



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:12 PM UTC

PDB ID : 9QZF / pdb_00009qzf
EMDB ID : EMD-53471
Title : Proximal A-C linker of Tetrahymena centriole, six repeating units
Authors : Cai, B.; Xu, J.W.; Luo, L.; Aarts, E.; Leitner, A.; Ishikawa, T.; Beltro, P.;
Pilhofer, M.; Wieczorek, M.
Deposited on : 2025-04-22
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

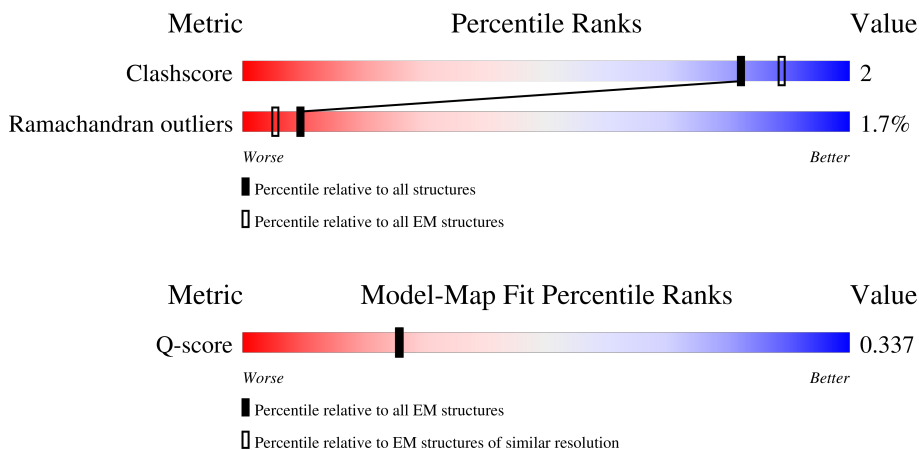
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



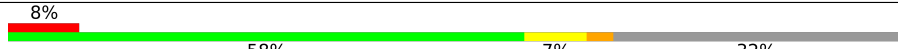
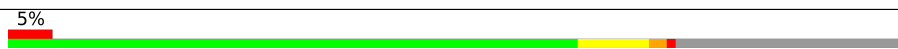
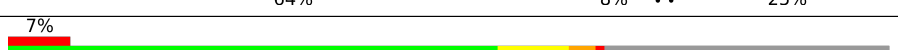
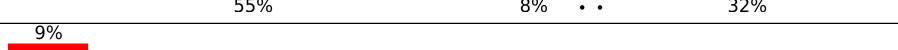
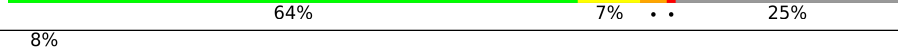
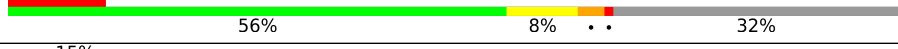
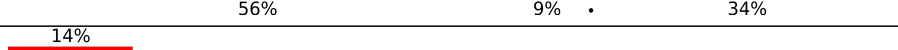
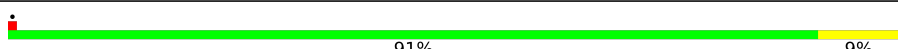
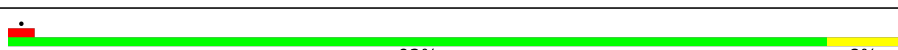
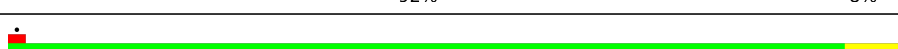
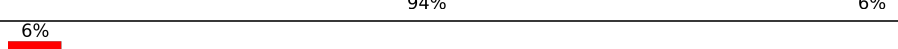
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	452	11% 83% 10% 5%
1	BD	452	6% 83% 11% 5%
1	C	452	10% 82% 11% 5%
1	CP	452	5% 82% 11% 5%
1	Ca	452	11% 82% 11% 5%

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Mol	Chain	Length	Quality of chain
1	i	452	
2	BK	380	
2	BR	380	
2	CW	380	
2	Cd	380	
2	Ch	380	
2	D	380	
2	f	380	
2	k	380	
2	q	380	
2	s	380	
2	y	380	
2	z	380	
3	1	937	
3	7	937	
3	BY	937	
3	E	937	
3	I	937	
3	n	937	
4	BO	151	
4	BZ	151	
4	Bw	151	
4	F	151	
4	d	151	
4	o	151	

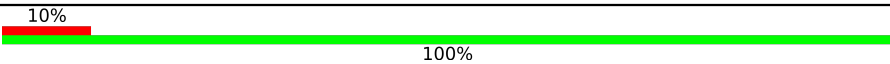
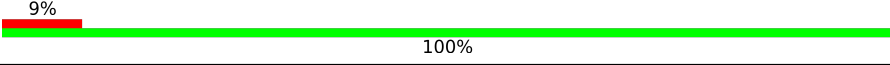
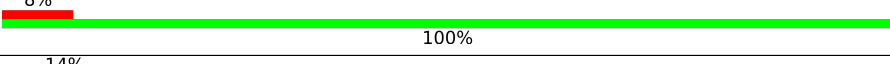
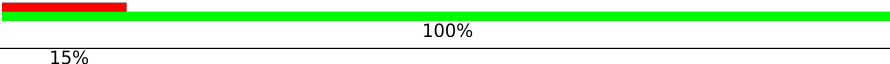
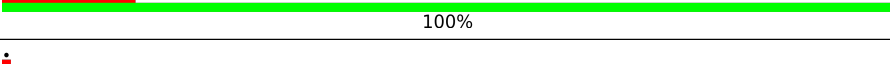
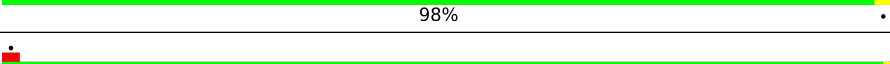
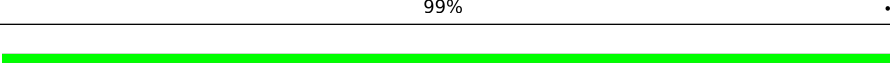
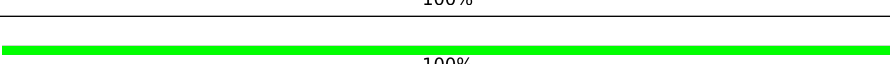
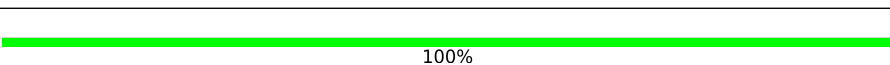
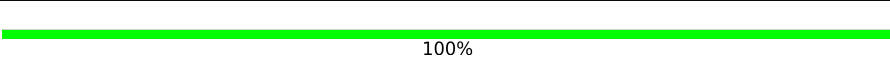
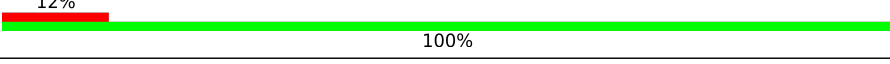
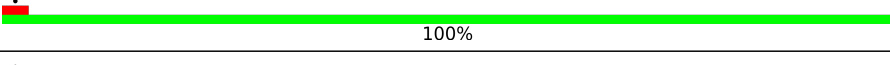
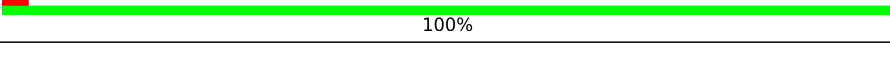
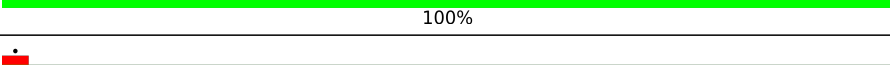
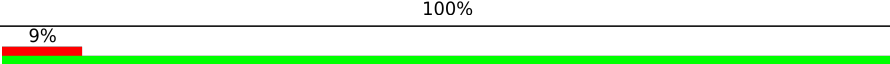
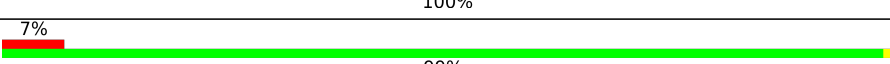
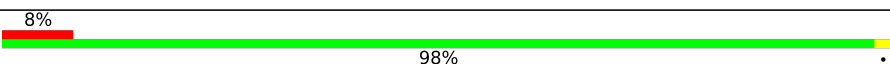
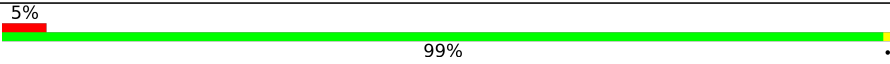
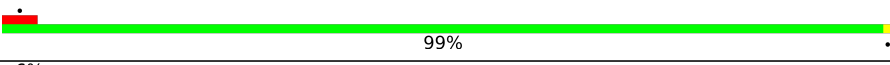
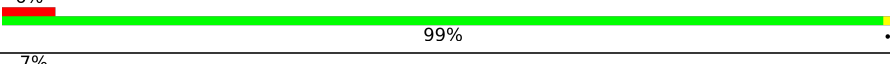
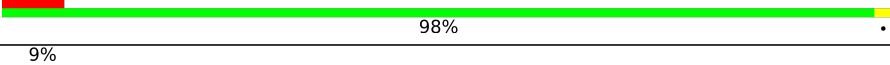
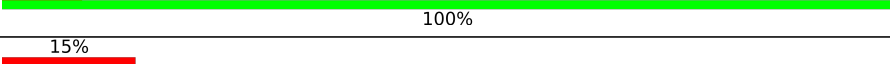
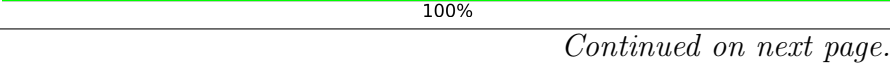
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Mol	Chain	Length	Quality of chain
5	9	1202	
5	AB	1202	
5	AE	1202	
5	AO	1202	
5	AU	1202	
5	Bf	1202	
5	Bt	1202	
5	G	1202	
5	L	1202	
5	M	1202	
5	R	1202	
5	v	1202	
6	B4	164	
6	BV	164	
6	Bg	164	
6	H	164	
6	l	164	
6	w	164	
7	4	634	
7	AG	634	
7	AM	634	
7	Bm	634	
7	J	634	
7	O	634	
8	5	167	

