110.49
1	A	183	ALA	N-CA-CB	6.30	121.14	110.49
1	A	168	TYR	N-CA-CB	-6.29	100.90	110.77
1	E	375	LYS	N-CA-C	-6.29	106.14	113.88
1	A	163	HIS	CE1-NE2-CD2	-6.27	102.73	109.00
1	E	323	ALA	CA-C-N	6.27	126.24	119.78
1	E	323	ALA	C-N-CA	6.27	126.24	119.78
2	H	257	GLU	CA-C-N	6.27	128.69	120.28
2	H	257	GLU	C-N-CA	6.27	128.69	120.28
1	I	323	ALA	CA-C-N	6.27	126.24	119.78
1	I	323	ALA	C-N-CA	6.27	126.24	119.78
1	A	372	VAL	N-CA-C	6.27	117.77	110.62
1	A	375	LYS	N-CA-C	-6.26	106.18	113.88
1	E	372	VAL	N-CA-C	6.26	117.76	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ALA	CA-C-N	6.26	126.22	119.78
1	A	323	ALA	C-N-CA	6.26	126.22	119.78
1	E	163	HIS	CE1-NE2-CD2	-6.26	102.74	109.00
1	F	323	ALA	CA-C-N	6.24	126.20	119.78
1	F	323	ALA	C-N-CA	6.24	126.20	119.78
2	H	99	LEU	CA-C-O	6.23	127.36	120.82
1	B	323	ALA	CA-C-N	6.21	126.18	119.78
1	B	323	ALA	C-N-CA	6.21	126.18	119.78
2	G	133	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	F	45	VAL	CA-C-O	6.21	127.41	120.95
1	E	347	ILE	N-CA-C	-6.20	104.47	110.42
1	E	139	GLN	CA-C-N	6.20	129.10	120.29
1	E	139	GLN	C-N-CA	6.20	129.10	120.29
1	A	347	ILE	N-CA-C	-6.20	104.47	110.42
2	G	141	MET	CA-C-N	6.20	128.58	120.28
2	G	141	MET	C-N-CA	6.20	128.58	120.28
2	H	143	ILE	CA-C-N	6.19	128.58	120.28
2	H	143	ILE	C-N-CA	6.19	128.58	120.28
1	E	328	LYS	CA-C-O	-6.19	114.23	121.16
2	H	98	GLU	N-CA-CB	6.18	119.31	110.16
1	F	64	ARG	NH1-CZ-NH2	-6.17	111.27	119.30
1	A	328	LYS	CA-C-O	-6.17	114.25	121.16
1	E	111	PRO	N-CA-CB	6.17	108.66	103.17
1	A	111	PRO	N-CA-CB	6.17	108.66	103.17
2	H	145	GLU	CA-C-O	-6.17	114.01	120.55
1	A	139	GLN	CA-C-N	6.17	129.04	120.29
1	A	139	GLN	C-N-CA	6.17	129.04	120.29
2	G	119	ALA	CA-C-N	6.16	129.04	120.29
2	G	119	ALA	C-N-CA	6.16	129.04	120.29
1	I	64	ARG	NH1-CZ-NH2	-6.16	111.29	119.30
1	I	219	CYS	N-CA-CB	6.16	119.04	110.17
1	I	45	VAL	CA-C-O	6.15	127.35	120.95
2	G	152	LYS	N-CA-CB	6.15	118.98	110.07
2	H	238	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	D	219	CYS	N-CA-CB	6.14	119.00	110.17
1	E	219	CYS	N-CA-CB	6.13	118.99	110.17
1	A	219	CYS	N-CA-CB	6.12	118.99	110.17
1	E	109	GLU	CA-C-N	6.12	129.19	120.49
1	E	109	GLU	C-N-CA	6.12	129.19	120.49
1	B	219	CYS	N-CA-CB	6.12	118.98	110.17
1	F	219	CYS	N-CA-CB	6.11	118.97	110.17
1	C	219	CYS	N-CA-CB	6.11	118.97	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	258	ARG	N-CA-CB	6.11	119.10	110.12
2	H	103	GLN	OE1-CD-NE2	6.10	128.70	122.60
1	B	186	ASP	CA-C-N	6.09	128.44	120.28
1	B	186	ASP	C-N-CA	6.09	128.44	120.28
1	A	109	GLU	CA-C-N	6.08	129.13	120.49
1	A	109	GLU	C-N-CA	6.08	129.13	120.49
1	I	234	SER	N-CA-CB	6.08	119.12	110.67
1	A	258	ARG	N-CA-CB	6.08	119.06	110.12
2	H	159	ASP	CB-CA-C	-6.08	100.70	110.79
1	C	258	ARG	N-CA-CB	6.07	119.05	110.12
1	D	258	ARG	N-CA-CB	6.07	119.05	110.12
1	F	234	SER	N-CA-CB	6.07	119.11	110.67
1	C	224	ASP	CA-C-N	6.07	128.33	120.44
1	C	224	ASP	C-N-CA	6.07	128.33	120.44
1	F	258	ARG	N-CA-CB	6.07	119.04	110.12
1	B	258	ARG	N-CA-CB	6.07	119.04	110.12
1	D	214	ILE	N-CA-C	6.06	116.72	110.36
1	D	224	ASP	CA-C-N	6.06	128.32	120.44
1	D	224	ASP	C-N-CA	6.06	128.32	120.44
1	E	258	ARG	N-CA-CB	6.06	119.03	110.12
1	A	234	SER	N-CA-CB	6.05	119.09	110.67
1	B	224	ASP	CA-C-N	6.05	128.31	120.44
1	B	224	ASP	C-N-CA	6.05	128.31	120.44
1	C	234	SER	N-CA-CB	6.05	119.09	110.67
2	G	203	ASN	CA-C-O	-6.05	114.10	120.63
1	I	215	LYS	CA-C-N	6.05	128.88	120.29
1	I	215	LYS	C-N-CA	6.05	128.88	120.29
1	B	215	LYS	CA-C-N	6.05	128.88	120.29
1	B	215	LYS	C-N-CA	6.05	128.88	120.29
2	G	259	GLU	CA-C-N	6.04	128.38	120.28
2	G	259	GLU	C-N-CA	6.04	128.38	120.28
1	A	186	ASP	CA-C-N	6.04	128.38	120.28
1	A	186	ASP	C-N-CA	6.04	128.38	120.28
2	G	202	ASN	N-CA-C	6.04	117.53	111.07
1	I	224	ASP	CA-C-N	6.04	128.29	120.44
1	I	224	ASP	C-N-CA	6.04	128.29	120.44
1	A	234	SER	N-CA-C	-6.04	106.24	113.97
1	E	214	ILE	N-CA-C	6.04	116.70	110.36
2	H	160	ARG	O-C-N	6.04	128.29	122.07
1	E	234	SER	N-CA-CB	6.04	119.06	110.67
1	B	214	ILE	N-CA-C	6.04	116.70	110.36
2	H	115	GLU	CA-C-N	6.04	128.86	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	115	GLU	C-N-CA	6.04	128.86	120.29
1	E	186	ASP	CA-C-N	6.03	128.37	120.28
1	E	186	ASP	C-N-CA	6.03	128.37	120.28
1	F	186	ASP	CA-C-N	6.03	128.37	120.28
1	F	186	ASP	C-N-CA	6.03	128.37	120.28
2	H	162	TYR	CA-CB-CG	-6.03	103.05	113.90
1	C	215	LYS	CA-C-N	6.03	128.85	120.29
1	C	215	LYS	C-N-CA	6.03	128.85	120.29
1	D	215	LYS	CA-C-N	6.03	128.85	120.29
1	D	215	LYS	C-N-CA	6.03	128.85	120.29
1	E	215	LYS	CA-C-N	6.03	128.85	120.29
1	E	215	LYS	C-N-CA	6.03	128.85	120.29
1	F	224	ASP	CA-C-N	6.02	128.27	120.44
1	F	224	ASP	C-N-CA	6.02	128.27	120.44
1	D	234	SER	N-CA-C	-6.02	106.26	113.97
1	D	234	SER	N-CA-CB	6.02	119.04	110.67
1	F	185	ARG	CA-C-N	6.02	128.35	120.28
1	F	185	ARG	C-N-CA	6.02	128.35	120.28
2	H	117	GLU	CA-C-N	6.02	128.27	120.44
2	H	117	GLU	C-N-CA	6.02	128.27	120.44
1	E	224	ASP	CA-C-N	6.02	128.26	120.44
1	E	224	ASP	C-N-CA	6.02	128.26	120.44
1	F	214	ILE	N-CA-C	6.02	116.68	110.36
1	I	186	ASP	CA-C-N	6.02	128.34	120.28
1	I	186	ASP	C-N-CA	6.02	128.34	120.28
1	A	224	ASP	CA-C-N	6.01	128.26	120.44
1	A	224	ASP	C-N-CA	6.01	128.26	120.44
1	E	234	SER	N-CA-C	-6.01	106.27	113.97
1	F	234	SER	N-CA-C	-6.01	106.28	113.97
2	H	120	ALA	N-CA-C	-6.01	104.65	111.14
1	B	234	SER	N-CA-CB	6.01	119.02	110.67
1	F	215	LYS	CA-C-N	6.01	128.82	120.29
1	F	215	LYS	C-N-CA	6.01	128.82	120.29
2	G	249	LEU	N-CA-C	6.01	117.83	111.28
1	I	214	ILE	N-CA-C	6.01	116.67	110.36
1	B	234	SER	N-CA-C	-6.00	106.28	113.97
1	I	234	SER	N-CA-C	-6.00	106.28	113.97
1	A	215	LYS	CA-C-N	6.00	128.81	120.29
1	A	215	LYS	C-N-CA	6.00	128.81	120.29
1	C	214	ILE	N-CA-C	5.99	116.65	110.36
2	G	126	GLY	CA-C-N	5.99	128.23	120.44
2	G	126	GLY	C-N-CA	5.99	128.23	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ILE	N-CA-C	5.99	116.65	110.36
1	E	327	MET	CA-C-N	5.98	129.37	120.87
1	E	327	MET	C-N-CA	5.98	129.37	120.87
1	I	185	ARG	CA-C-N	5.98	128.30	120.28
1	I	185	ARG	C-N-CA	5.98	128.30	120.28
1	C	234	SER	N-CA-C	-5.98	106.32	113.97
2	H	257	GLU	N-CA-CB	5.96	118.88	110.12
2	G	99	LEU	CA-C-N	5.95	128.18	120.44
2	G	99	LEU	C-N-CA	5.95	128.18	120.44
1	A	327	MET	CA-C-N	5.94	129.31	120.87
1	A	327	MET	C-N-CA	5.94	129.31	120.87
1	C	253	GLY	CA-C-N	5.92	132.91	121.18
1	C	253	GLY	C-N-CA	5.92	132.91	121.18
1	E	253	GLY	CA-C-N	5.92	132.91	121.18
1	E	253	GLY	C-N-CA	5.92	132.91	121.18
1	E	172	ALA	N-CA-CB	5.92	118.67	109.97
1	A	172	ALA	N-CA-CB	5.91	118.66	109.97
1	A	219	CYS	CA-C-O	-5.90	115.13	121.56
1	B	253	GLY	CA-C-N	5.90	132.87	121.18
1	B	253	GLY	C-N-CA	5.90	132.87	121.18
1	D	253	GLY	CA-C-N	5.90	132.87	121.18
1	D	253	GLY	C-N-CA	5.90	132.87	121.18
1	E	219	CYS	CA-C-O	-5.90	115.13	121.56
2	G	205	LYS	CA-C-O	-5.90	114.30	120.55
2	H	123	SER	CA-C-N	5.90	128.67	120.29
2	H	123	SER	C-N-CA	5.90	128.67	120.29
1	A	253	GLY	CA-C-N	5.90	132.86	121.18
1	A	253	GLY	C-N-CA	5.90	132.86	121.18
2	G	238	ARG	CA-C-N	5.90	128.66	120.29
2	G	238	ARG	C-N-CA	5.90	128.66	120.29
1	A	154	VAL	CA-C-N	5.89	131.07	122.41
1	A	154	VAL	C-N-CA	5.89	131.07	122.41
1	I	253	GLY	CA-C-N	5.89	132.85	121.18
1	I	253	GLY	C-N-CA	5.89	132.85	121.18
1	B	219	CYS	CA-C-O	-5.89	115.14	121.56
1	F	253	GLY	CA-C-N	5.89	132.84	121.18
1	F	253	GLY	C-N-CA	5.89	132.84	121.18
1	E	154	VAL	CA-C-N	5.88	131.06	122.41
1	E	154	VAL	C-N-CA	5.88	131.06	122.41
1	D	219	CYS	CA-C-O	-5.88	115.15	121.56
2	G	258	ASP	CB-CA-C	-5.88	101.66	110.88
1	I	219	CYS	CA-C-O	-5.87	115.16	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	CYS	CA-C-O	-5.87	115.16	121.56
1	F	219	CYS	CA-C-O	-5.87	115.16	121.56
1	I	42	HIS	CA-C-N	5.87	131.26	122.99
1	I	42	HIS	C-N-CA	5.87	131.26	122.99
1	C	336	GLU	CA-C-N	5.87	129.99	120.60
1	C	336	GLU	C-N-CA	5.87	129.99	120.60
1	I	369	PRO	CA-C-N	5.86	128.94	120.38
1	I	369	PRO	C-N-CA	5.86	128.94	120.38
1	I	336	GLU	CA-C-N	5.86	129.97	120.60
1	I	336	GLU	C-N-CA	5.86	129.97	120.60
1	A	336	GLU	CA-C-N	5.85	129.96	120.60
1	A	336	GLU	C-N-CA	5.85	129.96	120.60
1	E	336	GLU	CA-C-N	5.84	129.95	120.60
1	E	336	GLU	C-N-CA	5.84	129.95	120.60
2	H	96	GLU	CA-C-N	5.84	128.11	120.28
2	H	96	GLU	C-N-CA	5.84	128.11	120.28
1	B	336	GLU	CA-C-N	5.83	129.93	120.60
1	B	336	GLU	C-N-CA	5.83	129.93	120.60
1	F	42	HIS	CA-C-N	5.83	131.21	122.99
1	F	42	HIS	C-N-CA	5.83	131.21	122.99
1	F	336	GLU	CA-C-N	5.83	129.93	120.60
1	F	336	GLU	C-N-CA	5.83	129.93	120.60
1	E	141	VAL	O-C-N	5.82	127.52	121.87
1	F	319	ILE	N-CA-C	5.82	116.60	110.72
2	H	235	ALA	CA-C-O	-5.82	114.39	120.55
2	H	236	GLU	N-CA-C	5.82	117.29	111.07
2	H	256	LEU	CB-CA-C	-5.82	100.96	110.85
1	A	168	TYR	O-C-N	-5.81	116.47	123.27
1	E	168	TYR	O-C-N	-5.81	116.52	123.31
1	A	6	GLU	CA-C-N	5.80	129.07	120.95
1	A	6	GLU	C-N-CA	5.80	129.07	120.95
2	G	162	TYR	CA-C-N	5.80	128.05	120.28
2	G	162	TYR	C-N-CA	5.80	128.05	120.28
1	A	319	ILE	N-CA-C	5.80	116.58	110.72
2	G	223	GLU	CA-C-N	5.79	127.97	120.44
2	G	223	GLU	C-N-CA	5.79	127.97	120.44
1	E	319	ILE	N-CA-C	5.79	116.57	110.72
1	B	41	ARG	NE-CZ-NH2	5.79	124.41	119.20
2	H	183	ALA	CB-CA-C	-5.78	101.76	110.90
2	H	171	ILE	CA-C-N	5.78	128.38	120.46
2	H	171	ILE	C-N-CA	5.78	128.38	120.46
1	I	275	GLY	N-CA-C	5.78	119.93	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	161	LYS	CA-C-N	5.77	128.01	120.28
2	H	161	LYS	C-N-CA	5.77	128.01	120.28
1	I	119	GLU	N-CA-C	5.76	117.56	111.28
1	A	275	GLY	N-CA-C	5.76	119.91	112.54
1	F	275	GLY	N-CA-C	5.75	119.91	112.54
2	G	214	TYR	N-CA-C	-5.75	105.09	111.36
1	A	141	VAL	O-C-N	5.75	127.44	121.87
1	B	119	GLU	N-CA-C	5.75	117.55	111.28
1	A	119	GLU	N-CA-C	5.75	117.54	111.28
1	E	6	GLU	CA-C-N	5.74	128.99	120.95
1	E	6	GLU	C-N-CA	5.74	128.99	120.95
1	E	82	ASP	CA-CB-CG	5.74	118.34	112.60
1	E	275	GLY	N-CA-C	5.74	119.89	112.54
2	H	202	ASN	CA-CB-CG	5.74	118.34	112.60
1	E	377	PHE	N-CA-C	-5.74	94.94	111.00
1	I	48	GLY	N-CA-C	-5.74	107.75	115.21
2	H	144	GLN	CA-C-O	-5.73	114.47	120.55
1	B	275	GLY	N-CA-C	5.73	119.87	112.54
1	A	377	PHE	N-CA-C	-5.73	94.97	111.00
1	E	119	GLU	N-CA-C	5.72	117.52	111.28
1	E	168	TYR	N-CA-CB	-5.72	100.90	110.80
2	H	98	GLU	CB-CA-C	-5.72	101.13	110.85
2	G	93	GLN	CB-CA-C	-5.72	101.30	110.79
1	E	273	SER	N-CA-C	5.71	118.55	110.50
1	F	119	GLU	N-CA-C	5.71	117.50	111.28
2	H	229	SER	CA-C-N	5.71	127.86	120.44
2	H	229	SER	C-N-CA	5.71	127.86	120.44
2	G	196	GLU	CA-C-O	-5.71	114.83	120.82
1	E	326	THR	N-CA-C	-5.70	106.37	113.38
1	E	142	LEU	O-C-N	5.69	128.15	122.12
1	D	326	THR	N-CA-C	5.69	121.50	113.02
2	G	260	LEU	CA-C-N	5.69	127.90	120.28
2	G	260	LEU	C-N-CA	5.69	127.90	120.28
2	H	246	VAL	CA-CB-CG2	-5.68	100.74	110.40
1	I	273	SER	N-CA-C	5.68	118.51	110.50
2	H	133	ARG	N-CA-CB	5.67	118.56	110.16
1	F	48	GLY	N-CA-C	-5.67	107.84	115.21
1	A	326	THR	N-CA-C	-5.67	106.41	113.38
1	A	27	ASP	N-CA-C	-5.66	105.58	112.88
1	E	27	ASP	N-CA-C	-5.66	105.58	112.88
1	A	162	THR	O-C-N	-5.65	116.62	123.29
1	A	290	ASP	N-CA-C	5.65	118.21	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	THR	CA-C-N	5.65	128.42	120.28
2	H	201	THR	C-N-CA	5.65	128.42	120.28
1	E	162	THR	O-C-N	-5.65	116.62	123.29
1	E	314	ARG	CA-C-N	5.65	127.85	120.28
1	E	314	ARG	C-N-CA	5.65	127.85	120.28
1	I	339	TYR	CA-CB-CG	5.64	124.06	113.90
1	C	27	ASP	N-CA-C	-5.64	105.61	112.88
1	A	142	LEU	O-C-N	5.64	128.09	122.12
1	B	121	MET	CB-CA-C	-5.63	101.44	110.79
1	E	290	ASP	N-CA-C	5.63	118.19	111.71
1	C	314	ARG	CA-C-N	5.63	127.82	120.28
1	C	314	ARG	C-N-CA	5.63	127.82	120.28
2	G	259	GLU	O-C-N	-5.63	115.73	122.15
1	B	27	ASP	N-CA-C	-5.63	105.62	112.88
1	C	339	TYR	CA-CB-CG	5.63	124.03	113.90
1	F	339	TYR	CA-CB-CG	5.63	124.03	113.90
