



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:11 PM UTC

PDB ID : 9I8M / pdb_00009i8m
EMDB ID : EMD-52729
Title : NEDD1-bound native vertebrate gamma-tubulin ring complex from *Xenopus laevis*, focused reconstruction
Authors : Vermeulen, B.J.A.; Pfeffer, S.
Deposited on : 2025-02-05
Resolution : 4.30 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:

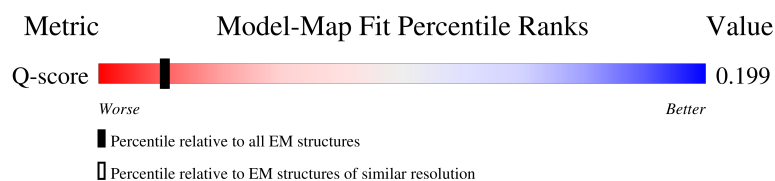
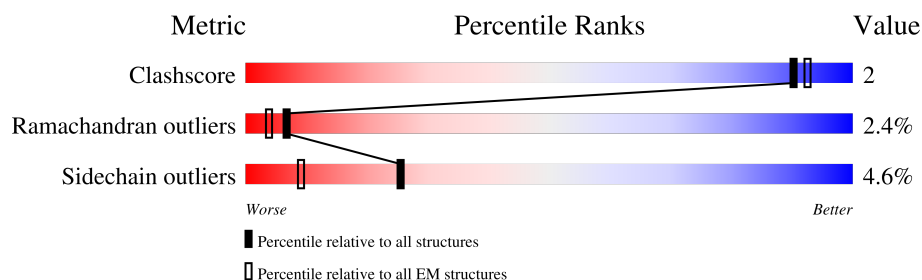
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.30 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	4585 (3.80 - 4.80)

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	896	13% 14% 14% . 69%
1	C	896	7% 13% 13% . 72%
1	E	896	16% 12% 14% . 72%
1	G	896	7% 14% 12% . 72%

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Mol	Chain	Length	Quality of chain
2	B	906	
2	D	906	
2	F	906	
2	H	906	
2	O	906	
2	Q	906	
2	R	906	
2	S	906	
2	T	906	
3	I	666	
3	K	666	
4	J	1019	
5	L	1698	
6	U	671	
6	V	671	
6	W	671	
6	X	671	
7	o	72	
7	p	72	
7	q	72	
7	r	72	
7	s	72	
7	t	72	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 37358 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 Gamma-tubulin complex component.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	275	Total	C	N	O	S	0	0
			2211	1412	369	421	9		
1	C	250	Total	C	N	O	S	0	0
			2014	1289	336	382	7		
1	E	253	Total	C	N	O	S	0	0
			2038	1306	340	385	7		
1	G	250	Total	C	N	O	S	0	0
			2014	1289	336	382	7		

- Molecule 2 is a protein called Gamma-tubulin complex component 3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	294	Total	C	N	O	S	0	0
			2363	1517	401	434	11		
2	D	254	Total	C	N	O	S	0	0
			2059	1324	351	375	9		
2	F	242	Total	C	N	O	S	0	0
			1964	1263	337	355	9		
2	H	263	Total	C	N	O	S	0	0
			2135	1374	363	389	9		
2	O	93	Total	C	N	O	S	0	0
			753	480	137	134	2		
2	Q	109	Total	C	N	O	S	0	0
			878	557	160	159	2		
2	R	98	Total	C	N	O	S	0	0
			794	503	144	145	2		
2	S	109	Total	C	N	O	S	0	0
			878	557	160	159	2		
2	T	93	Total	C	N	O	S	0	0
			753	480	137	134	2		

- Molecule 3 is a protein called Gamma-tubulin complex component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	287	Total	C	N	O	S	0	0
			2325	1500	394	418	13		
3	K	287	Total	C	N	O	S	0	0
			2325	1500	394	418	13		

- Molecule 4 is a protein called Gamma-tubulin complex component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	352	Total	C	N	O	S	0	0
			2909	1881	493	522	13		

- Molecule 5 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	478	Total	C	N	O	S	0	0
			3794	2449	613	713	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	392	ASP	GLU	conflict	UNP A0A974HT83
L	394	VAL	ILE	conflict	UNP A0A974HT83

- Molecule 6 is a protein called NEDD1 gamma-tubulin ring complex targeting factor L homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
6	V	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
6	W	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
6	X	75	Total	C	N	O	S	0	0
			634	396	112	122	4		

- Molecule 7 is a protein called Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	o	52	Total	C	N	O	S	0	0
			403	248	71	79	5		
7	p	56	Total	C	N	O	S	0	0
			429	263	73	89	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	56	Total	C	N	O	S	0	0
			432	266	76	86	4		
7	r	59	Total	C	N	O	S	0	0
			454	278	80	91	5		
7	s	59	Total	C	N	O	S	0	0
			451	277	79	90	5		
7	t	58	Total	C	N	O	S	0	0
			446	274	78	89	5		

[illegible]

- Molecule 1: Gamma-tubulin complex component

[illegible][illegible][illegible]

ASN
GLN
LYS
SER
ALA
PRO
LEU
LEU
GLY
PRO
ALA
GLN
HIS
ALA
VAL
SER
THR
LYS

- Molecule 1: Gamma-tubulin complex component



ALA PRO ASN THR SER LYS ILE SER MET GLN LEU LEU GLU GLU GLU GLU THR ALA THR THR VAL VAL ALA VAL SER SER HIS GLN PRO PRO VAL VAL VAL LEU ARG ASP LYS LEU ASN LYS LYS HIS HIS GLY GLY VAL PRO PRO VAL VAL VAL LEU ARG ARG ASP LYS ASN LYS LYS THR THR GLY PHE VAL PRO PRO TRP VAL

[illegible][illegible]

E373	L374	C375	A381	A382	A383	A384	A385	A386	F387	D388	L389	L390	E391	R392	A393	L394	Y395	R396	G397	L398	L399	M400	D401	P402	Y403	Y404	A405	F406	M407	V408	E409	E410	H411	GLU	LEU	GLN	LYS	LYS	GLU	LYS	LYS	ILE	GLN	GLU	ASP	TYR	ASN	ASP	LYS	TYR	W427	D428	Q429	R430	Y431	T432	T433	L434	Q435	Q436
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Q437	I438	P439	S440	F441	L442	Q443	K444	V445	A446	D447	K448	I449	L450	S451	T452	G453	K454	V455	L456	N457	V458	VAL	ARG	GLU	CYS	GLY	GLY	HIS	ASP	ASP	ALA	LYS	GLU	ILE	THR	TYR	TYR	LEU	LYS	LYS	GLU	Q481	A482	V483	V484	E485	R486	I487	E488	A489	Y491	N492	Y493	A494	S495
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V497	LEU	ASP	ASP	ASP	PHE	PHE	MET	GLU	GLU	GLU	GLU	LEU	VAL	ALA	HIS	HIS	LEU	ARG	SER	ILE	LYS	HIS	TYR	PHE	PHE	LEU	MET	ASP	GLN	GLY	ASP	ASP	PHE	PHE	VAL	HIS	HIS	PHE	MET	MET	ASP	LEU	THR	GLU	GLU	GLU	LEU	LYS	LYS	PRO	VAL	ASP	ASP	ILE	ILE	PRO	THR	ARG	LEU	GLU	ALA	LEU	GLU
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ALA LEU ARG MET SER THR ALA ASN THR ASP PRO PHE LYS ASP LEU TLE GLU LEU MET PRO HIS ASP LEU THR GLN LEU LEU ANG VAL LEU LEU TLE GLU THR HIS GLN GLU LYS ALA LEU TLE ASN SER ASP PRO THR GLU LEU ALA SER GLY LEU SER PHE

PHE	ASP	TYR	ILE	VAL	LYS	TRP	PRO	LEU	SER	LEU	ILE	ILE	ASN	ARG	LYS	ALA	LEU	THR	TYR	GLN	MET	MET	PHE	PHE	ARG	HIS	HIS	VAL	VAL	GLU	ARG	LEU	LEU	CYS	CYS	ASN	VAL	TRP	ILE	SER	ASN	LYS	LYS	THR	ALA	LYS	GLN	PHE	PHE	LEU	HIS	SER	ALA	LYS	TRP	PHE	ALA
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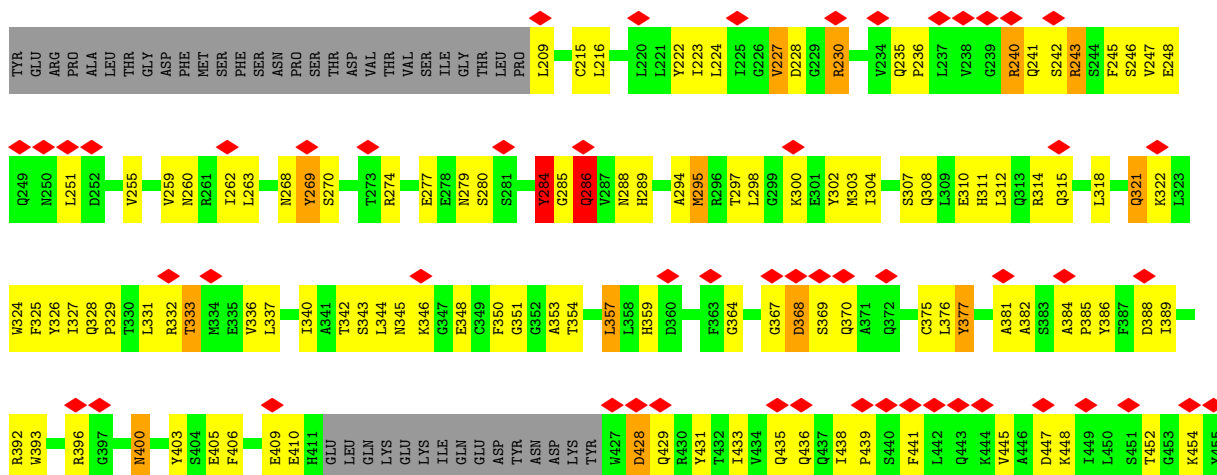
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MET	LEU	THR	THR	ASN	PRO	GLU	LEU	LEU	LEU	ILE	LYS	PHE	SER	LYS	LEU	MET	MET	SER	VAL	CYS	CYS	LEU	GLN	ARG	PHE	THR	GLN	SER	MET	GLN	VAL	GLN	THR	GLU	GLU	GLU	LEU	LEU	THR	HIS	LEU	THR	THR	THR	GLN	CYS	GLU	GLU	ARG	THR	THR	GLU	GLU
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- Molecule 1: Gamma-tubulin complex component



ALA	PRO	ASN	THR	SER	LYS	ILE	SER	MET	GLN	GLU	LEU	GLU	GLU	LEU	ARG	ARG	GLN	LEU	LEU	THR	ALA	THR	THR	VAL	ALA	VAL	SER	SER	CYS	HIS	GLN	PRO	PRO	VAL	GLU	VAL	LEU	LEU	ARG	ASP	LYS	LEU	ASN	LYS	LYS	HIS	THR	GLY	HIS	PRO	PRO	VAL	VAL	PHE	PRO	SER	SER	TRP	VAL
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[illegible]

LYS	HIS	TYR	PHE	LEU	MET	ASP	GLN	GLY	ASP	PHE	PHE	VAL	HIS	PHE	MET	ASP	LEU	THR	GLU	GLU	GLU	LEU	LYS	LYS	PRO	VAL	ASP	ASP	ILE	ILE	PRO	PRO	THR	ARG	LEU	GLU	ALA	LEU	LEU	GLU	LEU	ALA	LEU	ARG	MET	SER	THR	ALA	ASN	THR	ASP	PRO	PHE	LYS	ASP	ASP	LEU	LYS	ILE	ILE
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LEU MET PRO HIS ASP LEU THR GLN LEU ARG VAL LEU ALA ILE GLU THR HIS GLN LYS GLY ALA LEU ILE ASN SER ASP PRO THR GLJ LEU ALA LEU SER GLY LEU GLJ SER SER PHE PHE TYR TYP ILE VAL LYS TRP PRO LEU SER SER SER PHE ASN ARG LYS ALA LEU THR

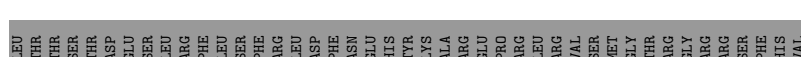
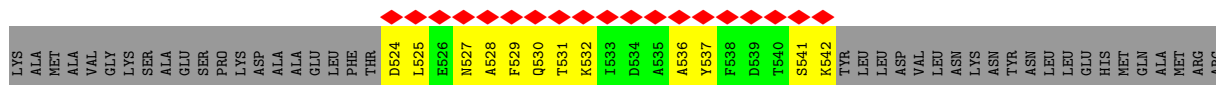
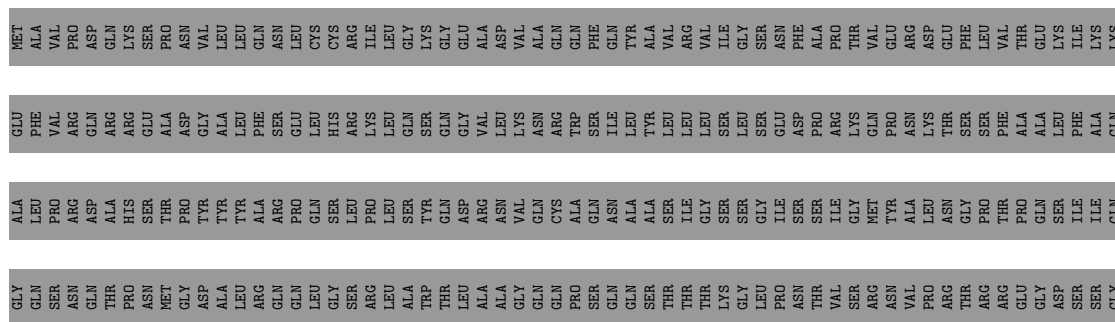
ARG	TYR	GLN	MET	LEU	PHE	ARG	HIS	MET	PHE	TYR	CYS	LYS	HIS	VAL	GLU	ARG	LEU	LEU	CYS	ASN	VAL	TRP	ILE	SER	ASN	LYS	THR	ALA	ALA	LYS	GLN	PHE	GLN	SER	SER	LEU	LEU	HIS	SER	ALA	ALA	LYS	TRP	TRP	ALA	ALA	GLY	ALA	PHE	THR	THR	LEU	LEU	ARG	GLN	GLN	ARG	MET	LEU	MET	ASN	ASN	VAL	PHE	PHE	VAL	GLN	ILE	ILE	GLN	GLN	TYR	TYR
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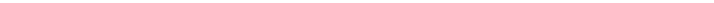
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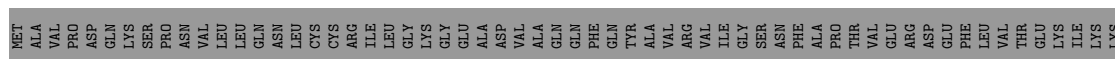
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SER	SER	PHE	GLY	PHE	GLU	SER	THR	THR	ILE	ASN	ASN	PHE	ASP	SER	ASN	PHE	SER	SER	THR	SER	ASP	CYS	GLU	HIS	MET	MET	ILE	ILE	TYR	ARG	LEU	ASP	PHE	ASN	ASN	GLY	PHE	THR	TYR	THR	GLU	ARG	LEU	LYS	GLN	LEU	SER
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- Chain F:  14% 12% 13% 73%



- Molecule 2: Gamma-tubulin complex component 3 homolog



- Molecule 2: Gamma-tubulin complex component 3 homolog

[illegible]



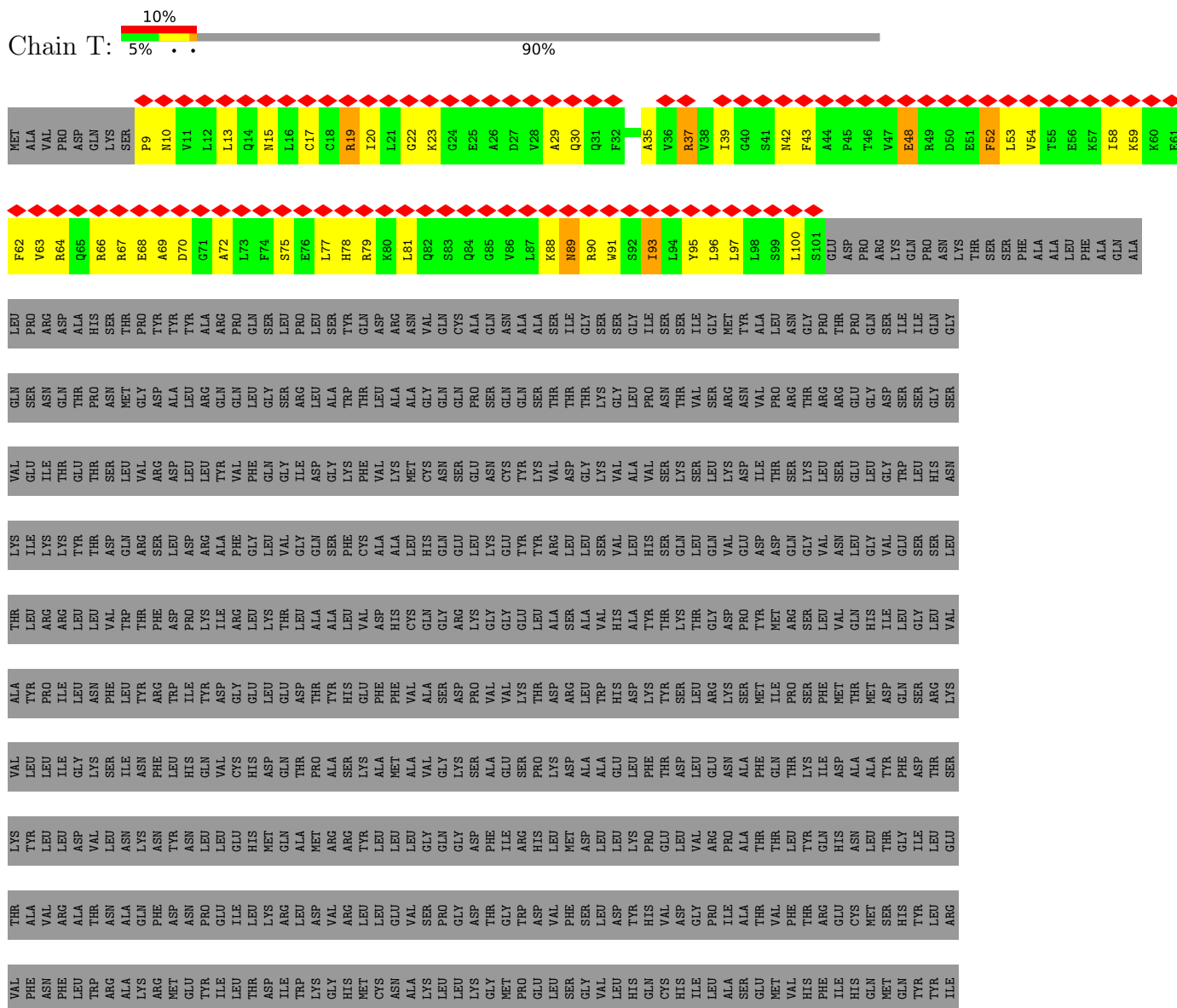
[illegible]

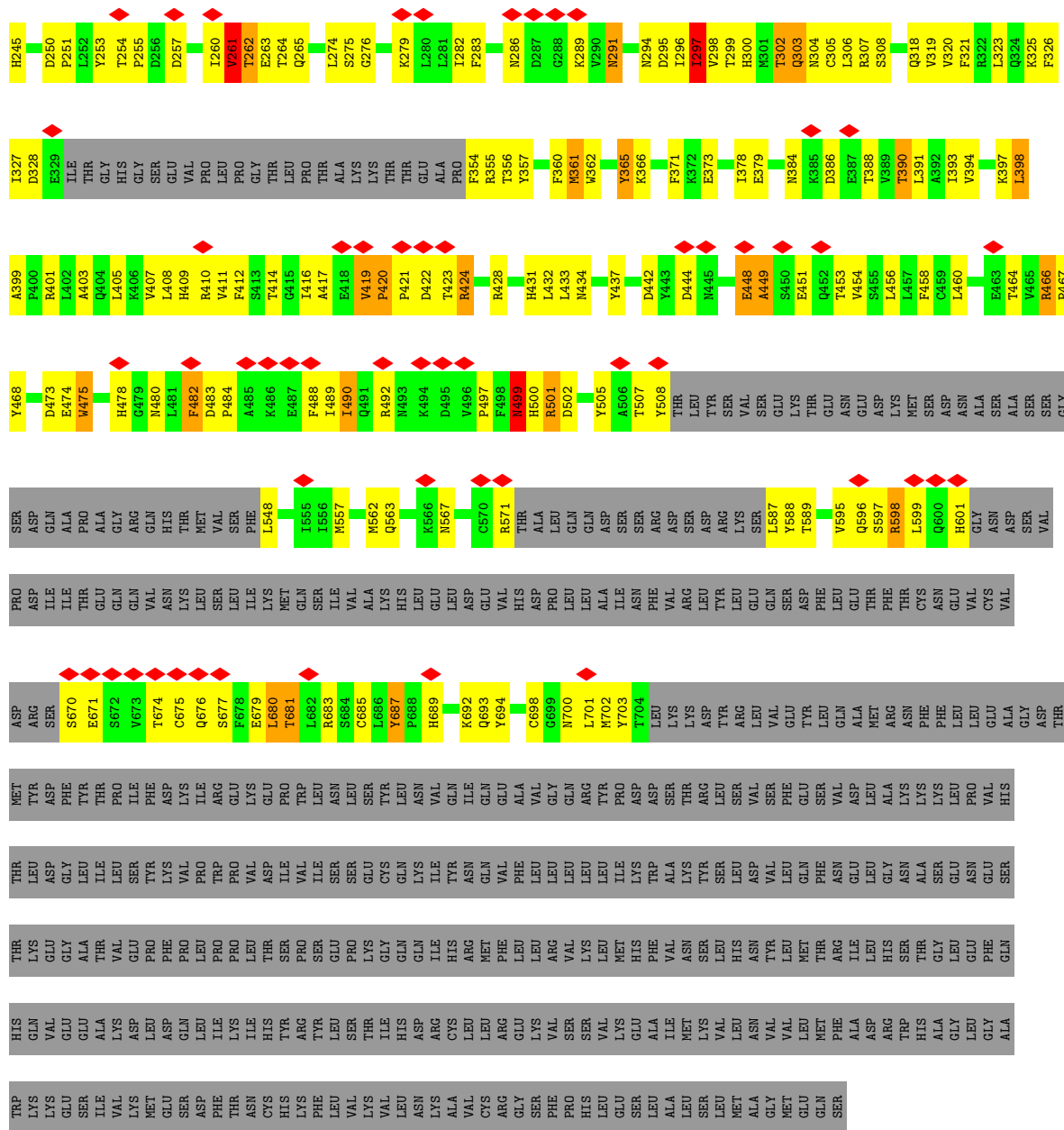
- Molecule 2: Gamma-tubulin complex component 3 homolog



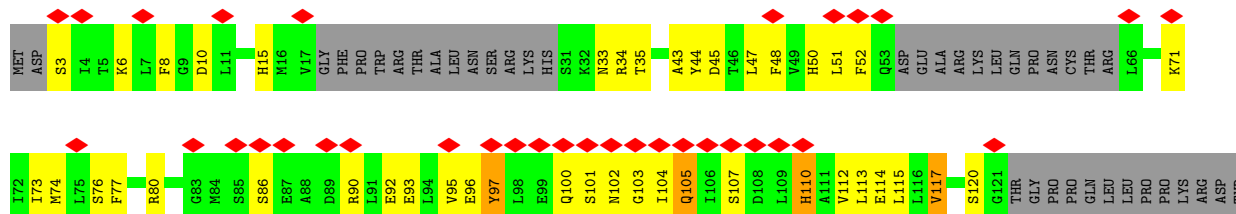
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GLN	LEU	GLN	GLY	THR	LEU	VAL	GLY	GLY	ASP	LEU	LEU	ARG	TYR	A69	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	GLY	ASP	LEU	LEU	ARG	ALA	D70	
CYS	LEU	GLN	GLY	THR	LEU	VAL	GLY	PHE	VAL	GLN	LEU	GLN	PRO	G71	
HIS	LEU	GLN	GLY	THR	LEU	VAL	GLY	GLY	GLY	ASP	LEU	GLN	GLN	A72	
ASP	LEU	GLN	GLY	THR	LEU	VAL	GLY	GLY	ASP	SER	LEU	SER	LEU	L73	
GLN	LEU	GLN	GLY	THR	LEU	VAL	GLY	ILE	ASP	ARG	PRO	LEU	LEU		
THR	LEU	GLN	GLY	THR	LEU	VAL	GLY	ILE	ASP	ARG	PRO	LEU	LEU	H78	
PRO	LEU	GLN	GLY	THR	LEU	VAL	GLY	GLY	ASP	LEU	LEU	SER	GLN	R79	
ALA	LEU	GLN	GLY	THR	LEU	VAL	GLY	GLY	ASP	ALA	THR	TYR	TYR	K80	
SER	LEU	GLN	GLY	THR	LEU	VAL	GLY	PHE	THR	THR	THR	GLN	GLN	L81	
LYS	LEU	GLN	GLY	THR	LEU	VAL	GLY	PHE	THR	THR	LEU	ASP	ASP	Q82	
LYS	LEU	GLN	GLY	THR	LEU	VAL	GLY	VAL	THR	ALA	ALA	ARG	ARG	S83	
ALA	LEU	GLN	GLY	THR	LEU	VAL	GLY	LYS	THR	ALA	ALA	ASN	ASN	N15	
MET	LEU	GLN	GLY	THR	LEU	VAL	GLY	MET	THR	ALA	ALA	ASN	ASN	L16	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	L19	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	ASN	THR	ALA	ALA	GLN	GLN	G84	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	ASN	THR	ALA	ALA	GLN	GLN	G85	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	V86	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	L87	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	R88	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	N89	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	R90	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	K91	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	S92	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	I93	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	L94	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	Y95	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	SER	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	L96	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN	L97	
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS	THR	ALA	ALA	GLN	GLN		
VAL	LEU	GLN	GLY	THR	LEU	VAL	GLY	CYS							

- Molecule 2: Gamma-tubulin complex component 3 homolog



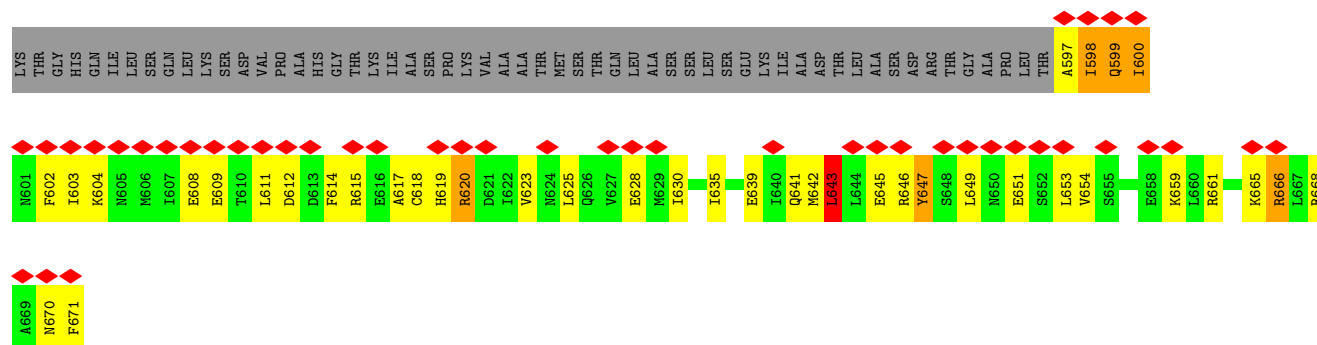


• Molecule 5: Gamma-tubulin complex component 6

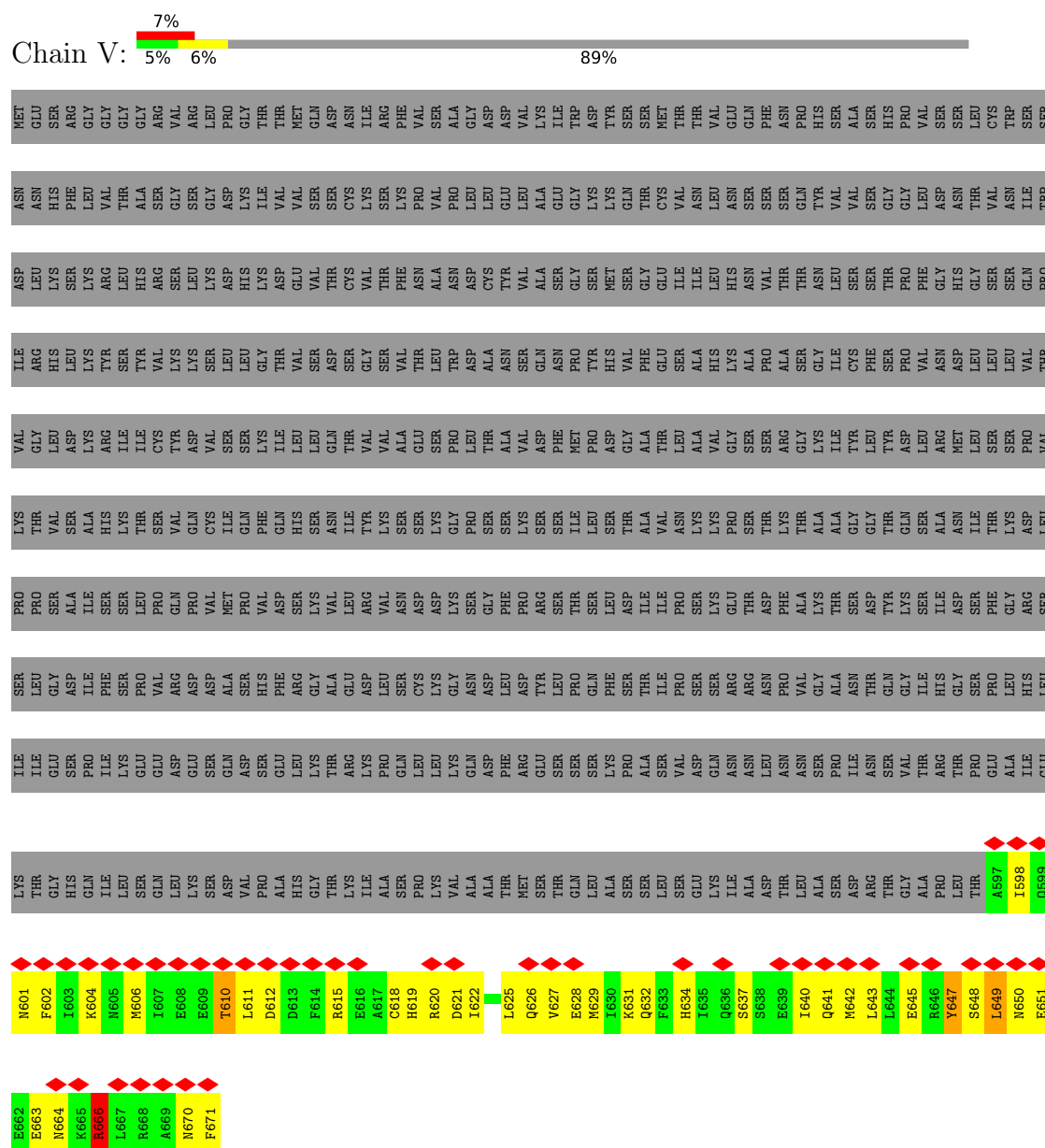




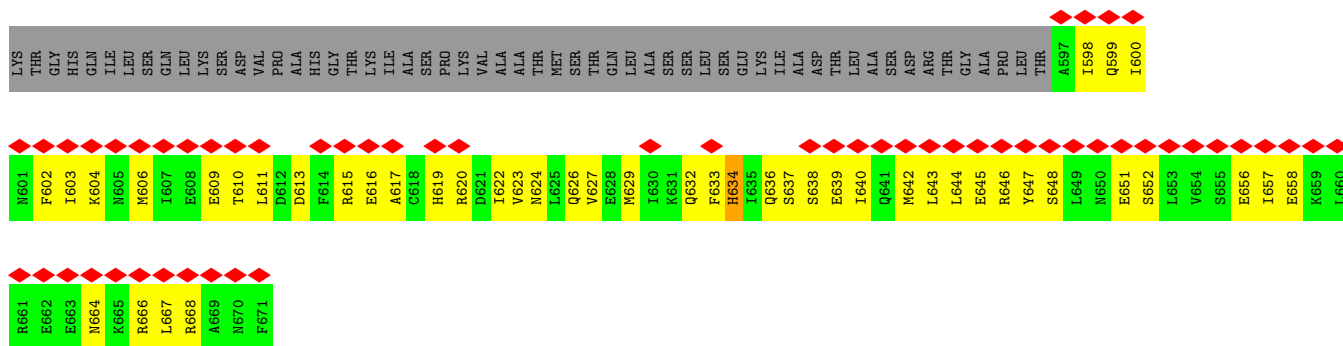


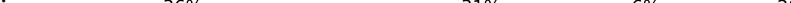


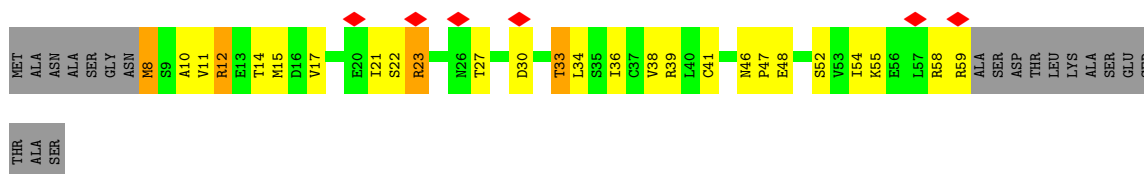
- Molecule 6: NEDD1 gamma-tubulin ring complex targeting factor L homeolog

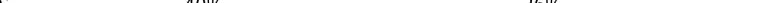


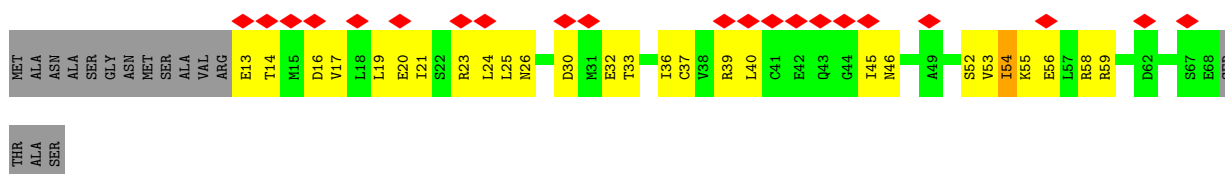
- Molecule 6: NEDD1 gamma-tubulin ring complex targeting factor L homeolog

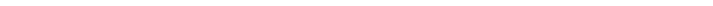


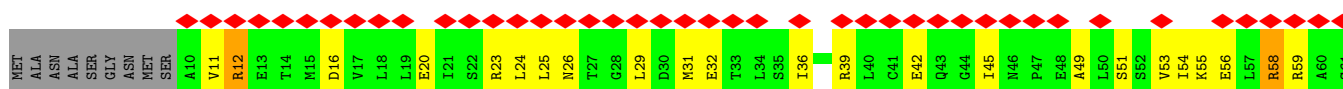
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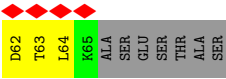


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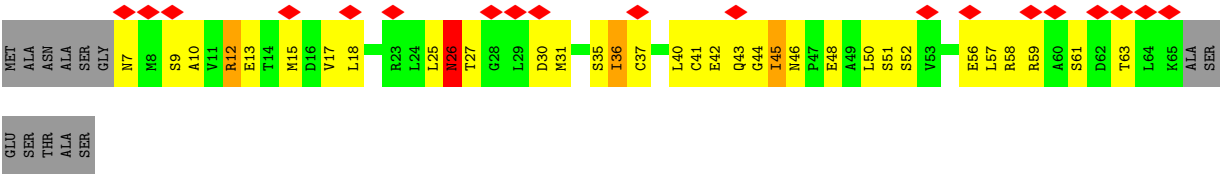


Chain q: 

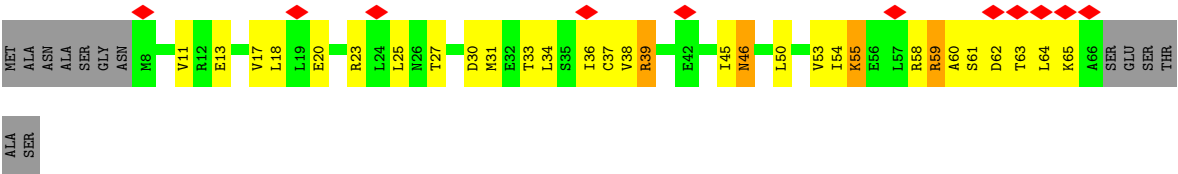




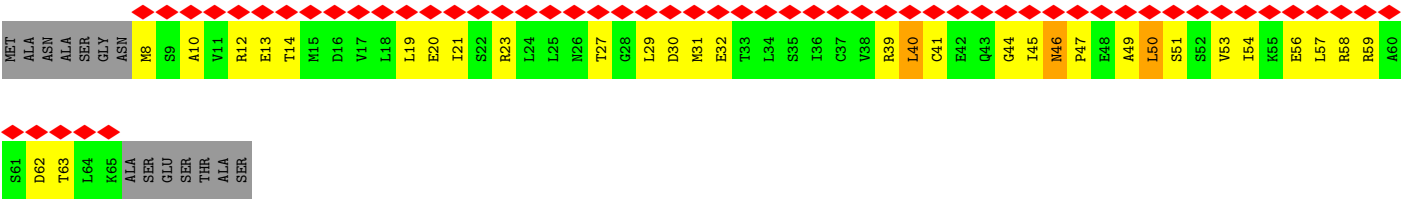
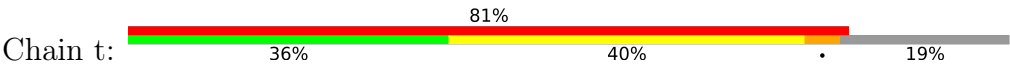
• Molecule 7: Mitotic-spindle organizing protein 1



• Molecule 7: Mitotic-spindle organizing protein 1



• Molecule 7: Mitotic-spindle organizing protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	299022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.286	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0421	Depositor
Map size (Å)	365.9392, 365.9392, 365.9392	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.42945, 1.42945, 1.42945	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.24	75/2254 (3.3%)	2.41	150/3055 (4.9%)
1	C	2.26	80/2053 (3.9%)	2.42	121/2781 (4.4%)
1	E	2.24	63/2077 (3.0%)	2.38	135/2813 (4.8%)
1	G	2.22	64/2053 (3.1%)	2.35	112/2781 (4.0%)
2	B	2.22	81/2413 (3.4%)	2.32	113/3257 (3.5%)
2	D	2.20	68/2101 (3.2%)	2.33	121/2831 (4.3%)
2	F	2.18	71/2004 (3.5%)	2.33	101/2700 (3.7%)
2	H	2.18	71/2178 (3.3%)	2.34	108/2936 (3.7%)
2	O	2.21	21/764 (2.7%)	2.60	69/1026 (6.7%)
2	Q	2.23	27/892 (3.0%)	2.61	82/1199 (6.8%)
2	R	2.30	30/805 (3.7%)	2.45	41/1081 (3.8%)
2	S	2.23	25/892 (2.8%)	2.53	69/1199 (5.8%)
2	T	2.27	25/764 (3.3%)	2.59	53/1026 (5.2%)
3	I	2.25	70/2377 (2.9%)	2.38	154/3212 (4.8%)
3	K	2.24	81/2377 (3.4%)	2.30	116/3212 (3.6%)
4	J	2.45	98/2976 (3.3%)	2.43	176/4037 (4.4%)
5	L	2.22	143/3862 (3.7%)	2.42	257/5228 (4.9%)
6	U	2.24	19/640 (3.0%)	2.66	62/854 (7.3%)
6	V	2.18	18/640 (2.8%)	2.65	53/854 (6.2%)
6	W	2.27	21/640 (3.3%)	2.44	41/854 (4.8%)
6	X	2.29	26/640 (4.1%)	2.61	49/854 (5.7%)
7	o	2.26	14/403 (3.5%)	2.45	27/541 (5.0%)
7	p	2.27	12/429 (2.8%)	2.66	42/577 (7.3%)
7	q	2.32	18/432 (4.2%)	2.50	24/581 (4.1%)
7	r	2.28	16/454 (3.5%)	2.65	41/610 (6.7%)
7	s	2.38	25/451 (5.5%)	2.40	31/606 (5.1%)
7	t	2.24	12/446 (2.7%)	2.72	41/599 (6.8%)
All	All	2.25	1274/38017 (3.4%)	2.42	2389/51304 (4.7%)

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	C	0	6
1	E	0	8
1	G	0	10
2	B	0	5
2	D	0	6
2	F	0	10
2	H	0	11
2	O	0	2
2	Q	0	2
2	R	0	3
2	S	0	3
2	T	0	2
3	I	0	9
3	K	0	6
4	J	0	16
5	L	0	20
6	U	0	4
6	V	0	2
6	W	0	4
6	X	0	4
7	o	0	2
7	q	0	2
7	r	0	1
7	s	0	1
7	t	0	1
All	All	0	146