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Mol	Chain	Length	Quality of chain
8	Bc	167	
8	Bn	167	
8	CA	167	
8	K	167	
8	t	167	
9	2	161	
9	AC	161	
9	Bj	161	
9	Bu	161	
9	CH	161	
9	N	161	
10	AJ	32	
10	AW	32	
10	Ac	32	
10	B1	32	
10	P	32	
10	U	32	
11	0	105	
11	AK	105	
11	B2	105	
11	Bq	105	
11	CO	105	
11	Q	105	
12	AR	33	
12	Ae	33	

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Mol	Chain	Length	Quality of chain
12	Ak	33	12% 100%
12	B8	33	6% 100%
12	S	33	6% 100%
12	X	33	12% 100%
13	AH	127	98% .
13	AS	127	22% 99% .
13	B9	127	98% .
13	Bx	127	98% .
13	CV	127	98% .
13	T	127	98% .
14	AZ	153	9% 95% 5% .
14	Am	153	33% 90% 10%
14	As	153	95% 5% .
14	CE	153	95% 5% .
14	V	153	6% 96% ..
14	a	153	8% 95% 5% .
15	AP	102	6% 94% 5% .
15	Aa	102	21% 98% .
15	B5	102	96% ..
15	CF	102	95% ..
15	Cc	102	97% ..
15	W	102	7% 97% ..
16	A7	230	7% 57% 10% 31% .
16	Ai	230	8% 54% 8% 34% .
16	An	230	10% 55% 8% 34% .

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Mol	Chain	Length	Quality of chain
16	Aq	230	
16	Av	230	
16	Az	230	
16	CB	230	
16	CI	230	
16	CM	230	
16	CT	230	
16	Z	230	
16	c	230	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 130144 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 WD repeat WRAP73-like protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	429	Total	C	N	O	0	0
			2129	1271	429	429		
1	C	429	Total	C	N	O	0	0
			2129	1271	429	429		
1	i	429	Total	C	N	O	0	0
			2129	1271	429	429		
1	BD	429	Total	C	N	O	0	0
			2129	1271	429	429		
1	CP	429	Total	C	N	O	0	0
			2129	1271	429	429		
1	Ca	429	Total	C	N	O	0	0
			2129	1271	429	429		

- Molecule 2 is a protein called Centrosomal protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	284	Total	C	N	O	0	0
			1415	847	284	284		
2	f	258	Total	C	N	O	0	0
			1288	772	258	258		
2	k	284	Total	C	N	O	0	0
			1415	847	284	284		
2	q	284	Total	C	N	O	0	0
			1415	847	284	284		
2	s	258	Total	C	N	O	0	0
			1288	772	258	258		
2	y	258	Total	C	N	O	0	0
			1288	772	258	258		
2	BK	284	Total	C	N	O	0	0
			1415	847	284	284		
2	BR	258	Total	C	N	O	0	0
			1288	772	258	258		
2	CW	284	Total	C	N	O	0	0
			1415	847	284	284		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	Cd	258	Total	C	N	O	0	0
			1288	772	258	258		
2	Ch	284	Total	C	N	O	0	0
			1415	847	284	284		
2	z	258	Total	C	N	O	0	0
			1288	772	258	258		

- Molecule 3 is a protein called Rab-GAP TBC domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	724	Total	C	N	O	0	0
			3597	2149	724	724		
3	I	813	Total	C	N	O	0	0
			4040	2414	813	813		
3	n	665	Total	C	N	O	0	0
			3302	1972	665	665		
3	1	621	Total	C	N	O	0	0
			3082	1840	621	621		
3	7	813	Total	C	N	O	0	0
			4040	2414	813	813		
3	BY	773	Total	C	N	O	0	0
			3841	2295	773	773		

- Molecule 4 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	151	Total	C	N	O	0	0
			755	453	151	151		
4	d	151	Total	C	N	O	0	0
			755	453	151	151		
4	o	151	Total	C	N	O	0	0
			755	453	151	151		
4	BO	151	Total	C	N	O	0	0
			755	453	151	151		
4	BZ	151	Total	C	N	O	0	0
			755	453	151	151		
4	Bw	151	Total	C	N	O	0	0
			755	453	151	151		

- Molecule 5 is a protein called TBC1 domain family member 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	414	Total	C	N	O	0	0
			2064	1236	414	414		
5	L	518	Total	C	N	O	0	0
			2584	1548	518	518		
5	M	354	Total	C	N	O	0	0
			1752	1044	354	354		
5	R	354	Total	C	N	O	0	0
			1752	1044	354	354		
5	v	359	Total	C	N	O	0	0
			1790	1072	359	359		
5	9	303	Total	C	N	O	0	0
			1510	904	303	303		
5	AB	354	Total	C	N	O	0	0
			1752	1044	354	354		
5	AE	518	Total	C	N	O	0	0
			2584	1548	518	518		
5	AO	354	Total	C	N	O	0	0
			1752	1044	354	354		
5	AU	354	Total	C	N	O	0	0
			1752	1044	354	354		
5	Bf	468	Total	C	N	O	0	0
			2334	1398	468	468		
5	Bt	354	Total	C	N	O	0	0
			1752	1044	354	354		

- Molecule 6 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	164	Total	C	N	O	0	0
			820	492	164	164		
6	l	164	Total	C	N	O	0	0
			820	492	164	164		
6	w	164	Total	C	N	O	0	0
			820	492	164	164		
6	BV	164	Total	C	N	O	0	0
			820	492	164	164		
6	Bg	164	Total	C	N	O	0	0
			820	492	164	164		
6	B4	164	Total	C	N	O	0	0
			820	492	164	164		

- Molecule 7 is a protein called POC1 centriolar protein homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	365	Total	C	N	O	0	0
			1806	1076	365	365		
7	O	365	Total	C	N	O	0	0
			1806	1076	365	365		
7	4	365	Total	C	N	O	0	0
			1806	1076	365	365		
7	AG	365	Total	C	N	O	0	0
			1806	1076	365	365		
7	AM	365	Total	C	N	O	0	0
			1806	1076	365	365		
7	Bm	365	Total	C	N	O	0	0
			1806	1076	365	365		

- Molecule 8 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	167	Total	C	N	O	0	0
			835	501	167	167		
8	t	167	Total	C	N	O	0	0
			835	501	167	167		
8	5	167	Total	C	N	O	0	0
			835	501	167	167		
8	Bc	167	Total	C	N	O	0	0
			835	501	167	167		
8	Bn	167	Total	C	N	O	0	0
			835	501	167	167		
8	CA	167	Total	C	N	O	0	0
			835	501	167	167		

- Molecule 9 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	161	Total	C	N	O	0	0
			805	483	161	161		
9	2	161	Total	C	N	O	0	0
			805	483	161	161		
9	AC	161	Total	C	N	O	0	0
			805	483	161	161		
9	Bj	161	Total	C	N	O	0	0
			805	483	161	161		
9	Bu	161	Total	C	N	O	0	0
			805	483	161	161		
9	CH	161	Total	C	N	O	0	0
			805	483	161	161		

- Molecule 10 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	P	32	Total	C	N	O	0	0
			160	96	32	32		
10	U	32	Total	C	N	O	0	0
			160	96	32	32		
10	AJ	32	Total	C	N	O	0	0
			160	96	32	32		
10	AW	32	Total	C	N	O	0	0
			160	96	32	32		
10	Ac	32	Total	C	N	O	0	0
			160	96	32	32		
10	B1	32	Total	C	N	O	0	0
			160	96	32	32		

- Molecule 11 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Q	105	Total	C	N	O	0	0
			525	315	105	105		
11	0	105	Total	C	N	O	0	0
			525	315	105	105		
11	AK	105	Total	C	N	O	0	0
			525	315	105	105		
11	Bq	105	Total	C	N	O	0	0
			525	315	105	105		
11	B2	105	Total	C	N	O	0	0
			525	315	105	105		
11	CO	105	Total	C	N	O	0	0
			525	315	105	105		

- Molecule 12 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	S	33	Total	C	N	O	0	0
			165	99	33	33		
12	X	33	Total	C	N	O	0	0
			165	99	33	33		
12	AR	33	Total	C	N	O	0	0
			165	99	33	33		
12	Ae	33	Total	C	N	O	0	0
			165	99	33	33		
12	Ak	33	Total	C	N	O	0	0
			165	99	33	33		

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Mol	Chain	Residues	Atoms				AltConf	Trace
12	B8	33	Total	C	N	O	0	0
			165	99	33	33		

- Molecule 13 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	T	127	Total	C	N	O	0	0
			635	381	127	127		
13	AH	127	Total	C	N	O	0	0
			635	381	127	127		
13	AS	127	Total	C	N	O	0	0
			635	381	127	127		
13	Bx	127	Total	C	N	O	0	0
			635	381	127	127		
13	B9	127	Total	C	N	O	0	0
			635	381	127	127		
13	CV	127	Total	C	N	O	0	0
			635	381	127	127		