1	B	339	TYR	CA-CB-CG	5.62	124.02	113.90
1	A	314	ARG	CA-C-N	5.62	127.81	120.28
1	A	314	ARG	C-N-CA	5.62	127.81	120.28
1	A	121	MET	CB-CA-C	-5.61	101.47	110.79
2	H	200	VAL	O-C-N	-5.61	116.41	121.91
1	A	282	ASN	CA-CB-CG	-5.61	106.99	112.60
1	F	121	MET	CB-CA-C	-5.61	101.48	110.79
1	F	314	ARG	CA-C-N	5.61	127.80	120.28
1	F	314	ARG	C-N-CA	5.61	127.80	120.28
1	E	339	TYR	CA-CB-CG	5.61	123.99	113.90
1	I	121	MET	CB-CA-C	-5.59	101.50	110.79
1	E	121	MET	CB-CA-C	-5.58	101.52	110.79
2	G	96	GLU	O-C-N	-5.58	116.20	122.12
2	H	175	ASP	CB-CA-C	-5.58	101.36	110.85
1	D	314	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	F	54	SER	N-CA-C	-5.58	98.82	108.69
1	B	314	ARG	NE-CZ-NH1	-5.57	115.93	121.50
2	H	172	ILE	O-C-N	5.56	127.27	121.87
1	C	314	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	I	54	SER	N-CA-C	-5.56	98.85	108.69
1	I	314	ARG	NE-CZ-NH1	-5.55	115.95	121.50
2	H	197	LEU	CA-C-N	5.55	127.71	120.28
2	H	197	LEU	C-N-CA	5.55	127.71	120.28
1	E	314	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	F	314	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	A	314	ARG	NE-CZ-NH1	-5.53	115.97	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASN	OD1-CG-ND2	5.53	128.13	122.60
1	E	282	ASN	CA-CB-CG	-5.53	107.07	112.60
2	H	170	VAL	CB-CA-C	-5.52	104.69	112.14
2	H	196	GLU	N-CA-C	5.52	116.98	111.07
2	H	230	ASP	CA-CB-CG	5.52	118.12	112.60
2	H	239	ALA	N-CA-C	-5.52	105.27	111.28
1	E	352	SER	N-CA-CB	5.51	118.83	110.28
1	E	32	VAL	N-CA-CB	5.50	119.50	112.34
1	F	227	ASN	OD1-CG-ND2	5.50	128.10	122.60
1	D	32	VAL	N-CA-CB	5.50	119.49	112.34
1	F	32	VAL	N-CA-CB	5.50	119.49	112.34
2	H	218	GLU	CA-C-N	5.50	127.96	120.54
2	H	218	GLU	C-N-CA	5.50	127.96	120.54
1	C	32	VAL	N-CA-CB	5.49	119.48	112.34
1	A	352	SER	N-CA-CB	5.48	118.78	110.28
1	I	32	VAL	N-CA-CB	5.48	119.46	112.34
1	C	227	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	E	227	ASN	OD1-CG-ND2	5.47	128.07	122.60
2	H	238	ARG	CA-C-N	5.47	127.61	120.28
2	H	238	ARG	C-N-CA	5.47	127.61	120.28
1	I	227	ASN	OD1-CG-ND2	5.47	128.07	122.60
2	H	175	ASP	CA-C-N	5.46	127.54	120.44
2	H	175	ASP	C-N-CA	5.46	127.54	120.44
1	D	227	ASN	OD1-CG-ND2	5.46	128.06	122.60
2	G	212	GLU	O-C-N	5.45	127.90	122.12
1	B	227	ASN	OD1-CG-ND2	5.45	128.05	122.60
1	E	165	VAL	CA-C-N	5.45	126.29	120.13
1	E	165	VAL	C-N-CA	5.45	126.29	120.13
1	A	375	LYS	CB-CA-C	5.44	117.84	109.03
2	H	227	VAL	N-CA-C	-5.43	105.08	110.62
1	I	44	GLY	N-CA-C	-5.43	107.29	114.95
2	G	136	LYS	CA-C-N	5.43	128.00	120.29
2	G	136	LYS	C-N-CA	5.43	128.00	120.29
1	A	82	ASP	CA-CB-CG	5.43	118.03	112.60
2	G	253	ILE	CA-C-N	5.42	127.49	120.44
2	G	253	ILE	C-N-CA	5.42	127.49	120.44
1	A	165	VAL	CA-C-N	5.42	126.25	120.13
1	A	165	VAL	C-N-CA	5.42	126.25	120.13
1	F	44	GLY	N-CA-C	-5.42	107.31	114.95
1	E	375	LYS	CB-CA-C	5.41	117.80	109.03
1	A	299	ASN	OD1-CG-ND2	5.39	127.99	122.60
1	I	325	SER	O-C-N	-5.38	112.66	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	THR	CB-CA-C	5.37	118.99	109.75
2	H	151	ALA	CB-CA-C	-5.37	101.87	110.79
1	I	326	THR	CB-CA-C	5.37	119.45	110.44
2	H	133	ARG	CA-C-O	-5.36	114.74	120.42
2	G	225	ILE	O-C-N	5.35	127.06	121.87
2	G	244	ARG	NE-CZ-NH1	-5.35	116.15	121.50
2	H	95	VAL	CB-CA-C	-5.35	104.84	112.22
1	E	299	ASN	OD1-CG-ND2	5.34	127.94	122.60
1	I	87	ILE	N-CA-CB	5.33	116.79	110.55
2	H	114	GLU	CB-CG-CD	-5.33	103.55	112.60
1	D	210	ILE	CA-C-N	5.32	127.75	120.46
1	D	210	ILE	C-N-CA	5.32	127.75	120.46
1	F	87	ILE	N-CA-CB	5.32	116.77	110.55
2	H	263	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	A	375	LYS	N-CA-CB	-5.30	103.54	110.59
1	E	157	SER	N-CA-C	-5.30	98.59	108.02
1	I	64	ARG	O-C-N	-5.30	116.51	122.12
1	A	157	SER	N-CA-C	-5.29	98.59	108.02
1	B	195	LEU	CA-C-N	5.29	127.37	120.28
1	B	195	LEU	C-N-CA	5.29	127.37	120.28
1	E	375	LYS	N-CA-CB	-5.29	103.55	110.59
1	F	64	ARG	O-C-N	-5.29	116.51	122.12
2	G	243	GLU	N-CA-CB	5.29	117.69	110.01
1	E	351	LEU	N-CA-CB	5.29	118.05	110.06
2	G	221	TYR	CA-C-N	5.29	127.37	120.28
2	G	221	TYR	C-N-CA	5.29	127.37	120.28
2	H	144	GLN	CB-CG-CD	-5.29	103.61	112.60
1	E	195	LEU	CA-C-N	5.29	127.37	120.28
1	E	195	LEU	C-N-CA	5.29	127.37	120.28
1	F	195	LEU	CA-C-N	5.29	127.36	120.28
1	F	195	LEU	C-N-CA	5.29	127.36	120.28
1	D	31	ALA	N-CA-CB	5.28	119.48	110.71
1	I	190	TYR	CB-CG-CD2	5.28	128.72	120.80
1	I	233	ALA	CA-C-N	5.28	130.77	122.11
1	I	233	ALA	C-N-CA	5.28	130.77	122.11
1	D	195	LEU	CA-C-N	5.28	127.36	120.28
1	D	195	LEU	C-N-CA	5.28	127.36	120.28
1	A	190	TYR	CB-CG-CD2	5.28	128.72	120.80
2	G	216	GLN	CG-CD-NE2	-5.28	108.48	116.40
2	H	175	ASP	N-CA-CB	5.28	117.97	110.16
1	C	233	ALA	CA-C-N	5.27	130.76	122.11
1	C	233	ALA	C-N-CA	5.27	130.76	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	193	LYS	N-CA-C	5.27	116.71	111.07
1	A	351	LEU	N-CA-CB	5.26	118.01	110.06
1	E	193	LYS	N-CA-C	5.26	116.70	111.07
1	F	233	ALA	CA-C-N	5.26	130.74	122.11
1	F	233	ALA	C-N-CA	5.26	130.74	122.11
1	A	195	LEU	CA-C-N	5.26	127.33	120.28
1	A	195	LEU	C-N-CA	5.26	127.33	120.28
1	A	233	ALA	CA-C-N	5.26	130.74	122.11
1	A	233	ALA	C-N-CA	5.26	130.74	122.11
1	A	298	ASN	CB-CG-ND2	-5.26	108.51	116.40
1	C	190	TYR	CB-CG-CD2	5.25	128.68	120.80
1	E	233	ALA	CA-C-N	5.25	130.73	122.11
1	E	233	ALA	C-N-CA	5.25	130.73	122.11
1	E	298	ASN	CB-CG-ND2	-5.25	108.52	116.40
1	B	233	ALA	CA-C-N	5.25	130.72	122.11
1	B	233	ALA	C-N-CA	5.25	130.72	122.11
1	C	82	ASP	CA-CB-CG	5.25	117.85	112.60
1	F	190	TYR	CB-CG-CD2	5.25	128.68	120.80
2	G	216	GLN	N-CA-C	5.25	117.75	111.71
1	I	195	LEU	CA-C-N	5.25	127.31	120.28
1	I	195	LEU	C-N-CA	5.25	127.31	120.28
1	D	233	ALA	CA-C-N	5.24	130.71	122.11
1	D	233	ALA	C-N-CA	5.24	130.71	122.11
2	G	217	LYS	CA-C-N	5.24	127.25	120.44
2	G	217	LYS	C-N-CA	5.24	127.25	120.44
1	I	212	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	B	190	TYR	CB-CG-CD2	5.24	128.65	120.80
1	E	315	MET	CA-C-O	5.23	126.10	120.55
2	G	192	GLU	CB-CG-CD	-5.23	103.70	112.60
1	A	212	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	H	93	GLN	CB-CG-CD	-5.23	103.71	112.60
1	E	190	TYR	CB-CG-CD2	5.23	128.64	120.80
1	A	315	MET	CA-C-O	5.22	126.09	120.55
1	B	262	THR	CA-C-N	5.22	128.25	120.31
1	B	262	THR	C-N-CA	5.22	128.25	120.31
1	D	190	TYR	CB-CG-CD2	5.22	128.63	120.80
1	E	212	ARG	NE-CZ-NH2	5.22	123.90	119.20
2	G	159	ASP	CA-C-O	-5.22	115.02	120.55
1	A	262	THR	CA-C-N	5.22	128.24	120.31
1	A	262	THR	C-N-CA	5.22	128.24	120.31
1	D	212	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	F	262	THR	CA-C-N	5.21	128.23	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	262	THR	C-N-CA	5.21	128.23	120.31
1	F	315	MET	CA-C-O	5.21	126.07	120.55
1	C	315	MET	CA-C-O	5.21	126.07	120.55
1	I	262	THR	CA-C-N	5.21	128.23	120.31
1	I	262	THR	C-N-CA	5.21	128.23	120.31
1	F	212	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	C	212	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	H	233	LYS	N-CA-CB	5.20	117.76	110.12
2	H	261	TYR	CA-C-N	5.20	127.24	120.28
2	H	261	TYR	C-N-CA	5.20	127.24	120.28
1	C	210	ILE	CA-C-N	5.19	127.58	120.46
1	C	210	ILE	C-N-CA	5.19	127.58	120.46
1	E	262	THR	CA-C-N	5.19	128.20	120.31
1	E	262	THR	C-N-CA	5.19	128.20	120.31
2	H	162	TYR	O-C-N	-5.19	116.62	122.12
1	I	247	GLY	N-CA-C	-5.19	104.41	112.45
2	H	257	GLU	CB-CG-CD	-5.19	103.78	112.60
1	E	31	ALA	N-CA-CB	5.18	119.52	110.81
1	E	358	TRP	CB-CA-C	-5.18	102.07	109.84
2	H	128	LYS	N-CA-C	5.18	116.93	111.28
2	H	105	ARG	CB-CA-C	-5.18	102.19	110.79
2	G	244	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	F	31	ALA	N-CA-CB	5.17	119.50	110.81
1	E	194	ILE	CA-C-N	5.17	127.63	120.29
1	E	194	ILE	C-N-CA	5.17	127.63	120.29
2	G	147	GLN	O-C-N	5.17	127.60	122.12
1	A	328	LYS	O-C-N	5.17	129.19	122.89
1	A	358	TRP	CB-CA-C	-5.17	102.09	109.84
1	C	261	GLU	CB-CG-CD	5.17	121.38	112.60
1	I	31	ALA	N-CA-CB	5.17	119.49	110.81
1	C	31	ALA	N-CA-CB	5.16	119.48	110.81
1	F	247	GLY	N-CA-C	-5.16	104.45	112.45
1	I	194	ILE	CA-C-N	5.16	127.62	120.29
1	I	194	ILE	C-N-CA	5.16	127.62	120.29
1	I	261	GLU	CB-CG-CD	5.16	121.37	112.60
1	B	261	GLU	CB-CG-CD	5.15	121.35	112.60
1	D	216	GLU	O-C-N	-5.15	116.28	122.15
1	E	261	GLU	CB-CG-CD	5.15	121.35	112.60
1	F	261	GLU	CB-CG-CD	5.14	121.35	112.60
1	I	216	GLU	O-C-N	-5.14	116.28	122.15
1	A	261	GLU	CB-CG-CD	5.14	121.33	112.60
2	H	152	LYS	CA-C-O	-5.14	115.43	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	216	GLU	O-C-N	-5.13	116.30	122.15
1	F	194	ILE	CA-C-N	5.13	127.58	120.29
1	F	194	ILE	C-N-CA	5.13	127.58	120.29
1	I	149	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	B	82	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	194	ILE	CA-C-N	5.13	127.58	120.29
1	B	194	ILE	C-N-CA	5.13	127.58	120.29
1	D	261	GLU	CB-CG-CD	5.13	121.33	112.60
1	D	194	ILE	CA-C-N	5.13	127.57	120.29
1	D	194	ILE	C-N-CA	5.13	127.57	120.29
1	E	271	MET	CG-SD-CE	-5.13	89.62	100.90
1	C	194	ILE	CA-C-N	5.12	127.57	120.29
1	C	194	ILE	C-N-CA	5.12	127.57	120.29
1	E	328	LYS	O-C-N	5.12	129.14	122.89
1	I	271	MET	CG-SD-CE	-5.11	89.65	100.90
1	C	216	GLU	O-C-N	-5.11	116.32	122.15
2	H	162	TYR	N-CA-CB	5.10	117.62	110.12
1	B	216	GLU	O-C-N	-5.10	116.33	122.15
2	G	136	LYS	N-CA-C	5.10	116.92	111.36
1	A	374	ARG	N-CA-C	-5.10	107.23	113.50
1	F	216	GLU	O-C-N	-5.10	116.34	122.15
1	B	235	SER	N-CA-C	-5.09	100.79	108.52
1	B	325	SER	O-C-N	-5.09	113.18	122.34
1	A	194	ILE	CA-C-N	5.08	127.51	120.29
1	A	194	ILE	C-N-CA	5.08	127.51	120.29
1	I	59	GLU	CA-C-N	5.08	127.50	120.29
1	I	59	GLU	C-N-CA	5.08	127.50	120.29
1	I	202	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	135	TYR	N-CA-C	-5.08	101.02	108.99
1	A	216	GLU	O-C-N	-5.08	116.36	122.15
1	F	202	PHE	CA-CB-CG	-5.07	108.73	113.80
1	I	235	SER	N-CA-C	-5.07	100.81	108.52
1	B	292	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	A	235	SER	N-CA-C	-5.06	100.82	108.52
1	E	374	ARG	N-CA-C	-5.06	107.27	113.50
2	G	116	ALA	CB-CA-C	-5.06	102.25	110.85
2	H	104	GLU	CA-C-N	5.05	127.05	120.28
2	H	104	GLU	C-N-CA	5.05	127.05	120.28
1	F	59	GLU	CA-C-N	5.05	127.47	120.29
1	F	59	GLU	C-N-CA	5.05	127.47	120.29
1	B	116	ALA	CA-C-N	5.05	127.46	120.29
1	B	116	ALA	C-N-CA	5.05	127.46	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	SER	N-CA-C	-5.05	100.84	108.52
1	E	135	TYR	N-CA-C	-5.05	101.06	108.99
2	G	167	ARG	CG-CD-NE	-5.05	100.89	112.00
2	H	127	MET	CG-SD-CE	-5.05	89.79	100.90
1	E	210	ILE	CA-C-N	5.05	127.38	120.46
1	E	210	ILE	C-N-CA	5.05	127.38	120.46
1	F	139	GLN	OE1-CD-NE2	-5.05	117.55	122.60
2	G	113	LEU	N-CA-CB	5.05	117.33	110.01
1	E	235	SER	N-CA-C	-5.04	100.85	108.52
1	A	11	VAL	N-CA-C	-5.04	100.39	107.75
1	A	116	ALA	CA-C-N	5.04	127.45	120.29
1	A	116	ALA	C-N-CA	5.04	127.45	120.29
2	H	266	LYS	O-C-N	5.04	127.47	122.12
1	E	116	ALA	CA-C-N	5.04	127.45	120.29
1	E	116	ALA	C-N-CA	5.04	127.45	120.29
1	E	11	VAL	N-CA-C	-5.04	100.39	107.75
1	I	116	ALA	CA-C-N	5.04	127.44	120.29
1	I	116	ALA	C-N-CA	5.04	127.44	120.29
1	I	326	THR	CA-CB-CG2	5.04	119.06	110.50
1	C	235	SER	N-CA-C	-5.03	100.87	108.52
1	F	235	SER	N-CA-C	-5.03	100.88	108.52
1	C	192	MET	O-C-N	-5.03	116.79	122.12
1	I	202	PHE	O-C-N	-5.02	117.43	123.31
2	G	125	ARG	CA-C-N	5.02	125.51	119.94
2	G	125	ARG	C-N-CA	5.02	125.51	119.94
1	F	116	ALA	CA-C-N	5.02	127.41	120.29
1	F	116	ALA	C-N-CA	5.02	127.41	120.29
2	H	184	GLU	O-C-N	5.01	127.43	122.12
1	E	107	LEU	N-CA-C	-5.01	102.10	110.17
1	A	107	LEU	N-CA-C	-5.01	102.11	110.17
2	H	127	MET	CA-C-O	-5.01	115.56	120.82
2	H	126	GLY	O-C-N	5.01	127.09	122.13
2	G	100	ASP	CA-C-N	5.00	126.99	120.28
2	G	100	ASP	C-N-CA	5.00	126.99	120.28
1	E	153	ILE	CA-C-O	-5.00	115.02	120.72
2	H	172	ILE	CA-C-O	-5.00	115.75	120.95