All (1274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	16	ILE	CG1-CD1	33.79	2.83	1.51
4	J	242	TRP	CD2-CE3	33.30	1.93	1.40
4	J	242	TRP	CZ2-CH2	26.19	1.87	1.37
4	J	242	TRP	CE2-CZ2	24.86	1.92	1.39
4	J	242	TRP	CD2-CE2	22.39	1.79	1.41
4	J	242	TRP	CZ3-CH2	16.81	1.82	1.40
4	J	242	TRP	CE3-CZ3	14.80	1.83	1.38
2	F	269	ASN	CA-C	-11.87	1.47	1.53
4	J	291	ASN	CA-C	-11.28	1.39	1.52
1	C	447	ASP	N-CA	-10.78	1.33	1.46
2	R	43	PHE	CA-C	-10.63	1.39	1.52
2	F	477	ASP	CA-C	-10.18	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	25	LEU	CA-CB	10.10	1.60	1.53
7	t	27	THR	C-N	9.94	1.40	1.33
1	C	227	VAL	CA-C	-9.67	1.42	1.52
3	I	295	ARG	NE-CZ	9.63	1.43	1.33
2	H	311	SER	C-N	9.45	1.42	1.32
2	B	360	SER	CA-C	-9.44	1.40	1.52
2	H	434	TYR	CA-C	-9.36	1.40	1.52
2	Q	57	LYS	CA-C	9.35	1.65	1.52
1	A	311	HIS	ND1-CE1	9.11	1.41	1.32
2	H	452	VAL	C-N	9.11	1.42	1.33
1	C	411	HIS	ND1-CE1	9.11	1.41	1.32
7	q	59	ARG	NE-CZ	9.06	1.43	1.33
1	G	454	LYS	CA-C	-9.01	1.41	1.52
2	B	310	ARG	NE-CZ	8.97	1.43	1.33
1	C	278	GLU	CA-C	-8.93	1.41	1.52
2	B	497	HIS	ND1-CE1	8.88	1.41	1.32
3	K	339	HIS	ND1-CE1	8.84	1.41	1.32
2	H	549	ASN	N-CA	-8.78	1.35	1.46
1	A	387	PHE	CA-CB	8.69	1.66	1.53
5	L	213	ARG	CD-NE	8.65	1.58	1.46
3	K	271	ARG	CZ-NH2	8.64	1.44	1.33
2	H	481	LYS	C-N	8.62	1.43	1.34
7	s	63	THR	N-CA	-8.58	1.35	1.46
2	B	346	GLN	CA-C	-8.57	1.41	1.52
2	O	66	ARG	CA-C	8.53	1.62	1.53
2	D	398	ALA	C-N	8.50	1.43	1.34
1	E	351	GLY	CA-C	-8.48	1.40	1.51
1	A	406	PHE	C-N	8.47	1.45	1.33
1	C	345	ASN	CA-C	-8.46	1.42	1.53
5	L	45	ASP	CA-C	-8.44	1.42	1.52
3	I	2	ILE	CA-CB	-8.39	1.44	1.54
1	C	314	ARG	NE-CZ	8.39	1.42	1.33
1	E	216	LEU	C-N	8.35	1.44	1.33
2	D	466	ARG	CA-C	-8.32	1.42	1.52
4	J	398	LEU	C-N	8.31	1.42	1.33
5	L	366	SER	CA-CB	8.30	1.66	1.53
5	L	383	GLY	CA-C	-8.29	1.41	1.52
2	Q	77	LEU	C-N	8.26	1.44	1.33
1	E	363	PHE	C-N	8.23	1.43	1.33
1	C	393	TRP	CA-CB	8.22	1.66	1.53
3	K	149	HIS	ND1-CE1	8.21	1.40	1.32
6	U	623	VAL	CA-C	8.15	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	SER	N-CA	-8.15	1.36	1.46
3	K	83	GLY	C-N	8.14	1.42	1.33
3	I	110	GLU	C-N	8.14	1.45	1.33
5	L	355	LYS	CA-C	-8.13	1.41	1.52
2	R	32	PHE	CA-CB	8.10	1.66	1.53
4	J	283	PHE	CA-C	-8.08	1.42	1.52
1	E	246	SER	CA-C	-8.05	1.43	1.52
2	H	287	LYS	CA-C	-8.05	1.42	1.52
3	I	278	PHE	CA-CB	7.99	1.66	1.53
4	J	475	TRP	NE1-CE2	-7.97	1.28	1.37
5	L	540	VAL	CA-C	7.95	1.62	1.52
7	o	58	ARG	NE-CZ	7.91	1.41	1.33
2	B	480	ARG	CD-NE	7.90	1.57	1.46
3	K	308	ALA	CA-C	-7.90	1.42	1.52
5	L	544	VAL	CA-C	-7.90	1.43	1.52
4	J	391	LEU	C-N	7.87	1.43	1.33
6	X	646	ARG	NE-CZ	7.85	1.41	1.33
6	U	609	GLU	CA-C	-7.84	1.42	1.52
3	K	315	LYS	CA-C	-7.83	1.42	1.52
3	K	284	GLN	N-CA	-7.82	1.36	1.46
2	F	449	SER	C-N	7.80	1.42	1.33
2	F	457	ARG	NE-CZ	7.78	1.41	1.33
4	J	693	GLN	CA-C	-7.78	1.42	1.52
3	I	169	ARG	CA-C	-7.76	1.42	1.52
6	W	669	ALA	CA-C	-7.73	1.46	1.52
2	F	450	ASP	C-O	-7.71	1.20	1.23
6	V	628	GLU	CA-C	-7.71	1.42	1.52
4	J	431	HIS	ND1-CE1	7.71	1.40	1.32
6	X	647	TYR	CA-CB	7.70	1.66	1.53
2	D	460	HIS	ND1-CE1	7.70	1.40	1.32
3	I	194	GLY	CA-C	7.69	1.62	1.51
3	K	204	PHE	CA-C	-7.68	1.43	1.52
1	C	359	HIS	ND1-CE1	7.67	1.40	1.32
2	D	288	ASP	C-N	7.64	1.42	1.34
6	V	637	SER	C-N	7.63	1.44	1.33
1	E	237	LEU	N-CA	-7.63	1.40	1.47
4	J	215	HIS	ND1-CE1	7.62	1.40	1.32
5	L	429	VAL	N-CA	-7.62	1.37	1.46
1	C	256	LYS	CA-CB	7.59	1.65	1.53
2	S	79	ARG	CD-NE	7.59	1.56	1.46
1	C	371	ALA	CA-C	-7.57	1.42	1.52
5	L	583	CYS	CA-CB	7.57	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	407	MET	N-CA	-7.57	1.36	1.46
5	L	413	HIS	CB-CG	7.56	1.60	1.50
3	I	346	GLU	N-CA	-7.56	1.36	1.46
7	r	25	LEU	C-N	7.55	1.44	1.33
2	H	344	GLN	CA-CB	7.55	1.66	1.53
2	D	466	ARG	CZ-NH2	7.54	1.43	1.33
7	s	59	ARG	NE-CZ	7.53	1.41	1.33
1	A	297	THR	N-CA	-7.50	1.37	1.46
7	q	64	LEU	CA-C	-7.50	1.43	1.52
1	A	279	ASN	N-CA	-7.49	1.36	1.46
2	B	517	ASP	C-N	7.48	1.43	1.33
1	E	387	PHE	CA-CB	7.48	1.66	1.53
1	A	268	ASN	CA-C	7.46	1.62	1.52
7	q	49	ALA	N-CA	-7.45	1.37	1.46
6	U	661	ARG	N-CA	-7.44	1.37	1.46
6	W	661	ARG	NE-CZ	7.44	1.41	1.33
3	K	205	VAL	CA-C	-7.43	1.43	1.52
6	W	612	ASP	CA-CB	7.43	1.64	1.53
1	C	359	HIS	CB-CG	7.43	1.60	1.50
5	L	1374	HIS	CE1-NE2	7.42	1.40	1.32
6	X	629	MET	CA-C	-7.42	1.43	1.52
2	D	473	PHE	N-CA	-7.40	1.36	1.46
2	H	447	VAL	CA-C	-7.39	1.43	1.52
7	q	12	ARG	C-N	7.38	1.43	1.33
2	R	37	ARG	CA-C	-7.37	1.43	1.52
2	R	92	SER	CA-C	-7.36	1.43	1.52
2	O	76	GLU	N-CA	-7.35	1.37	1.46
4	J	597	SER	C-N	7.33	1.43	1.33
2	H	246	GLU	C-N	7.32	1.43	1.33
1	G	332	ARG	NE-CZ	7.32	1.41	1.33
3	I	186	GLN	CA-C	-7.30	1.43	1.52
4	J	500	HIS	CG-ND1	7.29	1.46	1.38
2	T	67	ARG	NE-CZ	7.29	1.41	1.33
5	L	179	ARG	N-CA	7.29	1.55	1.46
2	D	257	PHE	N-CA	7.27	1.55	1.46
4	J	670	SER	C-N	7.26	1.43	1.33
3	I	165	LEU	CA-C	7.26	1.61	1.52
2	R	19	ARG	CA-C	-7.26	1.42	1.52
1	C	254	SER	C-N	7.25	1.42	1.33
5	L	117	VAL	CA-C	-7.25	1.43	1.52
5	L	404	TYR	CA-CB	7.25	1.64	1.53
1	C	405	GLU	CA-CB	7.24	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	431	ARG	NE-CZ	7.23	1.41	1.33
5	L	431	GLN	C-O	-7.23	1.15	1.24
4	J	356	THR	CA-C	-7.22	1.43	1.52
3	I	37	GLY	N-CA	-7.22	1.34	1.45
6	V	618	CYS	C-N	7.22	1.43	1.33
1	A	275	PHE	C-N	7.22	1.42	1.33
6	U	661	ARG	NE-CZ	7.21	1.41	1.33
7	q	51	SER	CA-C	-7.21	1.43	1.52
1	G	368	ASP	CA-CB	7.18	1.62	1.53
1	E	280	SER	CA-CB	-7.17	1.41	1.53
1	E	242	SER	N-CA	-7.17	1.37	1.46
3	K	341	TRP	NE1-CE2	-7.15	1.29	1.37
1	E	408	VAL	CA-CB	-7.15	1.46	1.54
5	L	582	ASP	CA-C	-7.14	1.43	1.52
2	R	61	GLU	CA-C	-7.14	1.43	1.52
2	T	17	CYS	CA-CB	7.13	1.64	1.53
1	G	289	HIS	ND1-CE1	7.11	1.39	1.32
1	A	477	THR	CA-C	7.11	1.62	1.52
6	X	636	GLN	N-CA	-7.10	1.37	1.46
6	U	618	CYS	CA-CB	7.10	1.64	1.53
7	o	55	LYS	CA-C	-7.09	1.43	1.52
1	G	388	ASP	C-N	7.08	1.42	1.33
5	L	343	PRO	CA-C	-7.08	1.42	1.52
7	o	47	PRO	C-O	-7.07	1.16	1.24
7	t	58	ARG	NE-CZ	7.07	1.40	1.33
2	F	426	LEU	C-N	7.07	1.43	1.33
1	C	346	LYS	C-N	7.06	1.42	1.33
3	K	174	LYS	CA-C	7.06	1.61	1.52
2	R	44	ALA	CA-C	-7.06	1.45	1.53
1	C	217	VAL	CA-C	7.05	1.61	1.52
2	F	272	ASN	CA-C	-7.05	1.43	1.52
1	A	312	LEU	C-N	7.04	1.43	1.33
4	J	321	PHE	CA-CB	7.03	1.64	1.53
7	s	11	VAL	CA-C	7.03	1.61	1.52
3	K	282	SER	C-N	7.02	1.43	1.34
2	O	96	LEU	N-CA	-7.02	1.38	1.46
2	D	334	TYR	N-CA	-7.01	1.37	1.46
5	L	517	ASN	CA-C	-7.01	1.43	1.52
2	H	281	ALA	CA-C	-7.01	1.43	1.52
5	L	546	ARG	NE-CZ	7.01	1.40	1.33
5	L	590	HIS	CA-C	6.99	1.62	1.52
7	o	54	ILE	N-CA	-6.99	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	41	CYS	N-CA	-6.99	1.37	1.46
4	J	507	THR	N-CA	-6.97	1.36	1.46
4	J	482	PHE	CA-CB	6.96	1.64	1.53
1	A	448	LYS	N-CA	-6.96	1.37	1.46
2	H	470	ILE	N-CA	-6.96	1.38	1.47
5	L	354	VAL	N-CA	6.95	1.55	1.46
3	I	260	ARG	CZ-NH1	6.95	1.42	1.32
5	L	540	VAL	N-CA	-6.95	1.37	1.46
2	D	488	SER	C-N	6.94	1.41	1.33
1	G	247	VAL	N-CA	-6.94	1.38	1.46
1	E	311	HIS	ND1-CE1	6.94	1.39	1.32
7	q	24	LEU	N-CA	-6.94	1.38	1.46
3	K	202	GLU	N-CA	-6.93	1.38	1.46
3	I	129	PHE	N-CA	-6.93	1.36	1.46
6	X	644	LEU	N-CA	-6.93	1.38	1.46
1	E	368	ASP	N-CA	-6.92	1.38	1.46
2	Q	79	ARG	NE-CZ	6.92	1.40	1.33
1	G	343	SER	N-CA	-6.91	1.37	1.46
1	C	224	LEU	CA-C	6.90	1.62	1.52
2	B	283	SER	CA-C	-6.89	1.44	1.52
2	T	42	ASN	CA-C	-6.88	1.44	1.52
4	J	466	ARG	NE-CZ	6.88	1.40	1.33
2	S	31	GLN	C-O	6.88	1.32	1.24
2	H	434	TYR	CA-CB	6.87	1.64	1.53
6	X	623	VAL	N-CA	6.87	1.54	1.46
2	H	318	LEU	C-N	6.86	1.42	1.33
3	I	169	ARG	CA-CB	6.85	1.64	1.53
4	J	320	VAL	CA-CB	-6.85	1.45	1.54
3	K	336	VAL	N-CA	6.84	1.54	1.46
3	K	176	LEU	N-CA	-6.83	1.38	1.46
2	Q	76	GLU	N-CA	-6.83	1.38	1.46
1	G	300	LYS	CA-CB	6.82	1.64	1.53
7	s	20	GLU	CA-C	-6.82	1.44	1.52
1	C	296	ARG	CD-NE	6.80	1.55	1.46
1	G	441	PHE	CA-C	-6.80	1.43	1.52
3	I	257	PHE	N-CA	-6.80	1.37	1.45
6	X	622	ILE	N-CA	-6.80	1.38	1.46
3	K	136	ILE	CA-CB	6.80	1.63	1.54
2	H	480	ARG	NE-CZ	6.79	1.40	1.33
6	W	629	MET	CA-C	-6.78	1.44	1.52
5	L	1373	SER	C-N	6.78	1.43	1.33
5	L	478	CYS	N-CA	-6.78	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	369	SER	N-CA	-6.77	1.38	1.46
1	A	442	LEU	CA-C	-6.77	1.44	1.52
1	G	286	GLN	CA-CB	6.77	1.62	1.53
1	E	319	SER	N-CA	6.77	1.54	1.45
5	L	441	LEU	C-N	6.77	1.43	1.34
6	U	646	ARG	CA-C	-6.76	1.44	1.52
2	H	291	SER	N-CA	-6.75	1.37	1.46
7	s	37	CYS	N-CA	-6.75	1.38	1.46
3	I	171	ALA	N-CA	-6.74	1.38	1.46
1	C	210	PRO	N-CD	-6.74	1.38	1.47
1	E	486	ARG	NE-CZ	6.74	1.40	1.33
2	T	15	ASN	CA-C	-6.73	1.44	1.52
4	J	598	ARG	N-CA	6.72	1.54	1.46
2	F	335	TYR	CA-C	-6.72	1.44	1.52
5	L	245	GLY	CA-C	6.70	1.59	1.52
4	J	323	LEU	CA-CB	6.70	1.65	1.53
2	F	302	LYS	CA-C	6.70	1.61	1.52
1	E	431	TYR	C-N	6.69	1.43	1.33
2	H	251	ARG	NE-CZ	6.69	1.40	1.33
5	L	410	ARG	NE-CZ	6.68	1.40	1.33
5	L	50	HIS	N-CA	-6.67	1.38	1.46
3	K	193	HIS	CE1-NE2	-6.66	1.25	1.32
3	K	120	SER	N-CA	-6.66	1.37	1.46
1	A	458	VAL	CA-C	-6.64	1.44	1.52
1	A	262	ILE	C-N	6.64	1.42	1.33
3	I	169	ARG	NE-CZ	6.64	1.40	1.33
5	L	590	HIS	ND1-CE1	6.63	1.39	1.32
1	G	223	ILE	CA-CB	-6.62	1.45	1.54
2	O	46	THR	CA-C	6.61	1.62	1.52
3	K	332	ILE	CA-CB	6.61	1.62	1.54
1	C	429	GLN	C-N	6.61	1.42	1.33
3	I	185	LYS	C-N	6.61	1.42	1.33
5	L	378	PHE	CA-CB	6.61	1.64	1.53
1	G	280	SER	CA-CB	6.60	1.63	1.53
3	K	145	SER	C-N	6.60	1.43	1.33
7	r	35	SER	CA-CB	6.60	1.63	1.53
4	J	403	ALA	C-N	6.58	1.43	1.34
2	Q	35	ALA	CA-C	-6.58	1.44	1.52
7	p	52	SER	CA-C	-6.58	1.44	1.52
6	U	647	TYR	CA-C	-6.58	1.43	1.52
5	L	317	ALA	N-CA	-6.57	1.38	1.46
1	C	369	SER	CA-C	-6.57	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	436	GLY	C-N	6.57	1.42	1.33
5	L	224	ARG	N-CA	-6.57	1.37	1.46
1	E	235	GLN	CA-C	-6.57	1.44	1.52
2	H	479	SER	CA-CB	6.57	1.64	1.53
2	H	300	HIS	ND1-CE1	6.56	1.39	1.32
4	J	499	ASN	C-N	6.56	1.41	1.33
2	F	252	ASP	N-CA	-6.56	1.38	1.46
1	A	432	THR	C-N	6.55	1.41	1.33
2	Q	67	ARG	CD-NE	6.55	1.55	1.46
3	I	198	ASP	CA-C	6.54	1.60	1.52
1	G	396	ARG	C-N	6.54	1.42	1.33
5	L	112	VAL	CA-CB	6.53	1.62	1.54
1	G	246	SER	N-CA	-6.51	1.38	1.46
3	K	292	ASN	CA-CB	6.51	1.63	1.53
5	L	521	LEU	C-N	6.51	1.42	1.33
7	r	9	SER	CA-CB	6.50	1.63	1.53
1	G	308	GLN	N-CA	-6.50	1.38	1.46
2	S	114	PHE	N-CA	-6.50	1.38	1.46
3	K	96	ILE	CA-CB	6.49	1.62	1.54
3	K	13	PRO	C-N	6.48	1.42	1.33
2	S	62	PHE	C-N	6.48	1.42	1.33
1	E	264	PRO	C-N	6.48	1.41	1.33
5	L	319	ARG	N-CA	-6.48	1.38	1.46
6	V	619	HIS	C-N	6.48	1.42	1.33
2	D	525	LEU	N-CA	-6.48	1.37	1.46
3	K	116	HIS	CA-C	-6.48	1.44	1.52
6	X	611	LEU	C-N	6.48	1.42	1.33
2	H	303	ILE	N-CA	-6.48	1.38	1.46
2	R	15	ASN	C-N	6.48	1.42	1.33
2	S	65	GLN	N-CA	6.48	1.54	1.46
4	J	265	GLN	C-N	6.47	1.41	1.33
3	K	111	PHE	N-CA	6.47	1.54	1.46
2	F	417	ILE	C-N	6.46	1.42	1.33
3	I	170	SER	C-N	6.46	1.42	1.33
2	H	361	LEU	CA-C	-6.46	1.44	1.52
1	A	311	HIS	C-N	6.46	1.43	1.33
1	G	274	ARG	CZ-NH2	6.46	1.41	1.33
2	B	430	TYR	CA-C	-6.45	1.43	1.52
5	L	215	SER	C-N	6.45	1.41	1.33
3	I	8	ALA	CA-C	-6.43	1.43	1.52
2	S	48	GLU	C-N	6.43	1.42	1.33
2	F	252	ASP	CA-CB	6.43	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	403	THR	N-CA	-6.43	1.38	1.46
1	E	439	PRO	CA-C	6.43	1.61	1.52
6	X	639	GLU	CA-C	-6.43	1.44	1.52
2	F	269	ASN	CA-CB	6.42	1.62	1.52
5	L	575	LEU	N-CA	-6.41	1.38	1.46
5	L	228	MET	CA-CB	6.41	1.62	1.53
2	F	313	ASP	CA-CB	6.40	1.63	1.53
1	A	366	THR	N-CA	6.40	1.53	1.45
5	L	504	TYR	C-N	6.40	1.43	1.33
1	C	311	HIS	ND1-CE1	6.39	1.39	1.32
2	D	426	LEU	N-CA	6.39	1.54	1.46
3	K	35	HIS	CA-C	-6.38	1.46	1.53
7	q	12	ARG	NE-CZ	6.38	1.40	1.33
3	K	155	GLU	N-CA	-6.38	1.38	1.46
1	E	323	LEU	C-N	6.37	1.42	1.34
5	L	567	ARG	CA-C	-6.37	1.44	1.52
2	F	435	ASP	CA-C	-6.37	1.45	1.52
5	L	571	HIS	CD2-NE2	6.36	1.44	1.37
2	D	532	LYS	N-CA	-6.36	1.37	1.46
1	A	286	GLN	C-N	6.36	1.41	1.34
2	O	20	ILE	CA-C	-6.36	1.45	1.52
7	t	57	LEU	C-N	6.36	1.42	1.33
1	G	439	PRO	C-N	6.35	1.42	1.33
5	L	498	GLY	C-N	6.35	1.41	1.34
7	p	40	LEU	N-CA	-6.35	1.38	1.46
7	r	12	ARG	N-CA	-6.35	1.38	1.46
2	B	366	LEU	N-CA	-6.35	1.37	1.46
2	F	306	TYR	CA-C	-6.35	1.44	1.52
1	A	269	TYR	CA-CB	6.34	1.63	1.53
1	C	325	PHE	N-CA	-6.34	1.37	1.46
2	T	30	GLN	CA-C	-6.34	1.44	1.52
5	L	47	LEU	CA-CB	6.33	1.63	1.53
3	K	46	CYS	C-N	6.32	1.42	1.33
4	J	282	ILE	CA-C	-6.31	1.45	1.52
2	R	38	VAL	C-N	6.31	1.41	1.33
4	J	410	ARG	NE-CZ	6.31	1.40	1.33
2	S	105	ARG	NE-CZ	6.31	1.40	1.33
2	B	434	TYR	C-N	6.31	1.42	1.33
2	F	278	GLY	CA-C	-6.31	1.43	1.51
1	G	216	LEU	CA-CB	6.30	1.63	1.53
7	s	27	THR	CA-C	-6.30	1.44	1.52
3	I	16	ILE	CB-CG1	6.30	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	10	ALA	CA-C	-6.30	1.44	1.52
1	C	256	LYS	CA-C	-6.29	1.44	1.52
2	F	276	VAL	N-CA	-6.29	1.38	1.46
5	L	539	TRP	NE1-CE2	-6.29	1.30	1.37
4	J	235	HIS	CB-CG	6.29	1.58	1.50
6	W	658	GLU	C-N	6.29	1.41	1.33
3	K	323	VAL	C-N	6.28	1.42	1.34
5	L	372	ASN	C-O	-6.28	1.16	1.24
2	F	489	ILE	CA-CB	6.28	1.62	1.54
5	L	249	LYS	N-CA	6.28	1.54	1.46
3	I	339	HIS	C-N	6.27	1.43	1.33
4	J	700	ASN	C-N	6.27	1.42	1.33
4	J	488	PHE	CA-C	-6.27	1.45	1.52
4	J	681	THR	C-N	6.27	1.42	1.34
2	F	479	SER	CA-CB	6.27	1.63	1.53
1	G	364	GLY	CA-C	-6.27	1.43	1.51
5	L	105	GLN	CA-C	-6.26	1.44	1.52
2	F	311	SER	N-CA	-6.25	1.38	1.46
2	D	310	ARG	CD-NE	6.25	1.54	1.46
1	G	285	GLY	N-CA	-6.25	1.36	1.45
2	T	93	ILE	C-N	6.25	1.42	1.33
2	D	323	PHE	CA-C	-6.24	1.44	1.52
6	V	601	ASN	CA-CB	6.24	1.63	1.53
2	B	328	HIS	CA-C	6.24	1.61	1.52
1	A	376	LEU	CA-CB	6.23	1.63	1.53
5	L	8	PHE	CA-CB	6.23	1.63	1.53
2	B	267	MET	CA-CB	6.23	1.62	1.53
2	D	257	PHE	CA-C	-6.23	1.44	1.52
2	O	63	VAL	CA-CB	-6.23	1.46	1.54
2	B	298	TRP	CA-CB	6.22	1.63	1.53
1	E	311	HIS	CB-CG	6.22	1.58	1.50
4	J	245	HIS	ND1-CE1	6.22	1.38	1.32
2	B	333	GLU	C-N	6.22	1.42	1.33
1	C	439	PRO	CA-C	-6.21	1.46	1.52
2	F	423	TYR	C-O	-6.21	1.16	1.24
2	B	364	ARG	CZ-NH1	6.20	1.41	1.32
5	L	322	PHE	N-CA	-6.20	1.38	1.46
2	B	382	ALA	CA-C	-6.19	1.44	1.52
2	D	307	THR	N-CA	-6.19	1.38	1.46
1	G	445	VAL	CA-CB	6.19	1.62	1.54
6	U	666	ARG	NE-CZ	6.19	1.39	1.33
3	I	87	ARG	N-CA	-6.18	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	387	CYS	CA-C	-6.18	1.45	1.52
3	K	120	SER	CA-C	-6.18	1.44	1.52
3	K	298	SER	N-CA	-6.18	1.39	1.46
3	K	206	ARG	C-N	6.18	1.42	1.33
2	S	29	ALA	CA-CB	6.18	1.62	1.53
2	B	260	ILE	N-CA	-6.17	1.38	1.46
3	K	168	VAL	C-N	6.17	1.43	1.33
4	J	442	ASP	N-CA	-6.17	1.38	1.46
4	J	235	HIS	C-N	6.17	1.43	1.33
3	K	205	VAL	N-CA	-6.16	1.38	1.46
5	L	224	ARG	CD-NE	6.15	1.54	1.46
2	B	528	ALA	CA-C	-6.15	1.44	1.52
2	B	493	HIS	ND1-CE1	6.15	1.38	1.32
2	B	532	LYS	N-CA	-6.15	1.37	1.46
6	W	653	LEU	N-CA	-6.14	1.39	1.46
2	D	431	ARG	CD-NE	6.14	1.54	1.46
4	J	407	VAL	CA-CB	-6.14	1.46	1.54
1	C	339	SER	CA-C	6.14	1.61	1.52
5	L	340	THR	N-CA	-6.14	1.38	1.46
7	r	58	ARG	NE-CZ	6.14	1.39	1.33
2	D	399	VAL	N-CA	-6.13	1.37	1.46
1	A	477	THR	N-CA	6.13	1.54	1.46
1	E	357	LEU	CA-C	-6.13	1.44	1.52
2	H	388	GLN	CA-C	-6.12	1.44	1.52
2	H	457	ARG	CZ-NH1	6.12	1.41	1.32
7	q	39	ARG	NE-CZ	6.12	1.39	1.33
1	A	314	ARG	NE-CZ	6.12	1.39	1.33
1	C	438	ILE	C-N	6.12	1.40	1.33
2	Q	112	SER	CA-C	-6.11	1.45	1.52
5	L	254	ILE	CB-CG1	6.11	1.65	1.53
1	G	302	TYR	CA-C	-6.11	1.45	1.52
2	T	35	ALA	C-N	6.11	1.41	1.33
2	F	281	ALA	N-CA	-6.10	1.38	1.46
2	D	339	SER	C-N	6.10	1.41	1.33
2	H	270	SER	CA-C	-6.10	1.44	1.52
1	E	341	ALA	CA-C	-6.09	1.45	1.52
2	R	22	GLY	C-N	6.09	1.42	1.33
6	W	602	PHE	CA-CB	6.09	1.62	1.53
1	C	217	VAL	N-CA	-6.09	1.39	1.46
5	L	168	TYR	N-CA	-6.09	1.38	1.46
1	A	299	GLY	C-N	6.09	1.42	1.33
1	E	242	SER	CA-C	-6.08	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	500	LYS	N-CA	-6.08	1.38	1.46
2	O	18	CYS	CA-CB	6.08	1.62	1.53
2	B	274	TYR	N-CA	-6.07	1.38	1.45
1	G	269	TYR	CA-CB	6.07	1.63	1.53
3	K	35	HIS	CE1-NE2	6.07	1.38	1.32
1	G	393	TRP	NE1-CE2	6.07	1.44	1.37
2	B	468	SER	C-O	6.07	1.28	1.23
3	K	44	ARG	CD-NE	6.07	1.54	1.46
1	G	385	PRO	CA-C	-6.07	1.43	1.52
2	T	9	PRO	C-N	6.07	1.41	1.33
4	J	589	THR	C-N	6.06	1.41	1.33
6	U	604	LYS	CA-CB	6.06	1.62	1.53
1	E	329	PRO	CA-CB	-6.06	1.44	1.53
2	H	361	LEU	N-CA	-6.05	1.38	1.46
1	G	230	ARG	NE-CZ	6.05	1.39	1.33
6	U	630	ILE	C-N	6.05	1.42	1.33
1	A	359	HIS	CB-CG	6.05	1.58	1.50
1	G	448	LYS	CA-C	-6.04	1.45	1.52
4	J	683	ARG	NE-CZ	6.04	1.39	1.33
5	L	598	CYS	CA-C	-6.04	1.44	1.52
3	K	11	GLY	C-N	6.04	1.39	1.33
5	L	364	VAL	CA-C	-6.04	1.45	1.52
1	E	276	VAL	CA-C	-6.03	1.44	1.52
1	G	409	GLU	CA-C	-6.03	1.45	1.52
2	T	20	ILE	C-O	-6.03	1.17	1.24
1	A	486	ARG	CD-NE	6.03	1.54	1.46
3	I	196	LEU	N-CA	-6.03	1.39	1.46
7	p	20	GLU	C-N	6.03	1.41	1.33
3	K	22	ARG	NE-CZ	6.02	1.39	1.33
1	G	351	GLY	CA-C	-6.02	1.43	1.51
7	p	46	ASN	CA-C	6.02	1.59	1.53
4	J	275	SER	CA-CB	6.01	1.63	1.53
3	K	294	SER	CA-C	-6.01	1.44	1.53
5	L	442	GLN	C-N	6.01	1.42	1.34
2	F	390	ARG	N-CA	-6.01	1.39	1.46
7	o	17	VAL	CA-CB	-6.01	1.47	1.54
1	C	245	PHE	C-N	6.01	1.41	1.33
1	E	371	ALA	CA-C	-6.00	1.44	1.52
2	D	485	ILE	CA-CB	-6.00	1.46	1.54
2	B	423	TYR	CA-CB	6.00	1.62	1.53
5	L	336	LEU	N-CA	-6.00	1.38	1.46
7	q	45	ILE	CA-C	-6.00	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	88	LYS	CA-C	-6.00	1.45	1.52
1	C	230	ARG	CA-C	-5.99	1.48	1.52
3	I	5	LEU	C-N	5.99	1.41	1.33
5	L	511	GLU	CA-CB	5.99	1.61	1.52
1	G	312	LEU	CA-C	5.99	1.60	1.52
4	J	489	ILE	CB-CG1	5.99	1.65	1.53
1	C	253	SER	C-N	5.99	1.42	1.33
1	G	433	ILE	N-CA	-5.99	1.39	1.46
7	r	31	MET	CA-C	5.98	1.60	1.52
4	J	228	PHE	CA-C	-5.98	1.45	1.52
2	F	288	ASP	N-CA	-5.98	1.38	1.46
1	G	243	ARG	CA-C	-5.98	1.45	1.52
4	J	448	GLU	CA-C	-5.98	1.44	1.52
5	L	249	LYS	C-N	5.97	1.38	1.32
7	r	57	LEU	C-O	-5.97	1.17	1.24
4	J	224	ARG	C-N	5.97	1.42	1.33
2	D	315	ALA	CA-CB	5.97	1.63	1.53
1	G	340	ILE	CA-CB	5.97	1.62	1.54
2	D	429	LEU	N-CA	-5.96	1.39	1.46
2	H	543	TYR	CA-CB	5.96	1.62	1.53
7	o	12	ARG	CD-NE	5.96	1.54	1.46
2	D	489	ILE	C-N	5.96	1.41	1.33
2	D	413	LEU	CA-C	-5.95	1.45	1.52
7	t	20	GLU	CA-C	-5.95	1.45	1.52
2	Q	105	ARG	CD-NE	5.95	1.54	1.46
6	V	615	ARG	CD-NE	5.95	1.54	1.46
2	B	526	GLU	CA-C	5.94	1.60	1.52
7	q	45	ILE	N-CA	5.94	1.53	1.46
7	p	58	ARG	CZ-NH1	5.94	1.41	1.32
1	C	361	ARG	CD-NE	5.93	1.54	1.46
1	G	384	ALA	C-O	-5.93	1.19	1.24
7	s	25	LEU	CA-C	-5.93	1.44	1.52
3	K	204	PHE	N-CA	5.93	1.52	1.46
2	F	400	HIS	CA-C	-5.92	1.44	1.52
7	s	33	THR	N-CA	-5.92	1.39	1.46
4	J	460	LEU	CA-C	-5.92	1.44	1.52
6	W	628	GLU	C-N	5.92	1.41	1.33
7	r	17	VAL	CA-C	-5.92	1.45	1.52
2	F	333	GLU	C-N	5.92	1.42	1.34
5	L	225	THR	N-CA	-5.91	1.38	1.45
5	L	472	ARG	CZ-NH2	5.91	1.41	1.33
7	s	39	ARG	CA-C	-5.91	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	296	ARG	CZ-NH2	5.91	1.41	1.33
2	D	302	LYS	CA-C	-5.91	1.45	1.52
1	E	293	ALA	N-CA	5.91	1.53	1.46
2	S	95	TYR	C-N	5.91	1.41	1.33
1	E	443	GLN	CA-CB	5.91	1.63	1.53
5	L	465	ARG	NE-CZ	5.91	1.39	1.33
7	o	12	ARG	NE-CZ	5.91	1.39	1.33
2	H	474	MET	N-CA	-5.90	1.38	1.46
5	L	447	CYS	CA-C	-5.90	1.44	1.52
2	O	100	LEU	N-CA	-5.90	1.39	1.46
7	o	12	ARG	C-N	5.90	1.41	1.33
2	F	367	LEU	N-CA	-5.90	1.39	1.46
7	q	25	LEU	CA-C	-5.90	1.44	1.52
7	s	46	ASN	CA-C	-5.90	1.46	1.53
2	Q	93	ILE	CA-C	-5.89	1.45	1.52
6	V	622	ILE	CA-C	-5.89	1.44	1.52
6	X	643	LEU	CA-CB	5.89	1.62	1.53
5	L	407	TYR	CA-CB	5.88	1.63	1.53
2	F	452	VAL	CA-C	-5.88	1.45	1.52
3	I	304	GLU	CA-C	-5.88	1.44	1.52
4	J	401	ARG	NE-CZ	5.88	1.39	1.33
5	L	432	ALA	C-N	5.88	1.42	1.33
2	B	270	SER	C-N	5.88	1.39	1.33
6	W	666	ARG	NE-CZ	5.88	1.39	1.33
2	B	325	ALA	CA-C	-5.87	1.45	1.52
5	L	567	ARG	CD-NE	5.87	1.54	1.46
2	B	258	GLN	CA-CB	5.87	1.63	1.53
5	L	346	VAL	N-CA	-5.87	1.39	1.46
2	H	416	HIS	CG-CD2	5.86	1.42	1.35
2	F	267	MET	C-N	5.86	1.41	1.33
6	X	638	SER	N-CA	-5.86	1.39	1.46
2	B	409	TYR	C-O	-5.85	1.17	1.24
2	H	423	TYR	CA-CB	5.85	1.61	1.53
2	Q	102	GLU	N-CA	-5.85	1.38	1.45
3	I	87	ARG	CD-NE	5.84	1.54	1.46
1	C	361	ARG	CA-C	-5.84	1.44	1.52
2	Q	104	PRO	CA-CB	5.84	1.60	1.53
5	L	535	PHE	C-N	5.84	1.40	1.33
1	E	438	ILE	CA-CB	5.83	1.61	1.54
2	R	62	PHE	CA-CB	5.83	1.62	1.53
2	D	342	HIS	ND1-CE1	5.83	1.38	1.32
3	I	166	PRO	CA-C	5.83	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	343	LEU	C-N	5.83	1.42	1.33
3	K	143	ILE	CA-C	-5.83	1.45	1.52
5	L	213	ARG	CA-C	-5.83	1.45	1.52
1	G	228	ASP	CA-CB	5.83	1.62	1.53
1	E	226	GLY	CA-C	-5.83	1.44	1.51
2	O	39	ILE	C-N	5.83	1.40	1.33
3	I	314	LEU	N-CA	-5.82	1.38	1.46
2	T	64	ARG	CD-NE	5.82	1.54	1.46
1	A	220	LEU	CA-CB	5.82	1.62	1.53
3	I	318	PRO	N-CA	-5.82	1.40	1.47
5	L	209	GLU	N-CA	-5.82	1.39	1.46
2	O	72	ALA	CA-C	-5.82	1.45	1.52
5	L	347	LEU	C-N	5.82	1.41	1.33
2	S	83	SER	N-CA	-5.82	1.38	1.46
1	E	230	ARG	C-N	5.81	1.41	1.33
5	L	165	THR	C-N	5.81	1.41	1.33
7	s	62	ASP	C-N	5.81	1.41	1.33
5	L	162	LEU	CA-C	-5.81	1.45	1.52
1	E	252	ASP	CA-C	-5.81	1.45	1.52
5	L	250	VAL	CA-C	-5.81	1.48	1.52
1	E	245	PHE	C-N	5.81	1.41	1.33
2	Q	55	THR	C-N	5.81	1.41	1.33
6	U	615	ARG	CA-C	-5.81	1.45	1.52
1	C	322	LYS	N-CA	-5.81	1.39	1.46
1	C	487	ILE	N-CA	-5.80	1.38	1.46
2	H	249	LEU	CA-C	-5.80	1.44	1.52
3	I	2	ILE	CA-C	5.80	1.60	1.52
2	D	306	TYR	C-N	5.80	1.42	1.33
2	F	295	GLU	CA-C	-5.80	1.44	1.52
1	C	282	PHE	CA-C	-5.80	1.45	1.52
3	I	302	ASN	CA-CB	5.80	1.61	1.53
2	B	248	SER	N-CA	-5.80	1.39	1.46
5	L	346	VAL	C-O	-5.80	1.18	1.24
2	F	486	GLY	CA-C	-5.80	1.45	1.52
4	J	464	THR	C-N	5.80	1.40	1.34
4	J	467	PRO	C-N	5.80	1.42	1.33
2	R	51	GLU	N-CA	-5.80	1.39	1.46
6	V	650	ASN	CG-ND2	5.80	1.45	1.33
1	C	487	ILE	C-N	5.79	1.42	1.33
1	A	342	THR	C-N	5.79	1.42	1.33
2	F	417	ILE	N-CA	-5.79	1.38	1.46
2	F	481	LYS	N-CA	-5.79	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	568	TYR	CA-C	-5.79	1.45	1.52
1	A	405	GLU	C-N	5.79	1.41	1.33
3	K	191	MET	C-N	5.79	1.41	1.33
7	q	23	ARG	CD-NE	5.79	1.54	1.46
2	O	51	GLU	C-O	-5.78	1.17	1.24
4	J	327	ILE	CA-CB	5.78	1.60	1.53
1	A	220	LEU	C-O	-5.78	1.16	1.24
1	C	228	ASP	N-CA	-5.77	1.38	1.46
2	F	257	PHE	CA-CB	5.77	1.62	1.53
5	L	92	GLU	N-CA	-5.77	1.39	1.46
5	L	103	GLY	CA-C	-5.77	1.45	1.52
2	H	314	ARG	NE-CZ	5.77	1.39	1.33
7	t	29	LEU	C-N	5.77	1.41	1.33
1	G	318	LEU	C-N	5.76	1.40	1.33
4	J	295	ASP	C-N	5.76	1.40	1.33
6	X	626	GLN	C-N	5.76	1.41	1.33
6	X	668	ARG	CA-CB	5.76	1.62	1.53
2	D	400	HIS	ND1-CE1	5.75	1.38	1.32
1	C	230	ARG	NE-CZ	5.75	1.39	1.33
2	F	446	PHE	CA-C	5.75	1.60	1.52
3	K	298	SER	C-N	5.75	1.41	1.33
5	L	421	ASP	N-CA	-5.74	1.39	1.46
5	L	454	SER	CA-C	-5.74	1.45	1.52
2	T	39	ILE	CA-C	5.74	1.61	1.52
1	C	255	VAL	N-CA	-5.74	1.39	1.46
2	Q	37	ARG	CA-CB	5.74	1.62	1.53
2	D	297	GLY	CA-C	-5.73	1.44	1.51
3	K	121	HIS	C-N	5.73	1.40	1.33
2	F	270	SER	CA-C	-5.73	1.45	1.52
2	F	413	LEU	CA-C	-5.73	1.45	1.52
1	A	438	ILE	CA-C	-5.73	1.46	1.52
2	B	509	GLY	C-N	5.72	1.41	1.33
3	K	173	GLU	CA-C	-5.72	1.44	1.52
5	L	400	GLN	CA-C	-5.72	1.45	1.52
2	F	485	ILE	C-N	5.72	1.40	1.33
3	I	201	GLU	N-CA	-5.72	1.38	1.46
3	K	21	LYS	N-CA	-5.72	1.38	1.46
2	Q	101	SER	CA-C	-5.72	1.45	1.52
7	t	54	ILE	CA-CB	-5.72	1.47	1.54
2	F	436	GLY	N-CA	-5.72	1.37	1.45
3	K	84	ILE	CA-CB	5.71	1.60	1.54
1	E	396	ARG	NE-CZ	5.71	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1360	PRO	N-CA	5.71	1.55	1.47
5	L	323	ASP	N-CA	-5.71	1.39	1.46
5	L	359	ASN	C-N	5.71	1.40	1.33
4	J	323	LEU	C-N	5.70	1.42	1.33
2	S	39	ILE	CA-C	-5.70	1.45	1.52
2	S	67	ARG	NE-CZ	5.70	1.39	1.33
2	D	311	SER	CA-C	-5.70	1.45	1.52
2	B	507	ALA	C-N	5.70	1.41	1.33
2	F	407	ASP	CA-CB	5.70	1.62	1.53
6	W	635	ILE	N-CA	-5.70	1.40	1.46
1	C	281	SER	C-N	5.69	1.41	1.33
1	E	351	GLY	C-N	5.69	1.40	1.33
4	J	243	ASP	CA-CB	5.69	1.62	1.53
6	W	647	TYR	CA-C	-5.68	1.44	1.52
2	B	251	ARG	CD-NE	5.68	1.54	1.46
4	J	242	TRP	C-N	5.68	1.41	1.33
3	K	175	THR	N-CA	5.68	1.53	1.46
6	U	642	MET	C-N	5.68	1.41	1.33
4	J	361	MET	CA-C	-5.68	1.45	1.52
1	C	450	LEU	CA-CB	5.68	1.62	1.53
3	K	143	ILE	CA-CB	-5.68	1.47	1.54
2	H	482	VAL	C-N	5.67	1.41	1.33
2	B	265	VAL	CA-CB	-5.67	1.47	1.54
5	L	567	ARG	C-N	5.67	1.41	1.33
7	s	59	ARG	CZ-NH1	5.67	1.40	1.32
4	J	702	MET	SD-CE	5.67	1.93	1.79
5	L	474	LEU	C-N	5.67	1.41	1.33
5	L	599	GLY	CA-C	-5.67	1.44	1.51
1	A	380	LYS	CA-CB	5.67	1.62	1.53
6	X	616	GLU	N-CA	-5.67	1.39	1.46
2	B	456	ASP	C-N	5.67	1.40	1.33
3	K	158	TYR	N-CA	-5.66	1.39	1.46
5	L	51	LEU	CA-CB	5.66	1.62	1.53
7	o	27	THR	CA-C	-5.66	1.45	1.52
1	A	411	HIS	ND1-CE1	5.66	1.38	1.32
1	A	497	VAL	C-N	5.66	1.41	1.33
2	F	466	ARG	CZ-NH2	5.66	1.40	1.33
1	E	497	VAL	C-N	5.65	1.41	1.33
3	K	189	ALA	CA-C	-5.65	1.45	1.52
1	C	457	ASN	C-O	5.65	1.30	1.24
2	F	439	GLU	C-N	5.65	1.41	1.33
2	B	536	ALA	C-N	5.65	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	243	ARG	NE-CZ	5.65	1.39	1.33
1	A	462	CYS	N-CA	-5.64	1.39	1.46
3	K	332	ILE	CA-C	-5.64	1.46	1.52
2	O	32	PHE	N-CA	-5.64	1.39	1.46
7	s	23	ARG	CD-NE	5.64	1.54	1.46
3	I	53	ILE	N-CA	5.64	1.53	1.46
2	Q	76	GLU	CA-C	5.64	1.60	1.52
2	T	19	ARG	NE-CZ	5.64	1.39	1.33
1	G	376	LEU	C-N	5.64	1.42	1.33
6	X	617	ALA	CA-C	5.64	1.59	1.52
3	I	155	GLU	C-N	5.63	1.41	1.33
1	A	352	GLY	CA-C	5.63	1.58	1.52
3	K	121	HIS	CG-CD2	5.63	1.42	1.35
1	C	402	PRO	C-N	5.63	1.41	1.33
7	p	33	THR	C-N	5.63	1.41	1.33
1	A	221	LEU	C-N	5.62	1.42	1.33
1	C	393	TRP	CA-C	-5.62	1.45	1.52
5	L	558	GLU	CA-C	-5.62	1.46	1.52
4	J	306	LEU	CA-CB	5.62	1.62	1.53
6	X	606	MET	N-CA	-5.62	1.39	1.46
6	X	658	GLU	N-CA	-5.62	1.39	1.46
2	F	385	ASP	N-CA	-5.62	1.39	1.46
2	B	457	ARG	CZ-NH1	5.62	1.40	1.32
1	E	304	ILE	CB-CG1	5.62	1.64	1.53
2	B	416	HIS	CA-C	-5.62	1.44	1.52
2	S	103	ASP	C-N	5.62	1.41	1.34
2	D	302	LYS	N-CA	-5.62	1.39	1.46
5	L	364	VAL	CA-CB	-5.61	1.46	1.55
2	B	495	VAL	CA-C	5.61	1.58	1.52
1	G	270	SER	C-N	5.61	1.41	1.34
3	K	100	TYR	N-CA	5.61	1.53	1.46
1	C	437	GLN	CA-C	-5.61	1.45	1.53
2	B	361	LEU	C-N	5.61	1.40	1.33
3	I	325	PHE	CA-CB	5.61	1.62	1.53
7	o	38	VAL	CA-C	-5.61	1.46	1.52
7	r	51	SER	CA-CB	5.61	1.62	1.53
1	E	387	PHE	N-CA	-5.60	1.38	1.46
6	V	602	PHE	C-N	5.60	1.41	1.33
3	I	296	THR	N-CA	-5.60	1.38	1.46
2	D	429	LEU	CA-C	-5.60	1.45	1.52
2	H	400	HIS	ND1-CE1	5.60	1.38	1.32
2	H	323	PHE	N-CA	-5.60	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	38	GLU	N-CA	-5.60	1.38	1.46
5	L	526	LYS	C-N	5.60	1.41	1.33
2	T	75	SER	N-CA	-5.60	1.39	1.46
1	A	382	ALA	CA-C	-5.59	1.45	1.52
2	D	541	SER	C-N	5.59	1.41	1.33
1	A	497	VAL	CA-C	-5.59	1.46	1.52
1	G	481	GLN	C-N	5.59	1.41	1.33
7	r	12	ARG	CZ-NH1	5.59	1.40	1.32
1	A	260	ASN	CA-C	-5.59	1.44	1.52
7	s	38	VAL	N-CA	-5.59	1.39	1.46
6	U	603	ILE	N-CA	-5.58	1.39	1.46
7	t	40	LEU	CA-C	5.58	1.59	1.52
1	E	229	GLY	C-N	5.58	1.41	1.33
5	L	365	VAL	N-CA	-5.58	1.39	1.46
6	U	623	VAL	CA-CB	-5.58	1.47	1.54
1	A	241	GLN	C-N	5.58	1.41	1.33
1	E	253	SER	CA-CB	5.58	1.63	1.53
3	K	270	VAL	C-O	-5.58	1.17	1.24
2	O	37	ARG	CD-NE	5.58	1.54	1.46
2	B	294	SER	CA-CB	5.58	1.61	1.53
3	I	135	SER	N-CA	-5.57	1.38	1.46
4	J	700	ASN	CA-C	-5.57	1.45	1.52
5	L	113	LEU	N-CA	5.57	1.53	1.46
1	A	440	SER	C-N	5.57	1.41	1.33
2	F	361	LEU	C-N	5.57	1.40	1.33
3	I	269	PRO	CA-CB	5.57	1.61	1.53
2	H	529	PHE	N-CA	-5.57	1.39	1.46
1	G	396	ARG	CZ-NH2	5.57	1.40	1.33
2	T	19	ARG	CZ-NH1	5.57	1.40	1.32
2	D	536	ALA	N-CA	-5.56	1.39	1.46
2	F	398	ALA	C-N	5.56	1.40	1.33
5	L	526	LYS	N-CA	-5.56	1.39	1.46
2	R	78	HIS	CA-C	5.56	1.60	1.52
4	J	681	THR	C-O	-5.56	1.17	1.24
4	J	703	TYR	CA-C	-5.56	1.45	1.52
3	K	337	ALA	N-CA	-5.56	1.38	1.46
2	D	445	PHE	CA-C	-5.56	1.45	1.52
4	J	701	LEU	CA-C	-5.56	1.45	1.52
7	s	54	ILE	CA-CB	5.56	1.61	1.54
1	E	445	VAL	CA-CB	-5.55	1.47	1.54
2	H	282	VAL	C-N	5.55	1.41	1.33
2	B	438	LEU	C-N	5.55	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	22	ARG	NE-CZ	5.55	1.39	1.33
2	D	463	TYR	CA-CB	5.55	1.63	1.53
7	s	64	LEU	CA-CB	5.55	1.61	1.53
5	L	375	LEU	CA-CB	5.54	1.62	1.53
3	I	259	LEU	CA-C	-5.54	1.45	1.52
2	T	68	GLU	CA-C	5.54	1.59	1.52
2	T	79	ARG	CA-CB	5.54	1.62	1.53
4	J	432	LEU	N-CA	-5.54	1.39	1.46
2	R	79	ARG	CD-NE	5.54	1.54	1.46
6	V	621	ASP	CA-CB	5.54	1.62	1.53
3	K	185	LYS	CA-C	-5.54	1.45	1.52
2	T	15	ASN	C-N	5.53	1.41	1.33
6	W	645	GLU	CA-CB	5.53	1.61	1.53
3	K	302	ASN	CA-CB	5.53	1.62	1.53
2	F	469	MET	C-N	5.53	1.39	1.33
5	L	179	ARG	CZ-NH1	5.53	1.40	1.32
7	t	56	GLU	CA-C	-5.53	1.45	1.52
2	D	280	VAL	C-N	5.52	1.40	1.33
3	K	26	GLN	N-CA	-5.52	1.39	1.45
3	K	254	LEU	CA-CB	5.52	1.60	1.53
5	L	374	ALA	CA-CB	5.52	1.60	1.53
1	C	293	ALA	CA-C	-5.52	1.45	1.52
2	F	251	ARG	CA-C	-5.52	1.45	1.52
2	F	473	PHE	N-CA	-5.52	1.38	1.46
2	F	364	ARG	NE-CZ	5.52	1.39	1.33
6	W	638	SER	C-N	5.52	1.41	1.33
2	R	33	GLN	N-CA	-5.52	1.39	1.46
6	W	652	SER	C-N	5.52	1.41	1.33
5	L	546	ARG	CZ-NH1	5.51	1.40	1.32
2	R	38	VAL	CA-CB	-5.51	1.47	1.54
1	C	236	PRO	CA-CB	-5.50	1.46	1.53
1	C	485	GLU	CA-C	-5.50	1.45	1.52
3	K	19	TRP	CA-C	5.50	1.59	1.52
1	E	272	VAL	N-CA	-5.50	1.39	1.46
1	E	396	ARG	CA-C	5.50	1.59	1.52
2	H	249	LEU	C-N	5.50	1.40	1.33
2	R	37	ARG	NE-CZ	5.50	1.39	1.33
1	C	331	LEU	N-CA	-5.50	1.39	1.46
1	E	321	GLN	CA-C	-5.50	1.45	1.52
3	I	54	ARG	CZ-NH2	5.50	1.40	1.33
2	S	19	ARG	C-N	5.50	1.40	1.33
1	C	243	ARG	CD-NE	5.50	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	357	VAL	C-O	-5.50	1.17	1.24
1	C	438	ILE	CB-CG1	5.49	1.64	1.53
2	H	319	VAL	CA-CB	-5.49	1.47	1.54
7	t	29	LEU	N-CA	-5.49	1.39	1.46
2	F	431	ARG	N-CA	-5.49	1.39	1.46
1	A	302	TYR	CA-CB	5.49	1.62	1.53
3	I	288	ASN	CA-CB	5.49	1.62	1.53
2	B	386	HIS	ND1-CE1	5.48	1.38	1.32
2	B	469	MET	CA-CB	5.48	1.62	1.53
7	s	60	ALA	C-O	-5.48	1.17	1.24
4	J	473	ASP	CA-CB	5.48	1.61	1.53
2	B	457	ARG	CZ-NH2	5.48	1.40	1.33
1	C	359	HIS	CG-CD2	5.48	1.41	1.35
1	E	238	VAL	N-CA	-5.47	1.39	1.46
2	F	333	GLU	N-CA	5.47	1.53	1.46
3	I	176	LEU	CA-C	-5.47	1.45	1.52
6	U	649	LEU	N-CA	-5.47	1.39	1.46
1	A	464	HIS	ND1-CE1	5.47	1.38	1.32
5	L	477	LEU	C-N	5.47	1.42	1.33
2	H	344	GLN	N-CA	-5.47	1.38	1.46
2	B	523	THR	CA-CB	-5.47	1.45	1.53
4	J	397	LYS	N-CA	-5.47	1.38	1.46
1	C	255	VAL	CA-C	-5.46	1.44	1.52
6	U	653	LEU	CA-C	-5.46	1.45	1.52
2	F	344	GLN	CA-CB	5.46	1.62	1.53
2	H	277	ASP	CA-C	-5.46	1.45	1.52
1	C	318	LEU	CA-C	5.46	1.59	1.52
3	I	118	SER	C-N	5.46	1.40	1.34
1	C	273	THR	C-N	5.46	1.41	1.33
1	C	289	HIS	CA-C	-5.46	1.45	1.52
7	q	63	THR	CA-C	-5.45	1.45	1.52
1	C	315	GLN	CD-NE2	5.45	1.44	1.33
1	G	377	TYR	CZ-OH	5.45	1.49	1.38
4	J	501	ARG	NE-CZ	5.45	1.39	1.33
6	W	624	ASN	C-N	5.45	1.41	1.33
2	R	19	ARG	NE-CZ	5.44	1.39	1.33
7	r	63	THR	C-N	5.44	1.40	1.33
7	s	36	ILE	CA-CB	-5.44	1.47	1.54
1	G	350	PHE	CA-CB	5.44	1.61	1.53
2	H	257	PHE	N-CA	-5.44	1.39	1.46
4	J	428	ARG	N-CA	-5.44	1.39	1.46
1	G	224	LEU	CA-C	-5.44	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	342	LYS	CA-CB	5.44	1.63	1.53
2	B	434	TYR	CA-CB	5.44	1.62	1.53
2	H	410	MET	CA-C	-5.44	1.45	1.52
1	E	350	PHE	C-N	5.43	1.40	1.33
2	O	53	LEU	CA-CB	5.43	1.61	1.53
7	p	17	VAL	N-CA	-5.43	1.40	1.46
3	K	128	GLN	CA-C	-5.43	1.45	1.52
1	C	225	ILE	N-CA	5.43	1.52	1.46
2	B	282	VAL	C-N	5.42	1.40	1.33
2	F	447	VAL	CA-CB	-5.42	1.47	1.54
2	H	469	MET	C-N	5.42	1.39	1.33
7	s	23	ARG	N-CA	5.42	1.53	1.46
2	B	534	ASP	CA-C	-5.41	1.46	1.52
2	H	258	GLN	CA-CB	5.41	1.62	1.53
1	G	268	ASN	C-O	-5.41	1.17	1.24
6	V	632	GLN	N-CA	-5.41	1.40	1.46
1	A	390	LEU	C-O	5.41	1.30	1.24
1	E	374	LEU	N-CA	-5.41	1.39	1.46
5	L	93	GLU	CA-C	-5.41	1.46	1.52
5	L	443	TYR	N-CA	-5.41	1.39	1.46
2	B	288	ASP	CA-CB	5.41	1.62	1.53
2	S	46	THR	CA-C	-5.41	1.45	1.52
3	I	34	LEU	C-N	5.40	1.41	1.33
4	J	599	LEU	N-CA	-5.40	1.39	1.46
7	t	31	MET	N-CA	-5.40	1.39	1.46
5	L	402	ALA	CA-CB	5.40	1.61	1.53
2	F	310	ARG	CA-C	5.40	1.60	1.52
2	S	73	LEU	CA-CB	5.40	1.61	1.53
1	A	383	SER	CA-CB	5.39	1.62	1.53
2	D	382	ALA	CA-CB	-5.39	1.44	1.53
2	B	398	ALA	C-N	5.39	1.40	1.33
5	L	324	LYS	C-O	-5.39	1.17	1.24
7	s	50	LEU	N-CA	-5.39	1.39	1.46
3	K	97	LEU	CA-C	-5.39	1.45	1.52
3	I	289	GLN	CA-CB	5.39	1.62	1.53
5	L	388	GLY	C-N	5.39	1.40	1.33
2	R	66	ARG	NE-CZ	5.39	1.39	1.33
2	B	266	LYS	C-N	5.38	1.41	1.33
3	I	337	ALA	C-N	5.38	1.41	1.33
4	J	456	LEU	CA-CB	5.38	1.61	1.53
7	p	23	ARG	CD-NE	5.38	1.53	1.46
2	Q	98	LEU	CA-CB	5.38	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	297	THR	N-CA	5.38	1.52	1.46
3	K	257	PHE	CA-CB	5.38	1.61	1.53
5	L	44	TYR	CA-CB	5.38	1.61	1.53
2	B	249	LEU	CA-CB	5.38	1.62	1.53
5	L	178	GLN	CA-C	-5.38	1.45	1.52
2	H	530	GLN	CA-CB	5.37	1.62	1.53
1	C	255	VAL	C-N	5.37	1.41	1.33
7	o	8	MET	C-N	5.37	1.41	1.33
2	R	62	PHE	N-CA	-5.37	1.39	1.46
1	A	276	VAL	C-N	5.37	1.41	1.33
2	D	332	LYS	N-CA	-5.37	1.39	1.46
2	H	453	VAL	CA-C	-5.37	1.45	1.52
1	G	392	ARG	NE-CZ	5.37	1.39	1.33
1	A	359	HIS	C-N	5.36	1.41	1.33
2	F	367	LEU	C-N	5.36	1.40	1.33
1	G	436	GLN	C-N	5.36	1.41	1.33
3	I	145	SER	CA-CB	5.36	1.62	1.53
4	J	567	ASN	CG-ND2	5.36	1.44	1.33
2	Q	108	PRO	N-CD	-5.36	1.40	1.47
2	D	438	LEU	CA-CB	5.36	1.63	1.53
4	J	675	CYS	C-N	5.36	1.40	1.33
2	D	464	SER	CA-CB	5.35	1.63	1.53
2	S	67	ARG	CD-NE	5.35	1.53	1.46
2	B	519	ALA	CA-C	-5.35	1.45	1.52
2	B	468	SER	CA-C	-5.35	1.48	1.52
5	L	437	LEU	CA-C	-5.35	1.45	1.52
5	L	160	ALA	N-CA	-5.35	1.39	1.46
2	B	493	HIS	CD2-NE2	5.35	1.43	1.37
5	L	561	LEU	CA-CB	5.35	1.61	1.54
2	D	294	SER	C-N	5.35	1.41	1.33
3	K	130	HIS	ND1-CE1	5.34	1.37	1.32
2	D	400	HIS	CG-CD2	5.34	1.41	1.35
2	B	457	ARG	CA-CB	5.34	1.62	1.53
1	G	487	ILE	CA-C	-5.34	1.45	1.52
2	H	285	SER	N-CA	-5.34	1.39	1.46
1	G	353	ALA	C-N	5.33	1.41	1.33
1	A	272	VAL	CA-C	-5.33	1.45	1.52
1	A	359	HIS	C-O	-5.33	1.18	1.24
3	I	27	VAL	C-N	5.33	1.40	1.33
2	R	10	ASN	CG-ND2	5.33	1.44	1.33
2	H	422	ALA	CA-C	-5.33	1.45	1.52
1	G	433	ILE	CA-C	-5.33	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	416	ILE	C-O	-5.33	1.18	1.24
3	K	320	PHE	N-CA	-5.33	1.39	1.46
6	V	640	ILE	CA-C	-5.33	1.45	1.52
7	p	46	ASN	C-N	5.33	1.40	1.34
2	B	485	ILE	N-CA	-5.33	1.40	1.46
1	C	298	LEU	C-N	5.33	1.40	1.33
2	R	16	LEU	C-N	5.32	1.41	1.33
2	S	64	ARG	NE-CZ	5.32	1.39	1.33
7	p	32	GLU	CA-C	-5.32	1.46	1.52
1	C	393	TRP	N-CA	-5.32	1.40	1.46
1	G	345	ASN	C-O	-5.32	1.17	1.24
6	V	651	GLU	CA-C	-5.32	1.45	1.52
2	F	311	SER	CA-CB	5.32	1.60	1.53
6	W	653	LEU	C-N	5.32	1.40	1.33
7	t	53	VAL	C-N	5.32	1.40	1.33
5	L	360	VAL	CA-C	5.31	1.61	1.52
1	A	245	PHE	N-CA	-5.31	1.39	1.46
2	B	544	LEU	CA-CB	5.31	1.62	1.53
2	Q	11	VAL	CA-CB	-5.31	1.47	1.54
2	R	28	VAL	N-CA	-5.31	1.39	1.46
2	S	52	PHE	CA-C	-5.31	1.46	1.52
2	B	263	LYS	CA-CB	5.31	1.62	1.53
2	O	56	GLU	C-N	5.31	1.40	1.33
5	L	543	GLY	N-CA	5.31	1.52	1.45
1	A	476	TYR	C-N	5.31	1.41	1.33
3	I	42	LEU	CA-C	-5.31	1.45	1.52
3	I	303	GLN	C-O	-5.31	1.17	1.24
4	J	497	PRO	N-CD	5.31	1.55	1.47
2	F	450	ASP	N-CA	-5.31	1.42	1.46
4	J	458	PHE	N-CA	-5.31	1.39	1.46
2	D	541	SER	CA-C	-5.30	1.45	1.52
2	Q	44	ALA	N-CA	-5.30	1.38	1.46
2	H	369	TRP	CZ2-CH2	5.30	1.47	1.37
4	J	484	PRO	N-CA	-5.30	1.40	1.47
6	W	654	VAL	N-CA	-5.30	1.40	1.46
7	q	20	GLU	C-N	5.30	1.40	1.33
1	G	262	ILE	CA-CB	5.30	1.61	1.54
5	L	76	SER	C-N	5.30	1.40	1.33
5	L	234	MET	N-CA	-5.29	1.37	1.45
5	L	464	PHE	N-CA	-5.29	1.39	1.46
2	H	378	LYS	CA-CB	-5.29	1.44	1.53
2	H	484	LEU	CA-C	-5.29	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	642	MET	CA-C	-5.29	1.46	1.52
2	D	425	ILE	CA-CB	5.29	1.60	1.54
1	E	255	VAL	CA-C	5.29	1.60	1.52
2	S	17	CYS	CA-CB	5.29	1.61	1.53
2	D	542	LYS	CA-CB	5.29	1.64	1.53
2	H	525	LEU	CA-CB	5.29	1.61	1.53
5	L	396	SER	CA-CB	5.29	1.61	1.53
1	C	491	TYR	N-CA	-5.28	1.39	1.46
3	I	91	ARG	CD-NE	5.28	1.53	1.46
3	I	318	PRO	C-N	5.28	1.41	1.33
1	A	377	TYR	C-N	5.28	1.41	1.33
4	J	233	HIS	CG-ND1	5.28	1.44	1.38
1	C	401	ASP	CA-C	-5.28	1.46	1.52
2	D	460	HIS	C-N	5.28	1.40	1.33
3	K	116	HIS	CD2-NE2	5.27	1.43	1.37
3	K	151	CYS	C-N	5.27	1.41	1.33
2	B	483	LEU	CA-CB	5.27	1.61	1.53
2	D	460	HIS	CA-CB	5.27	1.62	1.53
7	p	53	VAL	N-CA	-5.27	1.40	1.46
4	J	687	TYR	CA-C	-5.27	1.46	1.52
1	A	272	VAL	C-O	-5.27	1.17	1.24
2	D	489	ILE	CB-CG1	5.27	1.64	1.53
2	H	550	LYS	C-N	5.27	1.40	1.33
1	A	491	TYR	CA-CB	5.26	1.62	1.53
1	A	497	VAL	CA-CB	-5.26	1.48	1.54
6	V	620	ARG	CZ-NH2	5.26	1.40	1.33
6	W	649	LEU	CB-CG	5.26	1.64	1.53
6	X	613	ASP	CA-CB	5.26	1.61	1.53
1	A	224	LEU	C-N	5.26	1.40	1.33
2	B	462	LYS	N-CA	-5.26	1.39	1.46
2	D	407	ASP	C-N	-5.26	1.29	1.33
1	G	359	HIS	CE1-NE2	5.26	1.37	1.32
2	H	482	VAL	CA-C	-5.26	1.44	1.52
2	T	78	HIS	CG-CD2	5.26	1.41	1.35
1	G	435	GLN	CA-C	-5.26	1.46	1.53
1	A	336	VAL	N-CA	-5.25	1.39	1.46
2	F	390	ARG	CA-CB	-5.25	1.46	1.53
4	J	588	TYR	CA-CB	5.25	1.61	1.53
2	O	12	LEU	CA-CB	5.25	1.61	1.53
2	F	415	GLN	C-N	5.25	1.41	1.34
2	H	427	ASN	CA-CB	5.25	1.61	1.53
2	B	472	SER	C-N	5.25	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	ASP	N-CA	-5.24	1.39	1.46
1	A	386	TYR	CA-CB	5.24	1.61	1.53
5	L	45	ASP	N-CA	-5.24	1.40	1.46
7	t	54	ILE	C-N	5.24	1.40	1.33
5	L	514	SER	N-CA	-5.24	1.40	1.46
1	C	289	HIS	ND1-CE1	5.24	1.37	1.32
3	K	168	VAL	N-CA	-5.24	1.39	1.46
2	H	550	LYS	CA-CB	5.24	1.61	1.53
2	O	90	ARG	N-CA	-5.24	1.40	1.46
2	R	59	LYS	CA-CB	-5.24	1.45	1.53
1	C	267	THR	CB-OG1	5.24	1.52	1.43
2	D	364	ARG	NE-CZ	5.24	1.38	1.33
5	L	362	ILE	C-N	5.24	1.40	1.33
2	B	254	LEU	CA-CB	5.23	1.61	1.53
4	J	365	TYR	CZ-OH	5.23	1.49	1.38
1	C	330	THR	N-CA	-5.23	1.39	1.46
1	C	449	ILE	CA-C	-5.22	1.46	1.52
1	E	240	ARG	CZ-NH1	5.22	1.40	1.32
2	Q	99	SER	C-N	5.22	1.41	1.33
2	H	463	TYR	CA-C	5.22	1.59	1.52
4	J	422	ASP	CA-CB	5.22	1.61	1.53
4	J	587	LEU	CB-CG	5.22	1.63	1.53
6	X	652	SER	CA-C	-5.22	1.46	1.52
2	D	267	MET	CA-C	-5.21	1.46	1.52
1	E	359	HIS	ND1-CE1	5.21	1.37	1.32
4	J	286	ASN	CA-C	-5.21	1.46	1.52
3	K	176	LEU	CA-CB	5.21	1.61	1.53
7	s	27	THR	N-CA	5.21	1.52	1.46
2	D	408	PRO	N-CA	-5.21	1.42	1.47
2	F	394	GLU	N-CA	-5.21	1.39	1.46
3	I	87	ARG	CA-CB	5.21	1.61	1.53
7	r	17	VAL	N-CA	-5.21	1.40	1.46
1	E	432	THR	N-CA	5.21	1.52	1.46
2	T	53	LEU	C-N	5.21	1.40	1.33
3	I	22	ARG	C-N	5.21	1.40	1.33
2	F	399	VAL	CA-C	5.20	1.60	1.52
1	G	308	GLN	C-N	5.20	1.41	1.33
4	J	361	MET	N-CA	-5.20	1.39	1.46
3	K	158	TYR	C-O	-5.20	1.18	1.24
2	S	107	GLN	N-CA	-5.20	1.39	1.45
1	C	350	PHE	CA-C	5.20	1.59	1.52
2	H	470	ILE	C-O	-5.20	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	98	LEU	CA-CB	5.20	1.61	1.53
1	C	222	TYR	CA-CB	5.20	1.61	1.53
2	Q	66	ARG	CZ-NH1	5.20	1.40	1.32
2	S	90	ARG	NE-CZ	5.20	1.38	1.33
5	L	101	SER	N-CA	5.20	1.52	1.45
2	T	78	HIS	CB-CG	5.20	1.57	1.50
6	V	655	SER	N-CA	-5.20	1.39	1.46
6	X	613	ASP	C-O	-5.20	1.18	1.24
3	I	85	TYR	CA-C	-5.19	1.45	1.52
2	R	89	ASN	CA-CB	5.19	1.57	1.53
7	s	39	ARG	CZ-NH2	5.19	1.40	1.33
5	L	445	ARG	CA-C	-5.19	1.46	1.52
6	U	603	ILE	CA-C	5.19	1.59	1.52
1	E	240	ARG	CZ-NH2	5.19	1.40	1.33
2	Q	50	ASP	CA-C	-5.19	1.47	1.53
2	Q	108	PRO	C-N	5.19	1.40	1.33
2	B	264	PHE	CA-C	-5.18	1.46	1.52
1	G	215	CYS	N-CA	-5.18	1.39	1.46
1	G	247	VAL	C-O	-5.18	1.17	1.24
1	A	455	TYR	CA-C	-5.18	1.46	1.52
2	F	263	LYS	CA-CB	5.18	1.61	1.53
5	L	385	TYR	CA-C	-5.18	1.46	1.52
2	B	337	LEU	CA-C	5.18	1.59	1.52
1	E	453	GLY	C-N	5.18	1.41	1.33
4	J	378	ILE	C-N	5.18	1.41	1.34
1	G	288	ASN	C-O	-5.17	1.17	1.24
1	A	252	ASP	CA-C	-5.17	1.45	1.52
2	B	283	SER	N-CA	-5.17	1.39	1.45
1	G	262	ILE	N-CA	-5.17	1.40	1.46
2	R	98	LEU	CA-C	-5.17	1.46	1.52
1	G	294	ALA	CA-C	-5.17	1.46	1.52
5	L	335	ILE	CA-C	-5.17	1.46	1.52
2	Q	67	ARG	CZ-NH2	5.17	1.40	1.33
1	C	259	VAL	C-N	5.16	1.41	1.33
6	X	639	GLU	C-N	5.16	1.40	1.33
2	D	258	GLN	CA-CB	5.16	1.62	1.53
2	D	315	ALA	C-N	5.16	1.40	1.33
7	q	32	GLU	C-N	5.16	1.40	1.33
1	A	398	ILE	CA-C	-5.16	1.46	1.52
2	B	389	GLY	CA-C	-5.16	1.44	1.52
1	E	285	GLY	C-N	5.16	1.40	1.33
2	Q	68	GLU	N-CA	-5.16	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	631	LYS	CA-CB	5.16	1.61	1.53
7	r	12	ARG	CD-NE	5.16	1.53	1.46
5	L	368	THR	C-O	-5.16	1.17	1.24
1	A	428	ASP	CA-C	5.15	1.59	1.52
2	T	37	ARG	NE-CZ	5.15	1.38	1.33
1	A	410	GLU	CA-C	-5.15	1.46	1.53
1	C	260	ASN	CA-CB	5.15	1.62	1.53
2	H	466	ARG	CD-NE	5.15	1.53	1.46
2	D	302	LYS	CA-CB	5.15	1.61	1.53
1	E	394	ILE	C-N	5.15	1.41	1.33
3	I	327	SER	CA-C	-5.15	1.45	1.52
3	K	265	PRO	N-CA	-5.15	1.40	1.47
7	q	29	LEU	C-N	5.15	1.40	1.33
2	Q	82	GLN	CA-C	5.15	1.59	1.52
2	B	321	GLN	CA-C	5.14	1.59	1.52
2	D	247	THR	CA-C	-5.14	1.45	1.52
2	D	384	VAL	CA-C	-5.14	1.46	1.52
2	F	306	TYR	N-CA	-5.14	1.40	1.46
3	I	35	HIS	CG-CD2	-5.14	1.30	1.35
5	L	461	SER	N-CA	5.14	1.52	1.46
1	A	353	ALA	C-N	5.14	1.40	1.33
5	L	471	LEU	CA-CB	5.14	1.61	1.53
6	U	619	HIS	CD2-NE2	5.14	1.43	1.37
1	E	338	ALA	C-N	-5.14	1.26	1.33
1	A	430	ARG	NE-CZ	5.13	1.38	1.33
2	B	539	ASP	CA-CB	5.13	1.61	1.53
2	D	274	TYR	N-CA	-5.13	1.40	1.46
4	J	355	ARG	CD-NE	5.13	1.53	1.46
4	J	414	THR	N-CA	-5.13	1.39	1.46
1	E	374	LEU	C-N	5.13	1.41	1.34
3	K	3	HIS	CA-CB	5.13	1.61	1.53
7	r	50	LEU	CA-C	-5.13	1.46	1.52
1	E	257	GLU	CA-C	5.12	1.59	1.52
2	H	480	ARG	C-N	5.12	1.40	1.33
4	J	357	TYR	CA-C	-5.12	1.45	1.52
3	K	86	LEU	CA-C	-5.12	1.46	1.52
1	A	359	HIS	CA-C	-5.12	1.46	1.52
2	H	460	HIS	CB-CG	-5.12	1.43	1.50
4	J	474	GLU	CA-CB	5.12	1.61	1.53
4	J	409	HIS	CA-CB	5.12	1.61	1.53
2	D	313	ASP	CA-C	-5.11	1.45	1.52
1	A	247	VAL	CA-C	-5.11	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	ASN	C-N	5.11	1.40	1.33
4	J	597	SER	CA-C	5.11	1.59	1.52
7	q	42	GLU	N-CA	-5.11	1.39	1.46
2	T	58	ILE	CA-C	-5.11	1.46	1.52
3	I	46	CYS	C-N	5.11	1.41	1.33
2	B	265	VAL	N-CA	-5.11	1.40	1.46
2	D	416	HIS	N-CA	5.11	1.52	1.46
2	R	50	ASP	C-N	5.11	1.40	1.33
1	A	495	SER	C-N	5.10	1.41	1.33
1	E	436	GLN	N-CA	-5.10	1.40	1.46
6	U	645	GLU	C-O	-5.10	1.18	1.24
1	C	440	SER	N-CA	-5.10	1.40	1.46
2	R	9	PRO	N-CD	-5.10	1.40	1.47
2	B	427	ASN	C-N	5.10	1.41	1.33
1	C	217	VAL	CA-CB	-5.10	1.48	1.54
2	B	393	GLY	CA-C	-5.10	1.46	1.52
2	H	360	SER	CA-CB	5.10	1.62	1.53
2	S	82	GLN	N-CA	-5.10	1.40	1.46
2	F	377	LEU	N-CA	5.09	1.52	1.46
6	W	664	ASN	C-N	5.09	1.40	1.33
1	E	299	GLY	CA-C	5.09	1.58	1.51
5	L	475	ALA	CA-CB	5.09	1.61	1.53
7	q	42	GLU	CA-CB	5.09	1.62	1.53
2	H	542	LYS	C-N	5.09	1.40	1.33
5	L	434	THR	N-CA	-5.09	1.39	1.46
7	o	52	SER	CA-CB	-5.09	1.45	1.53
3	K	29	GLN	C-N	5.09	1.40	1.33
2	H	451	PRO	CA-C	-5.09	1.45	1.52
4	J	230	HIS	ND1-CE1	5.09	1.37	1.32
6	X	599	GLN	N-CA	-5.09	1.40	1.46
2	B	269	ASN	CA-CB	5.08	1.61	1.53
2	D	418	LEU	N-CA	-5.08	1.40	1.46
2	D	483	LEU	CB-CG	5.08	1.63	1.53
3	K	160	HIS	CG-ND1	5.08	1.43	1.38
3	K	338	GLU	CA-C	-5.08	1.45	1.52
1	C	266	ALA	CA-C	-5.08	1.46	1.52
7	p	32	GLU	C-N	5.08	1.40	1.33
1	A	364	GLY	CA-C	-5.08	1.46	1.52
1	G	375	CYS	N-CA	-5.08	1.39	1.46
3	K	186	GLN	CA-CB	5.08	1.61	1.53
2	B	457	ARG	NE-CZ	5.07	1.38	1.33
4	J	207	ASP	N-CA	5.07	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	38	VAL	N-CA	-5.07	1.40	1.46
2	H	325	ALA	N-CA	-5.07	1.40	1.46
6	X	610	THR	CA-CB	5.07	1.61	1.53
6	X	658	GLU	CA-C	-5.07	1.46	1.52
2	D	274	TYR	C-O	-5.07	1.18	1.24
3	K	256	GLN	C-N	5.07	1.40	1.33
2	S	60	LYS	CA-CB	5.07	1.61	1.53
4	J	685	CYS	CA-CB	5.06	1.61	1.53
5	L	43	ALA	C-O	5.06	1.30	1.24
5	L	326	TYR	CA-C	5.06	1.59	1.52
2	O	70	ASP	C-O	-5.06	1.18	1.24
2	Q	14	GLN	CA-CB	5.06	1.61	1.53
3	I	333	ARG	NE-CZ	5.06	1.38	1.33
1	A	325	PHE	CA-CB	5.05	1.61	1.53
2	F	260	ILE	C-N	5.05	1.40	1.33
2	F	322	SER	C-N	5.05	1.40	1.33
2	H	524	ASP	N-CA	5.05	1.55	1.46
3	I	289	GLN	N-CA	-5.05	1.40	1.46
5	L	377	SER	CA-C	-5.05	1.46	1.52
1	A	476	TYR	N-CA	5.05	1.51	1.45
4	J	411	VAL	N-CA	-5.05	1.40	1.46
4	J	571	ARG	CD-NE	5.05	1.53	1.46
2	B	251	ARG	NE-CZ	5.05	1.38	1.33
2	B	254	LEU	CA-C	-5.05	1.45	1.52
1	C	402	PRO	N-CD	-5.05	1.40	1.47
3	I	96	ILE	C-O	-5.05	1.19	1.24
2	S	57	LYS	CA-CB	5.05	1.61	1.53
7	s	17	VAL	N-CA	5.05	1.52	1.46
2	D	408	PRO	N-CD	5.05	1.54	1.47
3	K	269	PRO	CA-CB	-5.05	1.46	1.53
2	B	372	ASP	C-N	5.04	1.40	1.33
2	H	309	GLN	C-N	5.04	1.40	1.33
2	H	363	LEU	CA-CB	5.04	1.61	1.53
1	G	332	ARG	N-CA	-5.04	1.39	1.46
1	C	277	GLU	CA-CB	5.04	1.61	1.53
5	L	237	VAL	N-CA	-5.04	1.40	1.46
1	E	384	ALA	CA-C	5.04	1.59	1.52
2	F	296	LEU	C-N	5.04	1.40	1.34
5	L	580	VAL	C-N	5.04	1.40	1.33
5	L	587	PHE	C-O	5.04	1.30	1.24
1	C	211	SER	CA-CB	5.04	1.61	1.53
2	H	411	ARG	CD-NE	5.04	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	376	LEU	CB-CG	5.04	1.63	1.53
1	E	279	ASN	CA-CB	5.04	1.61	1.53
5	L	320	GLU	CA-CB	5.03	1.61	1.53
6	W	601	ASN	N-CA	-5.03	1.40	1.46
2	H	457	ARG	CD-NE	5.03	1.53	1.46
4	J	297	ILE	CA-CB	-5.03	1.46	1.55
1	A	483	TYR	CA-CB	5.03	1.62	1.53
1	G	342	THR	CA-CB	5.03	1.61	1.53
5	L	35	THR	N-CA	-5.03	1.40	1.46
2	T	93	ILE	CA-CB	5.03	1.60	1.54
7	s	38	VAL	CA-CB	-5.03	1.48	1.54
2	B	301	ASN	CG-ND2	5.03	1.43	1.33
5	L	33	ASN	C-O	-5.03	1.18	1.24
5	L	472	ARG	CA-CB	5.03	1.61	1.53
2	O	38	VAL	CA-C	5.03	1.59	1.52
2	F	463	TYR	CA-C	-5.03	1.46	1.52
3	I	327	SER	C-N	5.03	1.39	1.34
7	r	17	VAL	C-N	5.03	1.40	1.33
1	C	241	GLN	C-N	5.03	1.41	1.33
5	L	458	LEU	CA-CB	5.03	1.61	1.53
6	X	616	GLU	C-N	5.03	1.40	1.33
7	r	41	CYS	CA-C	-5.03	1.46	1.52
2	B	523	THR	N-CA	-5.02	1.40	1.46
2	D	437	GLU	CA-C	-5.02	1.46	1.52
6	V	619	HIS	ND1-CE1	5.02	1.37	1.32
1	E	433	ILE	C-O	-5.02	1.18	1.24
6	W	661	ARG	CA-C	5.02	1.59	1.52
3	I	279	VAL	CA-CB	-5.02	1.48	1.54
4	J	226	PRO	C-N	5.02	1.40	1.33
2	T	90	ARG	C-O	5.02	1.29	1.24
6	V	659	LYS	C-N	5.02	1.40	1.33
4	J	598	ARG	CZ-NH2	5.02	1.40	1.33
5	L	250	VAL	N-CA	-5.01	1.41	1.46
5	L	553	MET	N-CA	-5.01	1.39	1.46
5	L	73	ILE	C-O	-5.01	1.18	1.24
2	R	43	PHE	C-N	5.01	1.41	1.33
4	J	289	LYS	C-N	5.01	1.39	1.33
2	T	97	LEU	C-N	5.01	1.40	1.33
7	s	30	ASP	C-N	5.01	1.40	1.33
2	B	513	GLU	CA-CB	5.00	1.61	1.53
2	D	486	GLY	CA-C	-5.00	1.44	1.51
2	H	360	SER	N-CA	-5.00	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	473	PHE	C-N	5.00	1.40	1.33
3	K	181	GLY	C-N	5.00	1.40	1.33