- Molecule 14 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	V	153	Total	C	N	O	0	0
			765	459	153	153		
14	a	153	Total	C	N	O	0	0
			765	459	153	153		
14	AZ	153	Total	C	N	O	0	0
			765	459	153	153		
14	Am	153	Total	C	N	O	0	0
			765	459	153	153		
14	As	153	Total	C	N	O	0	0
			765	459	153	153		
14	CE	153	Total	C	N	O	0	0
			765	459	153	153		

- Molecule 15 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	W	102	Total	C	N	O	0	0
			510	306	102	102		
15	AP	102	Total	C	N	O	0	0
			510	306	102	102		

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Mol	Chain	Residues	Atoms				AltConf	Trace
15	Aa	102	Total	C	N	O	0	0
			510	306	102	102		
15	B5	102	Total	C	N	O	0	0
			510	306	102	102		
15	CF	102	Total	C	N	O	0	0
			510	306	102	102		
15	Cc	102	Total	C	N	O	0	0
			510	306	102	102		

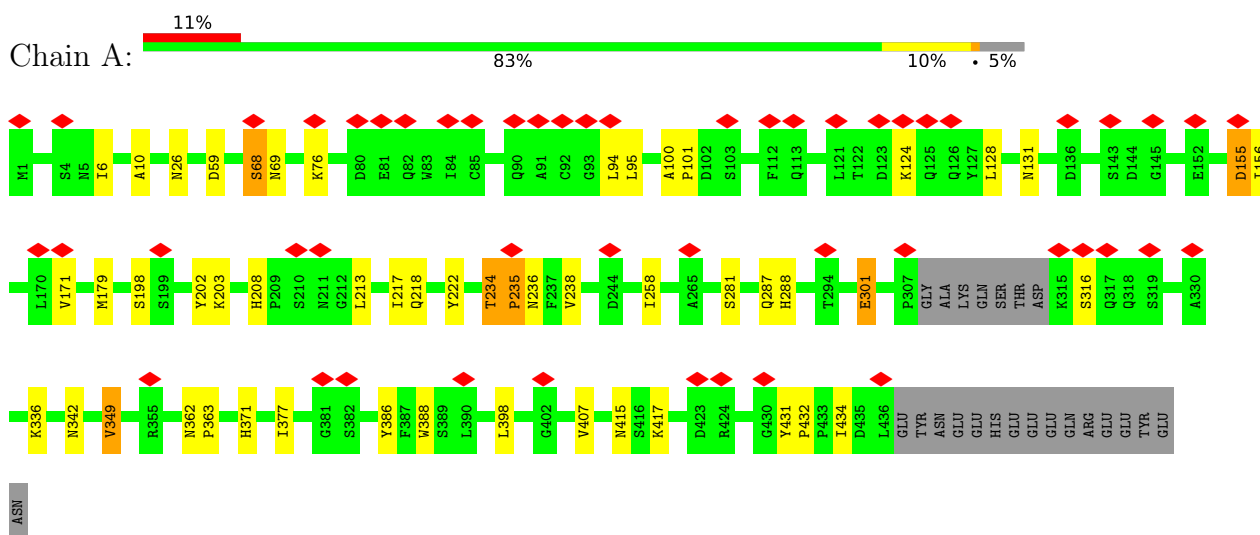
- Molecule 16 is a protein called SWIM-type domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Z	151	Total	C	N	O	0	0
			748	446	151	151		
16	c	158	Total	C	N	O	0	0
			783	467	158	158		
16	Ai	151	Total	C	N	O	0	0
			748	446	151	151		
16	An	151	Total	C	N	O	0	0
			748	446	151	151		
16	Aq	158	Total	C	N	O	0	0
			783	467	158	158		
16	Av	158	Total	C	N	O	0	0
			783	467	158	158		
16	Az	151	Total	C	N	O	0	0
			748	446	151	151		
16	A7	158	Total	C	N	O	0	0
			783	467	158	158		
16	CB	151	Total	C	N	O	0	0
			748	446	151	151		
16	CI	158	Total	C	N	O	0	0
			783	467	158	158		
16	CM	151	Total	C	N	O	0	0
			748	446	151	151		
16	CT	158	Total	C	N	O	0	0
			783	467	158	158		

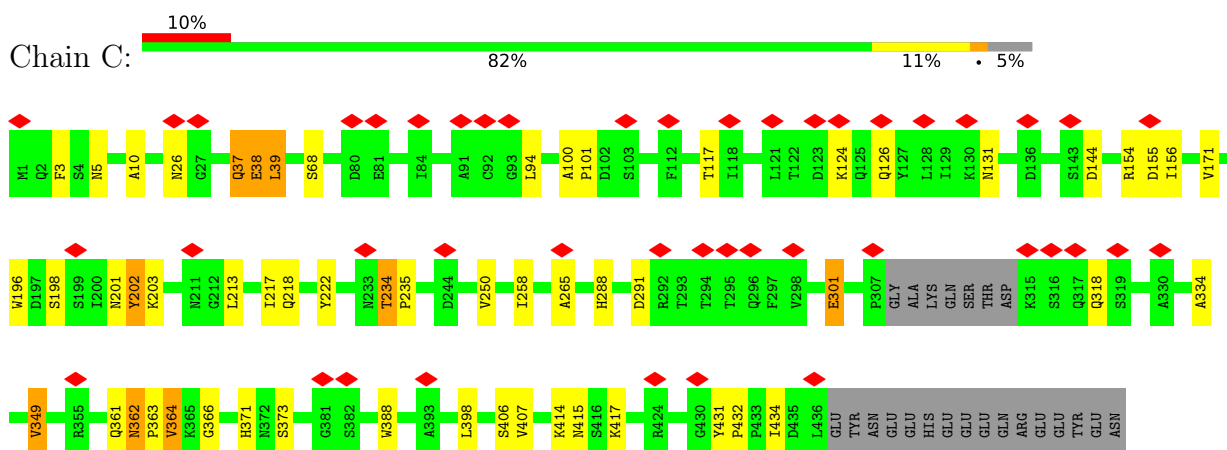
3 Residue-property plots

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

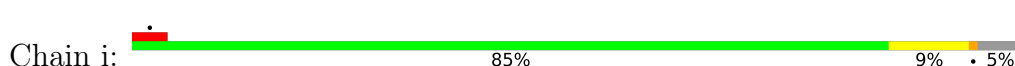
- Molecule 1: WD repeat WRAP73-like protein, putative

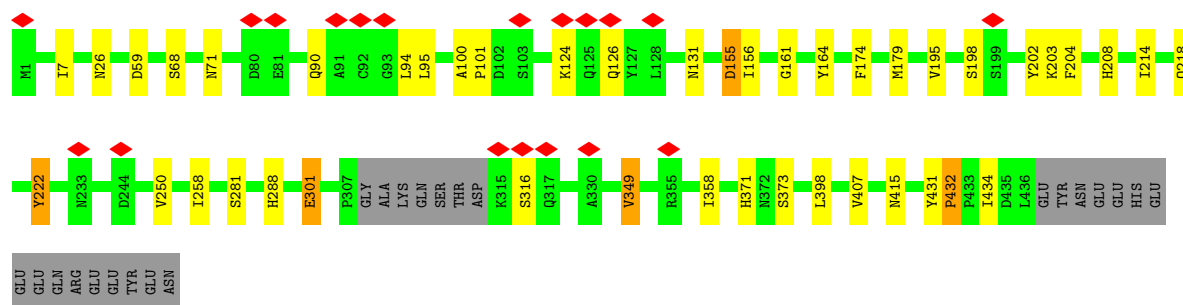


- Molecule 1: WD repeat WRAP73-like protein, putative

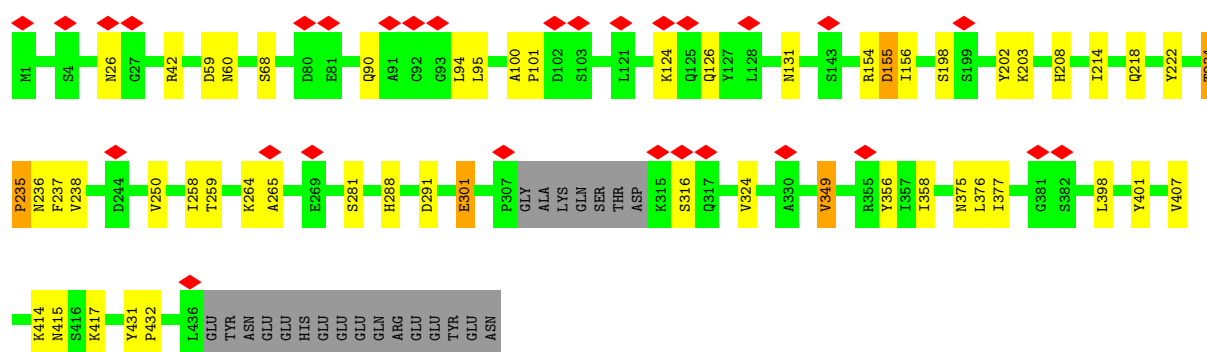
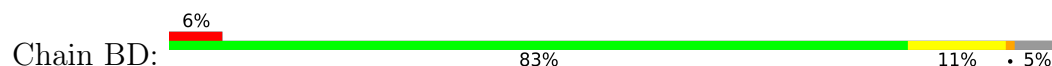