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	179	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	281	TYR	Sidechain
1	A	292	ARG	Sidechain
1	A	296	TYR	Sidechain
1	B	364	TYR	Sidechain
1	C	212	ARG	Sidechain
1	D	212	ARG	Sidechain
1	D	326	THR	Mainchain
1	E	168	TYR	Sidechain
1	E	179	ARG	Sidechain
1	E	212	ARG	Sidechain
1	E	281	TYR	Sidechain
1	E	292	ARG	Sidechain
1	E	296	TYR	Sidechain
1	E	71	TYR	Sidechain
1	F	212	ARG	Sidechain
1	F	364	TYR	Sidechain
1	F	71	TYR	Sidechain
2	G	105	ARG	Sidechain
2	G	160	ARG	Sidechain
2	H	214	TYR	Sidechain
2	H	267	TYR	Sidechain
1	I	212	ARG	Sidechain
1	I	71	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2907	0	2877	10	0
1	B	2907	0	2877	9	0
1	C	2907	0	2877	2	0
1	D	2907	0	2877	8	0
1	E	2907	0	2877	12	0
1	F	2907	0	2877	39	0
1	I	2907	0	2877	51	0
2	G	1458	0	1458	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1458	0	1458	22	0
All	All	23265	0	23055	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:GLU:C	1:I:115:LYS:HE2	1.56	1.31
1:E:330:LYS:NZ	2:G:257:GLU:CD	1.93	1.27
2:H:138:GLU:OE2	1:I:330:LYS:HD2	1.57	1.02
1:E:330:LYS:HZ1	2:G:257:GLU:CD	1.56	1.01
1:F:197:GLU:O	1:I:115:LYS:HE2	1.58	1.01
1:D:197:GLU:C	1:F:115:LYS:HE2	1.92	0.95
1:F:41:ARG:CZ	1:I:272:GLU:CD	2.44	0.91
1:E:330:LYS:NZ	2:G:257:GLU:OE2	1.95	0.90
2:H:138:GLU:CD	1:I:330:LYS:HD2	1.96	0.90
1:D:197:GLU:O	1:F:115:LYS:HE2	1.73	0.87
1:E:330:LYS:HZ3	2:G:257:GLU:CD	1.67	0.87
1:F:198:ARG:N	1:I:115:LYS:HE2	1.88	0.86
1:F:41:ARG:NE	1:I:272:GLU:OE2	2.09	0.84
2:H:138:GLU:CD	1:I:330:LYS:CE	2.52	0.82
1:F:197:GLU:O	1:I:115:LYS:HG3	1.78	0.82
2:H:138:GLU:OE1	1:I:330:LYS:CE	2.28	0.82
1:F:197:GLU:O	1:I:115:LYS:CE	2.28	0.80
1:F:198:ARG:HA	1:I:115:LYS:HE3	1.61	0.80
2:H:138:GLU:OE1	1:I:330:LYS:HE3	1.81	0.79
2:H:128:LYS:HG2	1:I:335:PRO:CB	2.12	0.79
1:F:41:ARG:NH2	1:I:272:GLU:HA	1.98	0.79
1:F:41:ARG:NH1	1:I:272:GLU:CD	2.41	0.78
2:H:138:GLU:OE1	1:I:330:LYS:NZ	2.18	0.76
1:F:198:ARG:HA	1:I:115:LYS:CE	2.16	0.75
2:H:138:GLU:CD	1:I:330:LYS:CD	2.59	0.75
1:F:41:ARG:CZ	1:I:272:GLU:CG	2.66	0.74
2:H:138:GLU:OE2	1:I:330:LYS:CD	2.35	0.74
2:H:138:GLU:CD	1:I:330:LYS:NZ	2.47	0.72
2:H:138:GLU:HB3	1:I:330:LYS:NZ	2.06	0.69
1:F:41:ARG:NH2	1:I:272:GLU:CB	2.57	0.68
1:F:197:GLU:O	1:I:115:LYS:CG	2.42	0.67
1:A:115:LYS:HE2	1:E:198:ARG:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ARG:CZ	1:I:272:GLU:OE2	2.46	0.60
1:A:197:GLU:O	1:B:115:LYS:HE2	2.02	0.60
1:F:41:ARG:NH2	1:I:272:GLU:CA	2.65	0.58
1:F:198:ARG:CA	1:I:115:LYS:CE	2.81	0.58
1:A:115:LYS:CE	1:E:198:ARG:HA	2.36	0.56
1:A:197:GLU:C	1:B:115:LYS:HE2	2.30	0.55
1:F:41:ARG:NH2	1:I:272:GLU:HB3	2.20	0.55
1:D:197:GLU:O	1:F:115:LYS:HG3	2.09	0.53
1:F:198:ARG:CA	1:I:115:LYS:HE2	2.38	0.53
1:D:198:ARG:HA	1:F:115:LYS:CE	2.39	0.53
2:H:128:LYS:HG2	1:I:335:PRO:HB3	1.88	0.52
1:A:175:HIS:CE1	1:E:270:GLY:HA3	2.45	0.52
1:D:197:GLU:O	1:F:115:LYS:CE	2.53	0.51
2:H:138:GLU:HB3	1:I:330:LYS:HZ1	1.74	0.51
1:D:198:ARG:N	1:F:115:LYS:HE2	2.26	0.51
1:A:115:LYS:HE2	1:E:197:GLU:O	2.12	0.50
1:B:217:LYS:HE2	2:G:195:GLU:OE1	2.12	0.50
1:F:198:ARG:N	1:I:115:LYS:CE	2.70	0.49
2:H:138:GLU:CB	1:I:330:LYS:NZ	2.74	0.49
1:B:327:MET:HE3	1:E:246:ASP:HA	1.95	0.49
2:H:138:GLU:CB	1:I:330:LYS:HZ1	2.26	0.48
1:A:198:ARG:HA	1:B:115:LYS:CE	2.45	0.47
1:D:198:ARG:HA	1:F:115:LYS:HE3	1.95	0.47
1:F:41:ARG:CZ	1:I:272:GLU:HG2	2.45	0.47
1:A:198:ARG:HA	1:B:115:LYS:HE2	1.97	0.46
1:F:41:ARG:NH2	1:I:272:GLU:CG	2.79	0.46
1:F:199:GLY:HA2	1:I:114:PRO:HB3	1.98	0.46
1:A:115:LYS:HE2	1:E:197:GLU:C	2.40	0.46
2:H:138:GLU:HB3	1:I:330:LYS:HZ2	1.79	0.46
1:F:41:ARG:CZ	1:I:272:GLU:CB	2.95	0.45
1:F:41:ARG:HH22	1:I:272:GLU:HB3	1.81	0.44
2:G:260:LEU:CD1	2:H:263:GLN:HG2	2.48	0.44
1:C:247:GLY:HA3	1:F:324:PRO:HB2	1.99	0.44
1:F:197:GLU:O	1:I:115:LYS:CD	2.65	0.44
1:B:327:MET:HA	1:B:327:MET:HE2	2.00	0.43
2:G:183:ALA:HA	2:H:183:ALA:HA	2.01	0.43
2:H:138:GLU:CG	1:I:330:LYS:NZ	2.82	0.43
1:F:41:ARG:NH1	1:I:272:GLU:OE1	2.52	0.42
2:H:128:LYS:HG2	1:I:335:PRO:HB2	1.94	0.42
2:G:169:LEU:HD13	2:H:169:LEU:HD13	2.01	0.42
1:I:125:MET:HA	1:I:125:MET:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:MET:HA	1:B:125:MET:HE2	2.02	0.42
1:E:125:MET:HA	1:E:125:MET:HE2	2.02	0.42
1:F:125:MET:HA	1:F:125:MET:HE2	2.02	0.42
1:A:125:MET:HA	1:A:125:MET:HE2	2.02	0.42
1:C:125:MET:HA	1:C:125:MET:HE2	2.02	0.42
1:F:41:ARG:CZ	1:I:272:GLU:HB3	2.50	0.42
1:F:41:ARG:HH22	1:I:272:GLU:CB	2.33	0.41
2:H:128:LYS:HG2	1:I:335:PRO:CG	2.50	0.41
1:B:326:THR:HB	1:E:247:GLY:HA2	2.02	0.41
1:D:247:GLY:HA3	1:I:324:PRO:HB2	2.03	0.41
1:F:41:ARG:HH22	1:I:272:GLU:HA	1.81	0.41
2:G:156:GLU:HB3	2:G:160:ARG:HH11	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/372 (100%)	351 (95%)	16 (4%)	3 (1%)	16	54
1	B	370/372 (100%)	352 (95%)	15 (4%)	3 (1%)	16	54
1	C	370/372 (100%)	352 (95%)	16 (4%)	2 (0%)	24	63
1	D	370/372 (100%)	349 (94%)	20 (5%)	1 (0%)	36	72
1	E	370/372 (100%)	353 (95%)	14 (4%)	3 (1%)	16	54
1	F	370/372 (100%)	355 (96%)	12 (3%)	3 (1%)	16	54
1	I	370/372 (100%)	356 (96%)	12 (3%)	2 (0%)	24	63
2	G	177/179 (99%)	177 (100%)	0	0	100	100
2	H	177/179 (99%)	175 (99%)	2 (1%)	0	100	100
All	All	2944/2962 (99%)	2820 (96%)	107 (4%)	17 (1%)	23	59