All (2389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	86	VAL	N-CA-C	-11.89	101.07	112.96
2	D	361	LEU	N-CA-C	-11.25	99.54	113.38
4	J	228	PHE	CA-CB-CG	11.13	124.93	113.80
1	E	441	PHE	CA-CB-CG	-11.03	102.77	113.80
1	A	327	ILE	N-CA-C	-10.53	102.54	111.91
2	H	364	ARG	NE-CZ-NH2	-10.52	109.73	119.20
5	L	249	LYS	CA-C-N	10.52	132.72	123.04
5	L	249	LYS	C-N-CA	10.52	132.72	123.04
1	C	245	PHE	CA-CB-CG	-10.36	103.44	113.80
4	J	308	SER	N-CA-C	-10.21	100.69	113.55
2	H	394	GLU	O-C-N	10.18	133.75	122.15
3	I	16	ILE	CB-CG1-CD1	10.10	135.00	113.80
2	F	524	ASP	CA-C-N	10.05	135.00	120.82
2	F	524	ASP	C-N-CA	10.05	135.00	120.82
2	H	313	ASP	N-CA-C	-10.01	101.06	113.28
5	L	518	TYR	CA-C-N	9.94	129.60	119.56
5	L	518	TYR	C-N-CA	9.94	129.60	119.56
1	A	369	SER	N-CA-C	-9.92	98.45	111.24
2	B	314	ARG	NE-CZ-NH2	9.85	128.06	119.20
2	H	314	ARG	NE-CZ-NH2	9.76	127.98	119.20
1	A	304	ILE	N-CA-C	-9.63	100.99	110.72
1	A	460	ARG	CA-C-N	9.60	133.15	120.28
1	A	460	ARG	C-N-CA	9.60	133.15	120.28
3	I	128	GLN	N-CA-C	-9.54	101.65	113.28
3	I	307	PHE	CA-CB-CG	-9.52	104.28	113.80
3	I	157	VAL	CA-C-O	9.51	130.74	120.47
6	X	657	ILE	CA-C-N	9.51	132.80	120.44
6	X	657	ILE	C-N-CA	9.51	132.80	120.44
1	C	246	SER	CA-C-N	9.50	134.62	120.75
1	C	246	SER	C-N-CA	9.50	134.62	120.75
6	W	650	ASN	CA-C-N	9.39	132.87	120.28
6	W	650	ASN	C-N-CA	9.39	132.87	120.28
1	A	289	HIS	CE1-NE2-CD2	-9.31	99.69	109.00
1	A	289	HIS	ND1-CE1-NE2	9.30	117.70	108.40
6	U	598	ILE	CA-C-N	9.29	133.49	120.29
6	U	598	ILE	C-N-CA	9.29	133.49	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	44	ALA	CA-C-N	9.29	129.33	119.76
2	Q	44	ALA	C-N-CA	9.29	129.33	119.76
4	J	454	VAL	O-C-N	-9.22	112.92	121.87
1	G	436	GLN	N-CA-C	-9.16	102.11	113.38
5	L	318	GLY	N-CA-C	9.13	122.07	110.38
2	H	318	LEU	N-CA-C	-9.13	102.72	114.04
4	J	355	ARG	CA-C-N	9.12	132.30	120.44
4	J	355	ARG	C-N-CA	9.12	132.30	120.44
7	p	16	ASP	CA-CB-CG	9.11	121.71	112.60
3	I	199	GLN	N-CA-C	-9.09	102.32	113.41
5	L	329	HIS	CA-CB-CG	9.08	122.88	113.80
7	o	59	ARG	NE-CZ-NH2	9.06	127.36	119.20
5	L	314	VAL	CA-C-N	9.05	133.14	120.29
5	L	314	VAL	C-N-CA	9.05	133.14	120.29
7	q	16	ASP	CA-CB-CG	9.02	121.62	112.60
1	G	222	TYR	CA-C-N	9.01	133.22	120.42
1	G	222	TYR	C-N-CA	9.01	133.22	120.42
2	D	441	THR	N-CA-C	-9.01	103.12	114.56
7	t	14	THR	CA-C-N	8.97	132.30	120.28
7	t	14	THR	C-N-CA	8.97	132.30	120.28
7	r	37	CYS	O-C-N	8.95	131.61	122.12
2	S	16	LEU	CA-C-N	8.95	132.07	120.44
2	S	16	LEU	C-N-CA	8.95	132.07	120.44
3	I	317	GLN	N-CA-C	-8.94	97.88	108.25
6	V	604	LYS	CA-C-N	8.91	132.02	120.44
6	V	604	LYS	C-N-CA	8.91	132.02	120.44
7	t	39	ARG	NE-CZ-NH2	8.88	127.19	119.20
6	V	661	ARG	NE-CZ-NH1	8.83	130.33	121.50
3	K	162	CYS	CA-C-N	8.83	132.53	121.06
3	K	162	CYS	C-N-CA	8.83	132.53	121.06
2	H	416	HIS	CA-CB-CG	8.82	122.62	113.80
2	Q	11	VAL	N-CA-C	-8.81	101.82	110.72
4	J	571	ARG	NE-CZ-NH1	8.81	130.31	121.50
1	A	438	ILE	CA-C-N	8.80	130.84	119.84
1	A	438	ILE	C-N-CA	8.80	130.84	119.84
1	C	303	MET	CG-SD-CE	-8.77	81.60	100.90
2	F	286	LEU	N-CA-C	-8.76	102.73	113.50
5	L	410	ARG	NE-CZ-NH1	8.73	130.23	121.50
1	C	343	SER	O-C-N	-8.73	111.53	122.27
2	F	465	LEU	N-CA-C	8.72	121.74	111.71
2	B	364	ARG	CA-C-N	8.70	132.89	120.79
2	B	364	ARG	C-N-CA	8.70	132.89	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	81	LEU	CA-C-N	8.69	131.93	120.28
2	O	81	LEU	C-N-CA	8.69	131.93	120.28
1	A	406	PHE	CA-CB-CG	-8.69	105.11	113.80
7	r	26	ASN	CA-CB-CG	8.69	121.29	112.60
2	D	452	VAL	N-CA-C	-8.67	93.50	107.28
3	K	88	ALA	N-CA-C	-8.64	101.80	111.82
4	J	451	GLU	CA-C-N	8.63	133.43	120.31
4	J	451	GLU	C-N-CA	8.63	133.43	120.31
2	H	450	ASP	CA-C-N	8.63	130.63	119.84
2	H	450	ASP	C-N-CA	8.63	130.63	119.84
6	V	649	LEU	N-CA-CB	8.60	125.02	110.49
1	C	440	SER	O-C-N	8.59	131.23	122.12
4	J	262	THR	N-CA-CB	8.58	126.09	111.50
7	s	62	ASP	CA-CB-CG	-8.55	104.05	112.60
3	I	263	MET	N-CA-C	-8.55	100.83	112.03
7	t	51	SER	CB-CA-C	-8.54	96.61	110.79
7	s	63	THR	O-C-N	8.54	131.88	122.15
5	L	15	HIS	CA-CB-CG	-8.47	105.33	113.80
1	G	311	HIS	ND1-CE1-NE2	8.47	116.87	108.40
5	L	396	SER	CA-C-N	8.46	132.31	120.29
5	L	396	SER	C-N-CA	8.46	132.31	120.29
1	A	472	LYS	N-CA-C	-8.44	101.44	112.41
2	R	78	HIS	CA-CB-CG	-8.44	105.36	113.80
2	T	69	ALA	CA-C-O	-8.43	111.61	120.55
7	r	12	ARG	CA-C-N	8.43	132.26	120.29
7	r	12	ARG	C-N-CA	8.43	132.26	120.29
2	Q	14	GLN	CA-C-N	8.42	131.56	120.28
2	Q	14	GLN	C-N-CA	8.42	131.56	120.28
1	E	298	LEU	CA-C-N	8.42	130.91	120.22
1	E	298	LEU	C-N-CA	8.42	130.91	120.22
5	L	465	ARG	NE-CZ-NH2	8.42	126.77	119.20
3	I	16	ILE	CA-CB-CG1	8.40	124.69	110.40
2	T	81	LEU	CA-C-N	8.40	131.54	120.28
2	T	81	LEU	C-N-CA	8.40	131.54	120.28
2	T	93	ILE	N-CA-C	8.40	119.18	110.62
4	J	689	HIS	ND1-CE1-NE2	8.36	116.76	108.40
2	B	440	ASP	CA-CB-CG	8.35	120.95	112.60
1	A	330	THR	N-CA-C	-8.34	102.54	112.89
1	C	273	THR	CA-C-N	8.31	131.42	120.28
1	C	273	THR	C-N-CA	8.31	131.42	120.28
5	L	96	GLU	CA-C-N	8.31	131.24	120.44
5	L	96	GLU	C-N-CA	8.31	131.24	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	281	ALA	N-CA-C	-8.30	93.30	107.99
1	E	243	ARG	CA-C-O	8.30	129.66	120.70
1	E	430	ARG	NE-CZ-NH2	8.29	126.67	119.20
6	V	618	CYS	CA-C-N	8.28	131.38	120.28
6	V	618	CYS	C-N-CA	8.28	131.38	120.28
1	G	406	PHE	CA-CB-CG	-8.28	105.52	113.80
2	H	551	ASN	CA-CB-CG	-8.28	104.32	112.60
1	G	405	GLU	N-CA-C	-8.28	102.39	114.39
4	J	500	HIS	CE1-NE2-CD2	-8.27	100.73	109.00
5	L	426	ASN	OD1-CG-ND2	-8.26	114.34	122.60
3	K	98	GLN	N-CA-CB	8.25	120.16	110.42
1	G	429	GLN	OE1-CD-NE2	8.22	130.82	122.60
1	E	307	SER	N-CA-C	8.21	121.34	111.82
1	C	261	ARG	CB-CA-C	8.20	123.92	109.65
1	G	263	LEU	CA-C-N	8.19	127.83	119.56
1	G	263	LEU	C-N-CA	8.19	127.83	119.56
2	B	518	ALA	N-CA-C	8.19	120.21	111.28
2	T	78	HIS	ND1-CE1-NE2	8.18	116.58	108.40
2	Q	90	ARG	NE-CZ-NH2	8.18	126.56	119.20
3	I	51	ASP	CA-CB-CG	8.17	120.77	112.60
2	D	306	TYR	O-C-N	8.14	131.43	122.15
1	G	369	SER	N-CA-C	-8.13	103.34	113.18
3	I	82	HIS	CA-CB-CG	8.13	121.93	113.80
5	L	34	ARG	CA-C-N	8.12	131.17	120.28
5	L	34	ARG	C-N-CA	8.12	131.17	120.28
5	L	102	ASN	N-CA-C	-8.13	96.16	109.40
2	R	24	GLY	CA-C-N	8.12	131.00	120.44
2	R	24	GLY	C-N-CA	8.12	131.00	120.44
2	Q	71	GLY	N-CA-C	8.12	122.47	112.73
6	U	628	GLU	N-CA-C	8.11	120.20	111.36
1	C	430	ARG	NE-CZ-NH2	8.11	126.50	119.20
6	X	645	GLU	N-CA-C	8.11	121.14	111.33
4	J	326	PHE	CA-CB-CG	-8.09	105.71	113.80
2	S	37	ARG	NE-CZ-NH2	8.09	126.48	119.20
1	E	263	LEU	CA-C-N	8.09	127.75	119.82
1	E	263	LEU	C-N-CA	8.09	127.75	119.82
2	H	264	PHE	CA-CB-CG	-8.09	105.71	113.80
4	J	398	LEU	CA-C-N	8.08	129.68	120.06
4	J	398	LEU	C-N-CA	8.08	129.68	120.06
4	J	501	ARG	NE-CZ-NH1	8.07	129.57	121.50
2	O	10	ASN	CA-C-N	8.05	130.70	120.56
2	O	10	ASN	C-N-CA	8.05	130.70	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	304	LYS	CA-C-N	8.03	132.52	120.31
2	D	304	LYS	C-N-CA	8.03	132.52	120.31
1	G	325	PHE	CA-CB-CG	8.02	121.82	113.80
2	F	462	LYS	N-CA-C	-8.02	100.27	113.50
2	T	77	LEU	O-C-N	-8.02	113.62	122.12
2	T	70	ASP	CA-C-N	8.01	128.87	119.98
2	T	70	ASP	C-N-CA	8.01	128.87	119.98
7	p	55	LYS	N-CA-C	8.01	120.00	111.28
2	T	100	LEU	CA-C-O	7.98	128.94	119.28
6	U	666	ARG	NE-CZ-NH2	-7.98	112.02	119.20
4	J	300	HIS	CA-CB-CG	7.98	121.78	113.80
1	G	487	ILE	N-CA-C	7.97	118.77	110.72
5	L	460	ILE	N-CA-C	-7.97	104.96	111.81
3	K	129	PHE	CA-CB-CG	-7.96	105.84	113.80
2	O	63	VAL	N-CA-C	7.96	118.74	110.62
5	L	413	HIS	CA-C-N	7.96	132.40	120.31
5	L	413	HIS	C-N-CA	7.96	132.40	120.31
2	R	71	GLY	CA-C-N	7.92	130.90	120.28
2	R	71	GLY	C-N-CA	7.92	130.90	120.28
6	V	598	ILE	CA-C-N	7.90	132.32	120.31
6	V	598	ILE	C-N-CA	7.90	132.32	120.31
2	F	311	SER	CA-C-N	7.90	136.08	122.81
2	F	311	SER	C-N-CA	7.90	136.08	122.81
7	r	44	GLY	N-CA-C	-7.90	103.58	111.56
7	o	36	ILE	N-CA-C	7.89	118.67	110.62
4	J	409	HIS	CE1-NE2-CD2	-7.88	101.11	109.00
4	J	420	PRO	N-CA-C	7.87	120.30	110.70
5	L	342	GLN	CA-C-N	7.85	129.66	119.84
5	L	342	GLN	C-N-CA	7.85	129.66	119.84
2	F	318	LEU	N-CA-C	-7.84	104.20	114.31
3	K	130	HIS	CA-CB-CG	7.83	121.63	113.80
3	I	35	HIS	CE1-NE2-CD2	-7.83	101.17	109.00
1	C	328	GLN	O-C-N	-7.81	112.33	121.32
2	O	91	TRP	CA-CB-CG	7.81	128.44	113.60
2	B	317	GLY	N-CA-C	-7.81	105.09	115.32
2	H	445	PHE	N-CA-C	-7.80	98.97	110.52
7	q	26	ASN	CA-CB-CG	-7.79	104.81	112.60
1	G	333	THR	CA-C-N	7.79	131.06	120.54
1	G	333	THR	C-N-CA	7.79	131.06	120.54
1	G	241	GLN	N-CA-C	-7.78	104.31	113.88
3	I	191	MET	CG-SD-CE	-7.78	83.78	100.90
1	E	482	ALA	N-CA-C	-7.78	100.46	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	27	ASP	CA-CB-CG	-7.78	104.82	112.60
4	J	500	HIS	CA-C-O	7.77	129.54	121.23
1	C	433	ILE	N-CA-CB	7.77	122.04	112.10
2	T	96	LEU	CA-C-N	7.76	130.68	120.28
2	T	96	LEU	C-N-CA	7.76	130.68	120.28
6	W	646	ARG	N-CA-C	7.74	120.70	111.33
1	C	328	GLN	CA-C-N	7.74	127.39	119.19
1	C	328	GLN	C-N-CA	7.74	127.39	119.19
2	H	314	ARG	NE-CZ-NH1	-7.74	113.76	121.50
6	U	639	GLU	CB-CA-C	-7.74	98.73	110.88
1	A	268	ASN	N-CA-CB	7.74	122.22	110.30
2	F	461	ASP	CA-CB-CG	7.74	120.33	112.60
3	K	339	HIS	CG-CD2-NE2	7.73	114.93	107.20
1	E	371	ALA	CA-C-N	7.72	132.04	120.31
1	E	371	ALA	C-N-CA	7.72	132.04	120.31
1	G	236	PRO	N-CA-CB	7.71	110.52	103.19
7	t	45	ILE	CA-C-N	7.71	135.73	121.69
7	t	45	ILE	C-N-CA	7.71	135.73	121.69
5	L	605	LEU	N-CA-C	-7.70	103.85	113.55
3	I	35	HIS	ND1-CE1-NE2	7.69	116.09	108.40
1	G	230	ARG	NE-CZ-NH2	-7.68	112.29	119.20
1	A	350	PHE	N-CA-C	-7.68	98.63	109.69
1	A	315	GLN	N-CA-C	-7.67	97.05	108.79
1	G	311	HIS	CE1-NE2-CD2	-7.67	101.33	109.00
3	K	319	LEU	N-CA-C	-7.67	97.34	109.23
7	o	22	SER	N-CA-C	7.67	119.64	111.28
2	B	445	PHE	N-CA-C	-7.66	97.59	109.76
5	L	455	LEU	N-CA-C	-7.66	103.48	114.12
5	L	209	GLU	O-C-N	7.65	130.23	122.12
1	G	289	HIS	CA-CB-CG	7.65	121.45	113.80
3	I	346	GLU	N-CA-C	-7.63	103.76	113.23
2	Q	95	TYR	CA-C-N	7.63	130.36	120.44
2	Q	95	TYR	C-N-CA	7.63	130.36	120.44
2	Q	28	VAL	N-CA-C	-7.63	105.41	112.43
1	G	457	ASN	CA-CB-CG	7.62	120.22	112.60
4	J	244	GLN	N-CA-CB	7.62	121.43	110.16
2	H	359	SER	CA-C-N	7.62	136.09	121.54
2	H	359	SER	C-N-CA	7.62	136.09	121.54
1	A	444	LYS	N-CA-C	7.59	119.56	111.28
5	L	52	PHE	CA-CB-CG	7.59	121.39	113.80
2	D	460	HIS	CA-CB-CG	7.58	121.38	113.80
4	J	424	ARG	NE-CZ-NH1	-7.58	113.92	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	31	ILE	CA-C-N	7.57	127.21	119.19
3	I	31	ILE	C-N-CA	7.57	127.21	119.19
4	J	698	CYS	CA-C-N	7.57	128.38	119.98
4	J	698	CYS	C-N-CA	7.57	128.38	119.98
1	A	224	LEU	CA-C-N	7.57	130.09	120.56
1	A	224	LEU	C-N-CA	7.57	130.09	120.56
1	C	360	ASP	CA-CB-CG	7.56	120.16	112.60
1	C	366	THR	N-CA-C	-7.55	103.00	112.90
2	T	78	HIS	CE1-NE2-CD2	-7.55	101.45	109.00
1	G	228	ASP	CA-CB-CG	7.54	120.14	112.60
6	X	648	SER	N-CA-CB	7.53	120.99	110.07
1	G	485	GLU	N-CA-C	7.53	120.55	111.82
4	J	207	ASP	CA-C-N	7.51	131.10	120.28
4	J	207	ASP	C-N-CA	7.51	131.10	120.28
3	K	164	GLY	O-C-N	7.51	132.47	122.70
6	X	622	ILE	O-C-N	7.51	129.16	121.87
3	I	142	GLN	N-CA-C	-7.50	103.12	111.82
2	B	325	ALA	N-CA-C	7.49	119.52	111.36
6	U	659	LYS	N-CA-C	7.48	119.08	111.07
1	A	399	ILE	N-CA-C	-7.48	97.71	108.48
2	H	261	ASP	CA-CB-CG	7.47	120.07	112.60
1	C	411	HIS	N-CA-CB	7.47	123.20	110.50
2	H	411	ARG	NE-CZ-NH2	-7.47	112.48	119.20
2	B	280	VAL	N-CA-C	-7.47	102.84	113.07
4	J	500	HIS	CG-CD2-NE2	7.46	114.66	107.20
1	C	314	ARG	N-CA-C	-7.46	104.58	112.93
3	I	177	ALA	CA-C-O	7.44	128.57	119.79
1	C	239	GLY	CA-C-N	7.44	132.68	122.19
1	C	239	GLY	C-N-CA	7.44	132.68	122.19
1	E	434	VAL	CA-C-O	-7.43	114.15	121.58
6	X	629	MET	N-CA-C	7.42	119.01	111.07
5	L	330	GLU	CA-C-N	7.41	128.33	120.03
5	L	330	GLU	C-N-CA	7.41	128.33	120.03
5	L	569	TRP	N-CA-C	-7.41	103.65	114.39
2	H	432	TRP	CB-CG-CD1	7.40	138.01	126.90
3	K	330	ASP	CA-CB-CG	7.40	120.00	112.60
5	L	92	GLU	N-CA-C	7.40	119.34	111.28
7	q	39	ARG	CA-C-N	7.40	130.19	120.28
7	q	39	ARG	C-N-CA	7.40	130.19	120.28
2	D	467	LYS	CA-C-N	7.39	130.79	120.29
2	D	467	LYS	C-N-CA	7.39	130.79	120.29
4	J	500	HIS	ND1-CE1-NE2	7.39	115.79	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	o	34	LEU	CA-C-O	-7.38	112.72	120.55
2	H	430	TYR	N-CA-CB	7.38	122.64	110.39
1	A	311	HIS	CG-CD2-NE2	7.38	114.58	107.20
6	U	617	ALA	CA-C-N	7.38	130.77	120.29
6	U	617	ALA	C-N-CA	7.38	130.77	120.29
2	T	89	ASN	N-CA-CB	7.37	122.95	110.49
3	K	121	HIS	CA-CB-CG	-7.37	106.44	113.80
2	S	41	SER	N-CA-CB	7.36	120.96	110.44
2	H	390	ARG	N-CA-C	-7.35	103.45	113.30
1	A	304	ILE	CA-C-O	-7.34	113.07	120.85
6	X	652	SER	N-CA-CB	7.34	120.65	110.01
4	J	488	PHE	CA-CB-CG	-7.32	106.48	113.80
1	A	304	ILE	O-C-N	7.32	129.37	121.83
2	H	258	GLN	N-CA-C	-7.32	104.33	113.18
2	R	89	ASN	N-CA-C	-7.32	95.41	109.24
3	I	109	GLN	CA-C-N	7.31	131.43	120.31
3	I	109	GLN	C-N-CA	7.31	131.43	120.31
2	T	96	LEU	O-C-N	-7.31	114.48	122.09
5	L	561	LEU	N-CA-C	-7.30	103.97	114.12
6	X	611	LEU	N-CA-C	-7.30	103.35	111.82
2	B	271	GLU	N-CA-C	7.29	118.79	108.00
7	r	7	ASN	CA-C-N	7.28	129.91	120.44
7	r	7	ASN	C-N-CA	7.28	129.91	120.44
2	H	287	LYS	N-CA-C	-7.28	104.65	113.97
2	D	288	ASP	CA-CB-CG	7.27	119.87	112.60
4	J	261	VAL	CA-C-N	7.27	134.79	121.70
4	J	261	VAL	C-N-CA	7.27	134.79	121.70
3	I	157	VAL	O-C-N	-7.27	113.59	121.80
5	L	240	ASN	CA-CB-CG	7.26	119.86	112.60
2	D	372	ASP	CA-C-N	7.26	126.96	119.56
2	D	372	ASP	C-N-CA	7.26	126.96	119.56
3	I	299	ILE	N-CA-C	-7.26	106.02	111.90
4	J	693	GLN	N-CA-C	-7.25	104.05	113.12
5	L	206	ASP	CB-CA-C	7.25	123.88	110.10
1	A	384	ALA	CA-C-O	-7.25	110.23	120.16
3	I	312	HIS	CA-C-N	7.25	129.99	120.28
3	I	312	HIS	C-N-CA	7.25	129.99	120.28
2	T	22	GLY	CA-C-N	7.25	131.41	121.05
2	T	22	GLY	C-N-CA	7.25	131.41	121.05
2	F	366	LEU	N-CA-C	-7.24	103.10	112.23
5	L	586	VAL	CB-CA-C	7.24	123.16	111.29
1	C	433	ILE	N-CA-C	-7.23	95.09	107.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	200	TYR	CA-C-N	7.23	135.35	121.54
3	I	200	TYR	C-N-CA	7.23	135.35	121.54
2	O	29	ALA	CA-C-N	7.23	130.56	120.29
2	O	29	ALA	C-N-CA	7.23	130.56	120.29
2	O	29	ALA	N-CA-C	7.22	118.80	111.07
2	R	28	VAL	N-CA-C	-7.22	105.31	112.17
3	K	256	GLN	CA-C-O	7.22	128.70	120.54
7	p	13	GLU	CA-C-N	7.21	129.95	120.28
7	p	13	GLU	C-N-CA	7.21	129.95	120.28
3	K	24	GLY	CA-C-N	7.21	131.62	121.24
3	K	24	GLY	C-N-CA	7.21	131.62	121.24
2	B	386	HIS	CA-C-N	7.21	132.89	122.44
2	B	386	HIS	C-N-CA	7.21	132.89	122.44
2	F	440	ASP	N-CA-CB	7.20	122.66	110.71
2	T	63	VAL	CA-C-N	7.20	129.93	120.28
2	T	63	VAL	C-N-CA	7.20	129.93	120.28
5	L	378	PHE	CA-CB-CG	-7.20	106.60	113.80
6	V	650	ASN	N-CA-C	-7.20	98.88	110.32
3	K	122	ILE	CA-C-N	7.19	129.92	120.28
3	K	122	ILE	C-N-CA	7.19	129.92	120.28
7	q	53	VAL	CA-C-N	7.19	130.63	120.42
7	q	53	VAL	C-N-CA	7.19	130.63	120.42
6	U	651	GLU	CA-C-N	7.19	129.79	120.44
6	U	651	GLU	C-N-CA	7.19	129.79	120.44
2	B	514	SER	CA-C-N	7.18	127.02	119.05
2	B	514	SER	C-N-CA	7.18	127.02	119.05
5	L	416	LEU	CA-C-N	7.18	129.90	120.28
5	L	416	LEU	C-N-CA	7.18	129.90	120.28
5	L	539	TRP	CA-C-O	-7.17	110.96	119.35
1	A	404	SER	CA-C-N	7.17	133.60	122.49
1	A	404	SER	C-N-CA	7.17	133.60	122.49
1	E	319	SER	N-CA-C	-7.17	99.25	110.36
4	J	262	THR	CB-CA-C	7.17	124.87	109.10
4	J	434	ASN	CA-CB-CG	7.16	119.76	112.60
5	L	393	ASN	CA-CB-CG	-7.16	105.44	112.60
2	Q	54	VAL	N-CA-C	7.16	117.29	110.42
2	D	529	PHE	CA-CB-CG	7.14	120.94	113.80
1	E	495	SER	O-C-N	-7.14	114.55	122.12
2	S	97	LEU	CA-C-N	7.14	129.72	120.44
2	S	97	LEU	C-N-CA	7.14	129.72	120.44
1	G	400	ASN	CA-CB-CG	7.14	119.74	112.60
2	F	441	THR	N-CA-C	-7.13	105.20	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	262	GLU	CA-C-O	7.13	127.67	119.18
5	L	587	PHE	CA-CB-CG	7.13	120.93	113.80
1	G	331	LEU	N-CA-C	-7.13	104.05	112.89
1	E	337	LEU	O-C-N	-7.11	114.05	122.15
3	I	112	LEU	N-CA-C	-7.11	104.87	113.97
3	K	112	LEU	CA-C-N	7.10	129.80	120.28
3	K	112	LEU	C-N-CA	7.10	129.80	120.28
1	A	315	GLN	O-C-N	-7.10	115.82	123.42
6	U	665	LYS	CA-C-N	7.10	129.79	120.28
6	U	665	LYS	C-N-CA	7.10	129.79	120.28
6	W	611	LEU	N-CA-C	-7.09	103.29	112.23
1	C	350	PHE	N-CA-C	-7.09	98.39	108.96
2	S	107	GLN	N-CA-C	-7.09	100.86	110.36
2	F	389	GLY	N-CA-C	-7.09	102.99	112.14
6	U	619	HIS	CA-C-N	7.09	129.78	120.28
6	U	619	HIS	C-N-CA	7.09	129.78	120.28
3	I	9	LEU	CA-C-O	-7.09	111.43	119.79
2	B	421	VAL	N-CA-C	-7.08	103.57	110.72
7	o	15	MET	CA-C-N	7.08	130.35	120.29
7	o	15	MET	C-N-CA	7.08	130.35	120.29
2	H	252	ASP	CA-CB-CG	7.08	119.68	112.60
7	p	46	ASN	CA-CB-CG	-7.08	105.52	112.60
3	I	123	ASN	CA-C-N	7.08	129.76	120.28
3	I	123	ASN	C-N-CA	7.08	129.76	120.28
3	K	287	GLU	CA-C-N	7.08	129.99	120.65
3	K	287	GLU	C-N-CA	7.08	129.99	120.65
4	J	279	LYS	N-CA-C	-7.08	97.37	108.90
5	L	585	PRO	N-CA-C	7.07	127.04	112.47
2	O	86	VAL	O-C-N	-7.07	116.48	121.85
1	E	400	ASN	CA-CB-CG	-7.06	105.54	112.60
1	E	450	LEU	CA-C-O	-7.06	113.43	120.70
2	B	548	LEU	N-CA-C	-7.06	103.34	112.23
1	A	494	ALA	CA-C-N	7.05	131.03	120.31
1	A	494	ALA	C-N-CA	7.05	131.03	120.31
2	B	402	TYR	CB-CG-CD2	-7.05	110.22	120.80
2	Q	89	ASN	CA-C-N	7.05	129.73	120.28
2	Q	89	ASN	C-N-CA	7.05	129.73	120.28
5	L	340	THR	CA-C-N	7.05	133.63	122.21
5	L	340	THR	C-N-CA	7.05	133.63	122.21
4	J	255	PRO	N-CA-CB	7.05	108.94	103.30
5	L	527	THR	N-CA-CB	7.05	120.59	110.16
2	T	35	ALA	CA-C-N	7.04	130.10	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	35	ALA	C-N-CA	7.04	130.10	120.46
1	C	449	ILE	CA-C-N	7.03	129.70	120.28
1	C	449	ILE	C-N-CA	7.03	129.70	120.28
2	Q	114	PHE	CA-C-O	-7.03	111.88	119.97
2	F	407	ASP	N-CA-CB	7.02	122.87	110.37
2	D	284	LYS	N-CA-CB	7.02	121.21	110.61
5	L	424	HIS	CA-CB-CG	-7.02	106.78	113.80
6	W	636	GLN	CA-C-N	7.02	129.68	120.28
6	W	636	GLN	C-N-CA	7.02	129.68	120.28
1	A	447	ASP	CA-CB-CG	-7.01	105.59	112.60
2	B	438	LEU	CA-C-O	7.00	128.90	121.33
5	L	326	TYR	N-CA-C	-7.00	103.65	111.28
6	U	659	LYS	CA-C-N	7.00	129.66	120.28
6	U	659	LYS	C-N-CA	7.00	129.66	120.28
3	I	37	GLY	O-C-N	-7.00	113.60	122.70
2	D	447	VAL	N-CA-C	-6.99	98.32	108.11
5	L	344	GLN	CA-C-N	6.99	131.91	120.94
5	L	344	GLN	C-N-CA	6.99	131.91	120.94
2	D	372	ASP	N-CA-CB	6.99	118.66	110.42
1	G	447	ASP	CA-CB-CG	-6.99	105.61	112.60
1	A	353	ALA	CA-C-N	6.98	129.52	120.44
1	A	353	ALA	C-N-CA	6.98	129.52	120.44
2	S	78	HIS	CA-CB-CG	6.98	120.78	113.80
1	G	246	SER	CA-C-O	-6.98	112.84	120.24
4	J	222	THR	CA-C-N	6.97	132.66	122.41
4	J	222	THR	C-N-CA	6.97	132.66	122.41
2	B	482	VAL	CA-C-O	6.97	128.01	119.58
5	L	48	PHE	CA-C-N	6.97	129.34	120.56
5	L	48	PHE	C-N-CA	6.97	129.34	120.56
2	H	529	PHE	N-CA-C	6.97	118.95	111.36
1	G	314	ARG	NE-CZ-NH2	6.96	125.46	119.20
2	B	417	ILE	N-CA-C	-6.95	103.42	111.00
6	U	646	ARG	N-CA-C	6.95	118.65	111.14
6	W	606	MET	N-CA-CB	6.95	120.34	110.12
2	H	457	ARG	NE-CZ-NH2	6.95	125.46	119.20
3	I	344	MET	CA-C-N	6.95	129.32	120.56
3	I	344	MET	C-N-CA	6.95	129.32	120.56
5	L	401	VAL	CA-C-N	6.95	130.16	120.29
5	L	401	VAL	C-N-CA	6.95	130.16	120.29
2	D	283	SER	N-CA-C	-6.95	98.48	108.07
3	I	96	ILE	N-CA-C	-6.95	103.18	113.39
2	B	490	ASN	CA-CB-CG	6.94	119.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	373	GLU	N-CA-C	6.94	118.85	111.28
2	T	90	ARG	NE-CZ-NH2	-6.94	112.95	119.20
6	X	643	LEU	CA-C-N	6.93	129.45	120.44
6	X	643	LEU	C-N-CA	6.93	129.45	120.44
4	J	298	VAL	N-CA-C	-6.93	98.14	108.46
3	I	109	GLN	CB-CG-CD	6.92	124.37	112.60
2	S	10	ASN	CA-C-N	6.92	129.28	120.56
2	S	10	ASN	C-N-CA	6.92	129.28	120.56
1	A	398	ILE	CA-C-N	6.92	132.61	123.06
1	A	398	ILE	C-N-CA	6.92	132.61	123.06
2	Q	66	ARG	NE-CZ-NH2	6.92	125.43	119.20
5	L	360	VAL	N-CA-C	-6.92	102.17	111.44
2	D	419	GLY	N-CA-C	6.91	122.27	114.67
7	p	25	LEU	CA-C-N	6.90	132.16	122.36
7	p	25	LEU	C-N-CA	6.90	132.16	122.36
1	E	486	ARG	O-C-N	-6.90	112.61	122.41
6	W	663	GLU	N-CA-CB	6.90	120.01	110.01
1	C	319	SER	CA-C-N	6.89	132.15	121.19
1	C	319	SER	C-N-CA	6.89	132.15	121.19
7	p	26	ASN	OD1-CG-ND2	6.89	129.49	122.60
7	s	53	VAL	N-CA-CB	6.89	119.91	110.54
1	C	493	TYR	N-CA-C	-6.89	103.00	111.40
6	X	633	PHE	CA-C-O	-6.89	113.12	120.42
3	I	321	SER	CA-C-O	6.89	127.89	120.38
2	H	483	LEU	CA-C-N	6.88	130.76	120.31
2	H	483	LEU	C-N-CA	6.88	130.76	120.31
1	A	492	ASN	CA-CB-CG	6.88	119.48	112.60
4	J	318	GLN	N-CA-C	-6.88	103.86	111.36
7	p	24	LEU	O-C-N	6.88	129.99	122.15
2	B	308	ASP	N-CA-C	-6.87	105.05	113.50
1	E	211	SER	CA-C-N	6.86	132.34	120.68
1	E	211	SER	C-N-CA	6.86	132.34	120.68
6	X	624	ASN	CA-C-O	-6.86	113.15	120.42
2	B	437	GLU	N-CA-C	6.86	119.68	110.35
4	J	362	TRP	CZ3-CH2-CZ2	6.86	130.42	121.50
2	B	495	VAL	N-CA-C	-6.86	98.71	108.65
4	J	250	ASP	CA-C-N	6.85	126.45	119.19
4	J	250	ASP	C-N-CA	6.85	126.45	119.19
2	O	14	GLN	CA-C-N	6.85	129.76	120.38
2	O	14	GLN	C-N-CA	6.85	129.76	120.38
6	X	637	SER	CA-C-N	6.85	129.34	120.44
6	X	637	SER	C-N-CA	6.85	129.34	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	p	40	LEU	CA-C-N	6.85	129.34	120.44
7	p	40	LEU	C-N-CA	6.85	129.34	120.44
6	V	661	ARG	NE-CZ-NH2	-6.85	113.04	119.20
1	A	409	GLU	N-CA-C	-6.84	99.83	110.17
4	J	390	THR	CA-C-N	6.84	129.78	120.54
4	J	390	THR	C-N-CA	6.84	129.78	120.54
2	Q	32	PHE	CA-C-O	-6.84	113.65	120.70
3	I	15	SER	CA-C-N	6.84	131.27	121.55
3	I	15	SER	C-N-CA	6.84	131.27	121.55
4	J	262	THR	CA-C-N	6.84	130.83	121.05
4	J	262	THR	C-N-CA	6.84	130.83	121.05
4	J	571	ARG	NE-CZ-NH2	-6.84	113.05	119.20
6	U	639	GLU	CA-C-N	6.84	129.83	120.46
6	U	639	GLU	C-N-CA	6.84	129.83	120.46
2	F	300	HIS	N-CA-C	-6.83	103.76	111.14
2	H	272	ASN	N-CA-C	-6.83	96.25	110.80
1	G	345	ASN	CA-CB-CG	6.83	119.43	112.60
2	S	32	PHE	CA-C-N	6.83	129.43	120.28
2	S	32	PHE	C-N-CA	6.83	129.43	120.28
5	L	10	ASP	CA-C-N	6.82	129.30	120.44
5	L	10	ASP	C-N-CA	6.82	129.30	120.44
1	E	328	GLN	CA-C-N	6.82	127.09	119.32
1	E	328	GLN	C-N-CA	6.82	127.09	119.32
2	H	278	GLY	O-C-N	6.82	130.30	122.33
2	B	325	ALA	CB-CA-C	-6.81	99.27	110.85
2	B	497	HIS	N-CA-CB	6.81	120.12	110.24
3	I	3	HIS	ND1-CE1-NE2	6.81	115.21	108.40
2	S	68	GLU	O-C-N	6.81	129.91	122.15
7	q	45	ILE	CA-C-O	6.81	128.19	120.90
6	U	666	ARG	CA-C-N	6.81	129.29	120.44
6	U	666	ARG	C-N-CA	6.81	129.29	120.44
3	I	141	GLU	CB-CG-CD	-6.80	101.04	112.60
2	D	291	SER	O-C-N	6.80	130.50	122.34
3	I	309	ALA	O-C-N	6.80	129.33	122.12
1	E	494	ALA	N-CA-C	6.79	118.69	111.28
3	K	112	LEU	N-CA-C	-6.79	105.12	113.41
5	L	249	LYS	N-CA-C	-6.79	99.46	110.20
3	K	84	ILE	CA-C-O	6.79	125.29	119.38
5	L	80	ARG	CA-C-N	6.79	131.44	120.30
5	L	80	ARG	C-N-CA	6.79	131.44	120.30
5	L	407	TYR	N-CA-C	-6.79	104.81	113.23
3	I	321	SER	O-C-N	-6.79	115.28	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	82	GLN	OE1-CD-NE2	6.79	129.39	122.60
2	S	28	VAL	CA-C-N	6.79	129.37	120.28
2	S	28	VAL	C-N-CA	6.79	129.37	120.28
6	X	667	LEU	N-CA-C	6.78	118.33	111.07
2	B	336	ARG	CD-NE-CZ	6.78	133.89	124.40
6	X	619	HIS	CE1-NE2-CD2	-6.78	102.22	109.00
1	G	251	LEU	N-CA-C	6.77	118.66	111.28
3	K	166	PRO	N-CA-C	6.77	118.96	110.70
4	J	240	ALA	CA-C-N	6.77	129.09	120.56
4	J	240	ALA	C-N-CA	6.77	129.09	120.56
5	L	212	THR	CA-C-N	6.77	129.90	120.29
5	L	212	THR	C-N-CA	6.77	129.90	120.29
5	L	542	SER	CB-CA-C	-6.76	100.28	109.28
3	I	152	GLN	CA-C-N	6.76	130.01	120.42
3	I	152	GLN	C-N-CA	6.76	130.01	120.42
2	B	460	HIS	CE1-NE2-CD2	-6.75	102.25	109.00
2	R	79	ARG	NE-CZ-NH2	-6.75	113.12	119.20
2	T	95	TYR	N-CA-CB	6.75	120.04	110.12
3	I	325	PHE	N-CA-CB	-6.74	100.18	110.16
7	p	54	ILE	N-CA-CB	6.74	118.44	110.55
2	B	319	VAL	CA-C-N	6.74	127.58	120.03
2	B	319	VAL	C-N-CA	6.74	127.58	120.03
2	B	466	ARG	N-CA-CB	6.74	121.88	110.49
4	J	397	LYS	N-CA-C	-6.74	105.69	114.04
2	T	52	PHE	N-CA-C	6.74	118.63	111.28
2	O	94	LEU	CA-C-N	6.74	129.20	120.44
2	O	94	LEU	C-N-CA	6.74	129.20	120.44
3	K	175	THR	CA-C-N	6.73	129.30	120.28
3	K	175	THR	C-N-CA	6.73	129.30	120.28
6	X	632	GLN	N-CA-C	6.73	119.45	111.71
2	O	68	GLU	CA-C-N	6.72	129.29	120.28
2	O	68	GLU	C-N-CA	6.72	129.29	120.28
2	R	54	VAL	CB-CA-C	-6.72	102.94	112.22
3	K	280	GLY	CA-C-N	6.72	130.53	120.31
3	K	280	GLY	C-N-CA	6.72	130.53	120.31
5	L	337	SER	N-CA-C	-6.72	104.56	112.89
6	V	619	HIS	CB-CG-CD2	-6.72	122.47	131.20
6	X	603	ILE	N-CA-CB	6.72	119.68	110.54
1	A	464	HIS	CA-CB-CG	6.71	120.51	113.80
3	K	296	THR	CA-C-N	6.71	134.55	121.41
3	K	296	THR	C-N-CA	6.71	134.55	121.41
2	F	267	MET	O-C-N	-6.70	115.61	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	90	ARG	O-C-N	6.70	129.22	122.12
1	C	279	ASN	CA-CB-CG	6.70	119.30	112.60
1	C	346	LYS	CA-C-N	6.70	127.37	120.00
1	C	346	LYS	C-N-CA	6.70	127.37	120.00
2	O	61	GLU	CA-C-N	6.70	129.15	120.44
2	O	61	GLU	C-N-CA	6.70	129.15	120.44
1	E	362	THR	CA-CB-OG1	6.69	119.64	109.60
7	s	58	ARG	CD-NE-CZ	-6.69	115.03	124.40
2	B	492	LEU	CB-CA-C	-6.69	102.77	111.40
2	D	380	LEU	CA-C-N	6.69	130.47	120.31
2	D	380	LEU	C-N-CA	6.69	130.47	120.31
2	Q	78	HIS	CA-C-N	6.69	129.24	120.28
2	Q	78	HIS	C-N-CA	6.69	129.24	120.28
4	J	366	LYS	CA-C-N	6.69	129.78	120.29
4	J	366	LYS	C-N-CA	6.69	129.78	120.29
3	K	271	ARG	NE-CZ-NH1	6.68	128.18	121.50
7	s	54	ILE	CA-C-N	6.68	129.77	120.29
7	s	54	ILE	C-N-CA	6.68	129.77	120.29
2	D	314	ARG	N-CA-CB	6.67	121.77	110.49
5	L	3	SER	CA-C-N	6.67	129.94	120.53
5	L	3	SER	C-N-CA	6.67	129.94	120.53
2	H	420	LEU	O-C-N	-6.67	114.25	122.25
7	p	36	ILE	CA-C-N	6.67	129.22	120.28
7	p	36	ILE	C-N-CA	6.67	129.22	120.28
2	Q	36	VAL	CA-C-N	6.67	129.11	120.44
2	Q	36	VAL	C-N-CA	6.67	129.11	120.44
2	Q	70	ASP	N-CA-CB	6.67	120.61	110.28
1	E	277	GLU	CA-C-N	6.66	129.21	120.28
1	E	277	GLU	C-N-CA	6.66	129.21	120.28
5	L	329	HIS	CA-C-N	6.66	129.21	120.28
5	L	329	HIS	C-N-CA	6.66	129.21	120.28
7	q	59	ARG	NH1-CZ-NH2	6.66	127.96	119.30
6	V	627	VAL	O-C-N	6.66	128.83	121.90
5	L	542	SER	CA-C-O	6.66	126.93	118.54
5	L	426	ASN	N-CA-C	-6.65	98.38	108.96
7	r	59	ARG	N-CA-C	6.65	118.53	111.28
3	K	290	ASN	CA-CB-CG	6.65	119.25	112.60
2	B	336	ARG	N-CA-C	6.64	119.53	111.82
5	L	468	GLY	CA-C-O	6.64	127.70	120.66
2	Q	81	LEU	N-CA-CB	6.64	119.89	110.12
1	C	326	TYR	N-CA-C	-6.64	104.21	112.90
5	L	226	ASN	N-CA-C	-6.63	105.09	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	r	17	VAL	N-CA-C	6.63	116.77	110.53
1	E	382	ALA	N-CA-C	-6.63	105.00	113.23
3	K	59	ILE	N-CA-C	-6.63	104.71	110.74
2	D	445	PHE	N-CA-C	-6.63	99.33	109.41
5	L	596	TYR	CA-C-N	6.63	131.17	120.30
5	L	596	TYR	C-N-CA	6.63	131.17	120.30
1	A	340	ILE	CB-CA-C	-6.62	103.20	112.14
2	B	517	ASP	N-CA-C	6.62	118.50	111.28
2	S	113	SER	CA-C-N	6.62	130.38	120.31
2	S	113	SER	C-N-CA	6.62	130.38	120.31
2	D	247	THR	CA-C-N	6.62	129.15	120.28
2	D	247	THR	C-N-CA	6.62	129.15	120.28
2	R	88	LYS	N-CA-C	-6.61	102.56	112.54
2	D	347	VAL	N-CA-CB	6.61	118.44	110.31
2	D	405	THR	CA-C-N	6.61	134.36	121.41
2	D	405	THR	C-N-CA	6.61	134.36	121.41
6	W	617	ALA	CA-C-N	6.61	129.13	120.28
6	W	617	ALA	C-N-CA	6.61	129.13	120.28
4	J	694	TYR	N-CA-C	6.60	119.48	111.82
1	A	384	ALA	CA-C-N	6.60	126.11	119.24
1	A	384	ALA	C-N-CA	6.60	126.11	119.24
3	K	34	LEU	N-CA-C	-6.60	97.52	108.34
2	H	448	ALA	N-CA-C	-6.59	99.92	110.14
2	S	91	TRP	CA-C-O	-6.59	113.51	120.63
1	G	318	LEU	CB-CA-C	6.59	120.24	110.62
3	K	13	PRO	CB-CA-C	-6.59	103.40	111.11
1	A	295	MET	CA-C-N	6.58	130.32	120.31
1	A	295	MET	C-N-CA	6.58	130.32	120.31
2	D	376	ARG	N-CA-C	6.58	121.52	112.04
4	J	236	SER	CA-C-O	6.58	126.94	119.18
3	K	341	TRP	CD2-CE2-CZ2	-6.58	115.82	122.40
6	U	614	PHE	CA-CB-CG	-6.58	107.22	113.80
2	B	427	ASN	N-CA-CB	6.58	121.30	110.39
1	E	329	PRO	O-C-N	6.58	129.80	122.24
4	J	410	ARG	N-CA-CB	6.57	120.42	110.30
2	B	403	THR	CA-C-N	6.57	129.61	120.29
2	B	403	THR	C-N-CA	6.57	129.61	120.29
1	E	311	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
2	S	52	PHE	CA-C-N	6.57	129.08	120.28
2	S	52	PHE	C-N-CA	6.57	129.08	120.28
1	A	328	GLN	O-C-N	-6.56	115.20	120.38
2	Q	55	THR	O-C-N	6.56	128.82	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	328	HIS	ND1-CE1-NE2	6.55	114.95	108.40
2	O	97	LEU	CA-C-N	6.55	129.06	120.28
2	O	97	LEU	C-N-CA	6.55	129.06	120.28
5	L	110	HIS	CE1-NE2-CD2	-6.55	102.45	109.00
3	K	343	LEU	N-CA-CB	6.54	119.68	110.07
3	I	322	LEU	N-CA-C	-6.54	104.95	113.12
7	r	30	ASP	CA-C-N	6.54	129.34	120.38
7	r	30	ASP	C-N-CA	6.54	129.34	120.38
1	G	431	TYR	CB-CG-CD2	6.53	130.60	120.80
1	E	291	LEU	CA-C-O	6.53	127.47	120.55
7	s	64	LEU	CA-C-O	-6.53	113.97	120.82
3	K	277	LEU	O-C-N	6.52	128.79	122.07
3	I	3	HIS	CE1-NE2-CD2	-6.52	102.48	109.00
4	J	241	ILE	N-CA-C	6.52	116.68	110.42
2	H	301	ASN	OD1-CG-ND2	6.52	129.12	122.60
1	A	257	GLU	CA-C-N	6.52	129.01	120.28
1	A	257	GLU	C-N-CA	6.52	129.01	120.28
5	L	325	LEU	CA-C-N	6.52	129.01	120.28
5	L	325	LEU	C-N-CA	6.52	129.01	120.28
5	L	97	TYR	O-C-N	6.51	128.78	122.07
2	F	277	ASP	CA-CB-CG	6.51	119.11	112.60
1	E	430	ARG	NE-CZ-NH1	-6.50	115.00	121.50
4	J	384	ASN	CA-C-O	-6.50	114.04	121.19
2	B	316	PHE	CA-CB-CG	-6.50	107.30	113.80
7	t	40	LEU	N-CA-CB	6.50	119.44	110.01
7	t	30	ASP	N-CA-CB	6.50	119.53	110.17
5	L	583	CYS	CB-CA-C	6.49	120.56	111.86
7	t	62	ASP	CA-C-N	6.49	129.51	120.29
7	t	62	ASP	C-N-CA	6.49	129.51	120.29
3	K	123	ASN	CA-C-N	6.49	129.27	120.44
3	K	123	ASN	C-N-CA	6.49	129.27	120.44
2	O	55	THR	N-CA-CB	6.49	119.42	110.01
1	E	236	PRO	N-CA-C	-6.49	100.22	111.32
5	L	115	LEU	CA-C-O	-6.48	114.02	120.82
2	T	64	ARG	N-CA-CB	6.48	119.64	110.12
2	B	328	HIS	CE1-NE2-CD2	-6.48	102.52	109.00
2	F	445	PHE	CA-CB-CG	6.48	120.28	113.80
1	G	280	SER	CA-CB-OG	6.48	124.06	111.10
2	T	78	HIS	CB-CG-CD2	-6.48	122.78	131.20
2	F	249	LEU	CA-C-N	6.48	129.62	120.42
2	F	249	LEU	C-N-CA	6.48	129.62	120.42
2	F	445	PHE	N-CA-C	-6.47	99.66	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	313	ASP	CA-C-N	6.47	133.90	121.54
2	D	313	ASP	C-N-CA	6.47	133.90	121.54
2	O	65	GLN	CA-C-N	6.47	132.61	122.78
2	O	65	GLN	C-N-CA	6.47	132.61	122.78
2	F	291	SER	N-CA-C	6.47	119.32	111.82
1	G	303	MET	CG-SD-CE	-6.46	86.69	100.90
1	C	290	ALA	CA-C-N	6.46	132.44	121.14
1	C	290	ALA	C-N-CA	6.46	132.44	121.14
6	X	638	SER	CA-C-N	6.46	128.83	120.44
6	X	638	SER	C-N-CA	6.46	128.83	120.44
1	C	388	ASP	CA-CB-CG	-6.45	106.15	112.60
2	O	40	GLY	O-C-N	-6.45	115.94	122.19
2	T	15	ASN	CA-C-N	6.45	128.82	120.44
2	T	15	ASN	C-N-CA	6.45	128.82	120.44
1	C	218	GLU	CA-C-N	6.45	130.11	120.31
1	C	218	GLU	C-N-CA	6.45	130.11	120.31
3	K	85	TYR	N-CA-C	-6.44	105.45	113.38
4	J	557	MET	N-CA-C	6.44	119.29	111.82
7	t	50	LEU	CA-C-N	6.44	128.91	120.28
7	t	50	LEU	C-N-CA	6.44	128.91	120.28
2	H	441	THR	N-CA-C	-6.44	107.28	114.62
5	L	383	GLY	O-C-N	-6.44	116.76	122.88
1	C	437	GLN	N-CA-C	-6.43	100.86	110.06
5	L	516	GLU	N-CA-C	-6.43	106.01	114.31
2	H	264	PHE	CA-C-N	6.43	129.85	120.91
2	H	264	PHE	C-N-CA	6.43	129.85	120.91
2	B	536	ALA	CA-C-N	6.43	128.89	120.28
2	B	536	ALA	C-N-CA	6.43	128.89	120.28
1	G	406	PHE	CA-C-N	6.43	128.89	120.28
1	G	406	PHE	C-N-CA	6.43	128.89	120.28
2	H	292	LYS	CA-C-O	6.43	127.36	119.97
2	H	440	ASP	CA-CB-CG	6.43	119.03	112.60
7	r	45	ILE	N-CA-CB	6.43	121.83	111.23
2	B	543	TYR	CA-C-N	6.42	130.07	120.31
2	B	543	TYR	C-N-CA	6.42	130.07	120.31
4	J	250	ASP	N-CA-CB	6.42	119.83	110.32
2	F	460	HIS	CA-CB-CG	6.42	120.22	113.80
4	J	224	ARG	NH1-CZ-NH2	6.42	127.65	119.30
3	I	89	PHE	CA-CB-CG	6.42	120.22	113.80
2	O	83	SER	N-CA-C	6.42	119.27	111.82
2	F	429	LEU	N-CA-CB	6.42	119.50	110.07
4	J	453	THR	CA-C-N	6.42	129.25	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	453	THR	C-N-CA	6.42	129.25	120.46
6	V	642	MET	CA-C-N	6.42	128.88	120.28
6	V	642	MET	C-N-CA	6.42	128.88	120.28
1	G	346	LYS	N-CA-C	-6.41	104.67	114.16
5	L	599	GLY	CA-C-O	6.41	127.36	120.30
2	B	525	LEU	N-CA-C	-6.41	98.77	108.96
2	B	498	ASP	CA-C-O	6.41	126.85	119.35
4	J	563	GLN	N-CA-C	6.41	118.35	111.36
1	E	317	LEU	O-C-N	-6.41	114.07	122.59
4	J	225	ALA	CA-C-N	6.41	126.36	120.21
4	J	225	ALA	C-N-CA	6.41	126.36	120.21
5	L	165	THR	CA-C-N	6.41	129.52	120.42
5	L	165	THR	C-N-CA	6.41	129.52	120.42
5	L	327	LYS	CA-C-N	6.41	129.16	120.44
5	L	327	LYS	C-N-CA	6.41	129.16	120.44
5	L	120	SER	CA-C-O	-6.41	114.14	121.19
6	V	671	PHE	CA-CB-CG	-6.40	107.40	113.80
2	D	448	ALA	CA-C-N	6.40	130.94	122.30
2	D	448	ALA	C-N-CA	6.40	130.94	122.30
1	E	409	GLU	N-CA-C	-6.40	98.47	108.90
4	J	257	ASP	N-CA-C	-6.40	98.11	108.41
4	J	689	HIS	CE1-NE2-CD2	-6.40	102.60	109.00
2	R	56	GLU	O-C-N	6.39	130.13	122.27
2	D	408	PRO	N-CA-C	-6.39	107.31	114.92
6	V	663	GLU	CA-C-N	6.39	128.84	120.28
6	V	663	GLU	C-N-CA	6.39	128.84	120.28
1	A	300	LYS	N-CA-CB	6.39	119.61	110.16
2	O	21	LEU	N-CA-CB	6.39	120.81	110.40
5	L	539	TRP	CA-CB-CG	6.38	125.73	113.60
2	B	431	ARG	CD-NE-CZ	-6.38	115.47	124.40
2	D	292	LYS	N-CA-C	-6.38	102.90	112.54
4	J	409	HIS	ND1-CE1-NE2	6.38	114.78	108.40
1	A	218	GLU	CA-C-N	6.38	130.00	120.31
1	A	218	GLU	C-N-CA	6.38	130.00	120.31
2	S	80	LYS	O-C-N	6.38	128.88	122.12
7	t	19	LEU	CA-C-N	6.38	128.73	120.44
7	t	19	LEU	C-N-CA	6.38	128.73	120.44
5	L	527	THR	N-CA-C	-6.37	104.42	111.36
1	A	428	ASP	N-CA-CB	6.37	121.25	110.49
2	H	283	SER	N-CA-CB	-6.37	101.97	110.57
5	L	587	PHE	O-C-N	6.37	128.87	122.12
7	r	36	ILE	N-CA-CB	6.37	118.00	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	VAL	CB-CA-C	6.37	119.50	110.84
1	G	493	TYR	N-CA-C	-6.37	103.83	113.89
4	J	379	GLU	N-CA-C	6.36	119.20	111.82
2	S	79	ARG	CA-C-O	6.36	127.29	120.55
6	W	619	HIS	CA-C-N	6.36	128.81	120.28
6	W	619	HIS	C-N-CA	6.36	128.81	120.28
6	U	666	ARG	N-CA-C	6.36	118.21	111.28
2	O	62	PHE	CA-CB-CG	-6.36	107.44	113.80