- Molecule 1: WD repeat WRAP73-like protein, putative

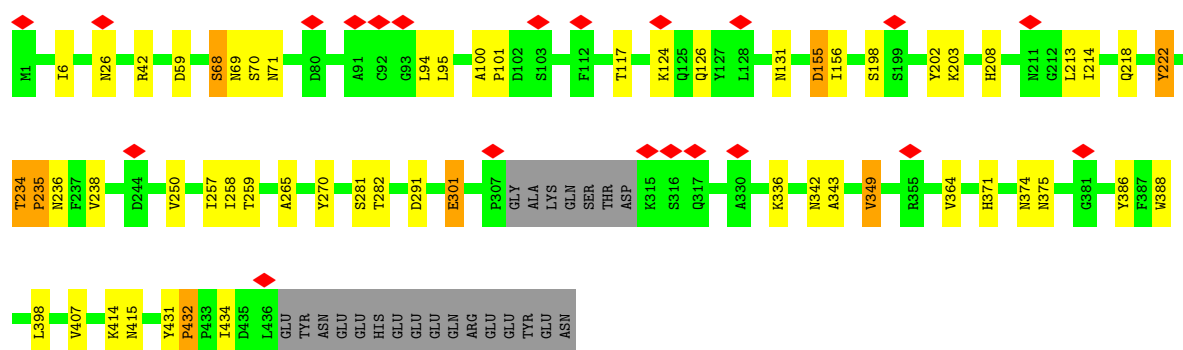
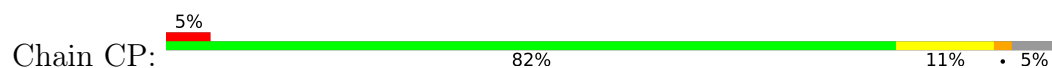




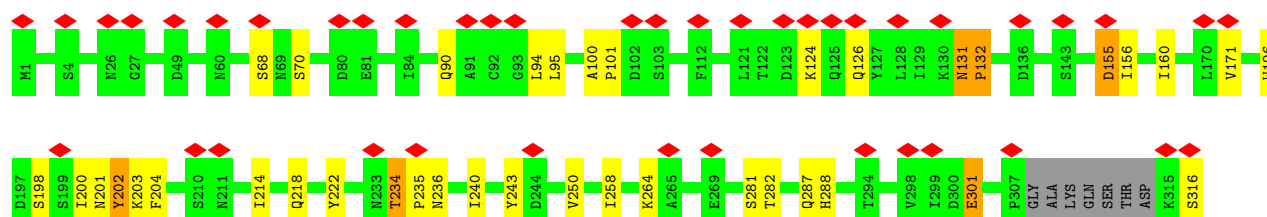
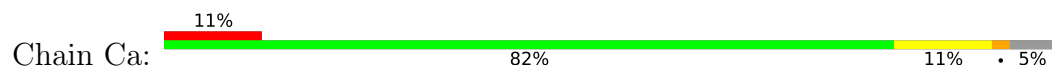
- Molecule 1: WD repeat WRAP73-like protein, putative



- Molecule 1: WD repeat WRAP73-like protein, putative

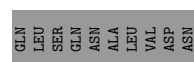
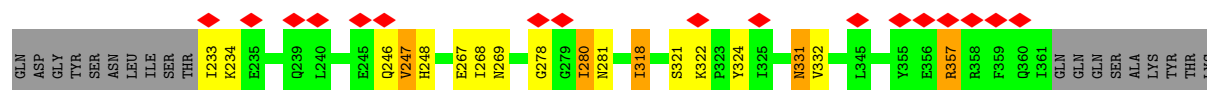
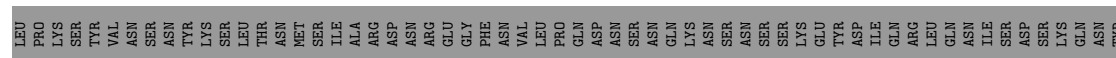
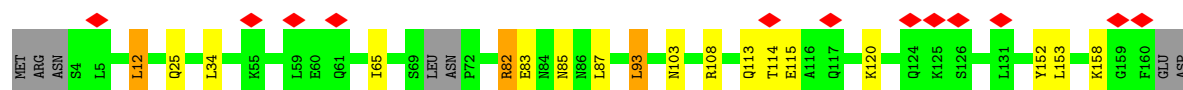


- Molecule 1: WD repeat WRAP73-like protein, putative

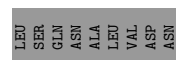
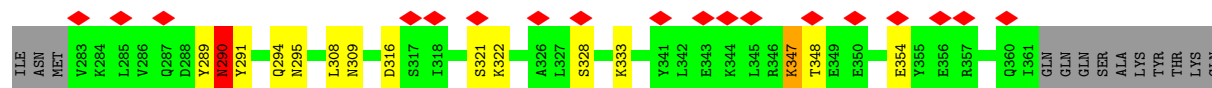
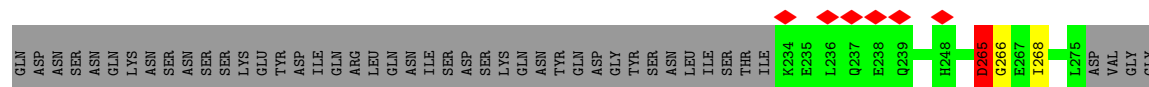
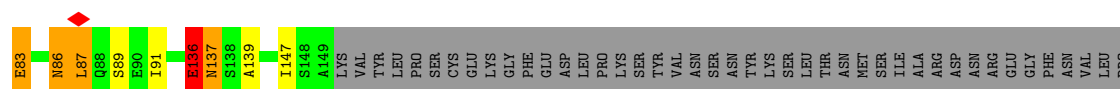




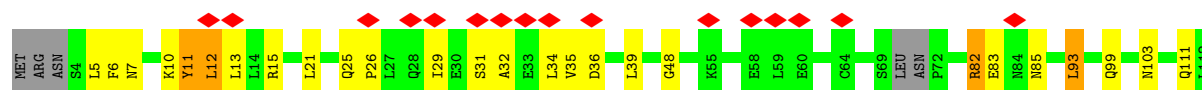
- Molecule 2: Centrosomal protein, putative