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	LEU
1	B	182	LEU
1	E	182	LEU
1	F	182	LEU
1	I	182	LEU
1	A	183	ALA
1	B	183	ALA
1	C	17	GLY
1	E	183	ALA
1	F	183	ALA
1	I	183	ALA
1	B	17	GLY
1	F	169	GLU
1	A	17	GLY
1	E	17	GLY
1	D	17	GLY
1	C	160	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/315 (100%)	312 (99%)	3 (1%)	68	78
1	B	315/315 (100%)	310 (98%)	5 (2%)	55	70
1	C	315/315 (100%)	312 (99%)	3 (1%)	68	78
1	D	315/315 (100%)	313 (99%)	2 (1%)	78	83
1	E	315/315 (100%)	312 (99%)	3 (1%)	68	78
1	F	315/315 (100%)	311 (99%)	4 (1%)	61	74
1	I	315/315 (100%)	309 (98%)	6 (2%)	50	67
2	G	156/156 (100%)	153 (98%)	3 (2%)	50	67
2	H	156/156 (100%)	152 (97%)	4 (3%)	40	62
All	All	2517/2517 (100%)	2484 (99%)	33 (1%)	59	74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	MET
1	A	346	SER
1	A	370	SER
1	B	125	MET
1	B	212	ARG
1	B	293	LYS
1	B	326	THR
1	B	346	SER
1	C	66	ILE
1	C	125	MET
1	C	204	THR
1	D	204	THR
1	D	328	LYS
1	E	125	MET
1	E	346	SER
1	E	370	SER
1	F	40	PRO
1	F	62	SER
1	F	87	ILE
1	F	125	MET
2	G	144	GLN
2	G	149	LYS
2	G	201	THR
2	H	99	LEU
2	H	108	THR
2	H	139	GLU
2	H	263	GLN
1	I	40	PRO
1	I	62	SER
1	I	87	ILE
1	I	125	MET
1	I	326	THR
1	I	370	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	139	GLN
1	A	175	HIS
1	A	248	GLN