3	I	55	PHE	N-CA-C	-6.36	105.18	113.12
3	I	121	HIS	ND1-CE1-NE2	6.36	114.75	108.40
2	S	37	ARG	N-CA-C	6.36	118.21	111.28
7	r	10	ALA	CA-C-N	6.36	129.44	120.42
7	r	10	ALA	C-N-CA	6.36	129.44	120.42
1	E	407	MET	N-CA-C	6.35	118.28	111.36
6	W	600	ILE	N-CA-CB	6.35	119.18	110.54
7	o	33	THR	N-CA-CB	6.35	119.56	110.16
1	E	392	ARG	N-CA-CB	6.35	120.75	110.40
1	A	267	THR	N-CA-C	6.35	118.20	111.28
1	G	336	VAL	CB-CA-C	-6.35	103.73	112.24
4	J	394	VAL	CG1-CB-CG2	6.35	124.76	110.80
2	F	462	LYS	CA-C-O	6.35	125.44	118.65
6	X	638	SER	CB-CA-C	-6.34	100.92	110.88
7	r	48	GLU	N-CA-C	6.34	118.27	111.36
4	J	221	TRP	N-CA-C	-6.34	106.13	114.31
4	J	499	ASN	CA-CB-CG	6.34	118.94	112.60
3	K	82	HIS	N-CA-C	-6.34	99.43	109.07
6	V	670	ASN	CA-C-O	6.34	126.69	119.27
2	D	525	LEU	N-CA-C	-6.34	99.31	109.96
2	B	285	SER	CA-C-N	6.34	129.40	120.28
2	B	285	SER	C-N-CA	6.34	129.40	120.28
7	t	40	LEU	O-C-N	-6.34	115.54	122.07
1	G	284	TYR	CB-CG-CD2	-6.33	111.30	120.80
2	Q	75	SER	CA-C-N	6.33	128.76	120.28
2	Q	75	SER	C-N-CA	6.33	128.76	120.28
7	t	44	GLY	N-CA-C	-6.33	105.95	115.32
1	E	491	TYR	N-CA-C	6.33	120.26	112.54
2	D	400	HIS	CE1-NE2-CD2	-6.33	102.67	109.00
2	T	59	LYS	CA-C-N	6.33	128.75	120.28
2	T	59	LYS	C-N-CA	6.33	128.75	120.28
1	G	310	GLU	CA-C-N	6.32	128.75	120.28
1	G	310	GLU	C-N-CA	6.32	128.75	120.28
2	D	274	TYR	CB-CA-C	-6.32	108.27	115.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	261	ARG	NE-CZ-NH1	-6.31	115.19	121.50
2	O	32	PHE	CA-C-N	6.31	128.74	120.28
2	O	32	PHE	C-N-CA	6.31	128.74	120.28
1	C	311	HIS	CA-C-O	6.31	127.24	120.55
2	F	289	ILE	O-C-N	6.31	128.46	121.90
3	K	293	MET	N-CA-C	-6.31	103.72	112.30
2	D	322	SER	CA-C-N	6.30	128.72	120.28
2	D	322	SER	C-N-CA	6.30	128.72	120.28
4	J	482	PHE	CA-CB-CG	-6.30	107.50	113.80
2	S	80	LYS	N-CA-C	6.30	118.14	111.28
2	Q	13	LEU	N-CA-CB	6.29	119.37	110.12
5	L	74	MET	CA-C-N	6.29	129.22	120.29
5	L	74	MET	C-N-CA	6.29	129.22	120.29
5	L	428	LEU	CA-C-N	6.29	129.35	120.42
5	L	428	LEU	C-N-CA	6.29	129.35	120.42
2	B	425	ILE	CA-C-O	-6.29	114.07	121.05
1	A	409	GLU	O-C-N	-6.28	114.51	122.43
5	L	425	SER	N-CA-C	-6.28	105.65	113.38
2	T	10	ASN	O-C-N	-6.28	115.46	122.12
1	A	349	CYS	CA-C-O	6.28	128.40	121.56
2	D	279	LYS	CA-C-O	-6.28	114.83	121.99
1	G	340	ILE	CA-C-O	-6.28	114.20	120.85
1	A	241	GLN	N-CA-CB	6.27	121.09	110.49
1	E	385	PRO	CA-C-N	6.27	128.97	120.44
1	E	385	PRO	C-N-CA	6.27	128.97	120.44
6	X	622	ILE	CA-C-O	-6.27	114.43	120.95
1	G	367	GLY	CA-C-N	6.27	130.99	122.84
1	G	367	GLY	C-N-CA	6.27	130.99	122.84
5	L	571	HIS	CA-CB-CG	-6.27	107.53	113.80
1	A	320	LEU	N-CA-CB	6.27	120.00	110.28
2	Q	62	PHE	CA-CB-CG	-6.26	107.54	113.80
2	F	425	ILE	O-C-N	6.26	128.28	121.83
2	S	87	LEU	CA-C-N	6.26	132.37	122.60
2	S	87	LEU	C-N-CA	6.26	132.37	122.60
1	G	298	LEU	CA-C-O	6.26	127.08	119.38
1	A	268	ASN	CA-C-N	6.26	128.57	120.44
1	A	268	ASN	C-N-CA	6.26	128.57	120.44
4	J	296	ILE	N-CA-CB	6.26	117.96	110.95
1	A	411	HIS	CE1-NE2-CD2	-6.25	102.75	109.00
2	H	429	LEU	N-CA-C	-6.25	103.17	111.24
2	F	452	VAL	N-CA-C	-6.25	99.20	108.45
2	Q	27	ASP	N-CA-CB	6.25	121.05	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	337	LEU	CA-C-N	6.25	129.16	120.29
1	E	337	LEU	C-N-CA	6.25	129.16	120.29
3	I	57	GLU	O-C-N	-6.25	114.59	122.27
1	C	319	SER	N-CA-C	-6.24	100.16	108.34
1	E	279	ASN	CB-CA-C	-6.24	100.24	110.85
6	W	601	ASN	N-CA-C	6.24	118.08	111.28
2	B	328	HIS	CG-CD2-NE2	6.24	113.44	107.20
7	p	14	THR	CA-C-N	6.24	129.79	120.31
7	p	14	THR	C-N-CA	6.24	129.79	120.31
1	C	212	GLN	CG-CD-NE2	-6.24	107.05	116.40
2	F	416	HIS	CE1-NE2-CD2	-6.23	102.77	109.00
3	I	133	PHE	CB-CG-CD1	6.23	131.30	120.70
2	O	43	PHE	N-CA-C	6.23	117.74	111.07
3	K	309	ALA	N-CA-C	6.23	118.07	111.28
2	Q	113	SER	CA-C-N	6.23	129.78	120.31
2	Q	113	SER	C-N-CA	6.23	129.78	120.31
1	E	318	LEU	CA-C-O	-6.23	113.95	121.05
5	L	523	SER	N-CA-C	-6.22	104.58	111.36
1	C	433	ILE	O-C-N	-6.22	116.99	123.03
1	G	382	ALA	N-CA-C	-6.22	104.58	111.36
1	A	443	GLN	N-CA-C	6.22	119.97	112.38
2	D	304	LYS	CA-C-O	6.22	127.14	120.55
6	V	663	GLU	N-CA-CB	6.22	119.26	110.12
2	O	11	VAL	N-CA-C	6.21	116.39	110.42
2	Q	24	GLY	CA-C-N	6.21	130.95	122.07
2	Q	24	GLY	C-N-CA	6.21	130.95	122.07
1	A	345	ASN	CB-CA-C	-6.21	98.37	109.24
3	I	186	GLN	OE1-CD-NE2	6.21	128.81	122.60
3	I	293	MET	N-CA-C	-6.21	104.87	112.88
5	L	213	ARG	CA-C-N	6.21	126.87	119.98
5	L	213	ARG	C-N-CA	6.21	126.87	119.98
7	q	62	ASP	CA-C-N	6.21	129.10	120.29
7	q	62	ASP	C-N-CA	6.21	129.10	120.29
2	H	276	VAL	N-CA-C	-6.20	96.82	107.24
2	H	311	SER	CA-C-N	6.20	129.77	123.13
2	H	311	SER	C-N-CA	6.20	129.77	123.13
4	J	483	ASP	CA-C-N	6.20	126.56	119.92
4	J	483	ASP	C-N-CA	6.20	126.56	119.92
2	O	50	ASP	CA-CB-CG	6.20	118.80	112.60
7	o	48	GLU	CA-C-N	6.20	128.50	120.44
7	o	48	GLU	C-N-CA	6.20	128.50	120.44
5	L	552	PHE	N-CA-C	-6.20	97.59	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	386	ASP	CA-C-N	6.20	129.41	120.79
4	J	386	ASP	C-N-CA	6.20	129.41	120.79
5	L	552	PHE	CA-C-N	6.19	133.36	121.54
5	L	552	PHE	C-N-CA	6.19	133.36	121.54
2	O	64	ARG	O-C-N	-6.19	115.56	122.12
1	E	431	TYR	N-CA-C	-6.19	104.90	112.88
2	Q	90	ARG	NE-CZ-NH1	-6.19	115.31	121.50
2	Q	79	ARG	NE-CZ-NH2	6.19	124.77	119.20
4	J	599	LEU	CA-C-O	-6.18	114.00	120.55
2	D	440	ASP	CA-CB-CG	6.18	118.78	112.60
2	H	485	ILE	O-C-N	6.18	128.20	121.83
5	L	524	LEU	N-CA-C	6.18	118.10	111.36
1	C	263	LEU	CA-C-N	6.18	127.56	119.84
1	C	263	LEU	C-N-CA	6.18	127.56	119.84
2	S	16	LEU	CB-CA-C	-6.18	101.18	110.88
1	G	318	LEU	CA-C-O	6.18	128.03	120.25
2	O	14	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	E	262	ILE	CA-CB-CG2	-6.18	100.00	110.50
1	E	274	ARG	CD-NE-CZ	6.18	133.05	124.40
2	R	34	TYR	CA-C-N	6.17	128.46	120.44
2	R	34	TYR	C-N-CA	6.17	128.46	120.44
2	S	9	PRO	CA-C-N	6.17	128.46	120.44
2	S	9	PRO	C-N-CA	6.17	128.46	120.44
5	L	426	ASN	CB-CG-OD1	6.16	133.12	120.80
2	F	460	HIS	CE1-NE2-CD2	-6.16	102.84	109.00
3	I	203	PHE	N-CA-C	-6.16	101.40	110.52
6	U	653	LEU	CA-C-N	6.16	128.90	120.46
6	U	653	LEU	C-N-CA	6.16	128.90	120.46
3	I	280	GLY	CA-C-N	6.16	129.67	120.31
3	I	280	GLY	C-N-CA	6.16	129.67	120.31
6	U	643	LEU	CA-C-N	6.16	128.53	120.28
6	U	643	LEU	C-N-CA	6.16	128.53	120.28
2	B	296	LEU	O-C-N	-6.16	115.44	122.09
2	S	47	VAL	N-CA-CB	6.16	121.39	111.23
1	A	434	VAL	N-CA-C	-6.16	99.56	108.36
1	E	351	GLY	CA-C-N	6.16	131.75	120.79
1	E	351	GLY	C-N-CA	6.16	131.75	120.79
7	o	38	VAL	CB-CA-C	6.16	119.85	111.97
2	D	482	VAL	CA-CB-CG1	-6.15	99.94	110.40
1	A	210	PRO	CA-C-N	6.15	129.66	120.31
1	A	210	PRO	C-N-CA	6.15	129.66	120.31
2	D	479	SER	N-CA-C	-6.15	104.12	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	308	ASP	N-CA-C	-6.15	104.48	112.23
7	r	10	ALA	N-CA-C	6.15	117.99	111.28
4	J	360	PHE	CA-CB-CG	6.15	119.95	113.80
5	L	34	ARG	NE-CZ-NH1	6.15	127.65	121.50
2	F	253	LEU	CA-C-N	6.15	129.13	120.28
2	F	253	LEU	C-N-CA	6.15	129.13	120.28
6	U	670	ASN	CA-C-O	6.14	125.75	118.69
3	I	309	ALA	CA-C-O	-6.14	114.04	120.55
6	W	631	LYS	CA-C-O	-6.14	114.37	120.82
2	H	260	ILE	CA-C-O	6.14	126.47	120.27
2	H	460	HIS	CA-C-O	-6.13	114.67	121.23
5	L	1374	HIS	CA-CB-CG	6.13	119.93	113.80
7	o	59	ARG	NH1-CZ-NH2	-6.13	111.33	119.30
3	K	108	GLU	CA-C-N	6.13	129.63	120.31
3	K	108	GLU	C-N-CA	6.13	129.63	120.31
2	O	88	LYS	CA-CB-CG	6.13	126.36	114.10
7	r	13	GLU	CA-C-N	6.13	128.41	120.44
7	r	13	GLU	C-N-CA	6.13	128.41	120.44
1	C	368	ASP	N-CA-CB	6.13	120.85	110.49
3	K	182	VAL	CA-CB-CG2	-6.13	99.98	110.40
7	t	54	ILE	N-CA-CB	6.13	117.72	110.55
2	F	468	SER	N-CA-C	-6.12	105.71	113.43
5	L	412	SER	CA-C-N	6.12	128.98	120.29
5	L	412	SER	C-N-CA	6.12	128.98	120.29
6	U	635	ILE	O-C-N	6.12	128.06	121.94
7	t	10	ALA	CA-C-N	6.12	128.85	120.46
7	t	10	ALA	C-N-CA	6.12	128.85	120.46
3	I	292	ASN	N-CA-C	-6.12	105.46	113.17
4	J	235	HIS	N-CA-C	-6.12	104.45	112.41
2	H	447	VAL	N-CA-C	-6.12	99.31	108.12
3	I	149	HIS	ND1-CE1-NE2	6.12	114.52	108.40
2	B	387	CYS	CA-C-O	6.12	127.95	120.25
4	J	419	VAL	CA-C-N	6.11	126.68	120.38
4	J	419	VAL	C-N-CA	6.11	126.68	120.38
3	K	91	ARG	CA-C-N	6.11	133.39	121.41
3	K	91	ARG	C-N-CA	6.11	133.39	121.41
5	L	220	LEU	N-CA-C	-6.11	99.76	109.23
2	S	43	PHE	CA-CB-CG	-6.11	107.69	113.80
1	C	433	ILE	CA-C-O	6.11	126.30	120.31
2	D	531	THR	N-CA-C	-6.11	103.95	111.40
1	E	213	GLU	CA-C-N	6.10	128.96	120.29
1	E	213	GLU	C-N-CA	6.10	128.96	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	479	SER	O-C-N	6.10	128.59	122.12
4	J	480	ASN	N-CA-C	-6.10	99.79	109.07
2	B	292	LYS	N-CA-CB	6.10	119.19	110.16
1	C	448	LYS	CA-C-N	6.10	128.37	120.56
1	C	448	LYS	C-N-CA	6.10	128.37	120.56
2	O	41	SER	CA-C-O	6.10	126.91	119.11
2	Q	102	GLU	N-CA-C	-6.09	99.81	109.07
3	I	257	PHE	CA-CB-CG	-6.09	107.71	113.80
2	F	289	ILE	N-CA-C	-6.09	104.81	110.53
7	o	46	ASN	O-C-N	-6.09	115.52	121.18
4	J	685	CYS	N-CA-C	-6.08	104.93	112.90
2	H	301	ASN	CA-C-N	6.08	129.56	120.31
2	H	301	ASN	C-N-CA	6.08	129.56	120.31
1	G	350	PHE	CA-CB-CG	-6.08	107.72	113.80
1	C	228	ASP	CA-CB-CG	6.08	118.68	112.60
5	L	393	ASN	CB-CA-C	-6.08	98.62	110.11
5	L	104	ILE	CA-CB-CG2	-6.07	100.17	110.50
2	Q	86	VAL	CA-C-O	-6.07	114.59	121.75
5	L	416	LEU	CA-C-O	-6.07	112.99	119.97
7	o	23	ARG	NE-CZ-NH1	-6.07	115.43	121.50
2	H	386	HIS	N-CA-C	-6.07	105.37	112.89
3	K	328	VAL	CA-C-O	-6.07	112.26	119.54
2	Q	78	HIS	N-CA-CB	6.07	118.87	110.07
1	G	230	ARG	N-CA-C	-6.07	105.54	113.12
3	K	4	GLU	N-CA-C	-6.07	105.84	113.18
6	W	626	GLN	N-CA-C	6.07	117.56	111.07
7	r	27	THR	N-CA-C	-6.07	100.10	109.14
1	A	359	HIS	ND1-CE1-NE2	6.06	114.46	108.40
6	U	603	ILE	CA-C-N	6.06	128.32	120.44
6	U	603	ILE	C-N-CA	6.06	128.32	120.44
5	L	373	GLN	OE1-CD-NE2	-6.06	116.54	122.60
6	W	633	PHE	N-CA-C	6.06	117.55	111.07
2	H	466	ARG	CA-C-O	6.05	128.73	121.65
3	I	16	ILE	N-CA-C	-6.05	104.49	113.39
3	I	8	ALA	N-CA-CB	6.05	120.27	110.40
5	L	100	GLN	OE1-CD-NE2	6.05	128.65	122.60
5	L	428	LEU	N-CA-C	-6.05	104.25	111.69
2	R	61	GLU	CA-C-O	-6.05	114.14	120.55
6	U	618	CYS	CB-CA-C	-6.05	100.56	110.85
7	p	36	ILE	CA-C-O	-6.05	114.44	120.85
3	I	136	ILE	CA-C-N	6.05	128.39	120.28
3	I	136	ILE	C-N-CA	6.05	128.39	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	254	THR	O-C-N	-6.05	114.42	120.83
2	B	485	ILE	CA-C-N	6.05	127.90	120.22
2	B	485	ILE	C-N-CA	6.05	127.90	120.22
2	B	286	LEU	O-C-N	-6.05	115.15	122.22
3	K	345	VAL	CB-CA-C	-6.05	104.10	112.02
6	X	604	LYS	O-C-N	6.04	128.30	122.07
7	q	58	ARG	CA-C-O	-6.04	114.47	120.82
3	I	273	ALA	CA-C-O	6.04	126.92	119.97
2	Q	82	GLN	CA-C-N	6.04	128.98	120.28
2	Q	82	GLN	C-N-CA	6.04	128.98	120.28
2	B	365	ARG	N-CA-CB	6.04	119.00	109.82
3	I	180	HIS	CA-CB-CG	-6.04	107.76	113.80
4	J	466	ARG	CA-C-N	6.04	125.59	119.19
4	J	466	ARG	C-N-CA	6.04	125.59	119.19
1	E	402	PRO	N-CA-CB	6.04	109.31	103.51
5	L	606	LYS	N-CA-CB	6.04	120.98	111.20
7	p	39	ARG	NE-CZ-NH2	-6.04	113.77	119.20
1	E	368	ASP	CA-C-N	6.03	128.86	120.29
1	E	368	ASP	C-N-CA	6.03	128.86	120.29
3	I	81	LEU	CA-C-N	6.03	133.06	121.54
3	I	81	LEU	C-N-CA	6.03	133.06	121.54
2	O	89	ASN	N-CA-CB	6.03	120.68	110.49
2	D	433	ILE	CB-CA-C	-6.03	103.90	112.22
4	J	671	GLU	CB-CG-CD	6.03	122.85	112.60
3	K	114	ASP	N-CA-C	-6.03	102.80	108.22
2	S	109	ASN	N-CA-CB	6.03	120.67	110.49
7	t	12	ARG	NE-CZ-NH1	6.03	127.53	121.50
2	F	269	ASN	N-CA-C	-6.02	102.97	108.75
5	L	161	ASP	CA-CB-CG	6.02	118.62	112.60
7	p	39	ARG	NH1-CZ-NH2	6.02	127.13	119.30
5	L	563	PHE	CA-CB-CG	-6.02	107.78	113.80
2	D	250	VAL	CB-CA-C	-6.02	104.01	112.14
3	I	137	MET	N-CA-CB	6.02	118.97	110.12
1	E	436	GLN	N-CA-C	-6.02	107.76	114.62
3	K	204	PHE	N-CA-C	-6.02	105.26	114.16
5	L	502	LEU	N-CA-C	6.01	118.63	111.71
2	B	269	ASN	CA-CB-CG	-6.01	106.59	112.60
2	F	471	PRO	CB-CA-C	6.01	119.28	111.64
6	V	641	GLN	CA-C-N	6.01	128.34	120.28
6	V	641	GLN	C-N-CA	6.01	128.34	120.28
2	D	407	ASP	O-C-N	-6.01	114.41	121.32
4	J	229	SER	N-CA-C	-6.01	98.00	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	62	PHE	N-CA-CB	6.01	118.72	110.01
3	I	13	PRO	N-CA-C	6.01	120.66	111.11
2	S	39	ILE	CB-CA-C	6.00	120.51	112.22
3	I	322	LEU	CA-C-O	6.00	127.04	119.78
1	G	486	ARG	N-CA-CB	6.00	118.94	110.12
2	H	391	LYS	CA-C-N	6.00	125.80	120.10
2	H	391	LYS	C-N-CA	6.00	125.80	120.10
4	J	420	PRO	N-CA-CB	6.00	108.90	103.08
3	I	85	TYR	N-CA-C	-6.00	106.00	113.38
1	E	217	VAL	N-CA-C	-6.00	104.47	111.00
1	G	376	LEU	N-CA-CB	6.00	119.03	110.16
2	T	48	GLU	CA-C-N	6.00	131.37	122.74
2	T	48	GLU	C-N-CA	6.00	131.37	122.74
2	B	537	TYR	N-CA-C	-5.99	104.75	111.28
1	C	367	GLY	N-CA-C	-5.99	100.60	111.15
1	E	225	ILE	O-C-N	5.99	128.00	121.83
1	A	349	CYS	N-CA-CB	5.99	118.80	110.17
1	E	443	GLN	N-CA-C	5.99	119.85	112.54
2	F	380	LEU	CA-C-N	5.99	128.79	120.29
2	F	380	LEU	C-N-CA	5.99	128.79	120.29
2	O	38	VAL	CA-CB-CG1	5.98	120.57	110.40
1	C	428	ASP	N-CA-C	-5.98	105.28	113.30
1	E	269	TYR	N-CA-C	5.98	117.88	111.36
2	H	446	PHE	N-CA-C	-5.98	105.81	112.57
2	Q	13	LEU	CB-CA-C	-5.98	100.86	110.79
1	E	329	PRO	CA-C-O	-5.97	109.74	119.84
1	C	347	GLY	CA-C-O	5.97	126.99	120.66
2	D	284	LYS	O-C-N	5.97	129.47	122.24
2	H	432	TRP	CB-CG-CD2	-5.97	118.44	126.80
5	L	33	ASN	CA-CB-CG	-5.97	106.63	112.60
5	L	564	ARG	CB-CG-CD	5.97	125.04	111.30
2	D	296	LEU	N-CA-C	-5.97	104.83	114.09
1	C	342	THR	N-CA-CB	5.97	118.72	110.07
3	I	143	ILE	CB-CA-C	5.97	119.84	112.02
7	s	45	ILE	O-C-N	-5.97	116.31	122.82
2	D	411	ARG	N-CA-CB	5.97	118.99	110.16
6	U	670	ASN	O-C-N	-5.97	116.04	122.19
2	F	322	SER	N-CA-CB	5.97	119.55	110.42
2	F	463	TYR	CB-CA-C	-5.97	99.66	109.80
6	W	628	GLU	O-C-N	-5.97	115.80	122.12
1	A	428	ASP	CA-CB-CG	5.96	118.56	112.60
5	L	602	ILE	N-CA-C	-5.96	104.27	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	35	ALA	N-CA-C	5.96	117.58	111.14
7	p	30	ASP	CA-C-N	5.96	128.76	120.29
7	p	30	ASP	C-N-CA	5.96	128.76	120.29
1	E	223	ILE	CA-C-N	5.96	129.37	120.31
1	E	223	ILE	C-N-CA	5.96	129.37	120.31
4	J	323	LEU	N-CA-CB	5.96	120.28	110.39
2	Q	38	VAL	N-CA-CB	5.96	119.52	110.58
2	F	443	HIS	ND1-CE1-NE2	5.96	114.36	108.40
5	L	1359	LEU	CA-C-N	5.96	126.07	119.87
5	L	1359	LEU	C-N-CA	5.96	126.07	119.87
2	D	251	ARG	CD-NE-CZ	-5.96	116.06	124.40
3	I	169	ARG	NE-CZ-NH1	-5.95	115.55	121.50
1	A	289	HIS	CG-CD2-NE2	5.95	113.15	107.20
2	R	67	ARG	NE-CZ-NH2	5.95	124.56	119.20
4	J	596	GLN	CA-C-N	5.95	128.25	120.28
4	J	596	GLN	C-N-CA	5.95	128.25	120.28
2	R	43	PHE	N-CA-C	-5.95	100.28	109.14
6	U	661	ARG	CA-C-N	5.95	128.74	120.29
6	U	661	ARG	C-N-CA	5.95	128.74	120.29
6	W	598	ILE	O-C-N	5.95	127.64	121.87
1	E	335	GLU	N-CA-C	-5.95	104.88	111.36
3	I	162	CYS	CA-C-N	5.95	129.45	121.01
3	I	162	CYS	C-N-CA	5.95	129.45	121.01
3	K	312	HIS	CE1-NE2-CD2	-5.95	103.05	109.00
1	G	329	PRO	N-CA-C	5.94	121.57	113.84
2	D	280	VAL	N-CA-C	-5.94	104.52	111.00
2	S	69	ALA	CA-C-N	5.94	128.24	120.28
2	S	69	ALA	C-N-CA	5.94	128.24	120.28
2	D	309	GLN	CA-C-O	5.94	126.72	119.11
2	D	436	GLY	N-CA-C	-5.94	106.27	116.01
1	A	433	ILE	N-CA-CB	5.94	118.61	111.31
2	B	269	ASN	N-CA-C	-5.94	105.22	112.88
2	R	80	LYS	CA-C-N	5.94	128.24	120.28
2	R	80	LYS	C-N-CA	5.94	128.24	120.28
4	J	261	VAL	O-C-N	-5.93	116.85	123.26
5	L	212	THR	O-C-N	5.93	128.41	122.12
2	D	435	ASP	CA-CB-CG	-5.93	106.67	112.60
1	G	493	TYR	N-CA-CB	5.93	119.49	110.95
4	J	219	GLN	CA-C-O	-5.93	115.26	121.55
1	A	491	TYR	CA-C-N	5.93	129.32	120.31
1	A	491	TYR	C-N-CA	5.93	129.32	120.31
2	F	336	ARG	N-CA-C	5.93	118.69	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1359	LEU	N-CA-CB	5.93	118.29	110.29
2	B	296	LEU	CA-C-N	5.92	127.81	120.34
2	B	296	LEU	C-N-CA	5.92	127.81	120.34
2	D	328	HIS	CG-CD2-NE2	5.92	113.12	107.20
3	I	166	PRO	N-CA-C	5.92	117.93	110.70
2	S	72	ALA	CA-C-N	5.92	128.22	120.28
2	S	72	ALA	C-N-CA	5.92	128.22	120.28
6	U	620	ARG	NE-CZ-NH1	-5.92	115.58	121.50
6	V	606	MET	O-C-N	5.92	128.17	122.07
3	I	175	THR	CA-C-N	5.92	130.74	120.68
3	I	175	THR	C-N-CA	5.92	130.74	120.68
5	L	529	CYS	CA-C-N	5.91	127.48	120.09
5	L	529	CYS	C-N-CA	5.91	127.48	120.09
2	B	347	VAL	N-CA-C	5.91	118.14	109.63
2	D	273	CYS	CA-CB-SG	-5.91	100.81	114.40
2	H	467	LYS	N-CA-CB	5.91	118.66	109.85
3	K	306	THR	O-C-N	5.91	128.89	122.15
2	D	391	LYS	N-CA-C	-5.91	98.78	108.41
2	O	83	SER	CA-C-N	5.91	128.20	120.28
2	O	83	SER	C-N-CA	5.91	128.20	120.28
6	V	600	ILE	CB-CA-C	-5.91	104.28	112.02
7	t	23	ARG	CA-C-N	5.91	128.20	120.28
7	t	23	ARG	C-N-CA	5.91	128.20	120.28
1	E	357	LEU	N-CA-C	-5.91	104.92	111.36
1	G	381	ALA	N-CA-C	-5.90	105.17	112.90
2	D	537	TYR	CA-C-N	5.90	130.70	120.68
2	D	537	TYR	C-N-CA	5.90	130.70	120.68
3	K	289	GLN	O-C-N	5.90	128.95	122.11
5	L	570	THR	N-CA-C	-5.90	98.67	108.75
1	A	216	LEU	CA-C-N	5.89	127.99	120.56
1	A	216	LEU	C-N-CA	5.89	127.99	120.56
3	I	86	LEU	N-CA-C	-5.89	104.44	111.69
6	X	613	ASP	O-C-N	5.89	128.37	122.12
2	H	260	ILE	CA-CB-CG1	5.89	120.41	110.40
3	K	146	GLN	CA-C-O	5.89	125.86	119.15
2	R	90	ARG	N-CA-CB	5.89	118.78	110.12
2	O	66	ARG	NE-CZ-NH1	-5.89	115.61	121.50
4	J	422	ASP	N-CA-CB	5.88	118.94	110.06
4	J	500	HIS	O-C-N	-5.88	117.13	123.42
6	X	603	ILE	O-C-N	5.88	127.58	121.87
4	J	305	CYS	CA-C-N	5.88	128.16	120.28
4	J	305	CYS	C-N-CA	5.88	128.16	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	616	GLU	N-CA-C	5.88	117.77	111.36
3	I	169	ARG	N-CA-C	5.88	118.64	111.82
1	C	403	TYR	CB-CG-CD2	-5.88	111.98	120.80
1	G	389	ILE	CA-C-O	5.88	126.69	119.58
2	H	299	LEU	CA-C-N	5.87	128.63	120.29
2	H	299	LEU	C-N-CA	5.87	128.63	120.29
5	L	375	LEU	CA-C-O	-5.87	112.11	120.51
2	B	400	HIS	ND1-CE1-NE2	5.87	114.27	108.40
3	K	35	HIS	CA-C-N	5.87	125.74	119.28
3	K	35	HIS	C-N-CA	5.87	125.74	119.28
1	C	328	GLN	N-CA-C	5.87	122.78	109.81
3	K	341	TRP	NE1-CE2-CD2	5.87	115.03	107.40
3	K	16	ILE	N-CA-C	5.87	117.39	111.00
7	o	14	THR	N-CA-CB	5.87	118.84	110.16
7	r	15	MET	N-CA-CB	5.87	118.75	110.12
1	A	275	PHE	N-CA-C	-5.87	105.22	112.90
3	I	279	VAL	N-CA-C	-5.87	104.80	110.72
1	E	361	ARG	NE-CZ-NH2	-5.86	113.92	119.20
6	U	602	PHE	N-CA-CB	5.86	118.51	110.01
1	A	392	ARG	NE-CZ-NH1	5.86	127.36	121.50
3	K	121	HIS	CB-CG-ND1	5.86	131.49	122.70
5	L	220	LEU	CA-C-N	5.86	129.74	121.53
5	L	220	LEU	C-N-CA	5.86	129.74	121.53
7	r	61	SER	CA-C-N	5.86	128.61	120.29
7	r	61	SER	C-N-CA	5.86	128.61	120.29
1	C	429	GLN	N-CA-CB	5.86	118.58	109.97
1	G	245	PHE	N-CA-CB	5.86	118.60	110.17
4	J	488	PHE	N-CA-C	-5.86	101.06	110.14
2	F	460	HIS	ND1-CE1-NE2	5.85	114.25	108.40
5	L	449	LEU	N-CA-C	-5.85	106.10	113.18
6	V	626	GLN	N-CA-C	5.85	117.33	111.07
7	s	64	LEU	CA-C-N	5.85	128.40	120.44
7	s	64	LEU	C-N-CA	5.85	128.40	120.44
1	C	362	THR	N-CA-CB	5.85	119.34	110.28
2	Q	71	GLY	O-C-N	5.85	127.80	122.19
2	D	400	HIS	ND1-CE1-NE2	5.84	114.24	108.40
5	L	6	LYS	O-C-N	5.84	128.09	122.07
3	I	201	GLU	N-CA-CB	5.84	120.36	110.49
2	Q	13	LEU	CA-C-N	5.84	128.11	120.28
2	Q	13	LEU	C-N-CA	5.84	128.11	120.28
2	Q	19	ARG	N-CA-C	5.84	117.72	111.36
1	A	401	ASP	CA-C-N	5.83	125.21	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	ASP	C-N-CA	5.83	125.21	118.85
1	G	333	THR	CA-C-O	-5.83	114.23	120.42
2	O	74	PHE	N-CA-CB	5.83	118.81	110.06
1	A	263	LEU	CA-C-N	5.83	125.37	119.19
1	A	263	LEU	C-N-CA	5.83	125.37	119.19
4	J	250	ASP	N-CA-C	-5.83	102.44	109.72
5	L	1367	VAL	CA-C-N	5.83	128.57	120.29
5	L	1367	VAL	C-N-CA	5.83	128.57	120.29
5	L	175	THR	CA-C-N	5.83	128.01	120.44
5	L	175	THR	C-N-CA	5.83	128.01	120.44
2	Q	34	TYR	CA-C-N	5.83	128.37	120.44
2	Q	34	TYR	C-N-CA	5.83	128.37	120.44
1	A	298	LEU	N-CA-C	-5.83	105.43	112.54
1	C	409	GLU	CB-CA-C	5.83	119.42	110.62
7	t	13	GLU	O-C-N	5.82	128.79	122.15
3	I	106	ASP	N-CA-C	-5.82	105.67	112.89
1	E	209	LEU	CA-C-O	-5.82	110.91	120.80
2	S	52	PHE	CA-CB-CG	-5.82	107.98	113.80
6	V	627	VAL	N-CA-C	5.82	116.00	110.53
6	X	619	HIS	CA-C-N	5.82	128.07	120.28
6	X	619	HIS	C-N-CA	5.82	128.07	120.28
1	A	326	TYR	CB-CG-CD1	5.81	129.51	120.80
3	K	84	ILE	CB-CA-C	-5.80	104.55	110.93
2	H	466	ARG	NE-CZ-NH1	5.80	127.30	121.50
2	D	403	THR	N-CA-C	-5.80	106.24	113.38
5	L	457	LEU	N-CA-C	-5.80	106.16	113.18
5	L	531	PRO	N-CA-CB	5.80	109.67	103.52
5	L	566	LYS	N-CA-CB	5.80	120.30	110.49
7	q	59	ARG	NE-CZ-NH1	-5.80	115.70	121.50
7	s	31	MET	CB-CA-C	-5.80	101.77	110.88
2	F	302	LYS	O-C-N	-5.80	115.54	122.15
1	E	370	GLN	CG-CD-NE2	5.80	125.10	116.40
7	r	26	ASN	CA-C-O	5.80	128.80	120.51
7	t	46	ASN	CA-CB-CG	5.80	118.40	112.60
2	D	365	ARG	NE-CZ-NH1	-5.80	115.70	121.50
4	J	263	GLU	N-CA-CB	5.80	118.46	109.48
2	D	400	HIS	CA-CB-CG	5.79	119.59	113.80
2	F	418	LEU	CA-C-O	-5.79	114.41	120.55
5	L	415	SER	CA-C-N	5.79	129.12	120.31
5	L	415	SER	C-N-CA	5.79	129.12	120.31
6	V	610	THR	CA-C-O	-5.79	114.28	120.42
6	V	619	HIS	CB-CG-ND1	5.79	131.39	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	654	VAL	CA-C-N	5.79	128.04	120.28
6	U	654	VAL	C-N-CA	5.79	128.04	120.28
7	q	55	LYS	O-C-N	5.79	128.04	122.07
2	B	514	SER	N-CA-CB	5.79	120.67	110.37
2	D	344	GLN	N-CA-CB	5.79	119.15	110.53
6	X	667	LEU	CA-C-N	5.78	129.10	120.31
6	X	667	LEU	C-N-CA	5.78	129.10	120.31
5	L	580	VAL	CA-C-N	5.78	129.04	120.95
5	L	580	VAL	C-N-CA	5.78	129.04	120.95
2	Q	41	SER	CA-C-N	5.78	129.08	120.87
2	Q	41	SER	C-N-CA	5.78	129.08	120.87
2	B	254	LEU	N-CA-C	-5.78	104.95	112.23
2	B	431	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	G	245	PHE	CA-CB-CG	-5.78	108.02	113.80
5	L	114	GLU	CA-C-N	5.77	127.95	120.44
5	L	114	GLU	C-N-CA	5.77	127.95	120.44
1	C	450	LEU	O-C-N	5.77	128.24	122.12
2	F	328	HIS	CE1-NE2-CD2	-5.77	103.23	109.00
1	E	333	THR	O-C-N	-5.77	116.01	122.12
5	L	472	ARG	N-CA-C	5.77	117.57	111.28
7	s	58	ARG	CA-C-N	5.76	128.01	120.28
7	s	58	ARG	C-N-CA	5.76	128.01	120.28
1	A	264	PRO	CA-C-N	5.76	128.35	120.46
1	A	264	PRO	C-N-CA	5.76	128.35	120.46
1	A	441	PHE	CA-CB-CG	-5.76	108.04	113.80
2	B	493	HIS	N-CA-C	-5.76	104.97	113.61
2	T	58	ILE	N-CA-CB	5.76	118.38	110.54
1	E	340	ILE	CA-C-N	5.76	128.47	120.29
1	E	340	ILE	C-N-CA	5.76	128.47	120.29
2	F	267	MET	N-CA-CB	5.76	121.28	111.66
6	V	666	ARG	CA-C-N	5.76	128.00	120.28
6	V	666	ARG	C-N-CA	5.76	128.00	120.28
2	H	436	GLY	N-CA-C	-5.76	106.57	116.01
4	J	355	ARG	CA-C-O	-5.76	114.45	120.55
2	D	295	GLU	CA-C-N	5.76	130.59	121.44
2	D	295	GLU	C-N-CA	5.76	130.59	121.44
1	G	428	ASP	N-CA-C	-5.76	98.54	110.80
3	I	298	SER	CA-C-N	5.76	128.24	122.66
3	I	298	SER	C-N-CA	5.76	128.24	122.66
2	R	74	PHE	CA-CB-CG	5.76	119.56	113.80
1	A	371	ALA	CA-C-O	-5.75	114.77	120.70
7	p	17	VAL	N-CA-CB	5.75	117.28	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	465	LEU	N-CA-CB	5.75	119.79	110.41
2	D	466	ARG	CD-NE-CZ	-5.75	116.35	124.40
3	K	317	GLN	CB-CG-CD	-5.75	102.82	112.60
2	O	16	LEU	N-CA-C	5.75	117.55	111.28
2	T	10	ASN	CA-C-O	5.75	126.65	120.55
1	A	392	ARG	CD-NE-CZ	-5.75	116.35	124.40
7	t	31	MET	O-C-N	5.75	128.94	122.22
7	p	33	THR	CA-C-N	5.74	127.98	120.28
7	p	33	THR	C-N-CA	5.74	127.98	120.28
2	B	407	ASP	CA-C-O	-5.74	112.30	120.16
2	B	494	GLN	N-CA-C	-5.74	105.86	112.92
5	L	117	VAL	N-CA-C	5.74	116.47	110.62
1	C	342	THR	CA-CB-OG1	-5.74	100.99	109.60
1	C	355	LEU	CA-C-N	5.74	128.44	120.29
1	C	355	LEU	C-N-CA	5.74	128.44	120.29
2	Q	103	ASP	CA-CB-CG	-5.74	106.86	112.60
1	C	217	VAL	O-C-N	-5.74	116.31	121.87
3	I	155	GLU	N-CA-C	-5.74	105.39	112.90
1	A	211	SER	CA-C-O	5.73	126.56	119.97
1	G	289	HIS	N-CA-C	-5.73	105.01	112.23
7	o	41	CYS	N-CA-CB	5.73	118.55	110.12
7	q	29	LEU	N-CA-C	-5.73	100.59	109.24
7	q	23	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	A	394	ILE	N-CA-C	-5.73	106.17	113.22
2	H	435	ASP	N-CA-CB	5.73	119.29	110.81
1	E	450	LEU	N-CA-C	-5.72	104.96	111.14
5	L	594	GLU	CA-C-O	-5.72	112.75	119.05
2	D	360	SER	N-CA-C	-5.72	106.09	114.39
1	E	248	GLU	CA-C-O	5.72	128.34	121.88
4	J	464	THR	N-CA-CB	5.72	118.63	110.16
2	H	335	TYR	N-CA-CB	5.72	119.14	110.28
1	E	232	ILE	N-CA-C	-5.72	99.40	107.75
6	X	600	ILE	N-CA-CB	5.71	117.23	110.55
2	F	432	TRP	CA-C-N	5.71	128.53	120.42
2	F	432	TRP	C-N-CA	5.71	128.53	120.42
4	J	601	HIS	CE1-NE2-CD2	-5.71	103.29	109.00
3	K	130	HIS	CE1-NE2-CD2	-5.71	103.29	109.00
5	L	439	LYS	CA-C-N	5.71	130.39	120.68
5	L	439	LYS	C-N-CA	5.71	130.39	120.68
4	J	319	VAL	CA-CB-CG1	5.71	120.11	110.40
5	L	110	HIS	CB-CG-CD2	-5.71	123.78	131.20
7	o	34	LEU	O-C-N	5.71	128.17	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	364	ARG	NE-CZ-NH2	5.70	124.33	119.20
4	J	399	ALA	O-C-N	-5.70	115.33	120.92
4	J	557	MET	CG-SD-CE	-5.70	88.35	100.90
2	D	333	GLU	CA-C-N	5.70	128.97	120.31
2	D	333	GLU	C-N-CA	5.70	128.97	120.31
2	D	399	VAL	CA-C-N	5.70	131.12	121.14
2	D	399	VAL	C-N-CA	5.70	131.12	121.14
4	J	401	ARG	CA-C-N	5.70	128.38	120.29
4	J	401	ARG	C-N-CA	5.70	128.38	120.29
2	R	37	ARG	O-C-N	5.70	127.94	122.07
1	C	282	PHE	CA-C-N	5.70	132.42	121.54
1	C	282	PHE	C-N-CA	5.70	132.42	121.54
2	F	303	ILE	CA-CB-CG1	5.70	120.08	110.40
6	U	653	LEU	N-CA-C	5.70	117.17	111.07
4	J	265	GLN	N-CA-CB	5.70	119.29	110.80
4	J	444	ASP	CA-C-O	-5.70	114.38	120.42
3	K	268	ILE	CA-C-N	5.70	126.96	119.84
3	K	268	ILE	C-N-CA	5.70	126.96	119.84
7	s	63	THR	N-CA-CB	5.69	118.59	110.16
1	A	276	VAL	CA-CB-CG2	5.69	120.08	110.40
5	L	179	ARG	CA-C-N	5.69	128.37	120.29
5	L	179	ARG	C-N-CA	5.69	128.37	120.29
2	R	75	SER	N-CA-CB	-5.69	101.75	110.12
5	L	1370	PRO	O-C-N	5.69	129.06	122.23
4	J	215	HIS	CB-CG-ND1	5.69	131.23	122.70
7	t	51	SER	CA-C-O	-5.69	114.52	120.55
1	A	233	SER	O-C-N	5.68	129.38	122.96
2	Q	65	GLN	OE1-CD-NE2	5.68	128.28	122.60
2	T	66	ARG	NE-CZ-NH1	-5.68	115.81	121.50
2	B	432	TRP	CA-CB-CG	5.68	124.40	113.60
7	r	31	MET	O-C-N	5.68	128.14	122.12
2	D	458	LEU	N-CA-C	-5.68	106.01	113.17
2	F	388	GLN	CA-C-N	5.68	125.73	120.34
2	F	388	GLN	C-N-CA	5.68	125.73	120.34
2	H	443	HIS	CA-CB-CG	-5.68	108.12	113.80
2	H	443	HIS	N-CA-CB	5.68	120.09	110.49
3	I	149	HIS	CA-CB-CG	5.68	119.48	113.80
2	H	317	GLY	N-CA-C	-5.68	106.25	112.04
6	U	661	ARG	O-C-N	5.68	127.92	122.07
6	X	651	GLU	CA-C-N	5.68	127.82	120.44
6	X	651	GLU	C-N-CA	5.68	127.82	120.44
7	s	38	VAL	N-CA-C	5.68	116.45	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1374	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
7	r	37	CYS	CA-C-O	-5.67	114.50	120.63
7	p	58	ARG	CA-C-O	-5.67	114.86	120.82
5	L	336	LEU	CA-C-O	5.67	125.62	119.15
7	o	21	ILE	N-CA-CB	5.67	118.25	110.54
4	J	208	ALA	N-CA-C	5.67	118.23	111.71
1	A	220	LEU	CA-C-O	-5.67	113.45	119.97
7	o	52	SER	CA-C-N	5.67	127.70	120.56
7	o	52	SER	C-N-CA	5.67	127.70	120.56
3	K	193	HIS	CB-CG-CD2	5.67	138.57	131.20
2	R	59	LYS	N-CA-CB	5.67	118.54	110.16
2	F	400	HIS	CE1-NE2-CD2	-5.66	103.34	109.00
2	S	27	ASP	CA-C-N	5.66	131.51	122.56
2	S	27	ASP	C-N-CA	5.66	131.51	122.56
6	V	629	MET	N-CA-CB	5.66	118.44	110.12
1	G	350	PHE	N-CA-CB	5.66	119.15	110.49
2	O	54	VAL	CA-C-N	5.66	127.79	120.44
2	O	54	VAL	C-N-CA	5.66	127.79	120.44
1	E	485	GLU	N-CA-C	-5.66	106.04	113.17
3	I	302	ASN	N-CA-C	-5.66	104.80	112.26
6	U	599	GLN	CA-C-O	-5.65	114.43	120.42
2	B	475	THR	CA-CB-OG1	5.65	118.08	109.60
2	F	272	ASN	N-CA-CB	5.65	120.04	110.49
1	G	370	GLN	CB-CG-CD	-5.65	102.99	112.60
2	H	407	ASP	CA-C-N	5.65	125.18	119.19
2	H	407	ASP	C-N-CA	5.65	125.18	119.19
2	F	303	ILE	CA-C-O	-5.65	114.15	120.25
2	S	68	GLU	N-CA-CB	5.65	118.52	110.16
2	D	530	GLN	N-CA-C	-5.64	106.35	113.18
3	I	149	HIS	CE1-NE2-CD2	-5.64	103.36	109.00
4	J	251	PRO	N-CA-C	-5.64	106.18	113.57
4	J	260	ILE	N-CA-CB	5.64	117.27	110.95
4	J	490	ILE	CA-C-N	5.64	130.15	122.19
4	J	490	ILE	C-N-CA	5.64	130.15	122.19
1	A	310	GLU	O-C-N	5.64	130.25	122.46
1	A	474	ILE	O-C-N	5.64	130.50	122.04
1	C	368	ASP	CA-C-N	5.64	128.30	120.29
1	C	368	ASP	C-N-CA	5.64	128.30	120.29
2	F	398	ALA	N-CA-CB	5.64	118.48	110.13
2	F	470	ILE	CA-C-N	5.64	125.97	119.93
2	F	470	ILE	C-N-CA	5.64	125.97	119.93
7	r	58	ARG	NE-CZ-NH1	5.64	127.14	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	TYR	O-C-N	-5.64	114.69	122.30
1	G	308	GLN	CA-C-N	5.64	128.30	120.29
1	G	308	GLN	C-N-CA	5.64	128.30	120.29
1	G	381	ALA	N-CA-CB	5.64	118.79	110.33
3	I	108	GLU	CA-C-O	5.64	126.40	120.42
2	D	289	ILE	CA-CB-CG2	-5.64	100.92	110.50
1	G	240	ARG	N-CA-C	5.64	119.12	111.17
7	r	12	ARG	NE-CZ-NH2	5.64	124.27	119.20
7	t	63	THR	CA-C-N	5.64	127.77	120.44
7	t	63	THR	C-N-CA	5.64	127.77	120.44
3	I	160	HIS	CA-CB-CG	-5.63	108.17	113.80
2	R	16	LEU	CA-C-N	5.63	127.83	120.28
2	R	16	LEU	C-N-CA	5.63	127.83	120.28
1	G	222	TYR	CA-C-O	-5.63	114.45	120.42
5	L	114	GLU	N-CA-C	5.63	117.42	111.28
6	W	628	GLU	CA-C-O	5.63	126.52	120.55
6	W	666	ARG	O-C-N	-5.63	116.15	122.12
1	C	454	LYS	N-CA-C	5.63	117.41	111.28
7	q	56	GLU	CA-C-O	-5.63	114.59	120.55
7	r	43	GLN	OE1-CD-NE2	5.63	128.23	122.60
4	J	362	TRP	CE3-CZ3-CH2	-5.62	113.79	121.10
4	J	478	HIS	CA-C-O	-5.62	112.95	118.97
1	C	376	LEU	O-C-N	5.62	127.86	122.07
1	A	329	PRO	CB-CA-C	-5.62	103.48	111.68
3	I	160	HIS	CE1-NE2-CD2	-5.62	103.39	109.00
3	I	258	SER	CA-C-O	-5.62	115.43	121.38
6	X	664	ASN	O-C-N	-5.62	116.17	122.12
1	G	357	LEU	CA-C-N	5.61	130.22	120.68
1	G	357	LEU	C-N-CA	5.61	130.22	120.68
2	H	273	CYS	N-CA-C	-5.61	103.59	110.61
3	K	126	LEU	CA-C-N	-5.61	113.63	121.99
3	K	126	LEU	C-N-CA	-5.61	113.63	121.99
7	p	30	ASP	CA-CB-CG	5.61	118.21	112.60
1	G	274	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	G	240	ARG	NE-CZ-NH2	-5.61	114.15	119.20
7	s	45	ILE	N-CA-C	-5.61	99.74	108.44
2	B	390	ARG	NE-CZ-NH2	-5.61	114.15	119.20
2	D	467	LYS	N-CA-C	-5.61	106.44	113.28
3	K	311	LEU	CA-C-N	5.61	127.80	120.28
3	K	311	LEU	C-N-CA	5.61	127.80	120.28
7	s	39	ARG	CA-C-O	-5.61	114.93	120.82
2	F	255	TYR	CA-C-O	5.61	125.83	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	305	LYS	N-CA-CB	5.61	119.54	110.40
2	D	335	TYR	CA-C-N	5.61	128.83	120.31
2	D	335	TYR	C-N-CA	5.61	128.83	120.31
1	G	486	ARG	CG-CD-NE	-5.61	99.67	112.00
6	V	626	GLN	OE1-CD-NE2	5.61	128.21	122.60
7	p	19	LEU	N-CA-C	-5.61	105.32	111.82
4	J	291	ASN	CA-C-O	5.60	127.32	121.38
2	B	318	LEU	CA-C-N	5.60	132.05	121.97
2	B	318	LEU	C-N-CA	5.60	132.05	121.97
3	I	157	VAL	CA-CB-CG2	-5.60	100.88	110.40
1	C	236	PRO	CA-C-O	-5.60	114.42	120.97
1	G	354	THR	N-CA-C	-5.60	105.25	111.36
5	L	537	TYR	N-CA-C	-5.60	106.28	113.23
2	S	28	VAL	N-CA-C	-5.60	105.94	111.77
3	I	166	PRO	CA-C-N	5.60	124.95	118.85
3	I	166	PRO	C-N-CA	5.60	124.95	118.85
4	J	505	TYR	CA-C-N	5.60	128.80	120.90
4	J	505	TYR	C-N-CA	5.60	128.80	120.90
7	p	56	GLU	O-C-N	5.60	127.84	122.07
5	L	475	ALA	N-CA-C	-5.60	105.24	112.68
2	R	37	ARG	CA-C-O	-5.60	114.94	120.82
2	H	467	LYS	CA-C-O	-5.59	114.38	120.81
1	A	431	TYR	CA-C-O	5.59	128.48	121.66
5	L	459	THR	CA-C-N	5.59	128.95	122.35
5	L	459	THR	C-N-CA	5.59	128.95	122.35
2	Q	81	LEU	CB-CA-C	-5.59	101.51	110.79
2	R	79	ARG	NH1-CZ-NH2	5.59	126.57	119.30
2	R	96	LEU	O-C-N	-5.59	116.05	122.09
2	B	337	LEU	N-CA-C	-5.59	105.96	112.89
7	r	35	SER	N-CA-CB	5.59	118.11	110.01
6	V	628	GLU	CA-C-O	-5.58	114.63	120.55
4	J	211	TRP	O-C-N	5.58	128.52	122.15
2	O	67	ARG	N-CA-C	-5.58	102.08	110.06
6	V	661	ARG	CA-C-N	5.58	127.76	120.28
6	V	661	ARG	C-N-CA	5.58	127.76	120.28
2	B	287	LYS	CG-CD-CE	5.58	124.13	111.30
2	F	379	THR	CA-C-N	5.58	130.17	120.68
2	F	379	THR	C-N-CA	5.58	130.17	120.68
6	W	639	GLU	O-C-N	-5.58	116.21	122.12
1	E	315	GLN	CA-C-N	5.57	132.33	121.41
1	E	315	GLN	C-N-CA	5.57	132.33	121.41
3	I	268	ILE	CA-C-N	5.57	126.81	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	268	ILE	C-N-CA	5.57	126.81	119.84
6	V	631	LYS	N-CA-C	5.57	118.07	111.33
7	p	45	ILE	CA-C-N	5.57	128.14	120.39
7	p	45	ILE	C-N-CA	5.57	128.14	120.39
6	U	670	ASN	N-CA-C	-5.57	106.31	114.39
1	A	399	ILE	N-CA-CB	5.57	121.08	111.39
2	B	419	GLY	O-C-N	5.57	128.35	122.28
1	C	271	THR	CA-CB-OG1	5.57	117.96	109.60
2	H	455	THR	CA-C-N	5.57	128.75	120.90
2	H	455	THR	C-N-CA	5.57	128.75	120.90
4	J	302	THR	CA-C-N	5.57	127.75	120.28
4	J	302	THR	C-N-CA	5.57	127.75	120.28
2	R	25	GLU	N-CA-C	5.57	117.03	111.07
3	K	328	VAL	CG1-CB-CG2	5.56	123.04	110.80
3	K	2	ILE	N-CA-C	5.56	116.29	110.62
2	R	44	ALA	CA-C-O	-5.56	114.66	119.72
2	H	308	ASP	N-CA-C	-5.56	105.22	112.23
3	I	126	LEU	N-CA-C	-5.56	103.35	111.30
3	K	169	ARG	NE-CZ-NH2	-5.56	114.20	119.20
2	Q	22	GLY	O-C-N	-5.56	115.98	122.87
2	D	432	TRP	CA-CB-CG	5.56	124.16	113.60
2	S	46	THR	CA-C-N	5.55	131.97	121.97
2	S	46	THR	C-N-CA	5.55	131.97	121.97
2	B	479	SER	N-CA-CB	5.55	118.88	110.28
2	H	343	SER	N-CA-C	-5.55	106.01	112.89
1	C	315	GLN	O-C-N	-5.54	115.34	122.94
2	H	305	LYS	N-CA-C	-5.54	106.02	112.89
7	t	30	ASP	CA-C-N	5.54	128.26	120.28
7	t	30	ASP	C-N-CA	5.54	128.26	120.28
2	H	289	ILE	O-C-N	5.54	127.54	121.83
2	B	411	ARG	NE-CZ-NH2	5.54	124.19	119.20
4	J	449	ALA	CA-C-N	5.54	135.05	122.20
4	J	449	ALA	C-N-CA	5.54	135.05	122.20
5	L	45	ASP	N-CA-CB	5.54	118.04	110.01
1	C	241	GLN	CA-C-N	5.54	131.70	122.73
1	C	241	GLN	C-N-CA	5.54	131.70	122.73
3	K	203	PHE	N-CA-C	-5.54	99.01	110.80
2	B	443	HIS	CA-CB-CG	-5.53	108.27	113.80
2	H	293	LEU	CA-C-N	5.53	128.72	120.31
2	H	293	LEU	C-N-CA	5.53	128.72	120.31
3	I	123	ASN	CB-CA-C	-5.53	101.60	110.79
6	X	634	HIS	CB-CG-CD2	-5.53	124.00	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	307	SER	CA-C-N	5.53	128.15	120.29
1	G	307	SER	C-N-CA	5.53	128.15	120.29
2	H	326	ALA	O-C-N	-5.53	115.47	122.27
3	K	283	VAL	CA-C-O	5.53	125.89	119.36
2	S	94	LEU	CA-C-N	5.53	128.15	120.29
2	S	94	LEU	C-N-CA	5.53	128.15	120.29
1	C	231	TYR	N-CA-C	-5.53	106.42	112.72
1	C	396	ARG	N-CA-CB	5.53	118.20	110.07