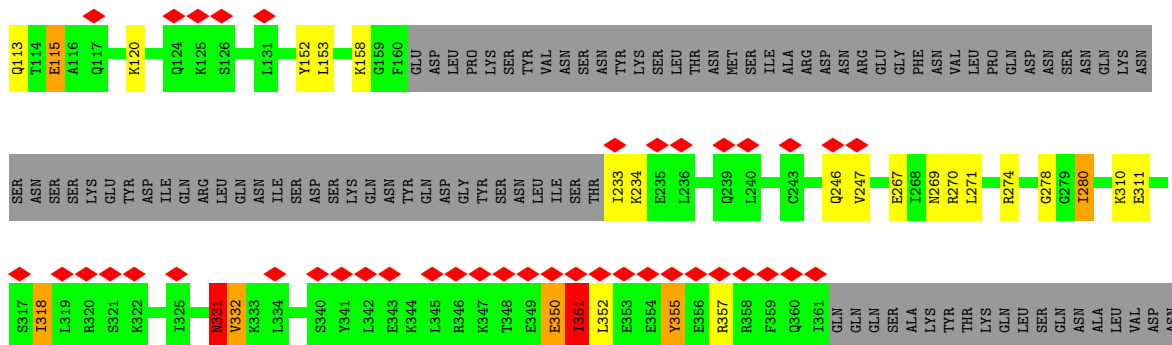


- Molecule 2: Centrosomal protein, putative

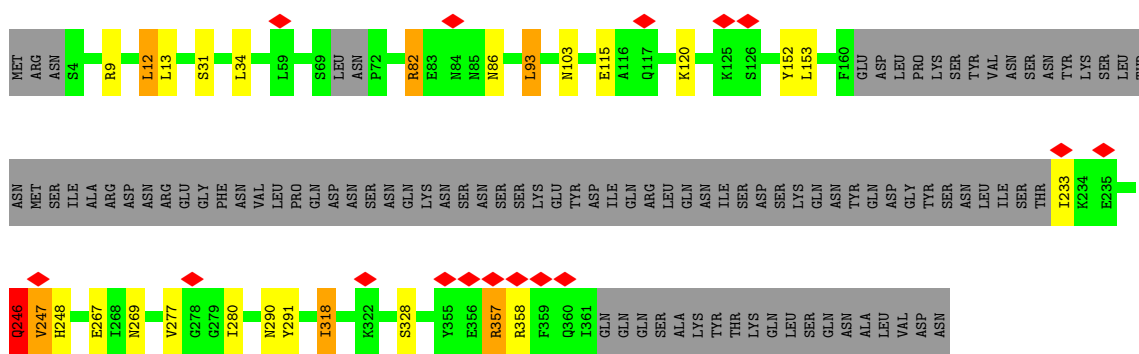


- Molecule 2: Centrosomal protein, putative

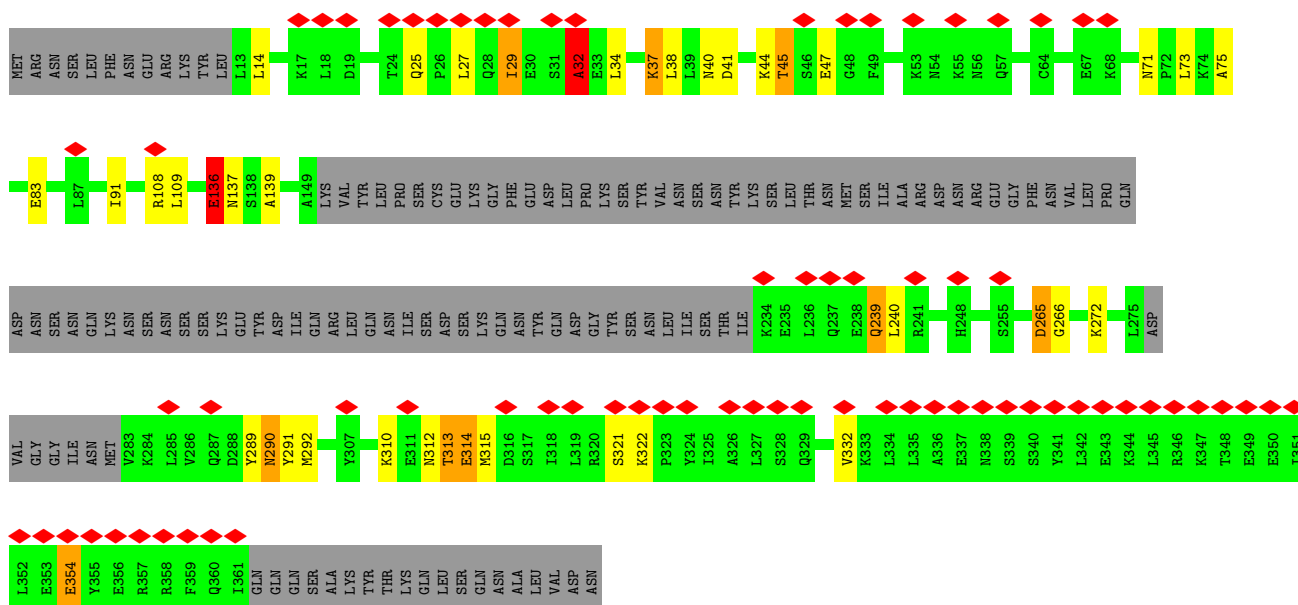




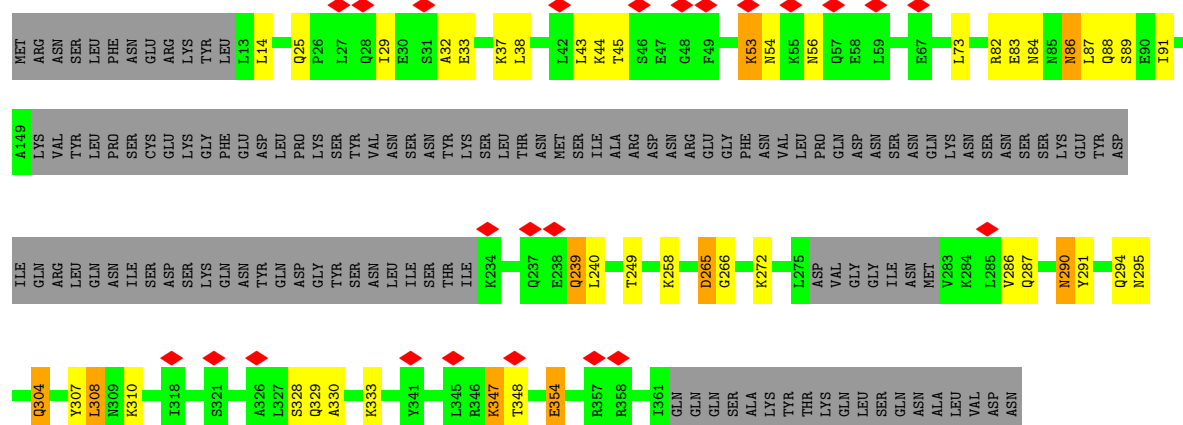
- Molecule 2: Centrosomal protein, putative



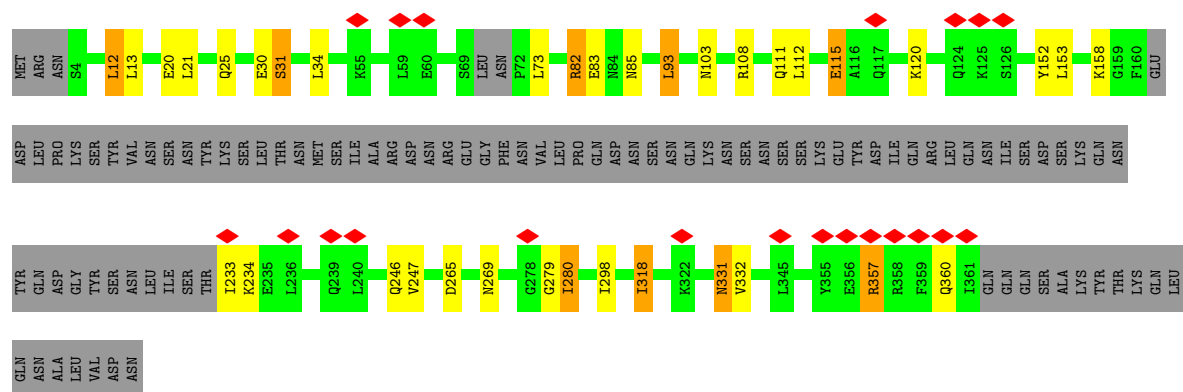
- Molecule 2: Centrosomal protein, putative



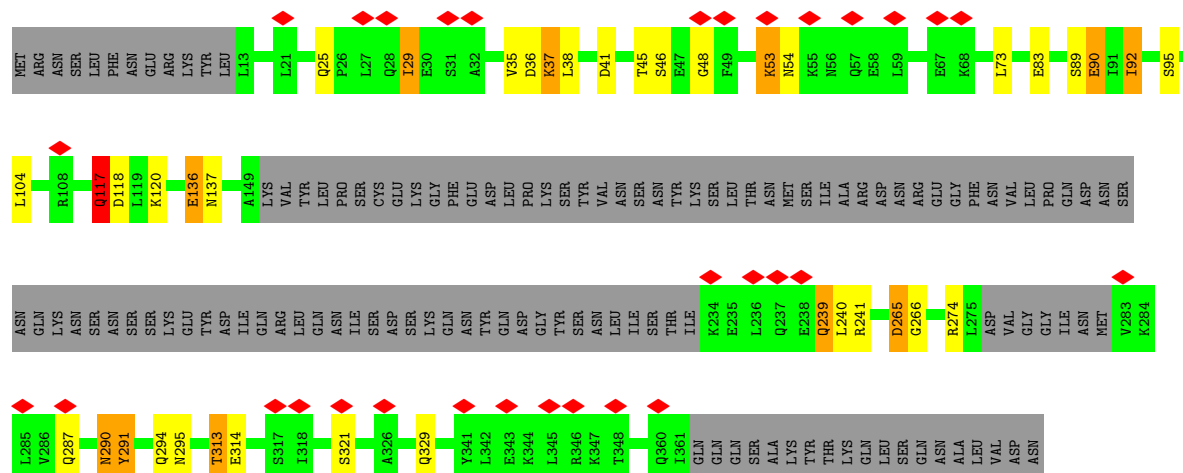
- Molecule 2: Centrosomal protein, putative



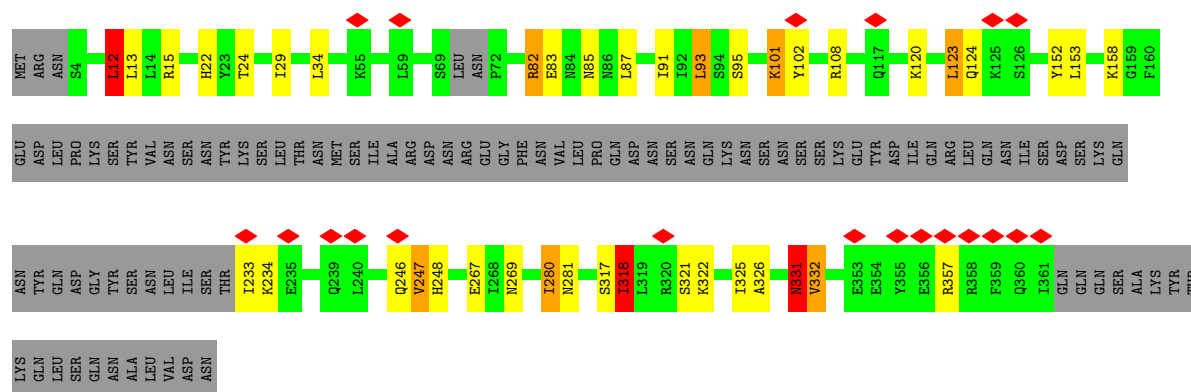
• Molecule 2: Centrosomal protein, putative



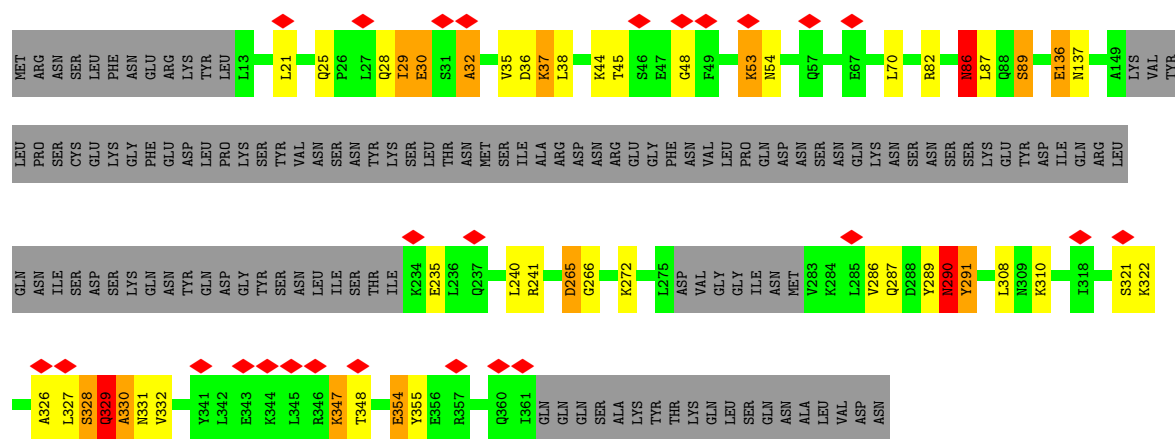
• Molecule 2: Centrosomal protein, putative