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Mol	Chain	Res	Type
1	A	316	GLN
1	B	42	HIS
1	B	90	HIS
1	B	130	ASN
1	B	163	HIS
1	B	298	ASN
1	B	299	ASN
1	B	316	GLN
1	C	90	HIS
1	C	123	GLN
1	D	90	HIS
1	D	123	GLN
1	D	139	GLN
1	D	299	ASN
1	D	316	GLN
1	E	90	HIS
1	E	130	ASN
1	E	139	GLN
1	E	316	GLN
1	F	130	ASN
1	F	248	GLN
1	F	316	GLN
2	G	135	GLN
2	G	153	HIS
2	G	210	GLN
2	G	216	GLN
2	H	153	HIS
1	I	130	ASN
1	I	163	HIS
1	I	248	GLN
1	I	316	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

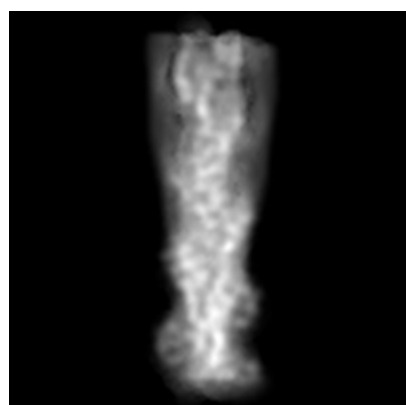
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18147. These allow visual inspection of the internal detail of the map and identification of artifacts.