2	F	310	ARG	N-CA-C	-5.53	105.66	112.90
3	I	206	ARG	N-CA-C	-5.53	101.57	110.14
2	D	390	ARG	CB-CA-C	-5.53	101.86	110.37
1	C	243	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	G	403	TYR	O-C-N	5.53	126.06	122.03
2	T	54	VAL	CA-C-O	-5.53	115.20	120.95
1	C	384	ALA	CA-C-O	-5.52	112.59	120.16
2	F	342	HIS	ND1-CE1-NE2	5.52	113.92	108.40
3	K	302	ASN	CA-CB-CG	5.52	118.12	112.60
6	V	637	SER	CA-C-N	5.52	127.68	120.28
6	V	637	SER	C-N-CA	5.52	127.68	120.28
7	q	11	VAL	CA-C-N	5.52	127.95	120.44
7	q	11	VAL	C-N-CA	5.52	127.95	120.44
1	A	471	ALA	N-CA-C	-5.52	106.32	113.16
2	R	59	LYS	CB-CA-C	-5.52	101.47	110.85
6	V	671	PHE	N-CA-CB	5.52	119.89	110.50
6	X	629	MET	N-CA-CB	5.52	118.01	110.01
1	A	474	ILE	N-CA-C	-5.52	104.57	112.35
1	E	286	GLN	CB-CG-CD	-5.52	103.22	112.60
4	J	242	TRP	CA-C-N	5.52	127.67	120.28
4	J	242	TRP	C-N-CA	5.52	127.67	120.28
2	D	528	ALA	N-CA-CB	5.51	118.75	110.53
3	I	205	VAL	CA-C-O	-5.51	114.28	120.95
4	J	242	TRP	O-C-N	-5.51	116.39	122.07
5	L	541	TYR	N-CA-C	-5.51	105.34	113.61
2	R	76	GLU	N-CA-CB	5.51	118.32	110.16
2	T	13	LEU	N-CA-CB	5.51	118.22	110.12
7	o	23	ARG	NH1-CZ-NH2	5.51	126.47	119.30
2	D	361	LEU	N-CA-CB	5.51	118.74	110.53
2	D	387	CYS	CA-C-O	5.51	128.18	120.52
4	J	434	ASN	CA-C-O	-5.51	113.63	119.97
2	T	72	ALA	CA-C-N	5.51	127.66	120.28
2	T	72	ALA	C-N-CA	5.51	127.66	120.28
2	F	310	ARG	CA-C-N	5.51	130.28	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	310	ARG	C-N-CA	5.51	130.28	122.24
1	E	436	GLN	CA-C-N	-5.50	115.23	122.99
1	E	436	GLN	C-N-CA	-5.50	115.23	122.99
2	F	413	LEU	CA-C-N	5.50	129.66	120.64
2	F	413	LEU	C-N-CA	5.50	129.66	120.64
5	L	531	PRO	CA-C-N	5.50	128.10	120.29
5	L	531	PRO	C-N-CA	5.50	128.10	120.29
1	A	467	THR	CA-C-N	5.50	126.97	120.09
1	A	467	THR	C-N-CA	5.50	126.97	120.09
5	L	406	THR	CA-C-O	5.50	126.28	119.79
1	A	233	SER	CA-C-N	5.50	130.34	123.14
1	A	233	SER	C-N-CA	5.50	130.34	123.14
1	A	395	TYR	N-CA-CB	5.50	119.78	110.49
1	E	243	ARG	O-C-N	-5.50	116.08	123.23
5	L	176	THR	N-CA-C	-5.50	105.19	111.07
5	L	553	MET	N-CA-CB	5.50	119.78	110.49
4	J	390	THR	N-CA-C	-5.50	101.37	109.18
2	T	29	ALA	CA-C-O	-5.50	114.59	120.42
1	E	429	GLN	N-CA-CB	5.50	119.78	110.49
2	D	280	VAL	CB-CA-C	5.49	119.60	112.24
2	S	86	VAL	CA-C-N	5.49	132.05	122.82
2	S	86	VAL	C-N-CA	5.49	132.05	122.82
3	K	91	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	C	362	THR	N-CA-C	-5.49	105.45	111.82
2	F	255	TYR	O-C-N	-5.49	114.94	122.46
2	Q	10	ASN	CA-CB-CG	-5.49	107.11	112.60
1	A	243	ARG	N-CA-C	-5.49	100.94	109.72
1	C	492	ASN	CA-CB-CG	-5.48	107.12	112.60
2	H	328	HIS	CA-C-N	5.48	127.63	120.28
2	H	328	HIS	C-N-CA	5.48	127.63	120.28
2	Q	28	VAL	CA-C-N	5.48	127.63	120.28
2	Q	28	VAL	C-N-CA	5.48	127.63	120.28
6	U	671	PHE	CA-CB-CG	-5.48	108.32	113.80
7	s	17	VAL	N-CA-CB	5.48	118.80	110.58
1	A	374	LEU	N-CA-C	-5.48	105.39	111.36
2	D	527	ASN	CB-CA-C	5.48	117.57	109.29
1	E	430	ARG	N-CA-CB	5.48	118.60	110.49
5	L	386	ILE	N-CA-C	-5.48	105.56	113.07
1	G	248	GLU	CA-C-O	-5.48	114.97	121.66
7	p	21	ILE	CB-CA-C	-5.48	104.75	112.14
7	p	59	ARG	N-CA-CB	5.48	117.95	110.01
1	A	457	ASN	CA-C-N	5.48	127.96	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ASN	C-N-CA	5.48	127.96	120.46
1	G	277	GLU	N-CA-CB	5.48	118.36	110.20
1	E	243	ARG	CG-CD-NE	-5.47	99.95	112.00
2	H	296	LEU	CA-C-N	5.47	127.23	120.34
2	H	296	LEU	C-N-CA	5.47	127.23	120.34
2	H	375	ILE	CA-CB-CG1	5.47	119.70	110.40
1	C	330	THR	CA-C-N	5.47	127.55	120.44
1	C	330	THR	C-N-CA	5.47	127.55	120.44
2	B	402	TYR	CA-C-O	5.46	125.89	119.28
2	D	362	THR	CA-CB-OG1	5.46	117.80	109.60
3	K	271	ARG	NE-CZ-NH2	-5.46	114.28	119.20
1	C	271	THR	O-C-N	5.46	127.71	122.03
1	G	242	SER	N-CA-C	-5.46	99.02	108.69
1	A	319	SER	CA-C-N	5.46	128.61	120.31
1	A	319	SER	C-N-CA	5.46	128.61	120.31
3	K	302	ASN	CA-C-N	5.46	127.60	120.28
3	K	302	ASN	C-N-CA	5.46	127.60	120.28
2	Q	80	LYS	CA-C-O	-5.46	114.76	120.55
2	B	423	TYR	CA-C-O	-5.46	112.68	120.16
7	r	37	CYS	N-CA-CB	5.46	118.25	110.06
2	Q	90	ARG	N-CA-C	5.46	117.23	111.28
5	L	346	VAL	CA-C-O	5.46	126.38	120.43
4	J	237	ASN	N-CA-C	-5.45	105.06	112.26
4	J	466	ARG	O-C-N	-5.45	115.05	121.32
3	I	56	THR	CA-C-N	5.45	128.59	120.31
3	I	56	THR	C-N-CA	5.45	128.59	120.31
1	G	236	PRO	N-CA-C	-5.45	102.01	111.32
4	J	291	ASN	OD1-CG-ND2	5.45	128.05	122.60
2	Q	79	ARG	O-C-N	-5.45	116.35	122.12
1	A	393	TRP	CA-CB-CG	5.44	123.94	113.60
1	C	259	VAL	N-CA-C	-5.44	104.93	112.50
1	C	218	GLU	N-CA-CB	5.44	118.21	110.16
2	O	73	LEU	CA-C-N	5.44	127.83	120.38
2	O	73	LEU	C-N-CA	5.44	127.83	120.38
1	C	408	VAL	CA-C-N	5.44	130.59	122.86
1	C	408	VAL	C-N-CA	5.44	130.59	122.86
1	E	444	LYS	CA-C-O	-5.44	113.72	119.97
6	V	625	LEU	CA-C-O	5.44	126.18	120.42
7	s	17	VAL	CA-C-N	5.44	127.56	120.28
7	s	17	VAL	C-N-CA	5.44	127.56	120.28
6	W	639	GLU	CA-C-N	5.44	127.91	120.46
6	W	639	GLU	C-N-CA	5.44	127.91	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	HIS	CB-CG-CD2	-5.43	124.14	131.20
2	B	477	ASP	N-CA-C	-5.43	106.60	113.18
2	F	405	THR	N-CA-CB	5.43	117.96	109.97
3	I	121	HIS	CE1-NE2-CD2	-5.43	103.57	109.00
2	B	439	GLU	O-C-N	5.43	129.81	122.59
2	B	460	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	G	488	GLU	N-CA-C	5.43	118.12	111.82
4	J	502	ASP	CB-CA-C	-5.43	98.93	109.68
4	J	676	GLN	O-C-N	-5.43	115.90	123.34
5	L	339	THR	CA-C-O	5.43	126.35	119.78
7	t	53	VAL	N-CA-CB	5.43	116.91	110.55
1	A	289	HIS	CA-CB-CG	5.43	119.23	113.80
3	I	317	GLN	CA-C-N	5.43	125.08	119.05
3	I	317	GLN	C-N-CA	5.43	125.08	119.05
5	L	227	ASP	CA-CB-CG	-5.43	107.17	112.60
2	S	79	ARG	CA-CB-CG	5.43	124.96	114.10
6	V	611	LEU	CA-C-N	5.43	127.56	120.28
6	V	611	LEU	C-N-CA	5.43	127.56	120.28
1	A	406	PHE	CA-C-N	5.43	127.81	120.38
1	A	406	PHE	C-N-CA	5.43	127.81	120.38
5	L	376	GLN	CA-C-N	5.43	131.00	122.21
5	L	376	GLN	C-N-CA	5.43	131.00	122.21
3	I	134	PRO	CA-C-N	5.42	129.78	120.72
3	I	134	PRO	C-N-CA	5.42	129.78	120.72
1	E	366	THR	CB-CA-C	5.42	118.81	110.62
3	I	312	HIS	CG-CD2-NE2	5.42	112.62	107.20
4	J	245	HIS	CG-CD2-NE2	5.42	112.62	107.20
2	D	451	PRO	N-CA-C	-5.42	106.64	114.18
5	L	544	VAL	N-CA-C	-5.42	100.25	108.17
2	O	30	GLN	CB-CG-CD	5.42	121.82	112.60
7	q	54	ILE	N-CA-C	5.42	116.20	110.72
1	C	258	LEU	CA-C-N	5.42	129.53	120.64
1	C	258	LEU	C-N-CA	5.42	129.53	120.64
3	K	26	GLN	CA-C-O	5.42	127.06	120.99
5	L	549	CYS	CB-CA-C	5.42	119.51	109.70
1	E	406	PHE	N-CA-C	-5.42	100.84	109.07
1	G	321	GLN	CA-C-N	5.42	127.54	120.28
1	G	321	GLN	C-N-CA	5.42	127.54	120.28
4	J	294	ASN	CB-CA-C	-5.42	104.32	111.74
5	L	208	PHE	CA-CB-CG	5.42	119.22	113.80
3	I	131	LEU	CB-CA-C	-5.41	101.33	110.64
2	O	64	ARG	N-CA-CB	5.41	118.08	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	o	30	ASP	N-CA-CB	5.41	117.61	110.25
2	D	455	THR	N-CA-C	-5.41	101.08	109.14
1	A	233	SER	CA-C-O	-5.41	115.25	121.47
2	D	376	ARG	CB-CA-C	-5.41	100.66	110.56
1	E	254	SER	N-CA-CB	5.41	117.91	110.07
3	I	35	HIS	CA-C-N	5.41	125.23	119.28
3	I	35	HIS	C-N-CA	5.41	125.23	119.28
5	L	334	GLN	OE1-CD-NE2	-5.41	117.19	122.60
2	R	10	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	A	266	ALA	CA-C-N	5.40	127.52	120.28
1	A	266	ALA	C-N-CA	5.40	127.52	120.28
1	C	385	PRO	N-CA-CB	5.40	108.92	103.25
5	L	210	LYS	N-CA-CB	5.40	118.06	110.12
2	B	332	LYS	CA-C-N	5.40	128.52	120.31
2	B	332	LYS	C-N-CA	5.40	128.52	120.31
1	C	288	ASN	OD1-CG-ND2	5.40	128.00	122.60
2	R	76	GLU	CB-CA-C	-5.40	101.67	110.85
1	A	447	ASP	CA-C-N	5.40	129.86	120.68
1	A	447	ASP	C-N-CA	5.40	129.86	120.68
7	p	23	ARG	CB-CG-CD	5.40	123.72	111.30
1	E	368	ASP	N-CA-C	-5.40	98.57	108.02
2	Q	63	VAL	CA-C-N	5.40	128.05	120.28
2	Q	63	VAL	C-N-CA	5.40	128.05	120.28
3	K	23	THR	CA-C-N	5.40	129.78	121.42
3	K	23	THR	C-N-CA	5.40	129.78	121.42
7	r	26	ASN	N-CA-CB	5.40	119.61	110.49
1	E	411	HIS	ND1-CE1-NE2	5.39	113.79	108.40
2	D	388	GLN	CA-C-N	5.39	126.32	120.44
2	D	388	GLN	C-N-CA	5.39	126.32	120.44
4	J	245	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
1	G	248	GLU	N-CA-C	-5.39	102.06	110.42
1	A	243	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	B	427	ASN	CA-CB-CG	-5.38	107.22	112.60
2	O	71	GLY	CA-C-N	5.38	127.50	120.28
2	O	71	GLY	C-N-CA	5.38	127.50	120.28
7	s	30	ASP	CA-C-N	5.38	127.44	120.44
7	s	30	ASP	C-N-CA	5.38	127.44	120.44
6	U	641	GLN	CB-CA-C	-5.38	102.43	110.88
5	L	181	LEU	N-CA-CB	5.38	118.03	110.12
2	S	65	GLN	N-CA-C	-5.38	106.69	113.20
2	H	364	ARG	N-CA-CB	5.38	118.40	110.33
4	J	571	ARG	N-CA-CB	5.38	119.64	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	386	HIS	CB-CG-CD2	-5.38	124.21	131.20
2	H	542	LYS	N-CA-CB	5.38	118.12	110.16
4	J	373	GLU	CB-CG-CD	-5.38	103.46	112.60
3	K	55	PHE	N-CA-CB	5.38	118.20	110.40
6	U	635	ILE	CA-C-O	-5.38	115.68	121.27
2	S	70	ASP	N-CA-C	5.38	117.14	111.28
2	S	86	VAL	CA-C-O	5.38	126.06	120.36
1	E	402	PRO	N-CD-CG	5.37	111.26	103.20
2	S	91	TRP	CA-C-N	5.37	127.92	120.29
2	S	91	TRP	C-N-CA	5.37	127.92	120.29
7	o	8	MET	CA-C-N	5.37	127.48	120.28
7	o	8	MET	C-N-CA	5.37	127.48	120.28
1	C	352	GLY	CA-C-N	5.36	128.00	120.28
1	C	352	GLY	C-N-CA	5.36	128.00	120.28
6	W	627	VAL	CA-C-N	5.36	127.47	120.28
6	W	627	VAL	C-N-CA	5.36	127.47	120.28
2	B	516	LYS	N-CA-C	5.36	117.12	111.28
1	E	444	LYS	O-C-N	5.36	128.87	122.27
1	A	285	GLY	CA-C-N	5.36	128.70	120.82
1	A	285	GLY	C-N-CA	5.36	128.70	120.82
1	G	295	MET	CA-C-O	-5.36	113.81	119.97
3	I	63	THR	N-CA-C	-5.36	99.38	110.80
6	W	628	GLU	CA-C-N	5.36	127.41	120.44
6	W	628	GLU	C-N-CA	5.36	127.41	120.44
1	A	270	SER	CA-C-O	-5.36	113.81	119.97
5	L	322	PHE	CA-C-N	5.36	127.46	120.28
5	L	322	PHE	C-N-CA	5.36	127.46	120.28
1	E	232	ILE	O-C-N	-5.36	117.52	123.20
2	B	446	PHE	N-CA-CB	5.35	118.08	110.16
2	F	300	HIS	ND1-CE1-NE2	5.35	113.75	108.40
7	p	16	ASP	O-C-N	5.35	128.25	122.15
3	K	98	GLN	N-CA-C	-5.35	105.18	112.35
1	C	379	THR	CA-CB-CG2	5.35	119.60	110.50
2	S	84	GLN	CB-CG-CD	-5.35	103.50	112.60
6	X	627	VAL	CA-C-N	5.35	127.45	120.28
6	X	627	VAL	C-N-CA	5.35	127.45	120.28
4	J	502	ASP	O-C-N	-5.35	117.15	123.41
2	H	287	LYS	CB-CA-C	-5.35	100.09	109.07
2	S	93	ILE	CA-C-N	5.35	127.88	120.29
2	S	93	ILE	C-N-CA	5.35	127.88	120.29
1	A	227	VAL	CA-C-N	5.34	128.82	120.75
1	A	227	VAL	C-N-CA	5.34	128.82	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	332	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	E	375	CYS	CB-CA-C	-5.34	100.41	110.67
1	G	327	ILE	CA-CB-CG2	5.34	119.58	110.50
4	J	225	ALA	O-C-N	-5.34	116.25	121.38
1	G	410	GLU	CA-C-N	5.34	131.31	121.70
1	G	410	GLU	C-N-CA	5.34	131.31	121.70
3	I	310	GLU	CA-C-N	5.34	127.70	120.44
3	I	310	GLU	C-N-CA	5.34	127.70	120.44
1	C	356	SER	N-CA-CB	5.34	118.06	110.16
1	G	304	ILE	O-C-N	-5.34	115.77	121.80
5	L	594	GLU	N-CA-C	-5.34	106.78	113.72
7	p	59	ARG	CD-NE-CZ	5.34	131.87	124.40
2	D	297	GLY	CA-C-N	5.33	127.87	120.29
2	D	297	GLY	C-N-CA	5.33	127.87	120.29
5	L	113	LEU	CA-C-N	5.33	127.43	120.28
5	L	113	LEU	C-N-CA	5.33	127.43	120.28
6	W	637	SER	O-C-N	5.33	127.78	122.12
1	A	248	GLU	CA-C-N	5.33	129.26	121.31
1	A	248	GLU	C-N-CA	5.33	129.26	121.31
5	L	592	ALA	N-CA-CB	5.33	118.55	110.28
5	L	429	VAL	CA-C-N	5.33	128.41	120.31
5	L	429	VAL	C-N-CA	5.33	128.41	120.31
2	D	393	GLY	N-CA-C	-5.33	107.86	115.64
2	F	407	ASP	CA-C-N	5.33	126.04	120.12
2	F	407	ASP	C-N-CA	5.33	126.04	120.12
2	F	312	LEU	O-C-N	5.33	130.25	123.11
1	G	285	GLY	N-CA-C	-5.33	100.55	113.18
2	F	443	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
6	X	598	ILE	CA-C-O	-5.32	115.53	121.17
4	J	264	THR	CA-C-N	5.32	130.59	122.29
4	J	264	THR	C-N-CA	5.32	130.59	122.29
5	L	311	GLU	CA-C-N	5.32	126.49	119.84
5	L	311	GLU	C-N-CA	5.32	126.49	119.84
1	E	320	LEU	N-CA-C	-5.32	106.57	113.16
1	G	260	ASN	OD1-CG-ND2	-5.32	117.28	122.60
4	J	394	VAL	N-CA-C	-5.32	106.24	111.77
2	O	23	LYS	CA-C-N	5.32	131.83	121.41
2	O	23	LYS	C-N-CA	5.32	131.83	121.41
2	O	84	GLN	N-CA-C	-5.32	105.48	111.28
6	V	620	ARG	CB-CA-C	-5.32	101.96	110.79
6	X	668	ARG	CA-C-N	5.32	128.39	120.31
6	X	668	ARG	C-N-CA	5.32	128.39	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	q	63	THR	CA-C-N	5.32	127.35	120.44
7	q	63	THR	C-N-CA	5.32	127.35	120.44
1	A	289	HIS	CA-C-N	5.32	128.39	120.31
1	A	289	HIS	C-N-CA	5.32	128.39	120.31
2	H	314	ARG	N-CA-C	-5.32	99.48	110.80
6	U	620	ARG	NH1-CZ-NH2	5.32	126.21	119.30
1	A	457	ASN	CA-CB-CG	5.31	117.91	112.60
2	B	264	PHE	CA-C-N	5.31	129.78	123.19
2	B	264	PHE	C-N-CA	5.31	129.78	123.19
4	J	371	PHE	CA-CB-CG	5.31	119.11	113.80
5	L	170	GLU	CA-C-N	5.31	127.40	120.28
5	L	170	GLU	C-N-CA	5.31	127.40	120.28
2	Q	17	CYS	CA-C-N	5.31	127.40	120.28
2	Q	17	CYS	C-N-CA	5.31	127.40	120.28
2	B	369	TRP	N-CA-C	5.31	117.75	111.33
1	G	227	VAL	CA-C-N	5.31	128.39	120.90
1	G	227	VAL	C-N-CA	5.31	128.39	120.90
3	K	30	ASP	N-CA-CB	5.31	119.46	110.49
5	L	169	GLN	CA-C-O	-5.31	114.92	120.55
1	E	348	GLU	CB-CG-CD	5.31	121.62	112.60
3	I	18	THR	CA-C-O	5.31	126.09	120.36
4	J	680	LEU	O-C-N	-5.31	115.14	122.46
7	r	42	GLU	CB-CA-C	-5.31	100.48	110.67
2	H	329	GLN	O-C-N	-5.30	116.50	122.12
3	K	109	GLN	CA-C-N	5.30	127.39	120.28
3	K	109	GLN	C-N-CA	5.30	127.39	120.28
6	V	648	SER	CA-C-N	5.30	131.67	121.54
6	V	648	SER	C-N-CA	5.30	131.67	121.54
7	t	51	SER	N-CA-CB	5.30	117.92	110.12
5	L	369	PHE	CA-C-N	5.30	130.81	123.07
5	L	369	PHE	C-N-CA	5.30	130.81	123.07
2	D	273	CYS	CA-C-O	-5.30	112.94	120.51
1	G	447	ASP	CA-C-N	5.30	127.81	120.29
1	G	447	ASP	C-N-CA	5.30	127.81	120.29
3	K	284	GLN	N-CA-C	-5.29	105.56	112.23
3	I	260	ARG	NE-CZ-NH2	-5.29	114.44	119.20
2	O	45	PRO	N-CA-CB	-5.29	98.59	103.25
2	B	326	ALA	N-CA-C	5.29	116.73	111.07
1	G	274	ARG	NE-CZ-NH2	-5.29	114.44	119.20
2	R	10	ASN	CA-C-N	5.29	127.33	120.56
2	R	10	ASN	C-N-CA	5.29	127.33	120.56
2	F	428	PHE	CA-CB-CG	5.29	119.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	r	52	SER	CB-CA-C	-5.29	102.58	110.88
2	S	89	ASN	CA-C-N	5.29	127.31	120.44
2	S	89	ASN	C-N-CA	5.29	127.31	120.44
7	q	36	ILE	N-CA-CB	5.29	117.73	110.54
7	t	23	ARG	CB-CG-CD	5.28	123.45	111.30
2	H	460	HIS	CG-CD2-NE2	5.28	112.48	107.20
1	E	389	ILE	O-C-N	-5.28	115.83	121.80
3	K	119	ILE	N-CA-C	-5.28	106.73	112.80
6	X	656	GLU	N-CA-CB	5.28	118.46	110.28
2	H	320	GLY	O-C-N	5.28	127.31	122.19
1	E	305	LEU	N-CA-CB	5.28	117.97	110.16
5	L	445	ARG	NE-CZ-NH1	5.28	126.78	121.50
7	p	16	ASP	CA-C-N	5.28	127.21	120.56
7	p	16	ASP	C-N-CA	5.28	127.21	120.56
1	C	266	ALA	N-CA-CB	5.28	117.88	110.12
2	B	304	LYS	CA-C-O	-5.27	113.90	119.97
2	Q	109	ASN	OD1-CG-ND2	5.27	127.87	122.60
6	W	615	ARG	NH1-CZ-NH2	-5.27	112.44	119.30
1	C	358	LEU	CA-C-N	5.27	129.64	120.68
1	C	358	LEU	C-N-CA	5.27	129.64	120.68
2	F	250	VAL	N-CA-C	-5.27	105.40	110.72
3	I	183	MET	CA-C-N	5.27	127.87	120.28
3	I	183	MET	C-N-CA	5.27	127.87	120.28
1	E	322	LYS	CA-C-N	5.27	129.51	120.72
1	E	322	LYS	C-N-CA	5.27	129.51	120.72
3	I	311	LEU	CA-C-N	5.27	127.77	120.29
3	I	311	LEU	C-N-CA	5.27	127.77	120.29
3	I	342	LYS	CB-CG-CD	5.27	123.42	111.30
3	K	193	HIS	CG-CD2-NE2	5.27	112.47	107.20
4	J	409	HIS	CG-CD2-NE2	5.27	112.47	107.20
7	t	12	ARG	NE-CZ-NH2	-5.26	114.46	119.20
1	E	299	GLY	CA-C-N	5.26	127.28	120.44
1	E	299	GLY	C-N-CA	5.26	127.28	120.44
2	F	442	TYR	N-CA-C	-5.26	106.37	114.16
3	I	3	HIS	CB-CG-CD2	-5.26	124.36	131.20
2	Q	88	LYS	N-CA-C	5.26	117.02	111.28
2	T	64	ARG	O-C-N	-5.26	116.54	122.12
6	U	612	ASP	CA-CB-CG	-5.26	107.34	112.60
2	B	378	LYS	N-CA-CB	5.26	118.43	110.28
6	U	635	ILE	N-CA-CB	5.26	116.35	110.51
1	A	497	VAL	N-CA-C	-5.26	105.92	113.07
2	Q	107	GLN	OE1-CD-NE2	-5.26	117.34	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	339	THR	N-CA-C	-5.26	106.55	113.12
3	I	305	ASP	N-CA-CB	5.25	118.39	110.30
1	A	435	GLN	N-CA-C	-5.25	106.92	113.38
2	F	382	ALA	N-CA-CB	5.25	118.39	110.30
1	G	235	GLN	CA-C-O	-5.25	114.33	119.69
4	J	274	LEU	O-C-N	-5.25	115.21	122.46
6	W	613	ASP	CA-C-N	5.25	127.32	120.28
6	W	613	ASP	C-N-CA	5.25	127.32	120.28
6	W	658	GLU	CB-CG-CD	-5.25	103.67	112.60
1	C	250	ASN	CB-CG-ND2	-5.25	108.53	116.40
5	L	366	SER	N-CA-C	-5.25	98.94	108.65
1	C	341	ALA	CA-C-N	5.25	127.57	120.44
1	C	341	ALA	C-N-CA	5.25	127.57	120.44
6	W	671	PHE	CA-CB-CG	5.25	119.05	113.80
1	E	261	ARG	NH1-CZ-NH2	5.25	126.12	119.30
2	F	346	GLN	N-CA-C	-5.24	102.63	110.23
5	L	1374	HIS	CA-C-N	5.24	128.90	120.30
5	L	1374	HIS	C-N-CA	5.24	128.90	120.30
2	Q	10	ASN	CA-C-N	5.24	127.86	120.42
2	Q	10	ASN	C-N-CA	5.24	127.86	120.42
1	A	223	ILE	O-C-N	5.24	127.23	121.83
4	J	562	MET	CG-SD-CE	-5.24	89.38	100.90
7	p	46	ASN	CB-CG-ND2	-5.24	108.54	116.40
3	I	142	GLN	N-CA-CB	5.24	118.40	110.28
7	r	40	LEU	CA-C-N	5.24	127.30	120.28
7	r	40	LEU	C-N-CA	5.24	127.30	120.28
1	A	361	ARG	N-CA-CB	5.24	117.91	110.16
2	O	52	PHE	CA-C-N	5.24	127.30	120.28
2	O	52	PHE	C-N-CA	5.24	127.30	120.28
1	G	409	GLU	N-CA-CB	5.23	118.72	110.56
7	s	55	LYS	CA-C-O	-5.23	114.87	120.42
2	B	453	VAL	N-CA-C	5.23	118.05	109.78
1	C	303	MET	CA-C-N	5.23	129.29	120.29
1	C	303	MET	C-N-CA	5.23	129.29	120.29
5	L	364	VAL	CA-C-N	5.23	131.06	122.64
5	L	364	VAL	C-N-CA	5.23	131.06	122.64
2	F	416	HIS	ND1-CE1-NE2	5.23	113.63	108.40
5	L	502	LEU	N-CA-CB	-5.23	102.16	110.22
2	S	14	GLN	CA-C-N	5.23	127.29	120.28
2	S	14	GLN	C-N-CA	5.23	127.29	120.28
3	I	325	PHE	N-CA-C	-5.23	105.66	111.36
2	T	79	ARG	CA-C-N	5.23	127.23	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	79	ARG	C-N-CA	5.23	127.23	120.44
7	r	56	GLU	O-C-N	-5.23	116.44	122.09
2	B	453	VAL	CA-C-O	-5.23	116.35	121.58
5	L	470	GLN	O-C-N	5.23	128.11	122.15
1	E	310	GLU	CA-C-O	-5.22	112.83	119.31
2	F	463	TYR	O-C-N	-5.22	117.02	123.44
2	H	341	LEU	O-C-N	5.22	128.11	122.15
4	J	466	ARG	CA-C-O	-5.22	113.00	120.16
3	K	309	ALA	CA-C-O	5.22	126.09	120.55
1	A	457	ASN	N-CA-C	-5.22	107.04	113.41
2	R	78	HIS	CA-C-N	5.22	127.28	120.28
2	R	78	HIS	C-N-CA	5.22	127.28	120.28
2	B	405	THR	N-CA-CB	5.22	117.71	110.04
2	Q	62	PHE	CA-C-N	5.22	127.61	120.46
2	Q	62	PHE	C-N-CA	5.22	127.61	120.46
2	R	34	TYR	CA-C-O	5.22	125.95	120.42
1	A	325	PHE	N-CA-C	-5.22	106.42	112.89
3	I	278	PHE	CA-C-N	5.22	127.83	120.42
3	I	278	PHE	C-N-CA	5.22	127.83	120.42
3	I	288	ASN	N-CA-CB	5.22	117.74	110.07
3	K	324	ASP	CA-CB-CG	5.22	117.82	112.60
1	E	313	GLN	N-CA-C	-5.21	105.66	112.23
4	J	260	ILE	CA-C-N	5.21	129.97	123.14
4	J	260	ILE	C-N-CA	5.21	129.97	123.14
3	K	205	VAL	CA-CB-CG2	-5.21	101.54	110.40
5	L	169	GLN	O-C-N	5.21	127.65	122.12
5	L	471	LEU	N-CA-CB	5.21	118.36	110.28
2	H	269	ASN	O-C-N	-5.21	115.66	122.59
6	U	600	ILE	CA-CB-CG1	5.21	119.26	110.40
2	B	291	SER	N-CA-C	-5.21	106.88	113.18
1	E	311	HIS	CG-CD2-NE2	5.21	112.41	107.20
1	C	374	LEU	N-CA-C	5.21	116.77	111.14
2	Q	52	PHE	CA-C-O	-5.21	115.03	120.55
7	r	31	MET	CA-C-O	-5.21	115.01	120.63
1	E	457	ASN	CA-CB-CG	5.21	117.81	112.60
4	J	253	TYR	N-CA-C	-5.21	100.91	109.40
6	V	645	GLU	CA-C-O	5.21	126.07	120.55
7	s	34	LEU	N-CA-CB	5.21	117.77	110.12
2	D	377	LEU	N-CA-C	-5.20	106.78	113.23
6	U	615	ARG	NE-CZ-NH2	-5.20	114.52	119.20
7	s	18	LEU	CA-C-N	5.20	128.22	120.31
7	s	18	LEU	C-N-CA	5.20	128.22	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	30	GLN	N-CA-CB	5.20	117.76	110.12
6	X	640	ILE	O-C-N	5.20	127.19	121.83
2	B	276	VAL	CA-C-O	-5.20	114.97	120.53
1	C	280	SER	N-CA-C	5.20	119.62	113.28
1	C	348	GLU	N-CA-CB	5.20	119.28	110.49
1	G	332	ARG	NE-CZ-NH2	-5.20	114.52	119.20
2	T	10	ASN	OD1-CG-ND2	5.20	127.80	122.60
6	U	597	ALA	CA-C-N	5.20	127.11	120.56
6	U	597	ALA	C-N-CA	5.20	127.11	120.56
6	V	612	ASP	O-C-N	5.20	127.63	122.12
1	A	278	GLU	N-CA-C	-5.20	107.49	113.88
7	o	38	VAL	O-C-N	5.19	127.00	121.91
2	S	93	ILE	CA-CB-CG2	-5.19	101.67	110.50
6	X	664	ASN	CB-CA-C	-5.19	102.17	110.79
2	D	321	GLN	OE1-CD-NE2	-5.19	117.41	122.60
2	F	467	LYS	O-C-N	5.19	128.65	122.26
6	V	664	ASN	CA-C-O	-5.19	115.05	120.55
5	L	585	PRO	CA-C-N	5.19	131.31	121.97
5	L	585	PRO	C-N-CA	5.19	131.31	121.97
1	E	288	ASN	N-CA-C	-5.19	106.21	112.54
2	O	71	GLY	N-CA-C	5.19	118.95	112.73
3	I	272	VAL	CA-C-N	5.19	128.19	120.31
3	I	272	VAL	C-N-CA	5.19	128.19	120.31
4	J	412	PHE	O-C-N	-5.19	115.38	122.33
3	K	152	GLN	N-CA-C	-5.19	106.73	113.16
5	L	95	VAL	CA-CB-CG1	5.18	119.21	110.40
2	Q	34	TYR	N-CA-C	5.18	116.93	111.28
1	C	310	GLU	N-CA-CB	5.18	118.31	110.28
4	J	263	GLU	CG-CD-OE2	-5.18	106.48	118.40
2	Q	36	VAL	N-CA-CB	5.18	117.59	110.54
2	D	288	ASP	CA-C-O	-5.18	113.43	118.97
2	D	321	GLN	CA-C-O	5.18	125.73	119.31
1	G	431	TYR	CB-CG-CD1	-5.18	113.03	120.80
2	H	256	VAL	CA-C-N	5.18	127.65	120.29
2	H	256	VAL	C-N-CA	5.18	127.65	120.29
2	D	536	ALA	CA-C-N	5.18	127.22	120.28
2	D	536	ALA	C-N-CA	5.18	127.22	120.28
2	O	98	LEU	CA-C-O	-5.18	115.06	120.55
2	O	77	LEU	N-CA-CB	5.18	117.73	110.12
1	C	263	LEU	O-C-N	-5.18	115.37	121.32
2	H	424	PRO	CA-C-N	5.18	127.08	120.56
2	H	424	PRO	C-N-CA	5.18	127.08	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	o	58	ARG	NE-CZ-NH2	-5.18	114.54	119.20
6	U	630	ILE	N-CA-C	5.17	115.94	110.72
4	J	227	ARG	NE-CZ-NH2	5.17	123.85	119.20
3	K	264	LEU	CA-C-N	5.17	125.17	119.89
3	K	264	LEU	C-N-CA	5.17	125.17	119.89
2	S	23	LYS	N-CA-CB	5.17	119.23	110.49
1	A	494	ALA	O-C-N	-5.17	115.50	122.43
3	I	335	THR	CA-C-N	5.17	129.62	121.09
3	I	335	THR	C-N-CA	5.17	129.62	121.09
5	L	226	ASN	O-C-N	-5.17	115.99	122.35
2	F	315	ALA	N-CA-CB	5.17	119.22	110.49
2	O	43	PHE	CB-CG-CD1	-5.17	111.92	120.70
2	B	469	MET	N-CA-CB	5.17	119.22	110.49
3	K	8	ALA	N-CA-C	-5.17	105.83	111.82
1	A	411	HIS	CG-CD2-NE2	5.16	112.36	107.20
1	E	454	LYS	N-CA-CB	5.16	117.80	110.16
5	L	539	TRP	N-CA-CB	-5.16	102.85	110.49
1	C	299	GLY	CA-C-O	-5.16	115.19	120.66
3	I	30	ASP	CA-C-O	5.16	126.37	120.54
6	V	619	HIS	CG-CD2-NE2	5.16	112.36	107.20
7	o	39	ARG	CD-NE-CZ	-5.16	117.18	124.40
5	L	110	HIS	ND1-CE1-NE2	5.16	113.56	108.40
2	S	34	TYR	CB-CG-CD2	-5.16	113.06	120.80
5	L	439	LYS	CG-CD-CE	5.16	123.16	111.30
2	S	25	GLU	CB-CG-CD	5.16	121.37	112.60
1	C	430	ARG	CA-C-O	-5.16	115.64	121.72
2	D	308	ASP	CB-CA-C	-5.16	102.09	110.85
1	E	257	GLU	CA-CB-CG	-5.16	103.79	114.10
3	K	294	SER	O-C-N	5.16	128.73	122.85
7	r	18	LEU	CA-C-N	5.16	127.61	120.29
7	r	18	LEU	C-N-CA	5.16	127.61	120.29
4	J	595	VAL	CA-C-N	5.15	127.45	120.44
4	J	595	VAL	C-N-CA	5.15	127.45	120.44
5	L	90	ARG	N-CA-CB	5.15	117.79	110.16
6	W	652	SER	CA-C-N	5.15	127.19	120.28
6	W	652	SER	C-N-CA	5.15	127.19	120.28
1	A	436	GLN	CA-C-N	5.15	130.18	122.86
1	A	436	GLN	C-N-CA	5.15	130.18	122.86
3	I	157	VAL	CA-C-N	5.15	127.61	120.29
3	I	157	VAL	C-N-CA	5.15	127.61	120.29
1	E	250	ASN	N-CA-C	-5.15	101.24	109.07
3	K	23	THR	N-CA-C	-5.15	106.40	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	251	PRO	N-CA-CB	-5.15	98.64	102.25
5	L	407	TYR	CB-CG-CD2	-5.15	113.08	120.80
5	L	421	ASP	N-CA-CB	5.15	117.78	110.16
6	X	646	ARG	NE-CZ-NH1	5.15	126.65	121.50
5	L	104	ILE	O-C-N	5.15	127.35	122.20
2	D	284	LYS	N-CA-C	-5.14	106.41	113.30
4	J	703	TYR	O-C-N	-5.14	115.94	122.27
3	K	339	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
2	T	20	ILE	CA-C-O	-5.14	115.40	120.85
6	V	625	LEU	CA-C-N	5.14	127.12	120.44
6	V	625	LEU	C-N-CA	5.14	127.12	120.44
6	X	652	SER	CA-C-N	5.14	127.12	120.44
6	X	652	SER	C-N-CA	5.14	127.12	120.44
2	D	395	LEU	CA-C-O	5.14	125.85	119.79
2	F	376	ARG	N-CA-CB	5.14	117.62	110.07
3	I	116	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
5	L	407	TYR	CA-C-N	5.14	127.59	120.29
5	L	407	TYR	C-N-CA	5.14	127.59	120.29
2	D	304	LYS	O-C-N	-5.14	116.68	122.12
2	H	416	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
3	I	283	VAL	CA-C-N	5.14	128.12	120.31
3	I	283	VAL	C-N-CA	5.14	128.12	120.31
6	W	637	SER	CA-C-O	-5.14	115.11	120.55
5	L	325	LEU	CA-C-O	-5.13	115.11	120.55
1	E	302	TYR	CA-C-O	-5.13	114.98	120.42
3	I	314	LEU	CA-C-N	5.13	127.16	120.28
3	I	314	LEU	C-N-CA	5.13	127.16	120.28
7	p	24	LEU	CA-C-O	-5.13	114.98	120.42
7	t	8	MET	CG-SD-CE	-5.13	89.61	100.90
2	Q	19	ARG	N-CA-CB	5.13	117.75	110.16
2	D	328	HIS	CA-CB-CG	5.13	118.93	113.80
1	E	324	TRP	CB-CG-CD1	-5.13	119.21	126.90
3	I	114	ASP	CA-C-N	5.13	126.25	119.84
3	I	114	ASP	C-N-CA	5.13	126.25	119.84
3	K	275	LYS	CA-C-O	5.13	125.67	119.31
7	r	36	ILE	CA-C-O	-5.13	115.73	121.17
4	J	224	ARG	NE-CZ-NH1	-5.13	116.37	121.50
2	T	89	ASN	CA-C-N	5.13	127.15	120.28
2	T	89	ASN	C-N-CA	5.13	127.15	120.28
2	D	273	CYS	N-CA-CB	5.12	119.15	110.49
1	E	483	TYR	N-CA-C	-5.12	105.92	113.61
3	I	290	ASN	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	493	HIS	N-CA-CB	5.12	118.43	110.80
3	I	287	GLU	CA-C-N	5.12	129.18	120.88
3	I	287	GLU	C-N-CA	5.12	129.18	120.88
3	K	53	ILE	O-C-N	-5.12	117.21	122.23
5	L	326	TYR	CA-C-N	5.12	127.14	120.28
5	L	326	TYR	C-N-CA	5.12	127.14	120.28
1	G	436	GLN	OE1-CD-NE2	5.12	127.72	122.60
3	K	172	LEU	N-CA-CB	-5.12	102.12	110.42
5	L	333	LEU	O-C-N	-5.12	115.47	122.33
1	A	492	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	C	355	LEU	O-C-N	5.12	127.55	122.12
1	C	432	THR	CA-CB-CG2	-5.12	101.80	110.50
1	G	328	GLN	OE1-CD-NE2	5.12	127.72	122.60
4	J	233	HIS	CA-C-O	-5.12	115.93	121.87
3	K	287	GLU	CA-C-O	5.12	125.83	119.79
5	L	210	LYS	CA-C-N	5.12	127.09	120.44
5	L	210	LYS	C-N-CA	5.12	127.09	120.44
2	B	257	PHE	CA-CB-CG	5.12	118.92	113.80
2	F	395	LEU	N-CA-C	-5.12	105.78	112.23
1	C	291	LEU	N-CA-C	-5.11	106.55	112.89
2	D	306	TYR	CA-C-O	-5.11	115.00	120.42
1	G	359	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
6	W	611	LEU	CA-C-O	-5.11	113.76	119.79
2	D	365	ARG	CA-CB-CG	5.11	124.32	114.10
5	L	566	LYS	CA-C-N	5.11	131.30	121.54
5	L	566	LYS	C-N-CA	5.11	131.30	121.54
1	A	448	LYS	CA-C-N	5.11	127.67	120.42
1	A	448	LYS	C-N-CA	5.11	127.67	120.42
2	F	472	SER	N-CA-C	-5.11	106.29	112.88
1	A	332	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
1	C	408	VAL	N-CA-CB	5.11	116.67	110.95
2	D	342	HIS	CB-CG-CD2	5.11	137.84	131.20
5	L	536	ILE	N-CA-C	-5.11	106.70	111.45
5	L	606	LYS	CA-C-O	-5.11	115.48	121.46
6	W	645	GLU	N-CA-CB	5.11	117.63	110.12
4	J	432	LEU	N-CA-C	-5.11	107.60	113.88
5	L	580	VAL	N-CA-CB	5.11	119.65	111.23
2	F	370	THR	N-CA-C	-5.10	107.10	113.38
2	H	284	LYS	N-CA-CB	5.10	118.69	111.19
2	H	330	GLU	N-CA-C	-5.10	105.80	112.23
5	L	315	THR	CA-C-O	-5.10	115.01	120.42
1	E	232	ILE	CA-C-O	5.10	125.69	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	488	GLU	CA-C-O	5.10	125.90	120.24
7	s	55	LYS	O-C-N	5.10	127.96	122.15
2	D	365	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	E	233	SER	CB-CA-C	-5.10	100.88	109.50
2	F	436	GLY	O-C-N	5.10	129.33	122.70
2	S	104	PRO	CA-C-N	5.10	129.85	121.39
2	S	104	PRO	C-N-CA	5.10	129.85	121.39
1	E	445	VAL	CA-C-N	5.10	127.53	120.29
1	E	445	VAL	C-N-CA	5.10	127.53	120.29
2	F	468	SER	CB-CA-C	-5.10	101.09	109.65
1	G	302	TYR	CA-CB-CG	5.10	123.07	113.90
2	D	254	LEU	CA-C-N	5.09	128.05	120.31
2	D	254	LEU	C-N-CA	5.09	128.05	120.31
1	E	263	LEU	CA-C-O	-5.09	113.18	120.16
2	F	300	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
3	K	121	HIS	ND1-CE1-NE2	5.09	113.50	108.40
5	L	86	SER	CA-C-N	5.09	127.52	120.29
5	L	86	SER	C-N-CA	5.09	127.52	120.29
1	E	312	LEU	CA-C-N	5.09	129.34	120.68
1	E	312	LEU	C-N-CA	5.09	129.34	120.68
6	W	627	VAL	CA-CB-CG1	5.09	119.06	110.40
1	A	301	GLU	CA-C-N	5.09	127.52	120.29
1	A	301	GLU	C-N-CA	5.09	127.52	120.29
2	F	454	LYS	N-CA-CB	5.09	117.45	109.97
7	q	49	ALA	N-CA-C	5.09	116.52	111.07
2	D	529	PHE	N-CA-C	-5.09	105.82	112.23
4	J	598	ARG	NE-CZ-NH2	-5.09	114.62	119.20
6	U	642	MET	N-CA-C	5.09	116.90	111.36
7	t	49	ALA	CA-C-O	-5.09	115.16	120.55
4	J	215	HIS	CG-CD2-NE2	5.08	112.28	107.20
7	t	41	CYS	CA-C-O	-5.08	114.12	119.97
2	D	295	GLU	N-CA-C	-5.08	106.59	112.89
2	H	250	VAL	O-C-N	-5.08	116.06	121.80
5	L	426	ASN	CA-CB-CG	-5.08	107.52	112.60
7	t	21	ILE	CA-C-N	5.08	127.09	120.28
7	t	21	ILE	C-N-CA	5.08	127.09	120.28
3	I	193	HIS	ND1-CE1-NE2	5.08	113.48	108.40
4	J	687	TYR	CA-C-N	5.08	124.69	119.56
4	J	687	TYR	C-N-CA	5.08	124.69	119.56
7	t	45	ILE	O-C-N	-5.08	117.32	122.75
1	E	438	ILE	CA-CB-CG1	5.08	119.03	110.40
2	F	400	HIS	CB-CG-CD2	-5.08	124.60	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	666	ARG	NH1-CZ-NH2	5.08	125.90	119.30
7	s	31	MET	CA-C-N	5.08	127.08	120.28
7	s	31	MET	C-N-CA	5.08	127.08	120.28
7	s	61	SER	CA-C-O	-5.08	115.49	120.82
1	G	438	ILE	CA-C-N	5.07	125.79	120.11
1	G	438	ILE	C-N-CA	5.07	125.79	120.11
2	H	365	ARG	N-CA-CB	5.07	117.67	110.16
7	p	26	ASN	O-C-N	-5.07	116.26	122.55
1	E	256	LYS	CA-C-O	-5.07	115.17	120.55
1	G	209	LEU	CA-C-O	-5.07	112.18	120.80
5	L	44	TYR	CA-C-N	5.07	127.03	120.44
5	L	44	TYR	C-N-CA	5.07	127.03	120.44
2	Q	99	SER	CB-CA-C	-5.07	102.37	110.79
1	E	388	ASP	CA-C-N	5.07	128.61	120.30
1	E	388	ASP	C-N-CA	5.07	128.61	120.30
4	J	468	TYR	CG-CD1-CE1	-5.07	113.60	121.20
1	A	216	LEU	O-C-N	-5.07	115.47	122.46
2	D	340	VAL	CA-CB-CG2	5.07	119.01	110.40
3	K	119	ILE	CA-CB-CG1	5.07	119.01	110.40
5	L	86	SER	O-C-N	5.07	127.92	122.15
2	T	54	VAL	N-CA-CB	5.07	117.43	110.54
6	U	653	LEU	CA-C-O	-5.07	115.50	120.82
5	L	167	ALA	CA-C-N	5.06	127.48	120.29
5	L	167	ALA	C-N-CA	5.06	127.48	120.29
1	C	211	SER	N-CA-C	5.06	116.88	111.36
2	O	17	CYS	CA-C-N	5.06	127.33	120.44
2	O	17	CYS	C-N-CA	5.06	127.33	120.44
2	F	312	LEU	CA-C-O	-5.06	115.54	121.46
5	L	104	ILE	N-CA-C	-5.06	107.00	113.22
5	L	222	HIS	ND1-CE1-NE2	5.06	113.46	108.40
5	L	241	ALA	N-CA-C	-5.06	106.52	113.30
6	W	619	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
5	L	251	PRO	CA-C-O	-5.06	115.80	121.97
2	B	530	GLN	OE1-CD-NE2	5.06	127.66	122.60
2	H	342	HIS	N-CA-CB	5.06	118.12	110.28
3	I	114	ASP	CB-CA-C	-5.05	100.68	109.32
5	L	1364	LYS	O-C-N	5.05	127.28	122.07
6	U	608	GLU	CA-C-N	5.05	127.05	120.28
6	U	608	GLU	C-N-CA	5.05	127.05	120.28
1	E	446	ALA	N-CA-C	-5.05	105.85	111.36
2	T	78	HIS	CA-CB-CG	5.05	118.85	113.80
1	C	217	VAL	CA-C-N	5.05	127.46	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	VAL	C-N-CA	5.05	127.46	120.29
3	K	2	ILE	N-CA-CB	5.05	117.41	110.54
2	Q	112	SER	CA-C-N	5.05	131.19	121.54
2	Q	112	SER	C-N-CA	5.05	131.19	121.54
5	L	586	VAL	N-CA-CB	5.05	119.56	111.23
3	K	184	TYR	N-CA-CB	5.05	118.10	110.28
7	o	52	SER	N-CA-CB	5.05	117.63	110.16
2	B	291	SER	CA-C-N	5.04	127.45	120.29
2	B	291	SER	C-N-CA	5.04	127.45	120.29
4	J	328	ASP	N-CA-C	-5.04	99.06	107.99
2	B	521	LEU	N-CA-C	-5.04	106.97	112.72
2	R	26	ALA	CA-C-O	-5.04	113.18	119.18
1	E	262	ILE	N-CA-C	-5.04	105.98	113.39
1	E	299	GLY	O-C-N	-5.04	116.79	122.28
2	F	331	LEU	N-CA-CB	5.04	118.09	110.28
5	L	253	SER	N-CA-C	5.04	117.32	111.02
2	T	75	SER	CA-C-N	5.04	127.44	120.29
2	T	75	SER	C-N-CA	5.04	127.44	120.29
2	F	474	MET	CA-C-N	5.04	127.30	120.65
2	F	474	MET	C-N-CA	5.04	127.30	120.65
2	H	524	ASP	CA-C-N	5.04	130.13	122.37
2	H	524	ASP	C-N-CA	5.04	130.13	122.37
2	F	400	HIS	ND1-CE1-NE2	5.04	113.44	108.40
1	A	357	LEU	N-CA-C	5.03	116.85	111.36
2	D	302	LYS	N-CA-C	-5.03	105.87	111.36
1	E	240	ARG	CA-C-N	5.03	129.95	121.14
1	E	240	ARG	C-N-CA	5.03	129.95	121.14
6	V	632	GLN	CB-CG-CD	-5.03	104.05	112.60
6	X	656	GLU	CB-CA-C	-5.03	101.01	110.67
7	p	14	THR	CA-C-O	-5.03	115.22	120.55
2	B	411	ARG	N-CA-CB	5.03	118.08	110.28
1	E	282	PHE	O-C-N	-5.03	116.79	123.13
2	H	251	ARG	CD-NE-CZ	5.03	131.44	124.40
5	L	224	ARG	CA-C-N	5.03	130.59	122.29
5	L	224	ARG	C-N-CA	5.03	130.59	122.29
6	U	614	PHE	CB-CA-C	5.03	118.78	110.88
1	C	396	ARG	CA-C-N	5.03	129.57	122.63
1	C	396	ARG	C-N-CA	5.03	129.57	122.63
3	I	119	ILE	CA-CB-CG1	5.03	118.95	110.40
3	K	35	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
1	C	402	PRO	N-CA-CB	5.03	108.53	103.25
2	T	53	LEU	CA-C-N	5.03	127.34	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	53	LEU	C-N-CA	5.03	127.34	120.46
6	X	640	ILE	N-CA-CB	5.03	118.12	110.58
4	J	303	GLN	CA-C-N	5.02	127.42	120.29
4	J	303	GLN	C-N-CA	5.02	127.42	120.29
6	U	611	LEU	CA-C-N	5.02	127.01	120.28
6	U	611	LEU	C-N-CA	5.02	127.01	120.28
1	C	370	GLN	OE1-CD-NE2	5.02	127.62	122.60
2	Q	30	GLN	CA-C-N	5.02	127.42	120.29
2	Q	30	GLN	C-N-CA	5.02	127.42	120.29
6	V	634	HIS	CA-C-N	5.02	126.89	120.56
6	V	634	HIS	C-N-CA	5.02	126.89	120.56
2	H	258	GLN	CA-CB-CG	5.02	124.14	114.10
3	K	265	PRO	N-CA-CB	5.02	107.54	103.32
5	L	50	HIS	CA-CB-CG	-5.02	108.78	113.80
2	O	67	ARG	CA-C-O	-5.02	116.16	121.78
1	E	345	ASN	N-CA-CB	5.02	117.59	110.16
1	G	346	LYS	CA-C-N	5.02	128.38	121.26
1	G	346	LYS	C-N-CA	5.02	128.38	121.26
1	A	350	PHE	CA-C-N	5.02	126.59	120.22
1	A	350	PHE	C-N-CA	5.02	126.59	120.22
2	H	419	GLY	N-CA-C	5.02	120.19	114.67
4	J	226	PRO	CA-C-O	-5.02	115.24	122.31
2	F	285	SER	CA-C-O	-5.01	113.34	120.51
5	L	334	GLN	CA-C-N	5.01	127.33	120.46
5	L	334	GLN	C-N-CA	5.01	127.33	120.46
7	p	32	GLU	CA-C-O	-5.01	115.54	120.70
1	G	484	VAL	CA-C-N	5.01	127.93	120.31
1	G	484	VAL	C-N-CA	5.01	127.93	120.31
3	K	93	LEU	CA-C-N	5.01	131.35	121.58
3	K	93	LEU	C-N-CA	5.01	131.35	121.58
3	I	86	LEU	CA-C-O	5.01	125.80	120.24
2	S	64	ARG	CA-C-O	-5.01	115.24	120.55
7	s	13	GLU	CA-C-O	-5.01	114.21	119.97
7	t	51	SER	O-C-N	5.01	127.43	122.12
1	E	483	TYR	O-C-N	5.01	128.11	122.20
2	O	35	ALA	N-CA-C	5.01	116.43	111.07
7	q	31	MET	O-C-N	5.01	127.50	122.09
5	L	173	ILE	N-CA-C	-5.01	105.51	110.62
2	H	316	PHE	N-CA-CB	5.00	117.35	109.69
1	E	249	GLN	OE1-CD-NE2	-5.00	117.60	122.60
3	I	174	LYS	CA-C-O	-5.00	114.22	119.97
1	G	340	ILE	CB-CA-C	-5.00	105.32	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	47	VAL	O-C-N	-5.00	117.78	123.03