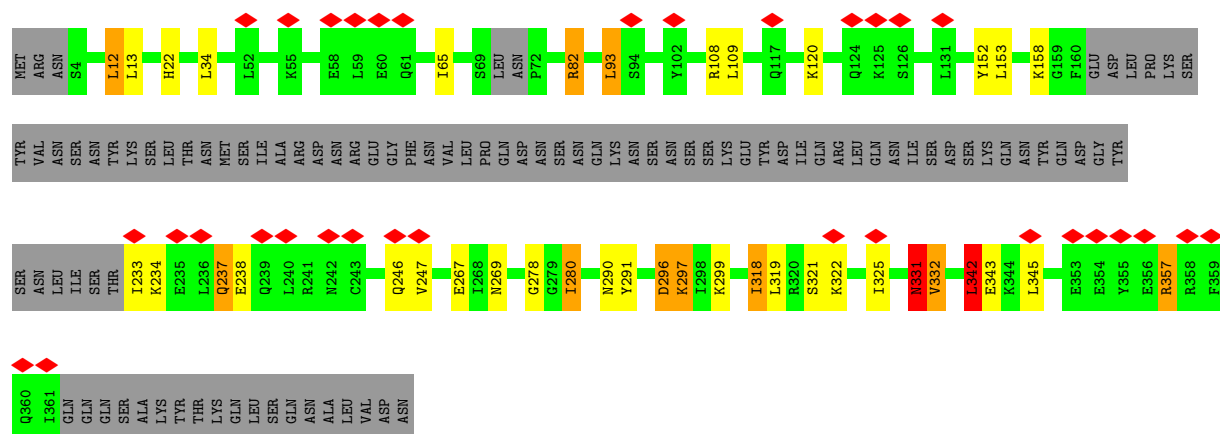
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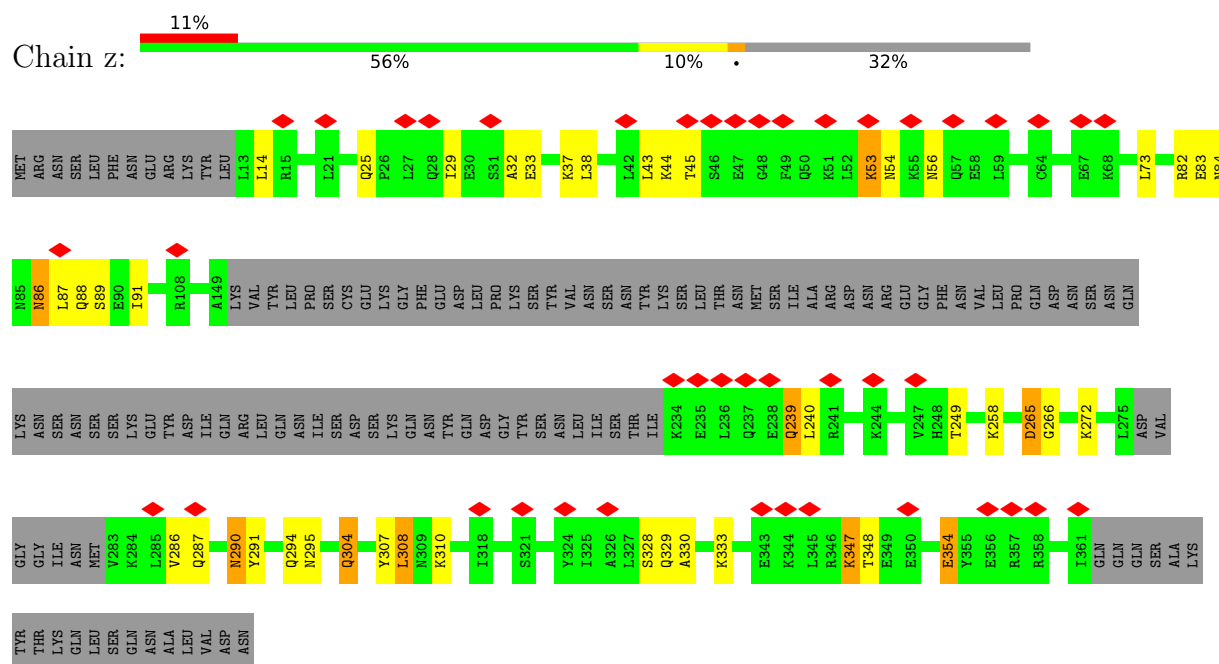
Chain Cd:



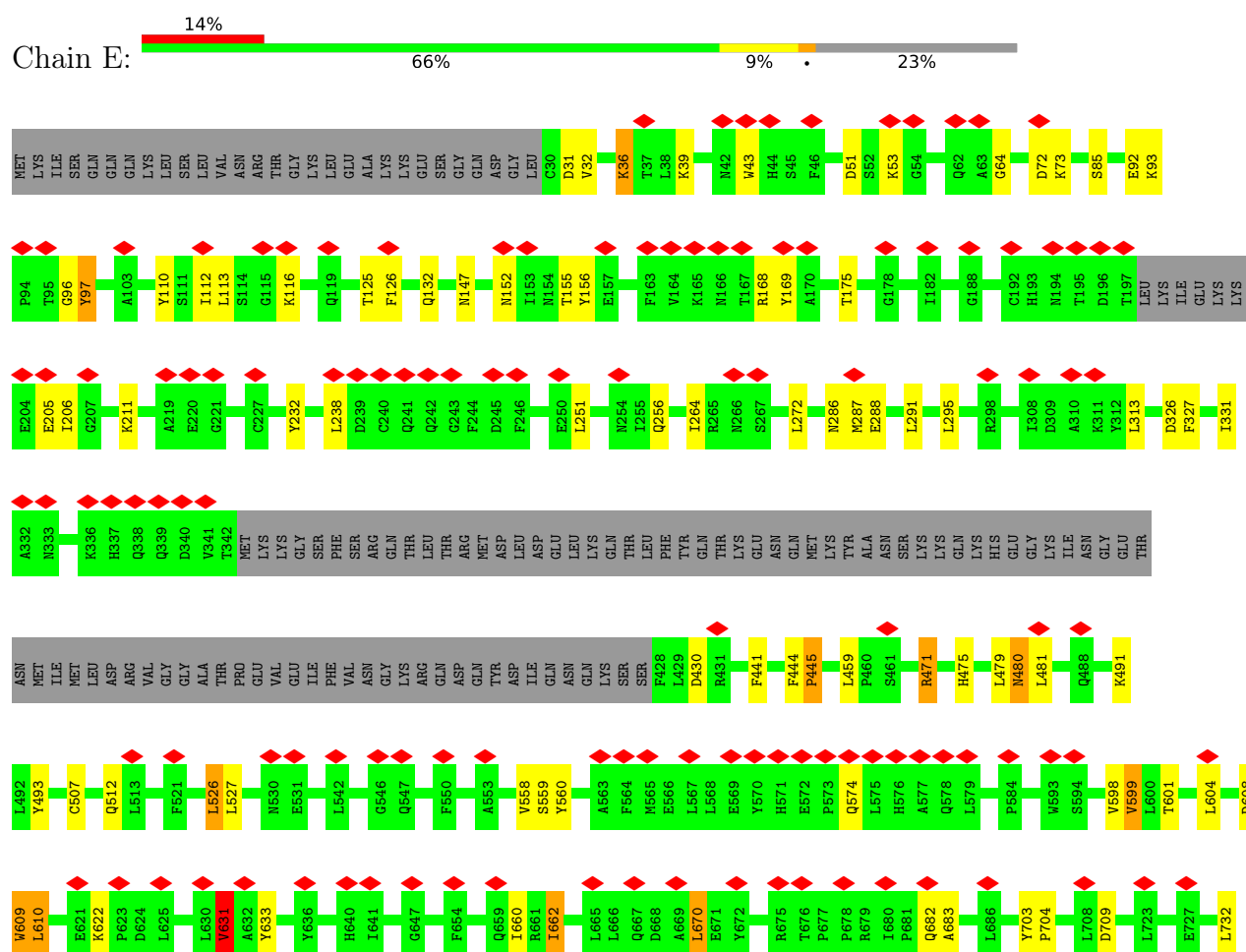
Chain Ch:



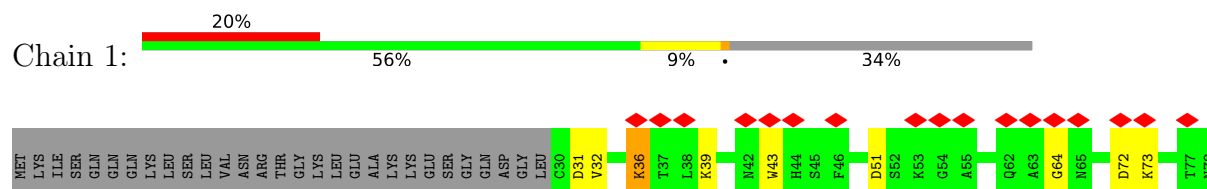
- Molecule 2: Centrosomal protein, putative