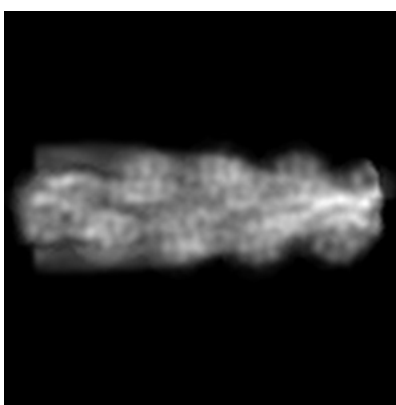
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

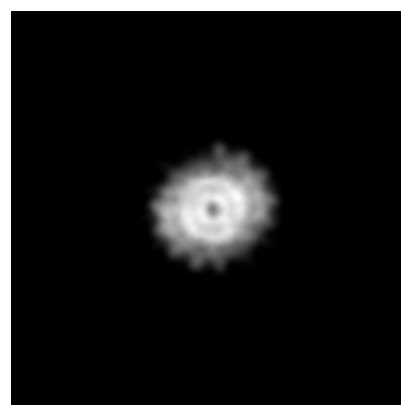
6.1.1 Primary map



X



Y

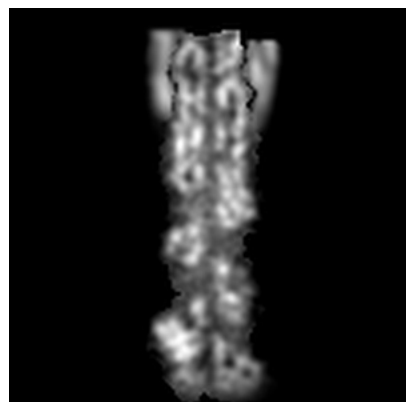


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 64



Y Index: 64

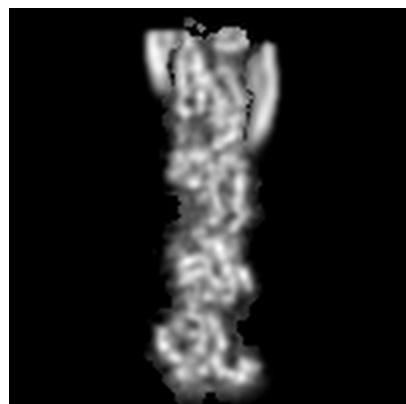


Z Index: 64

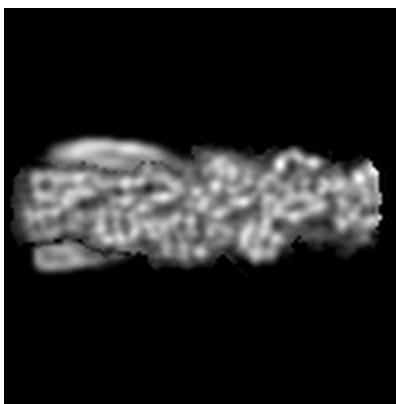
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 67



Y Index: 67

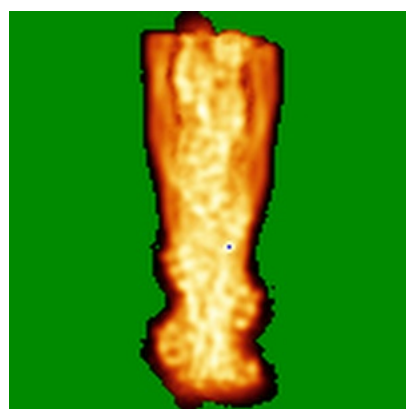


Z Index: 88

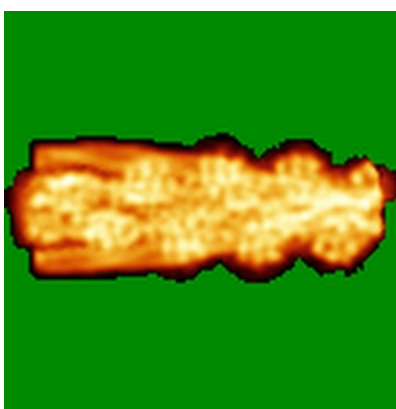
The images above show the largest variance slices of the map in three orthogonal directions.