There are no chirality outliers.

All (146) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	TYR	Sidechain
1	A	284	TYR	Sidechain
1	A	326	TYR	Sidechain
1	A	365	TYR	Sidechain
1	A	395	TYR	Sidechain
1	A	430	ARG	Sidechain
2	B	274	TYR	Sidechain
2	B	306	TYR	Sidechain
2	B	409	TYR	Sidechain
2	B	423	TYR	Sidechain
2	B	460	HIS	Sidechain
1	C	222	TYR	Sidechain
1	C	269	TYR	Sidechain
1	C	365	TYR	Sidechain
1	C	368	ASP	Sidechain
1	C	377	TYR	Sidechain
1	C	491	TYR	Sidechain
2	D	266	LYS	Peptide
2	D	306	TYR	Sidechain
2	D	313	ASP	Peptide
2	D	376	ARG	Sidechain
2	D	423	TYR	Sidechain
2	D	466	ARG	Sidechain
1	E	222	TYR	Sidechain
1	E	282	PHE	Peptide
1	E	363	PHE	Sidechain
1	E	365	TYR	Sidechain
1	E	395	TYR	Sidechain
1	E	431	TYR	Sidechain
1	E	433	ILE	Mainchain
1	E	483	TYR	Sidechain
2	F	257	PHE	Sidechain
2	F	306	TYR	Sidechain
2	F	335	TYR	Sidechain
2	F	402	TYR	Sidechain
2	F	423	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	F	430	TYR	Sidechain
2	F	446	PHE	Sidechain
2	F	463	TYR	Sidechain
2	F	473	PHE	Sidechain
2	F	529	PHE	Sidechain
1	G	240	ARG	Sidechain
1	G	243	ARG	Sidechain
1	G	269	TYR	Sidechain
1	G	284	TYR	Sidechain
1	G	326	TYR	Sidechain
1	G	348	GLU	Peptide
1	G	377	TYR	Sidechain
1	G	386	TYR	Sidechain
1	G	486	ARG	Sidechain
1	G	493	TYR	Sidechain
2	H	264	PHE	Sidechain
2	H	310	ARG	Sidechain
2	H	323	PHE	Sidechain
2	H	334	TYR	Sidechain
2	H	335	TYR	Sidechain
2	H	390	ARG	Sidechain
2	H	402	TYR	Sidechain
2	H	409	TYR	Sidechain
2	H	423	TYR	Sidechain
2	H	442	TYR	Sidechain
2	H	543	TYR	Sidechain
3	I	124	TYR	Sidechain
3	I	129	PHE	Sidechain
3	I	169	ARG	Sidechain
3	I	17	PHE	Sidechain
3	I	184	TYR	Sidechain
3	I	203	PHE	Sidechain
3	I	22	ARG	Sidechain
3	I	278	PHE	Sidechain
3	I	312	HIS	Sidechain
4	J	209	ARG	Sidechain
4	J	224	ARG	Sidechain
4	J	226	PRO	Peptide
4	J	261	VAL	Peptide
4	J	276	GLY	Peptide
4	J	291	ASN	Peptide
4	J	307	ARG	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
4	J	354	PHE	Sidechain
4	J	424	ARG	Peptide,Sidechain
4	J	466	ARG	Sidechain
4	J	482	PHE	Sidechain
4	J	508	TYR	Sidechain
4	J	677	SER	Peptide
4	J	687	TYR	Sidechain
3	K	129	PHE	Sidechain
3	K	257	PHE	Sidechain
3	K	267	TYR	Sidechain
3	K	295	ARG	Sidechain
3	K	33	PHE	Sidechain
3	K	54	ARG	Sidechain
5	L	110	HIS	Sidechain
5	L	224	ARG	Sidechain
5	L	313	TYR	Sidechain
5	L	326	TYR	Sidechain
5	L	347	LEU	Peptide
5	L	385	TYR	Mainchain,Peptide
5	L	413	HIS	Sidechain
5	L	443	TYR	Sidechain
5	L	444	TYR	Sidechain
5	L	504	TYR	Sidechain
5	L	506	TYR	Sidechain
5	L	541	TYR	Sidechain
5	L	552	PHE	Sidechain
5	L	573	TYR	Sidechain
5	L	580	VAL	Mainchain
5	L	585	PRO	Peptide
5	L	596	TYR	Sidechain
5	L	77	PHE	Sidechain
5	L	97	TYR	Sidechain
2	O	19	ARG	Sidechain
2	O	43	PHE	Sidechain
2	Q	19	ARG	Sidechain
2	Q	34	TYR	Sidechain
2	R	19	ARG	Sidechain
2	R	34	TYR	Sidechain
2	R	74	PHE	Sidechain
2	S	34	TYR	Sidechain
2	S	64	ARG	Sidechain
2	S	66	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	T	52	PHE	Sidechain
2	T	62	PHE	Sidechain
6	U	620	ARG	Sidechain
6	U	647	TYR	Sidechain
6	U	666	ARG	Sidechain
6	U	668	ARG	Sidechain
6	V	647	TYR	Sidechain
6	V	666	ARG	Sidechain
6	W	619	HIS	Sidechain
6	W	647	TYR	Sidechain
6	W	661	ARG	Sidechain
6	W	666	ARG	Sidechain
6	X	602	PHE	Sidechain
6	X	615	ARG	Sidechain
6	X	620	ARG	Sidechain
6	X	634	HIS	Sidechain
7	o	12	ARG	Sidechain
7	o	23	ARG	Sidechain
7	q	12	ARG	Sidechain
7	q	58	ARG	Sidechain
7	r	12	ARG	Sidechain
7	s	59	ARG	Sidechain
7	t	59	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2211	0	2199	6	0
1	C	2014	0	1998	5	0
1	E	2038	0	2031	5	0
1	G	2014	0	1998	6	0
2	B	2363	0	2379	6	0
2	D	2059	0	2080	8	0
2	F	1964	0	1988	8	0
2	H	2135	0	2160	3	0
2	O	753	0	779	1	0
2	Q	878	0	903	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	794	0	814	2	0
2	S	878	0	903	4	0
2	T	753	0	779	4	0
3	I	2325	0	2335	34	0
3	K	2325	0	2335	9	0
4	J	2909	0	2916	42	0
5	L	3794	0	3844	6	0
6	U	634	0	635	3	0
6	V	634	0	635	1	0
6	W	634	0	635	4	0
6	X	634	0	635	0	0
7	o	403	0	426	0	0
7	p	429	0	446	1	0
7	q	432	0	457	0	0
7	r	454	0	477	1	0
7	s	451	0	476	0	0
7	t	446	0	471	4	0
All	All	37358	0	37734	126	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 (126) 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)
4:J:242:TRP:CZ3	4:J:242:TRP:CE3	1.83	1.66
4:J:242:TRP:CZ2	4:J:242:TRP:CH2	1.87	1.61
4:J:242:TRP:CZ3	4:J:242:TRP:CH2	1.82	1.59
4:J:242:TRP:CZ2	4:J:242:TRP:CE2	1.92	1.57
4:J:242:TRP:CE3	4:J:242:TRP:CD2	1.93	1.56
4:J:242:TRP:CE2	4:J:242:TRP:CD2	1.79	1.53
3:I:16:ILE:CG1	4:J:242:TRP:CZ2	2.27	1.17
3:I:16:ILE:CG1	4:J:242:TRP:CE2	2.29	1.15
3:I:16:ILE:CG1	4:J:242:TRP:CD2	2.31	1.14
3:I:16:ILE:CD1	4:J:242:TRP:CE2	2.30	1.12
3:I:16:ILE:HG12	4:J:242:TRP:CE2	1.84	1.12
3:I:16:ILE:CG1	4:J:242:TRP:CH2	2.33	1.11
3:I:16:ILE:CD1	4:J:242:TRP:CD2	2.33	1.10
3:I:16:ILE:CG1	4:J:242:TRP:CE3	2.33	1.10
3:I:16:ILE:CD1	4:J:242:TRP:CZ2	2.35	1.10
3:I:16:ILE:CG1	4:J:242:TRP:CZ3	2.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:16:ILE:CD1	4:J:242:TRP:CE3	2.38	1.07
3:I:16:ILE:HG13	4:J:242:TRP:CE3	1.89	1.06
3:I:16:ILE:CD1	4:J:242:TRP:CH2	2.40	1.05
3:I:16:ILE:CD1	4:J:242:TRP:CZ3	2.40	1.04
3:I:16:ILE:HD11	4:J:242:TRP:CD2	2.00	0.95
3:I:16:ILE:HD13	4:J:242:TRP:CZ2	2.03	0.93
3:I:16:ILE:HD12	4:J:242:TRP:CZ3	2.05	0.92
3:I:16:ILE:HG13	4:J:242:TRP:CD2	2.11	0.84
3:I:16:ILE:CB	4:J:242:TRP:CH2	2.64	0.80
3:I:16:ILE:HG12	4:J:242:TRP:CZ2	2.20	0.76
3:I:16:ILE:HD11	4:J:242:TRP:CE2	2.24	0.72
3:I:16:ILE:HD12	4:J:242:TRP:CE3	2.29	0.68
1:C:320:LEU:HD22	1:C:320:LEU:H	1.63	0.63
3:I:16:ILE:HG12	4:J:242:TRP:CD2	2.33	0.62
2:D:364:ARG:HA	2:D:364:ARG:HE	1.65	0.62
2:R:58:ILE:HG12	2:R:98:LEU:HD13	1.84	0.60
1:G:284:TYR:HB3	1:G:286:GLN:H	1.65	0.60
3:I:16:ILE:HD13	4:J:242:TRP:CH2	2.36	0.59
3:K:193:HIS:CE1	3:K:294:SER:HB3	2.39	0.57
1:E:269:TYR:CE1	1:E:273:THR:HG21	2.39	0.57
3:I:16:ILE:CG2	4:J:242:TRP:CZ3	2.88	0.56
3:K:119:ILE:H	3:K:119:ILE:HD13	1.70	0.56
2:S:96:LEU:C	2:S:96:LEU:HD13	2.30	0.56
3:I:16:ILE:CG1	3:I:16:ILE:CD1	2.83	0.56
3:I:300:LEU:HD11	3:I:339:HIS:CE1	2.43	0.54
1:E:303:MET:HA	1:E:306:ILE:HD12	1.90	0.54
2:H:296:LEU:HD13	2:H:374:LYS:HD3	1.90	0.53
5:L:427:GLY:HA2	5:L:551:GLU:H	1.73	0.52
3:K:295:ARG:HH12	3:K:340:LEU:HB3	1.74	0.52
2:D:323:PHE:CG	2:D:395:LEU:HD22	2.46	0.51
7:t:40:LEU:HD13	7:t:50:LEU:HD13	1.93	0.51
3:I:16:ILE:CB	4:J:242:TRP:CZ3	2.94	0.50
4:J:492:ARG:HE	4:J:492:ARG:HA	1.76	0.50
6:U:598:ILE:HD12	6:U:598:ILE:H	1.77	0.50
2:B:340:VAL:HG11	5:L:216:LEU:HD13	1.94	0.49
2:F:253:LEU:HD22	2:F:290:THR:HG22	1.94	0.49
2:F:321:GLN:HA	2:F:324:CYS:SG	2.53	0.49
3:I:16:ILE:HA	4:J:242:TRP:CH2	2.48	0.49
2:S:90:ARG:HD2	2:S:91:TRP:H	1.78	0.49
2:B:465:LEU:HD23	2:B:465:LEU:H	1.78	0.48
1:E:311:HIS:CE1	2:F:365:ARG:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:419:VAL:HB	4:J:420:PRO:HD3	1.95	0.48
5:L:377:SER:HA	5:L:406:THR:HG23	1.95	0.48
1:E:396:ARG:HA	1:E:396:ARG:HE	1.79	0.48
1:G:295:MET:SD	1:G:337:LEU:HD22	2.55	0.47
2:T:37:ARG:HH12	6:W:635:ILE:HG21	1.79	0.47
2:D:293:LEU:C	2:D:293:LEU:HD23	2.38	0.47
2:D:475:THR:HG22	2:D:476:MET:H	1.79	0.47
3:I:138:VAL:HG12	3:I:160:HIS:CE1	2.50	0.47
2:F:276:VAL:HG12	2:F:278:GLY:H	1.80	0.46
3:K:86:LEU:HD21	3:K:149:HIS:HA	1.97	0.46
1:A:333:THR:HG23	1:A:374:LEU:HD22	1.96	0.46
2:F:334:TYR:CZ	2:F:338:LEU:HD11	2.51	0.46
1:G:255:VAL:O	1:G:259:VAL:HG23	2.16	0.46
2:R:12:LEU:HB3	7:r:36:ILE:HG23	1.98	0.45
2:H:447:VAL:HG13	2:H:463:TYR:HB3	1.97	0.45
5:L:586:VAL:HG13	5:L:588:LEU:HD21	1.99	0.45
2:D:372:ASP:HB3	2:D:373:PRO:HD3	1.98	0.45
4:J:209:ARG:CD	2:S:19:ARG:HH11	2.30	0.45
3:I:295:ARG:HA	3:I:339:HIS:CD2	2.53	0.44
4:J:302:THR:HG22	4:J:304:ASN:H	1.82	0.44
6:W:623:VAL:HA	6:W:626:GLN:HE21	1.81	0.44
3:I:139:VAL:HG22	3:I:160:HIS:CD2	2.52	0.44
3:K:38:GLU:O	3:K:42:LEU:HG	2.18	0.44
7:t:40:LEU:HD13	7:t:50:LEU:CD1	2.47	0.44
2:T:48:GLU:HA	2:T:91:TRP:CZ2	2.52	0.44
6:U:643:LEU:HD13	6:W:641:GLN:HE21	1.82	0.44
2:B:490:ASN:HA	2:B:493:HIS:CD2	2.53	0.44
1:C:212:GLN:H	1:C:212:GLN:HG2	1.58	0.44
2:D:428:PHE:HA	2:D:431:ARG:HE	1.83	0.44
2:T:43:PHE:HA	6:W:624:ASN:HD21	1.83	0.44
1:A:283:GLU:HB2	1:A:289:HIS:HB2	2.00	0.44
2:B:465:LEU:H	2:B:465:LEU:CD2	2.30	0.44
1:C:430:ARG:HA	1:C:430:ARG:HE	1.83	0.43
2:F:314:ARG:HH22	1:G:368:ASP:HB2	1.82	0.43
1:A:392:ARG:HE	1:A:398:ILE:HD11	1.82	0.43
2:H:363:LEU:HD12	2:H:363:LEU:H	1.83	0.43
2:D:418:LEU:HD22	2:D:524:ASP:N	2.34	0.43
3:K:180:HIS:CE1	3:K:320:PHE:CG	3.07	0.43
2:O:55:THR:HA	2:O:58:ILE:HD12	2.01	0.43
2:Q:108:PRO:HA	2:S:49:ARG:HE	1.83	0.43
1:E:261:ARG:H	1:E:261:ARG:HG2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:475:TRP:CE2	4:J:492:ARG:HD3	2.54	0.42
1:A:291:LEU:HD13	1:A:382:ALA:HB2	2.02	0.42
4:J:390:THR:H	4:J:393:ILE:HG22	1.83	0.42
7:p:37:CYS:SG	7:p:54:ILE:HD11	2.59	0.42
7:t:46:ASN:HD22	7:t:47:PRO:HD2	1.85	0.42
6:V:643:LEU:O	6:V:647:TYR:CD2	2.73	0.42
1:G:344:LEU:HD21	1:G:357:LEU:HD22	2.02	0.41
3:K:17:PHE:HB3	3:K:25:LEU:HD21	2.01	0.41
5:L:71:LYS:HE2	5:L:117:VAL:HG11	2.02	0.41
4:J:437:TYR:CG	4:J:548:LEU:HD11	2.55	0.41
3:I:110:GLU:HG2	3:I:121:HIS:CE1	2.56	0.41
2:T:19:ARG:HE	7:t:32:GLU:HB3	1.84	0.41
2:B:299:LEU:HA	2:B:302:LYS:HG2	2.02	0.41
1:C:227:VAL:HG13	1:C:228:ASP:O	2.20	0.41
6:U:599:GLN:H	6:U:599:GLN:CD	2.29	0.41
2:B:293:LEU:O	2:B:293:LEU:HD13	2.21	0.41
2:F:334:TYR:CE2	2:F:338:LEU:HD11	2.56	0.41
5:L:452:PRO:HA	5:L:453:ALA:HA	1.85	0.41
2:D:296:LEU:HA	2:D:299:LEU:HD23	2.03	0.41
4:J:365:TYR:CD1	3:K:131:LEU:HD23	2.55	0.41
1:C:337:LEU:HD13	1:C:378:LEU:HD11	2.04	0.40
2:F:410:MET:O	2:F:414:VAL:HG22	2.21	0.40
4:J:297:ILE:HG22	4:J:303:GLN:HB2	2.03	0.40
1:A:240:ARG:O	1:A:241:GLN:HG2	2.21	0.40
1:A:237:LEU:HD12	1:A:244:SER:H	1.86	0.40
1:G:321:GLN:HA	1:G:324:TRP:HB3	2.02	0.40
3:I:184:TYR:HB3	3:I:315:LYS:HE2	2.03	0.40
3:K:329:LEU:HA	3:K:332:ILE:HG22	2.04	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	271/896 (30%)	250 (92%)	14 (5%)	7 (3%)	4	25
1	C	244/896 (27%)	217 (89%)	21 (9%)	6 (2%)	4	26
1	E	247/896 (28%)	229 (93%)	12 (5%)	6 (2%)	4	27
1	G	244/896 (27%)	232 (95%)	11 (4%)	1 (0%)	30	66
2	B	290/906 (32%)	261 (90%)	20 (7%)	9 (3%)	3	22
2	D	248/906 (27%)	224 (90%)	17 (7%)	7 (3%)	4	24
2	F	236/906 (26%)	214 (91%)	13 (6%)	9 (4%)	2	19
2	H	257/906 (28%)	227 (88%)	20 (8%)	10 (4%)	2	19
2	O	91/906 (10%)	85 (93%)	5 (6%)	1 (1%)	11	45
2	Q	107/906 (12%)	97 (91%)	6 (6%)	4 (4%)	2	20
2	R	96/906 (11%)	90 (94%)	4 (4%)	2 (2%)	5	30
2	S	107/906 (12%)	96 (90%)	8 (8%)	3 (3%)	4	24
2	T	91/906 (10%)	85 (93%)	4 (4%)	2 (2%)	5	29
3	I	281/666 (42%)	255 (91%)	20 (7%)	6 (2%)	5	30
3	K	281/666 (42%)	259 (92%)	13 (5%)	9 (3%)	3	21
4	J	342/1019 (34%)	317 (93%)	15 (4%)	10 (3%)	3	23
5	L	462/1698 (27%)	422 (91%)	26 (6%)	14 (3%)	3	22
6	U	73/671 (11%)	73 (100%)	0	0	100	100
6	V	73/671 (11%)	72 (99%)	0	1 (1%)	9	39
6	W	73/671 (11%)	71 (97%)	1 (1%)	1 (1%)	9	39
6	X	73/671 (11%)	72 (99%)	1 (1%)	0	100	100
7	o	50/72 (69%)	50 (100%)	0	0	100	100
7	p	54/72 (75%)	54 (100%)	0	0	100	100
7	q	54/72 (75%)	53 (98%)	1 (2%)	0	100	100
7	r	57/72 (79%)	54 (95%)	1 (2%)	2 (4%)	3	20
7	s	57/72 (79%)	54 (95%)	3 (5%)	0	100	100
7	t	56/72 (78%)	55 (98%)	1 (2%)	0	100	100
All	All	4515/18903 (24%)	4168 (92%)	237 (5%)	110 (2%)	7	27