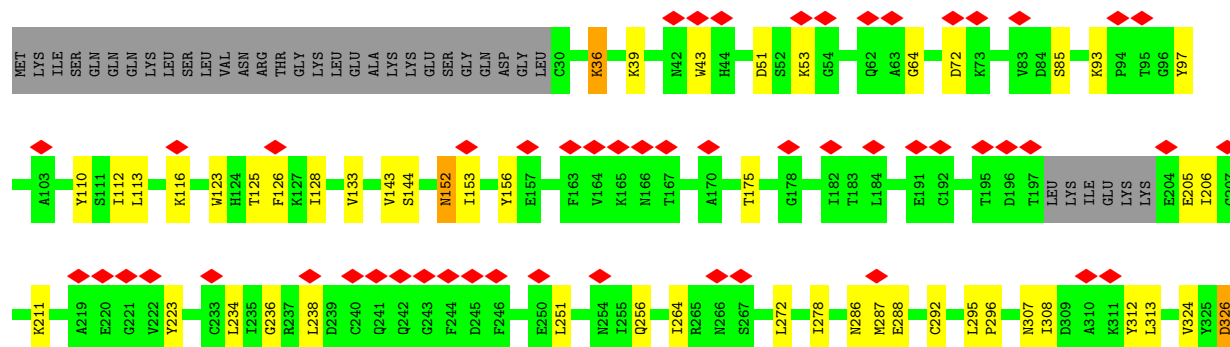


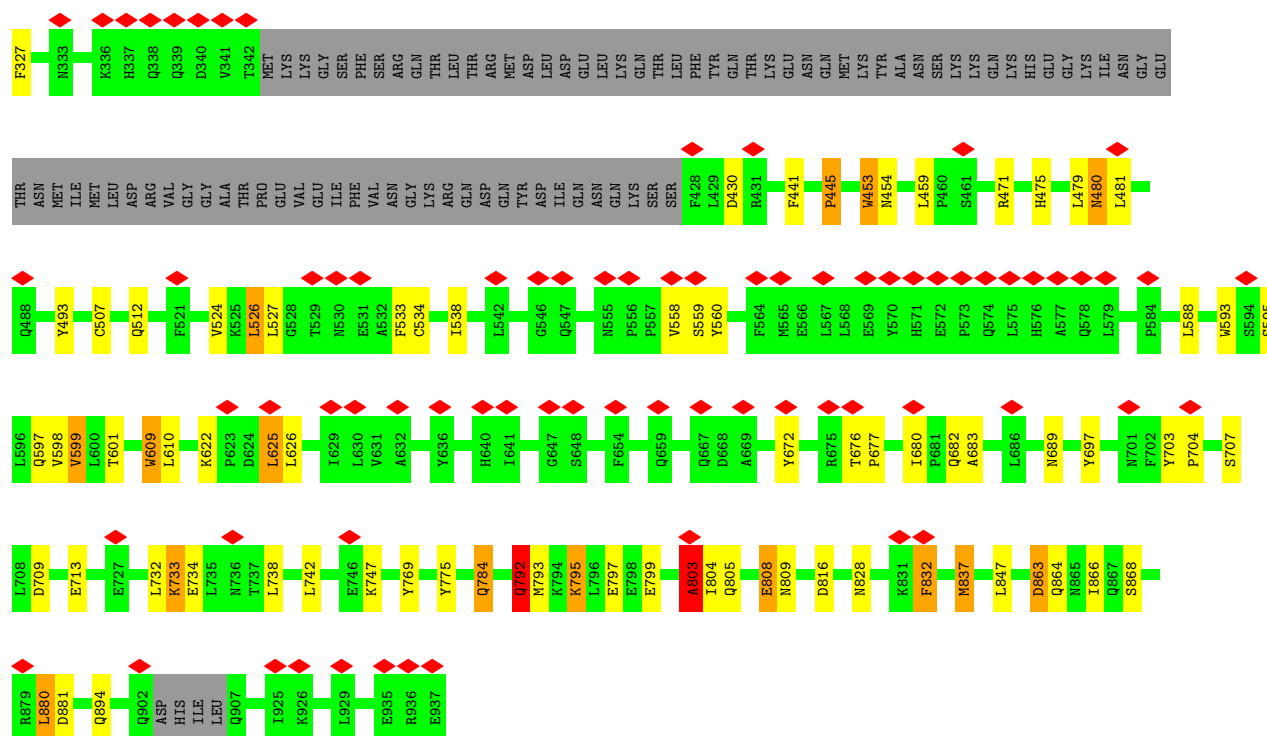
- Molecule 3: Rab-GAP TBC domain-containing protein



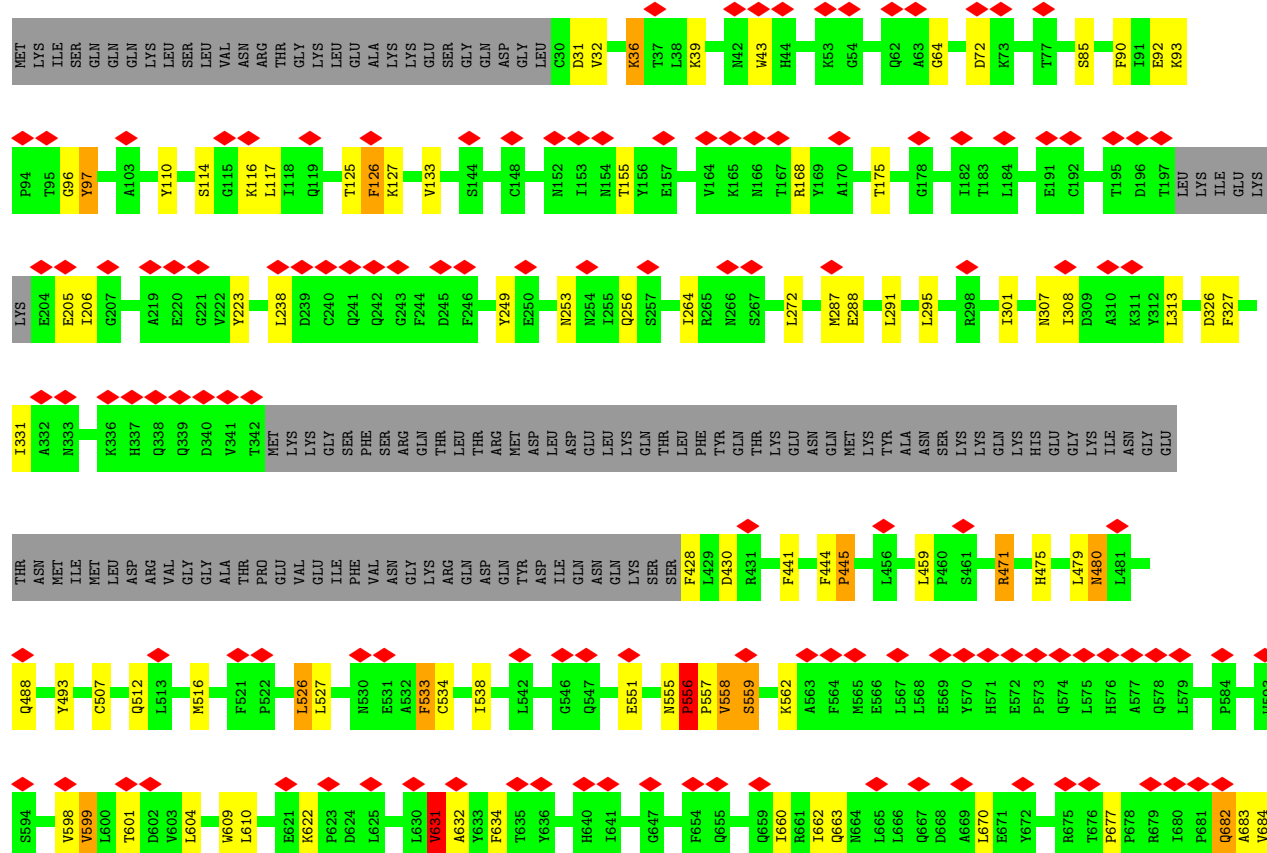
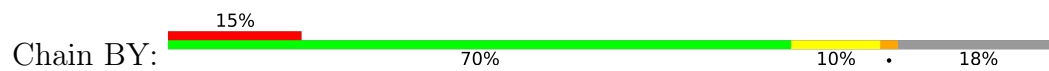
- Molecule 3: Rab-GAP TBC domain-containing protein

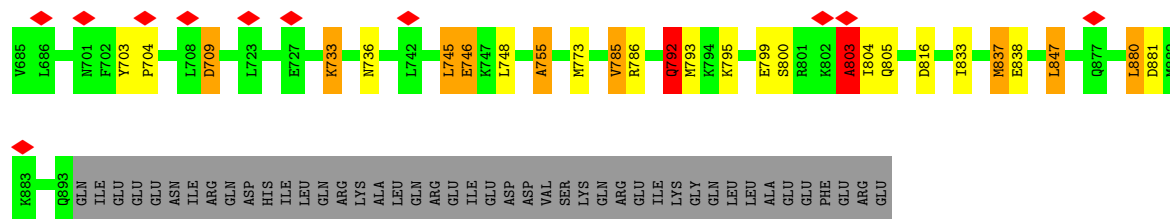






• Molecule 3: Rab-GAP TBC domain-containing protein

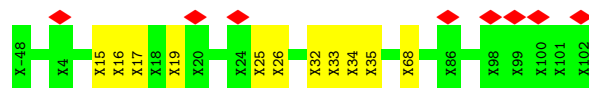
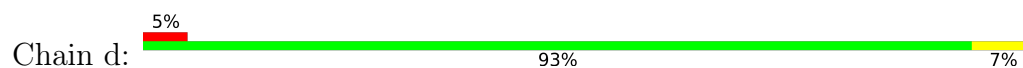