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

This section was not generated.

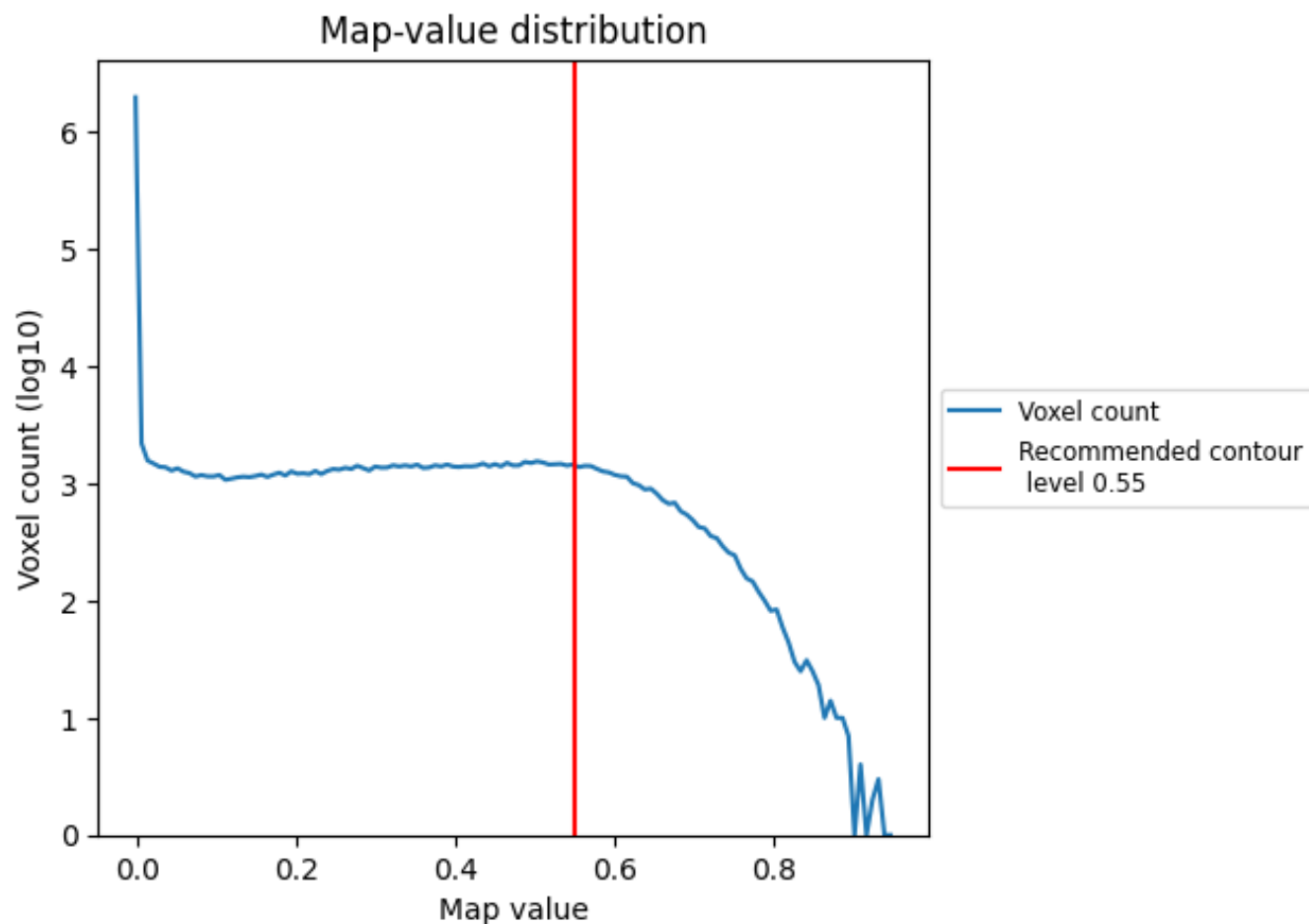
6.6 Mask visualisation

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

7 Map analysis [i](#)

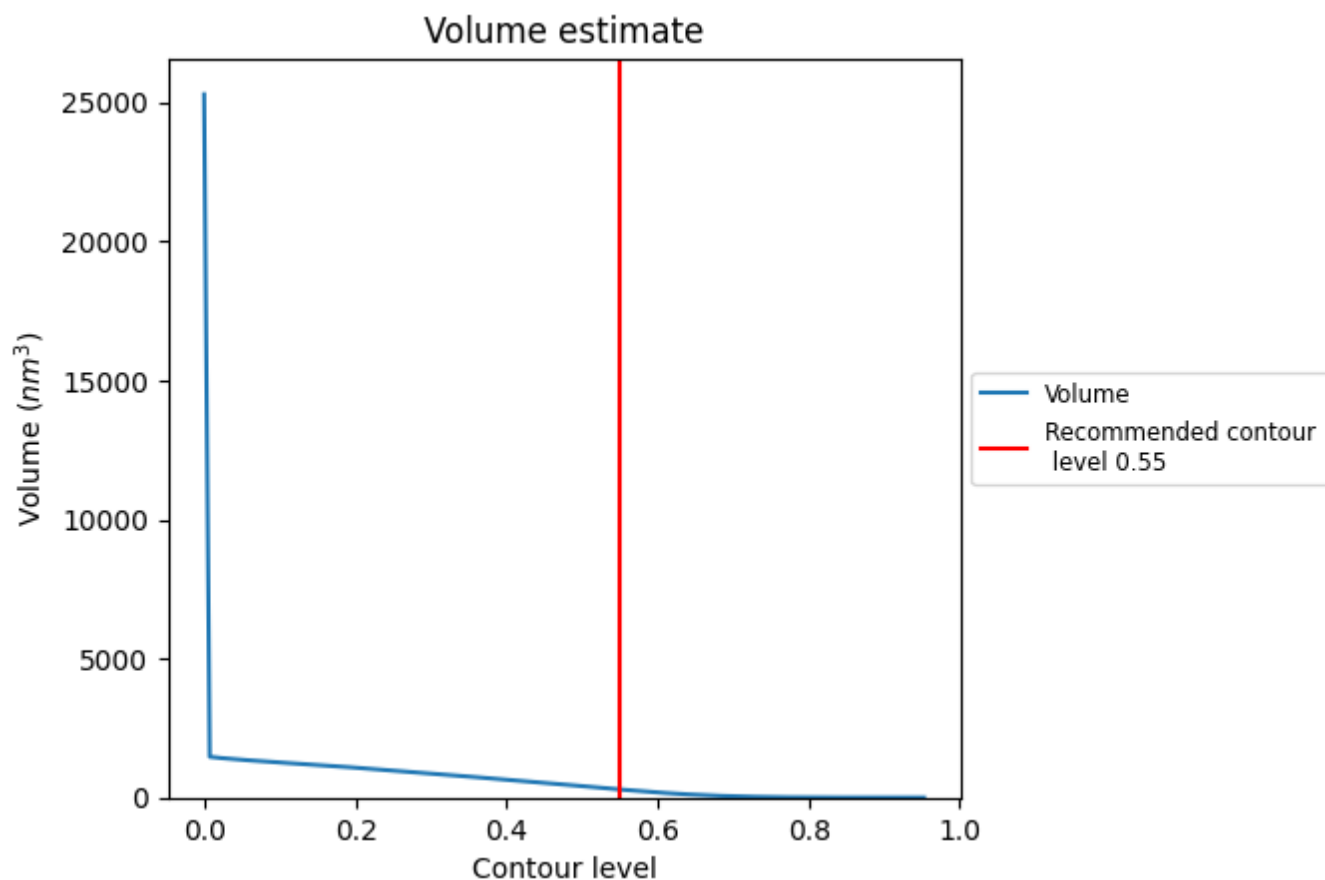
This section contains the results of statistical analysis of the map.

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.