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASP

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Mol	Chain	Res	Type
1	A	428	ASP
2	B	312	LEU
2	D	314	ARG
2	F	281	ALA
2	F	285	SER
2	F	314	ARG
2	F	476	MET
2	F	527	ASN
2	H	314	ARG
2	H	468	SER
3	I	82	HIS
3	I	254	LEU
3	I	298	SER
4	J	224	ARG
4	J	229	SER
4	J	417	ALA
4	J	449	ALA
3	K	128	GLN
3	K	203	PHE
5	L	571	HIS
5	L	580	VAL
2	Q	26	ALA
2	S	26	ALA
6	V	649	LEU
1	A	241	GLN
1	C	482	ALA
2	D	311	SER
2	D	315	ALA
2	D	406	GLY
2	D	459	TRP
1	E	231	TYR
1	E	432	THR
2	F	272	ASN
2	F	315	ALA
2	H	281	ALA
4	J	262	THR
4	J	388	THR
4	J	490	ILE
3	K	264	LEU
3	K	297	GLY
5	L	107	SER
5	L	547	ASP

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Mol	Chain	Res	Type
5	L	566	LYS
5	L	586	VAL
2	O	89	ASN
2	Q	105	ARG
2	S	23	LYS
2	S	47	VAL
2	T	88	LYS
1	A	439	PRO
2	B	263	LYS
2	B	462	LYS
1	C	402	PRO
2	D	407	ASP
1	E	317	LEU
2	F	316	PHE
1	G	428	ASP
2	H	269	ASN
2	H	285	SER
2	H	443	HIS
3	I	165	LEU
3	I	335	THR
4	J	448	GLU
4	J	499	ASN
3	K	193	HIS
5	L	375	LEU
5	L	564	ARG
2	R	7	LYS
2	B	407	ASP
1	C	283	GLU
2	D	261	ASP
2	F	407	ASP
2	H	270	SER
2	H	360	SER
2	H	407	ASP
4	J	423	THR
3	K	290	ASN
5	L	105	GLN
5	L	422	SER
5	L	607	LEU
2	Q	87	LEU
2	Q	113	SER
2	T	89	ASN
6	W	649	LEU

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Mol	Chain	Res	Type
7	r	26	ASN
7	r	45	ILE
1	A	249	GLN
1	A	470	ASP
2	B	443	HIS
2	B	469	MET
2	B	527	ASN
1	C	404	SER
1	C	442	LEU
1	E	429	GLN
3	K	165	LEU
3	K	195	LEU
5	L	222	HIS
5	L	340	THR
2	B	439	GLU
1	C	317	LEU
2	R	50	ASP
2	H	450	ASP
2	B	319	VAL
1	E	439	PRO
3	K	115	PRO
3	I	265	PRO
1	E	227	VAL
5	L	362	ILE
1	A	367	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	244/824 (30%)	230 (94%)	14 (6%)	18	41
1	C	221/824 (27%)	210 (95%)	11 (5%)	22	44
1	E	224/824 (27%)	214 (96%)	10 (4%)	24	47
1	G	221/824 (27%)	211 (96%)	10 (4%)	24	47
2	B	260/798 (33%)	249 (96%)	11 (4%)	26	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	227/798 (28%)	219 (96%)	8 (4%)	32	54
2	F	217/798 (27%)	202 (93%)	15 (7%)	14	37
2	H	236/798 (30%)	222 (94%)	14 (6%)	18	41
2	O	82/798 (10%)	80 (98%)	2 (2%)	43	63
2	Q	96/798 (12%)	94 (98%)	2 (2%)	47	65
2	R	87/798 (11%)	86 (99%)	1 (1%)	65	74
2	S	96/798 (12%)	87 (91%)	9 (9%)	8	27
2	T	82/798 (10%)	80 (98%)	2 (2%)	43	63
3	I	259/595 (44%)	245 (95%)	14 (5%)	20	43
3	K	259/595 (44%)	247 (95%)	12 (5%)	24	46
4	J	326/933 (35%)	308 (94%)	18 (6%)	19	43
5	L	431/1539 (28%)	414 (96%)	17 (4%)	28	50
6	U	72/598 (12%)	69 (96%)	3 (4%)	26	48
6	V	72/598 (12%)	70 (97%)	2 (3%)	38	59
6	W	72/598 (12%)	67 (93%)	5 (7%)	14	37
6	X	72/598 (12%)	70 (97%)	2 (3%)	38	59
7	o	48/62 (77%)	45 (94%)	3 (6%)	16	38
7	p	51/62 (82%)	51 (100%)	0	100	100
7	q	51/62 (82%)	51 (100%)	0	100	100
7	r	54/62 (87%)	52 (96%)	2 (4%)	30	51
7	s	53/62 (86%)	49 (92%)	4 (8%)	12	33
7	t	53/62 (86%)	53 (100%)	0	100	100
All	All	4166/16904 (25%)	3975 (95%)	191 (5%)	25	46

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	268	ASN
1	A	271	THR
1	A	288	ASN
1	A	309	LEU
1	A	333	THR
1	A	362	THR

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Mol	Chain	Res	Type
1	A	366	THR
1	A	394	ILE
1	A	398	ILE
1	A	430	ARG
1	A	438	ILE
1	A	467	THR
1	A	492	ASN
2	B	265	VAL
2	B	288	ASP
2	B	337	LEU
2	B	430	TYR
2	B	441	THR
2	B	460	HIS
2	B	465	LEU
2	B	474	MET
2	B	477	ASP
2	B	514	SER
2	B	532	LYS
1	C	267	THR
1	C	279	ASN
1	C	295	MET
1	C	320	LEU
1	C	321	GLN
1	C	328	GLN
1	C	357	LEU
1	C	433	ILE
1	C	438	ILE
1	C	450	LEU
1	C	481	GLN
2	D	293	LEU
2	D	299	LEU
2	D	301	ASN
2	D	363	LEU
2	D	364	ARG
2	D	375	ILE
2	D	404	LYS
2	D	475	THR
1	E	237	LEU
1	E	240	ARG
1	E	249	GLN
1	E	264	PRO
1	E	277	GLU

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Mol	Chain	Res	Type
1	E	358	LEU
1	E	427	TRP
1	E	443	GLN
1	E	444	LYS
1	E	493	TYR
2	F	254	LEU
2	F	279	LYS
2	F	286	LEU
2	F	287	LYS
2	F	299	LEU
2	F	370	THR
2	F	426	LEU
2	F	453	VAL
2	F	454	LYS
2	F	455	THR
2	F	465	LEU
2	F	467	LYS
2	F	470	ILE
2	F	473	PHE
2	F	478	GLN
1	G	227	VAL
1	G	230	ARG
1	G	279	ASN
1	G	286	GLN
1	G	315	GLN
1	G	322	LYS
1	G	333	THR
1	G	400	ASN
1	G	452	THR
1	G	493	TYR
2	H	275	LYS
2	H	279	LYS
2	H	282	VAL
2	H	300	HIS
2	H	305	LYS
2	H	318	LEU
2	H	395	LEU
2	H	405	THR
2	H	455	THR
2	H	458	LEU
2	H	467	LYS
2	H	475	THR

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Mol	Chain	Res	Type
2	H	525	LEU
2	H	540	THR
3	I	20	ASN
3	I	23	THR
3	I	27	VAL
3	I	36	PRO
3	I	39	THR
3	I	57	GLU
3	I	86	LEU
3	I	109	GLN
3	I	119	ILE
3	I	166	PRO
3	I	284	GLN
3	I	287	GLU
3	I	296	THR
3	I	300	LEU
4	J	261	VAL
4	J	297	ILE
4	J	299	THR
4	J	325	LYS
4	J	361	MET
4	J	398	LEU
4	J	405	LEU
4	J	408	LEU
4	J	421	PRO
4	J	433	LEU
4	J	499	ASN
4	J	501	ARG
4	J	598	ARG
4	J	674	THR
4	J	679	GLU
4	J	680	LEU
4	J	681	THR
4	J	692	LYS
3	K	2	ILE
3	K	25	LEU
3	K	109	GLN
3	K	117	LEU
3	K	119	ILE
3	K	134	PRO
3	K	147	LYS
3	K	265	PRO

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Mol	Chain	Res	Type
3	K	292	ASN
3	K	296	THR
3	K	322	LEU
3	K	340	LEU
5	L	224	ARG
5	L	240	ASN
5	L	335	ILE
5	L	340	THR
5	L	346	VAL
5	L	355	LYS
5	L	368	THR
5	L	381	LYS
5	L	382	GLN
5	L	452	PRO
5	L	471	LEU
5	L	474	LEU
5	L	519	PRO
5	L	573	TYR
5	L	575	LEU
5	L	606	LYS
5	L	1368	THR
2	O	36	VAL
2	O	45	PRO
2	Q	54	VAL
2	Q	107	GLN
2	R	16	LEU
2	S	12	LEU
2	S	16	LEU
2	S	23	LYS
2	S	80	LYS
2	S	88	LYS
2	S	90	ARG
2	S	96	LEU
2	S	110	LYS
2	S	113	SER
2	T	23	LYS
2	T	93	ILE
6	U	600	ILE
6	U	625	LEU
6	U	643	LEU
6	V	610	THR
6	V	666	ARG

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Mol	Chain	Res	Type
6	W	598	ILE
6	W	620	ARG
6	W	641	GLN
6	W	644	LEU
6	W	659	LYS
6	X	609	GLU
6	X	666	ARG
7	o	8	MET
7	o	11	VAL
7	o	33	THR
7	r	26	ASN
7	r	46	ASN
7	s	39	ARG
7	s	46	ASN
7	s	55	LYS
7	s	65	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	A	241	GLN
1	A	286	GLN
1	A	313	GLN
1	A	370	GLN
1	A	372	GLN
1	A	443	GLN
2	B	258	GLN
2	B	269	ASN
2	B	272	ASN
2	B	300	HIS
2	B	301	ASN
2	B	321	GLN
2	B	388	GLN
2	B	478	GLN
2	B	493	HIS
2	B	494	GLN
2	B	527	ASN
1	C	241	GLN
1	C	249	GLN
1	C	250	ASN
1	C	268	ASN

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Mol	Chain	Res	Type
1	C	279	ASN
1	C	288	ASN
1	C	308	GLN
1	C	311	HIS
1	C	328	GLN
1	C	345	ASN
1	C	370	GLN
1	C	372	GLN
1	C	411	HIS
1	C	436	GLN
1	C	437	GLN
2	D	258	GLN
2	D	300	HIS
2	D	342	HIS
2	D	416	HIS
2	D	427	ASN
2	D	460	HIS
2	D	490	ASN
1	E	250	ASN
1	E	286	GLN
1	E	311	HIS
1	E	313	GLN
1	E	345	ASN
1	E	400	ASN
1	E	429	GLN
1	E	481	GLN
2	F	300	HIS
2	F	321	GLN
2	F	342	HIS
2	F	443	HIS
1	G	308	GLN
1	G	311	HIS
1	G	315	GLN
1	G	321	GLN
1	G	328	GLN
1	G	372	GLN
1	G	411	HIS
1	G	457	ASN
2	H	258	GLN
2	H	301	ASN
2	H	321	GLN
2	H	415	GLN

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Mol	Chain	Res	Type
3	I	3	HIS
3	I	29	GLN
3	I	35	HIS
3	I	121	HIS
3	I	146	GLN
3	I	152	GLN
3	I	180	HIS
3	I	207	GLN
3	I	284	GLN
3	I	339	HIS
4	J	233	HIS
4	J	235	HIS
4	J	300	HIS
4	J	358	GLN
4	J	409	HIS
4	J	445	ASN
4	J	493	ASN
4	J	554	GLN
4	J	601	HIS
4	J	676	GLN
3	K	109	GLN
3	K	116	HIS
3	K	121	HIS
3	K	130	HIS
3	K	146	GLN
3	K	149	HIS
3	K	193	HIS
3	K	284	GLN
3	K	290	ASN
3	K	312	HIS
5	L	50	HIS
5	L	110	HIS
5	L	178	GLN
5	L	240	ASN
5	L	252	GLN
5	L	359	ASN
5	L	372	ASN
5	L	413	HIS
5	L	470	GLN
5	L	555	GLN
5	L	590	HIS
2	O	42	ASN

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Mol	Chain	Res	Type
2	Q	14	GLN
2	R	6	GLN
2	R	10	ASN
2	R	78	HIS
2	S	15	ASN
2	S	107	GLN
2	T	42	ASN
2	T	82	GLN
6	U	605	ASN
6	U	619	HIS
6	U	634	HIS
6	V	599	GLN
6	V	626	GLN
6	V	632	GLN
6	V	634	HIS
6	V	636	GLN
6	V	664	ASN
6	W	605	ASN
6	W	624	ASN
6	W	626	GLN
6	W	632	GLN
6	W	641	GLN
6	X	624	ASN
6	X	626	GLN
7	r	7	ASN
7	r	46	ASN
7	s	43	GLN
7	t	46	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

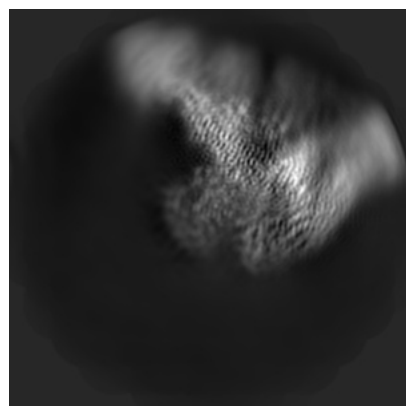
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52729. These allow visual inspection of the internal detail of the map and identification of artifacts.

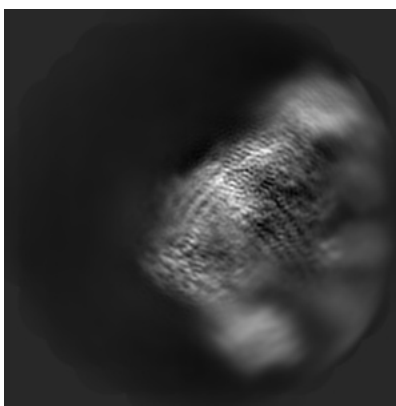
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

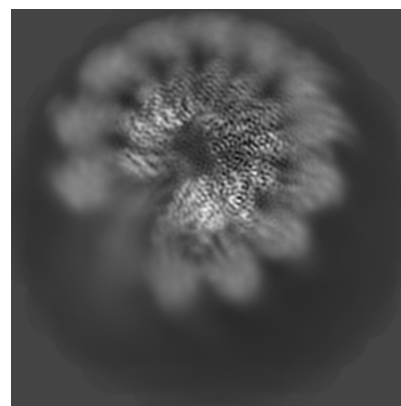
6.1.1 Primary map



X

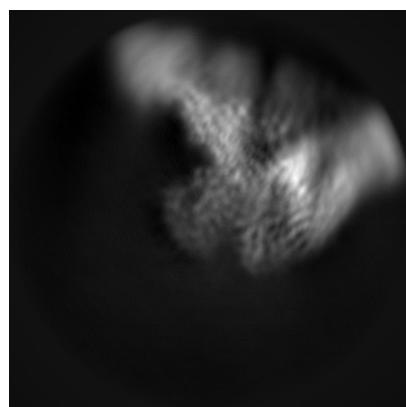


Y

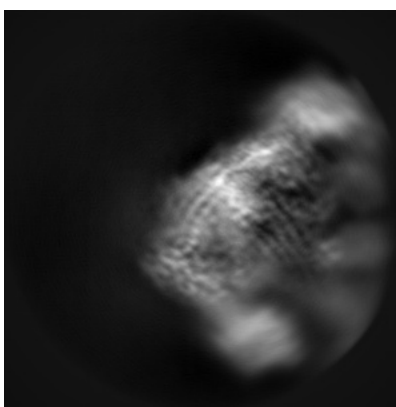


Z

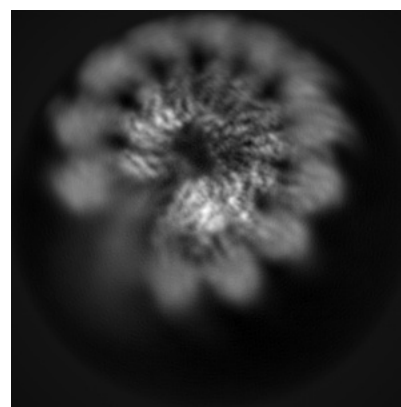
6.1.2 Raw map



X



Y

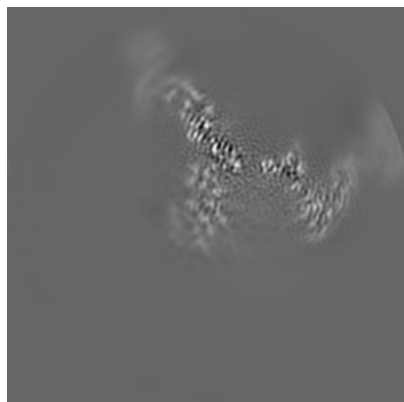


Z

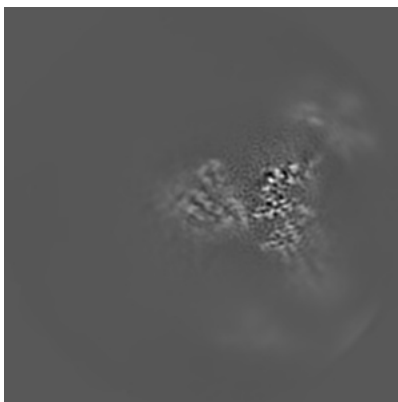
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

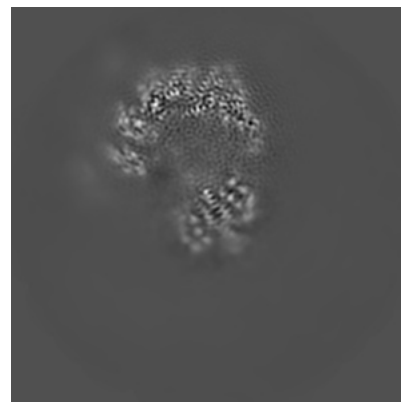
6.2.1 Primary map



X Index: 128

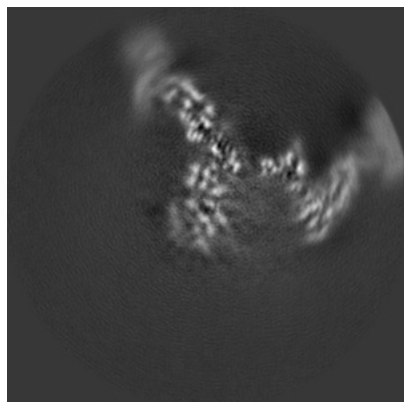


Y Index: 128

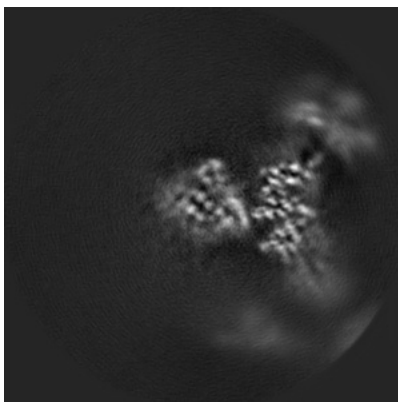


Z Index: 128

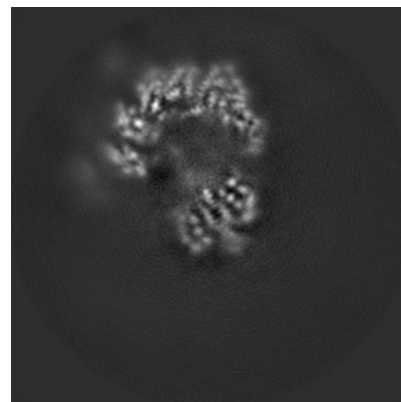
6.2.2 Raw map



X Index: 128



Y Index: 128

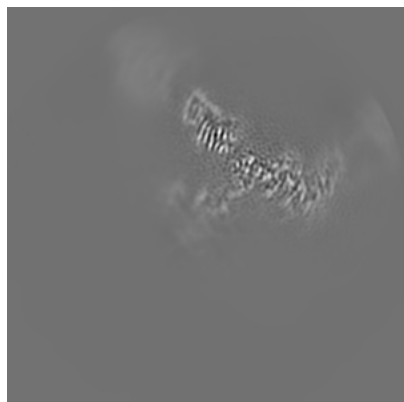


Z Index: 128

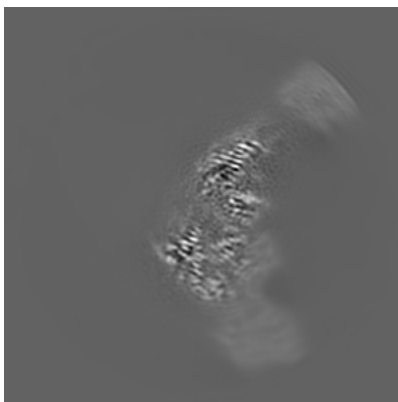
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

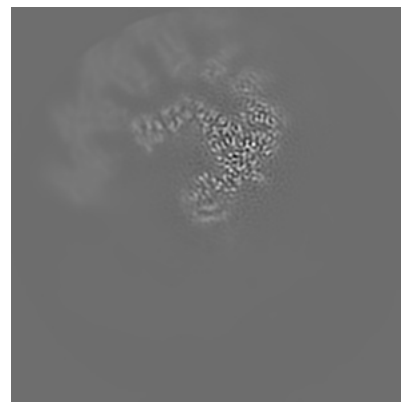
6.3.1 Primary map



X Index: 148

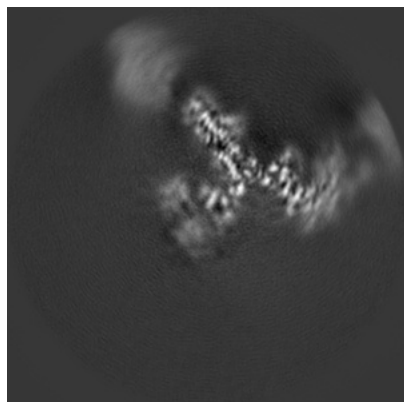


Y Index: 184

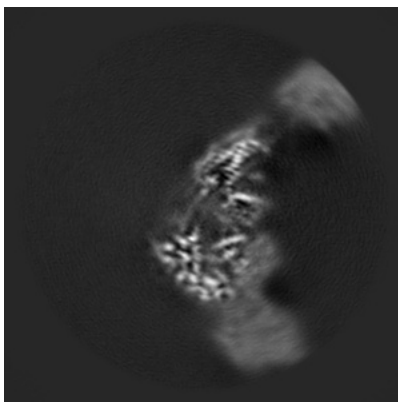


Z Index: 150

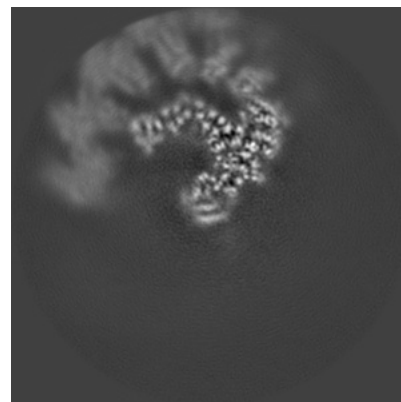
6.3.2 Raw map



X Index: 145



Y Index: 183

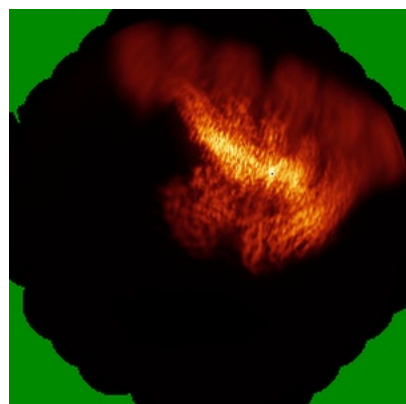


Z Index: 151

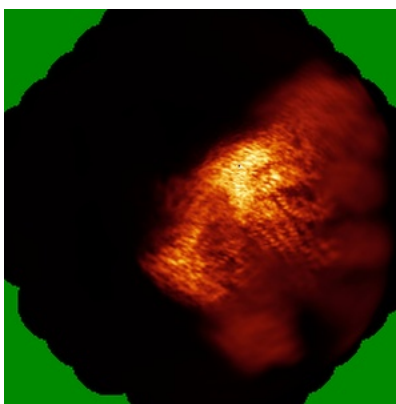
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

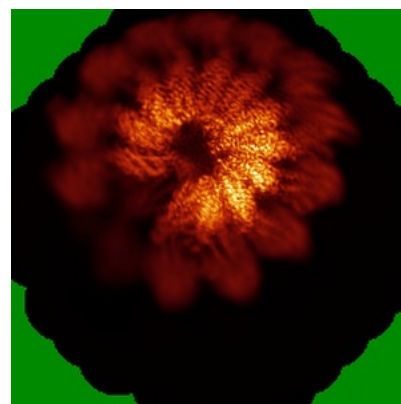
6.4.1 Primary map



X

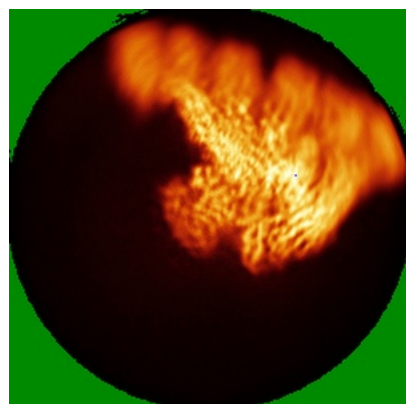


Y

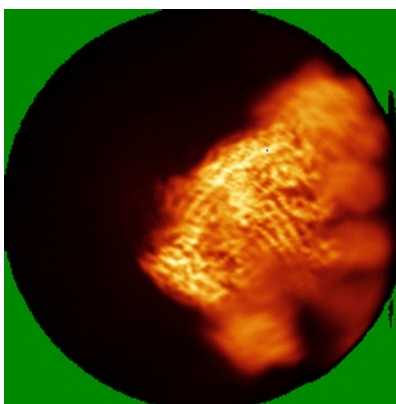


Z

6.4.2 Raw map



X



Y

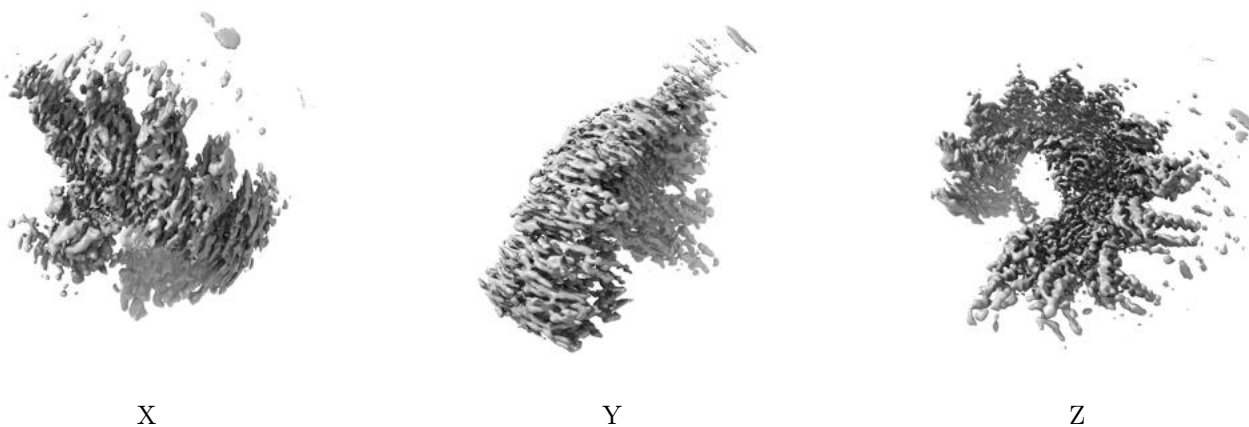


Z

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.

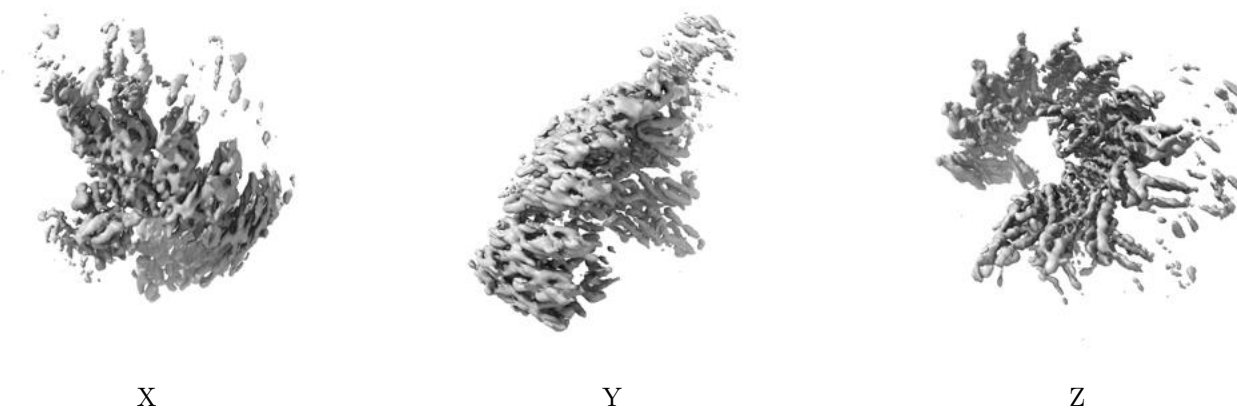
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0421. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

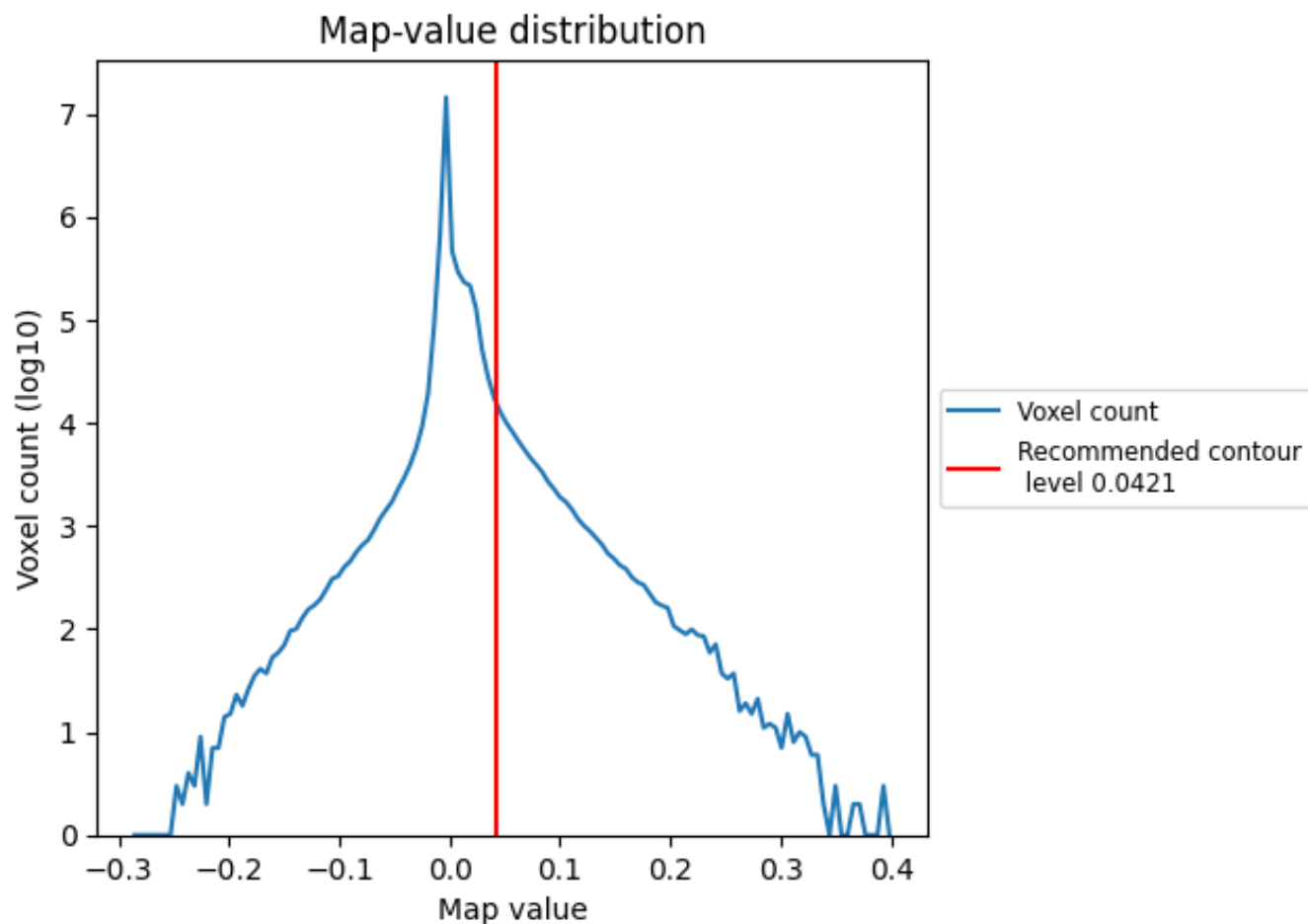
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

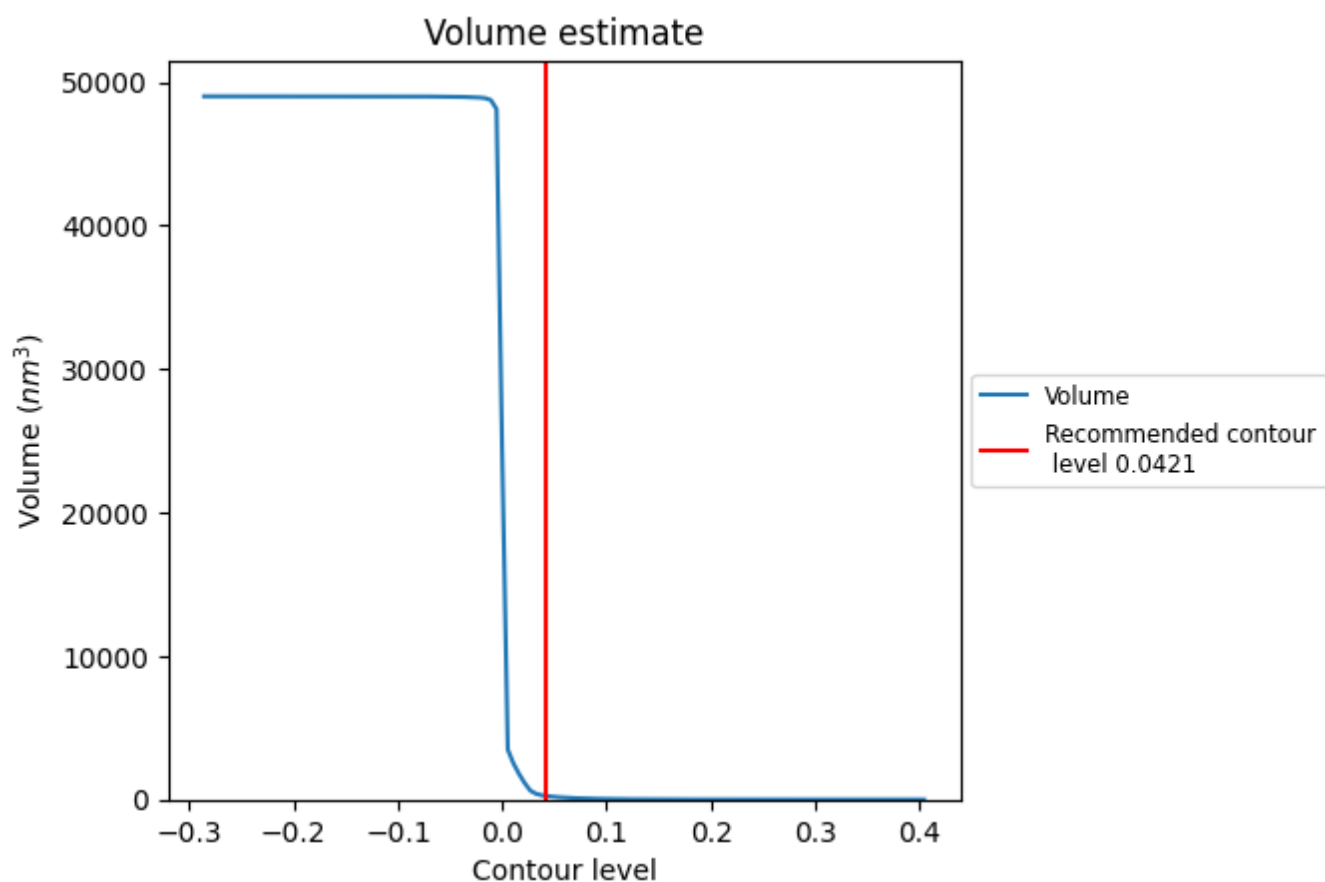
This section contains the results of statistical analysis of the map.

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.

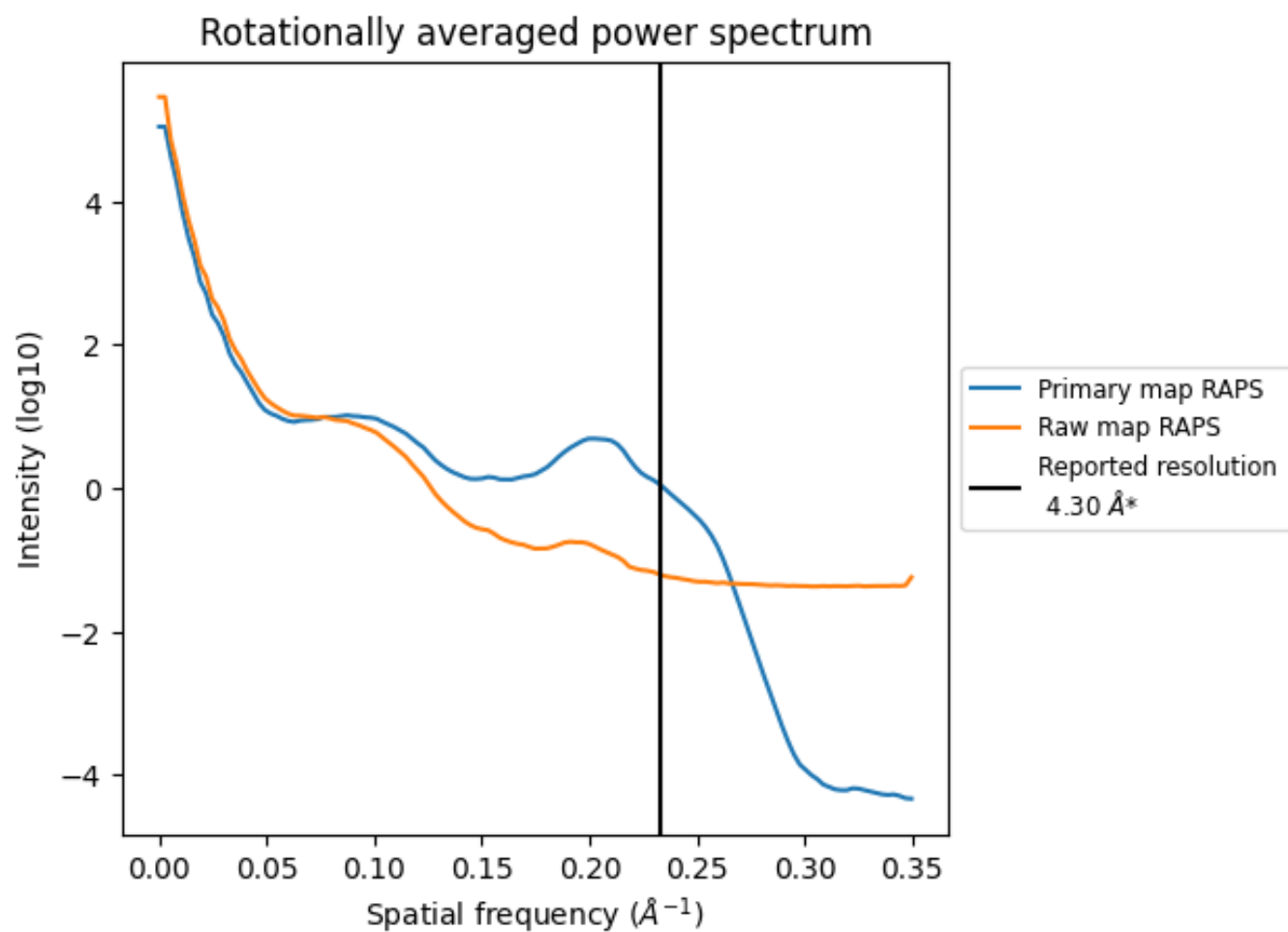
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm^3 ; this corresponds to an approximate mass of 227 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 ⓘ

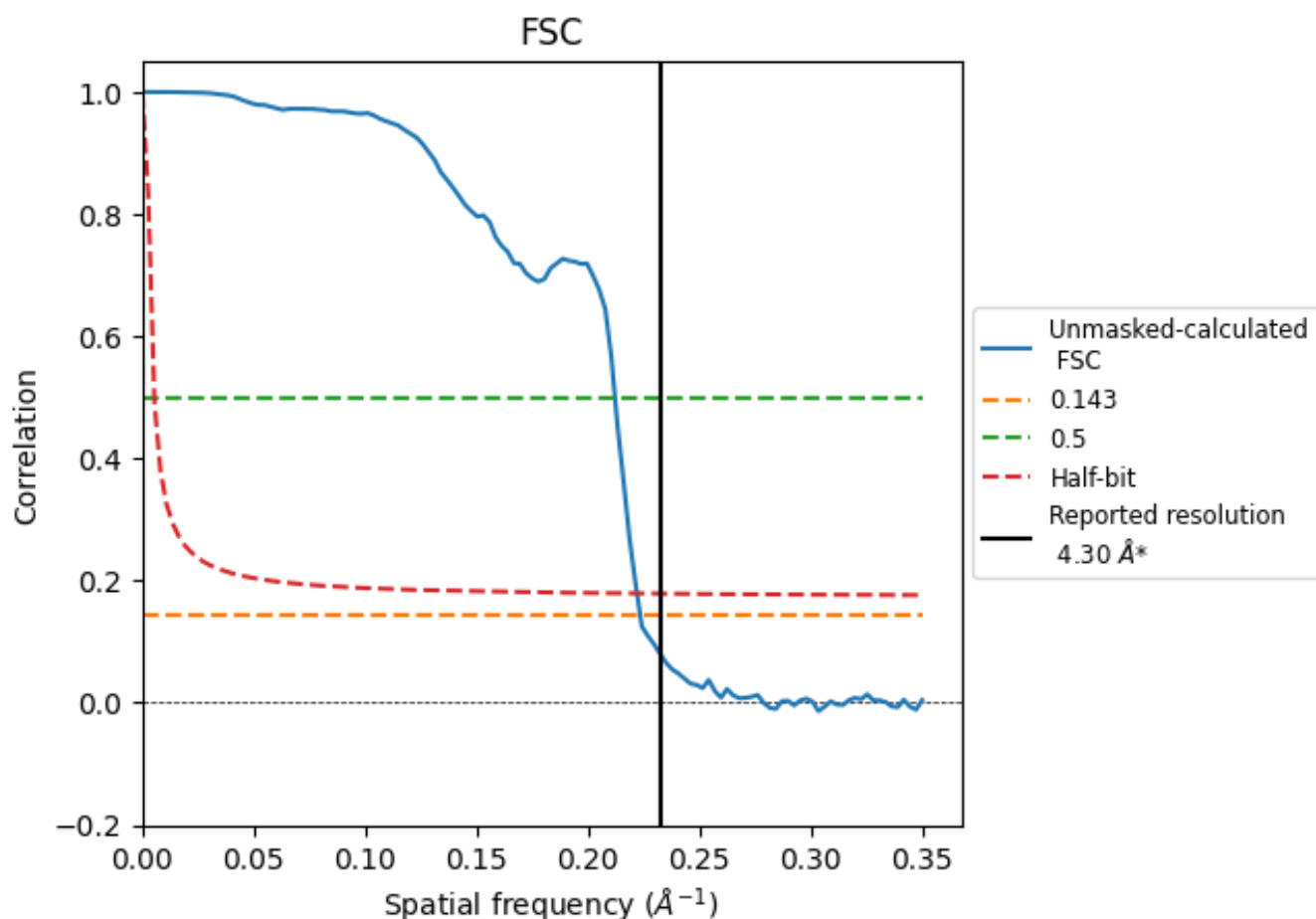


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

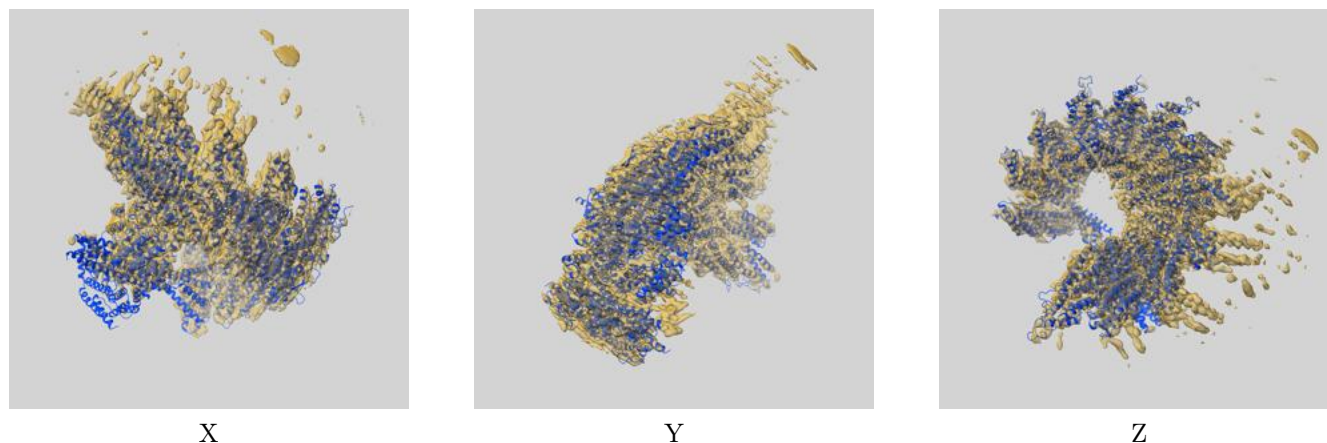
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.48	4.72	4.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

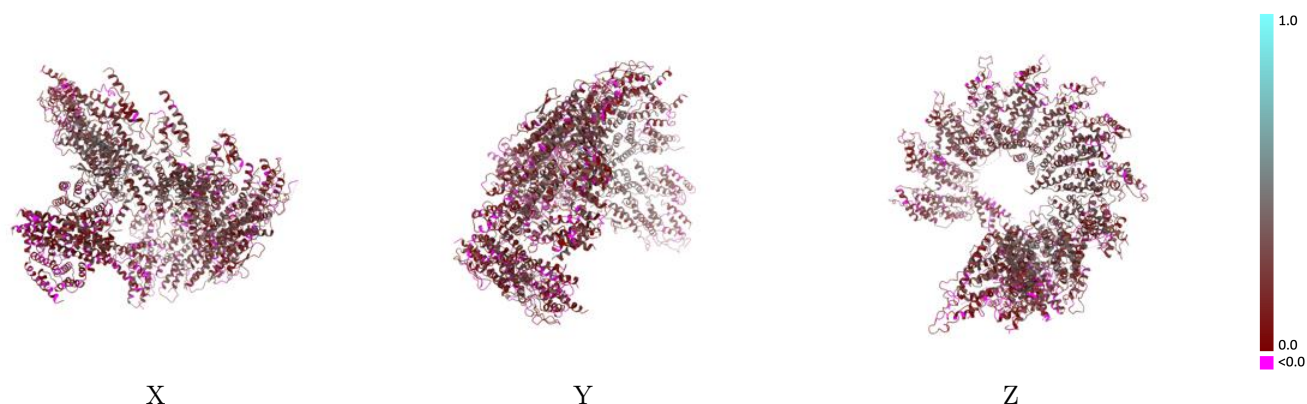
This section contains information regarding the fit between EMDB map EMD-52729 and PDB model 9I8M. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



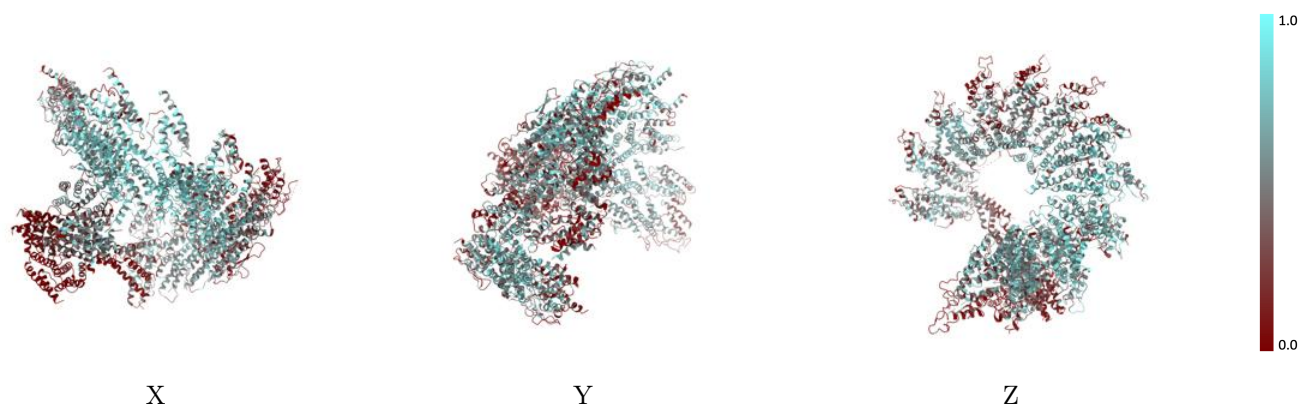
The images above show the 3D surface view of the map at the recommended contour level 0.0421 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



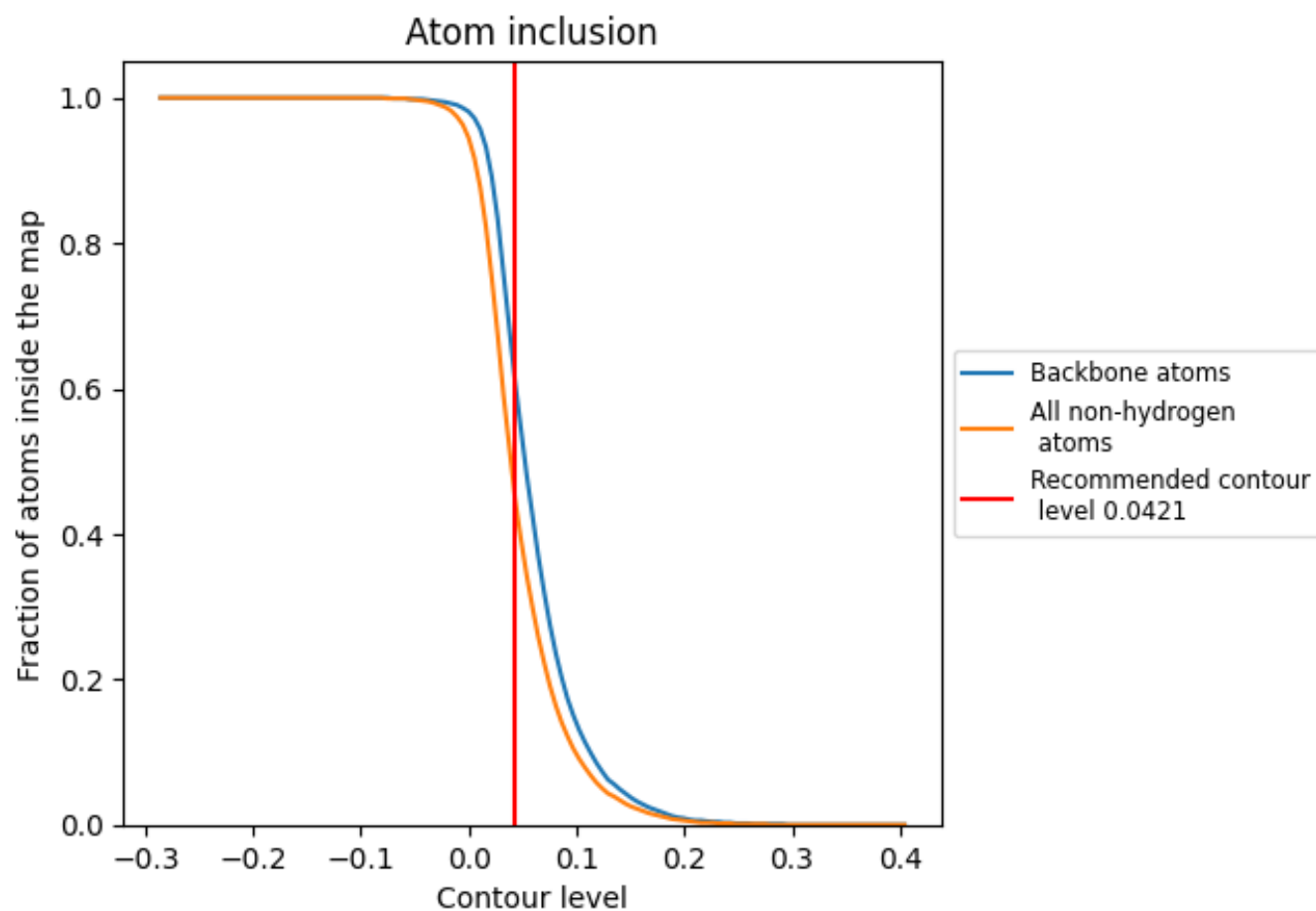
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0421).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 46% 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 (0.0421) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4610	 0.1990
A	 0.4370	 0.1340
B	 0.4790	 0.1530
C	 0.5550	 0.1810
D	 0.3590	 0.1690
E	 0.3630	 0.1960
F	 0.3810	 0.2020
G	 0.5550	 0.2200
H	 0.6540	 0.2460
I	 0.6440	 0.2650
J	 0.6320	 0.2690
K	 0.5640	 0.2530
L	 0.4320	 0.2020
O	 0.6400	 0.2920
Q	 0.1310	 0.1250
R	 0.3820	 0.1750
S	 0.4280	 0.1670
T	 0.0490	 0.0990
U	 0.3300	 0.1960
V	 0.2790	 0.1550
W	 0.2160	 0.1210
X	 0.1970	 0.1160
o	 0.6900	 0.3130
p	 0.4750	 0.2310
q	 0.1470	 0.0950
r	 0.4640	 0.1750
s	 0.5460	 0.1970
t	 0.0230	 0.1270