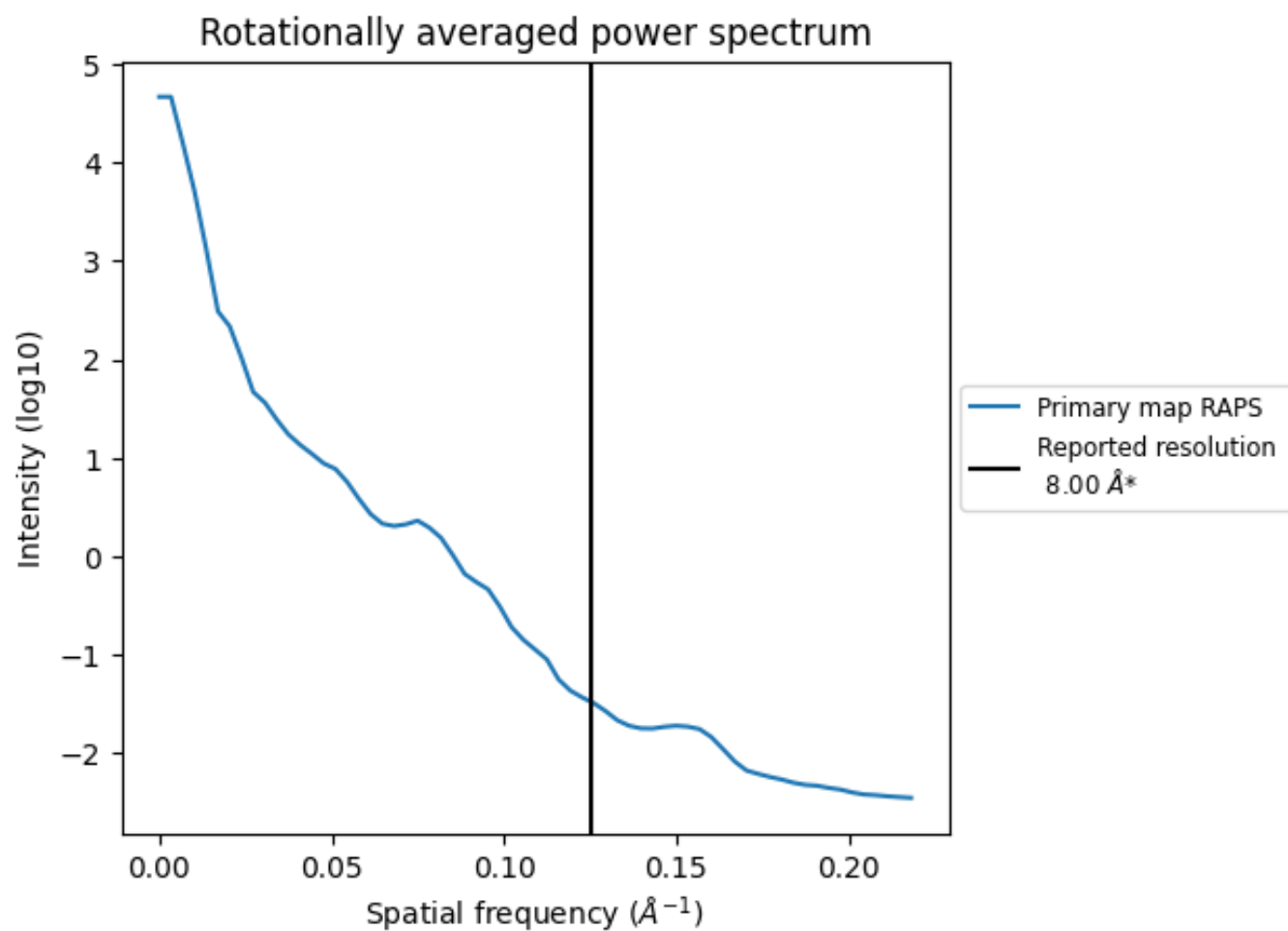
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 292 nm^3 ; this corresponds to an approximate mass of 264 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 0.125 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

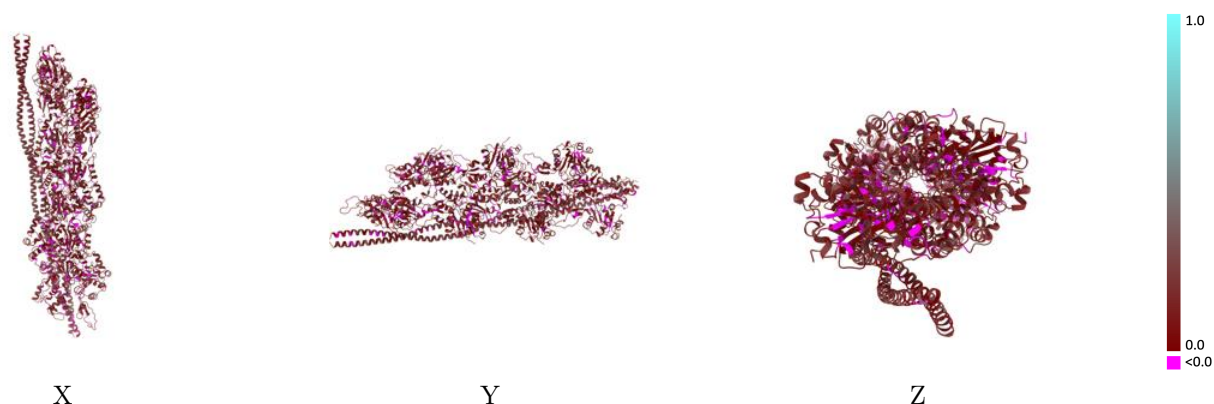
This section contains information regarding the fit between EMDB map EMD-18147 and PDB model 8Q4G. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.55 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](#)

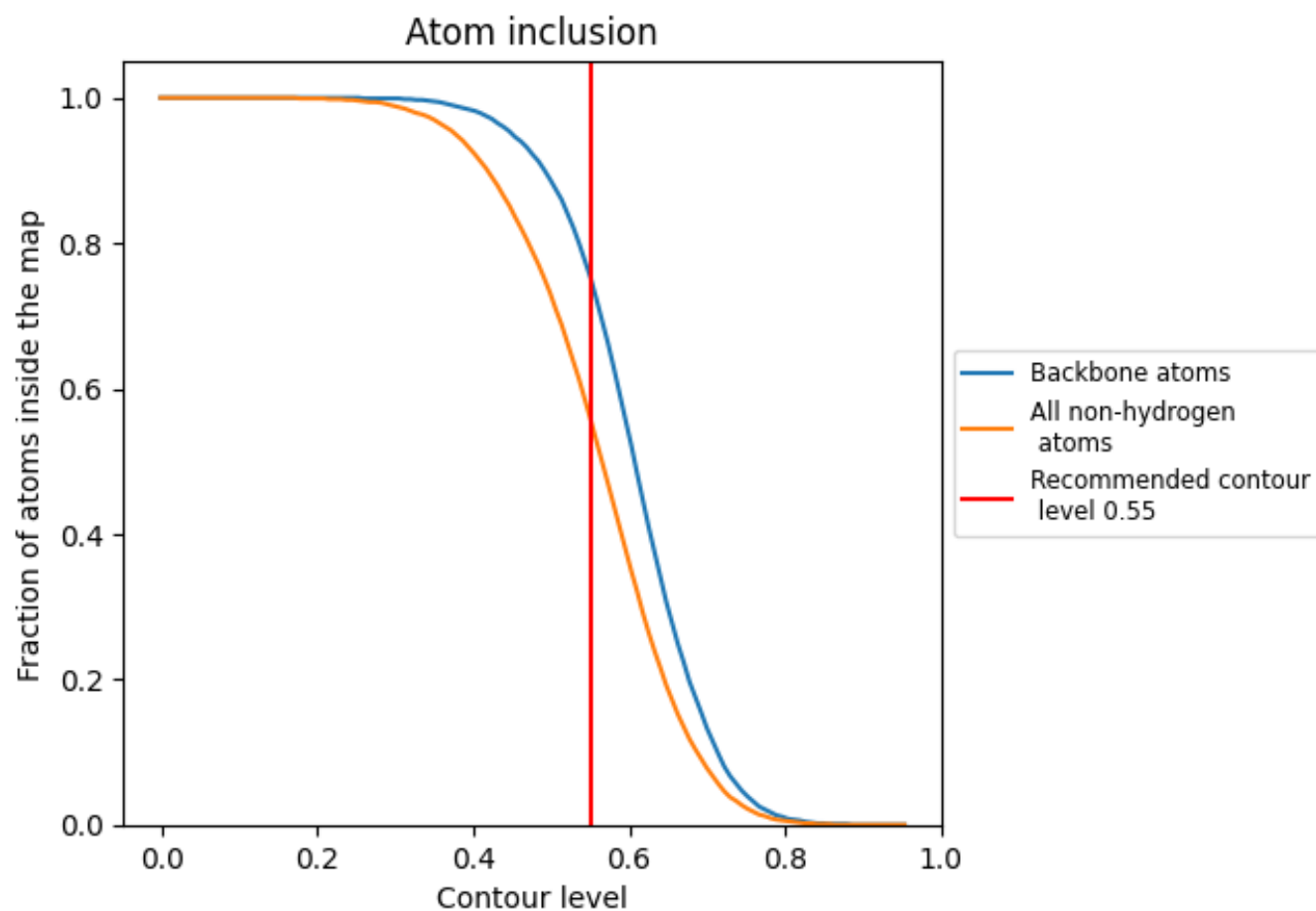


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 56% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5590	0.1290
A	0.5660	0.1270
B	0.5530	0.1260
C	0.5460	0.1220
D	0.5530	0.1240
E	0.5250	0.1220
F	0.5570	0.1240
G	0.6130	0.1630
H	0.6360	0.1650
I	0.5460	0.1240

1.0

0.0

<0.0