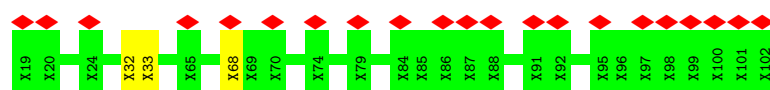
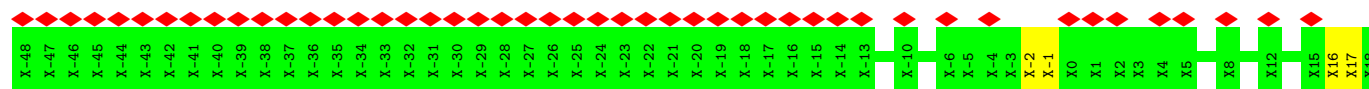
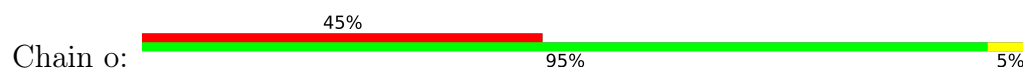
- Molecule 4: Unknown Protein Chain



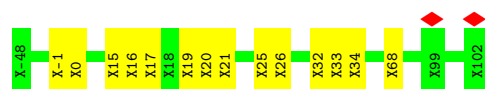
- Molecule 4: Unknown Protein Chain



- Molecule 4: Unknown Protein Chain



- Molecule 4: Unknown Protein Chain



- Molecule 4: Unknown Protein Chain



- Molecule 4: Unknown Protein Chain

Category	Percentage
Used a mobile app to manage their account	94%
Did not use a mobile app to manage their account	6%



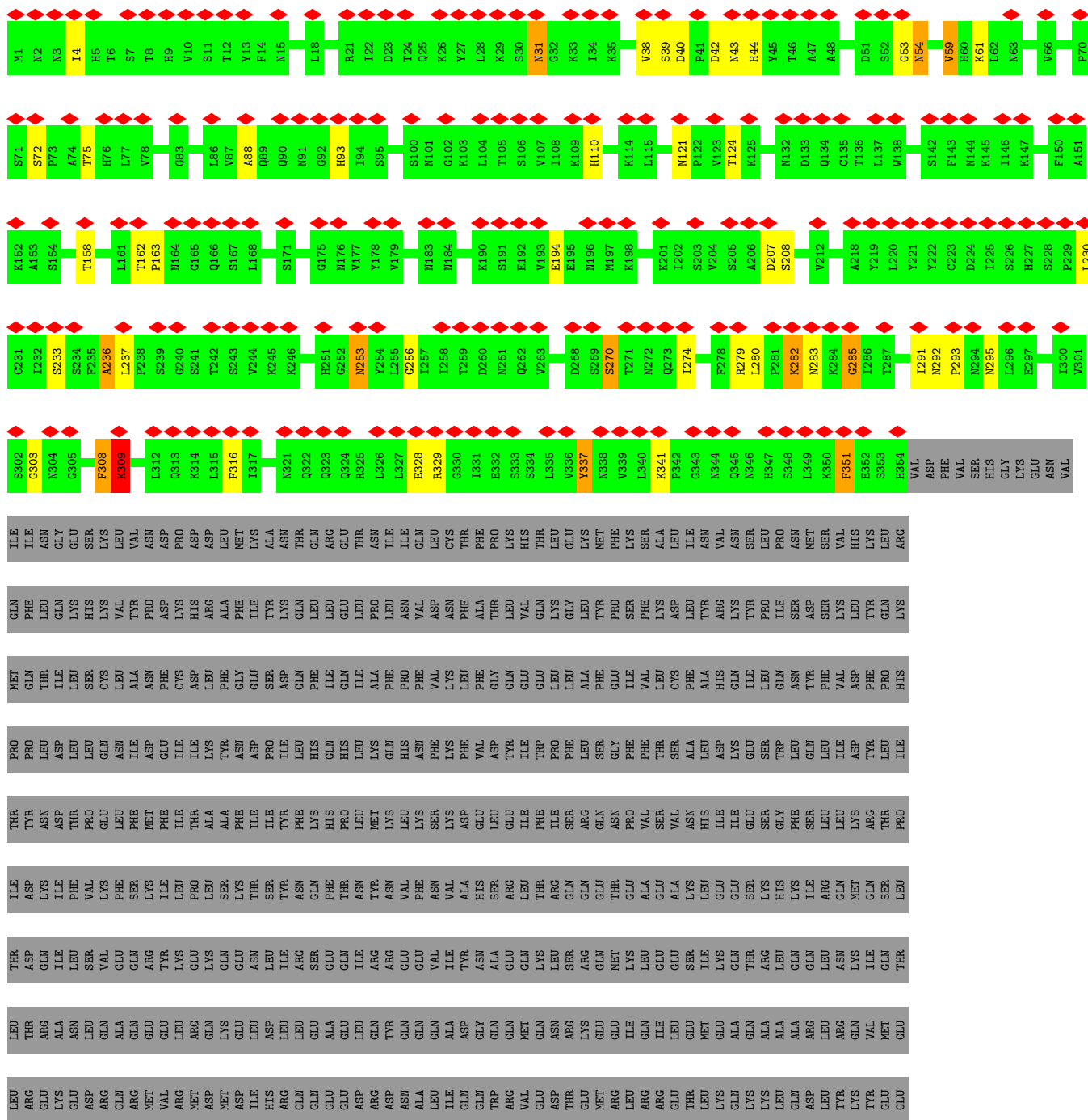
Group	Percentage
All respondents	29%
Men	29%
Women	66%





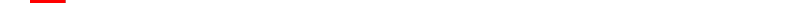
ASN	PHE	GLN	ARG	ASN	GLU	HIS	THR	LYS	MET	PRO	SER	GLY	ILE	ASN	GLN	GLU	GLY	GLY	GLN	THR	ASP	MET	GLU	GLN
GLN	ARG	LEU	GLN	GLU	GLN	MET	GLN	LEU	GLN	ILE	ARG	GLU	THR	ASP	GLN	MET	ASN	GLN	LYS	LEU	GLU	THR	ILE	GLN

- Molecule 5: TBC1 domain family member 31



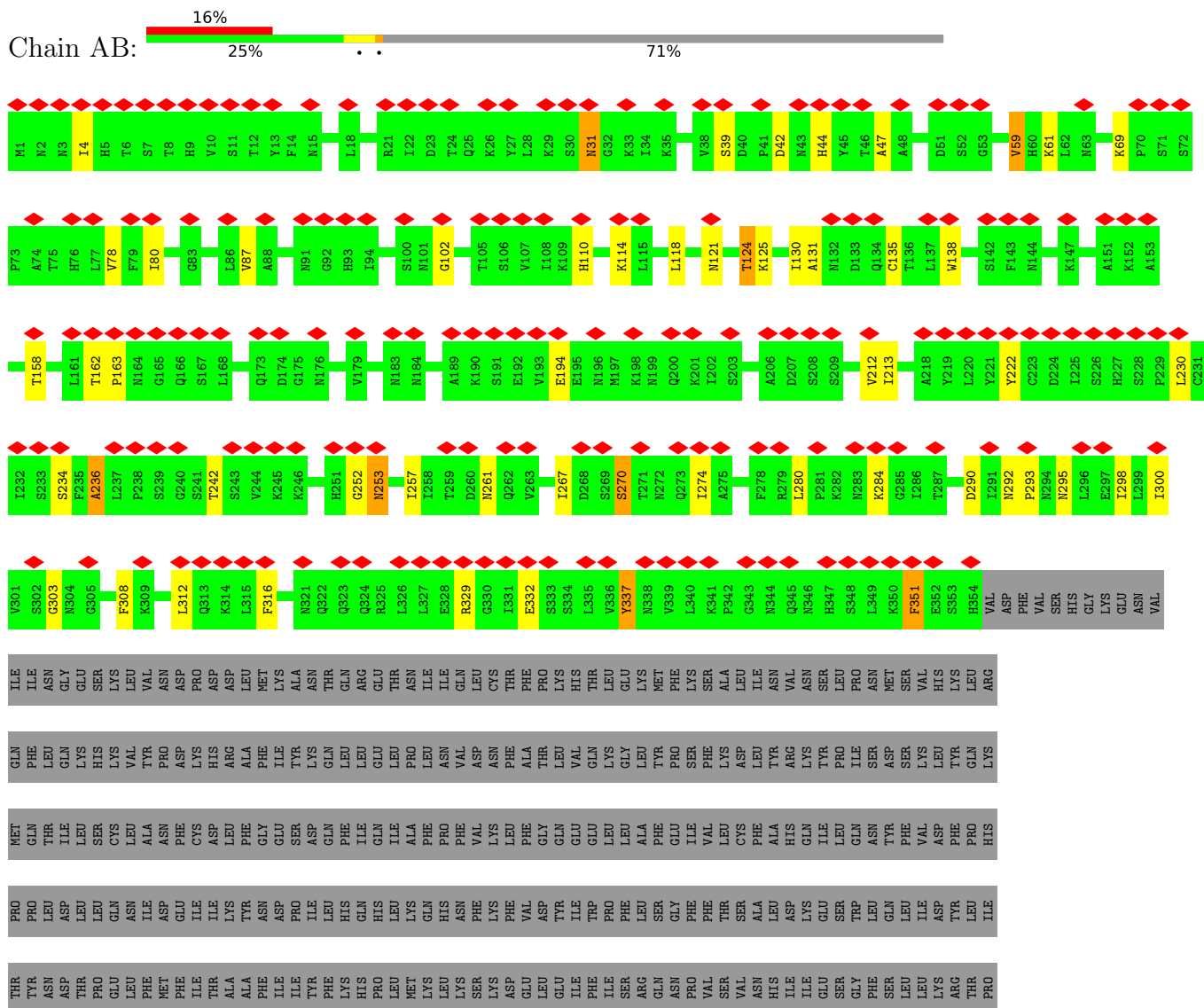
[illegible]

- Molecule 5: TBC1 domain family member 31

Chain γ : 

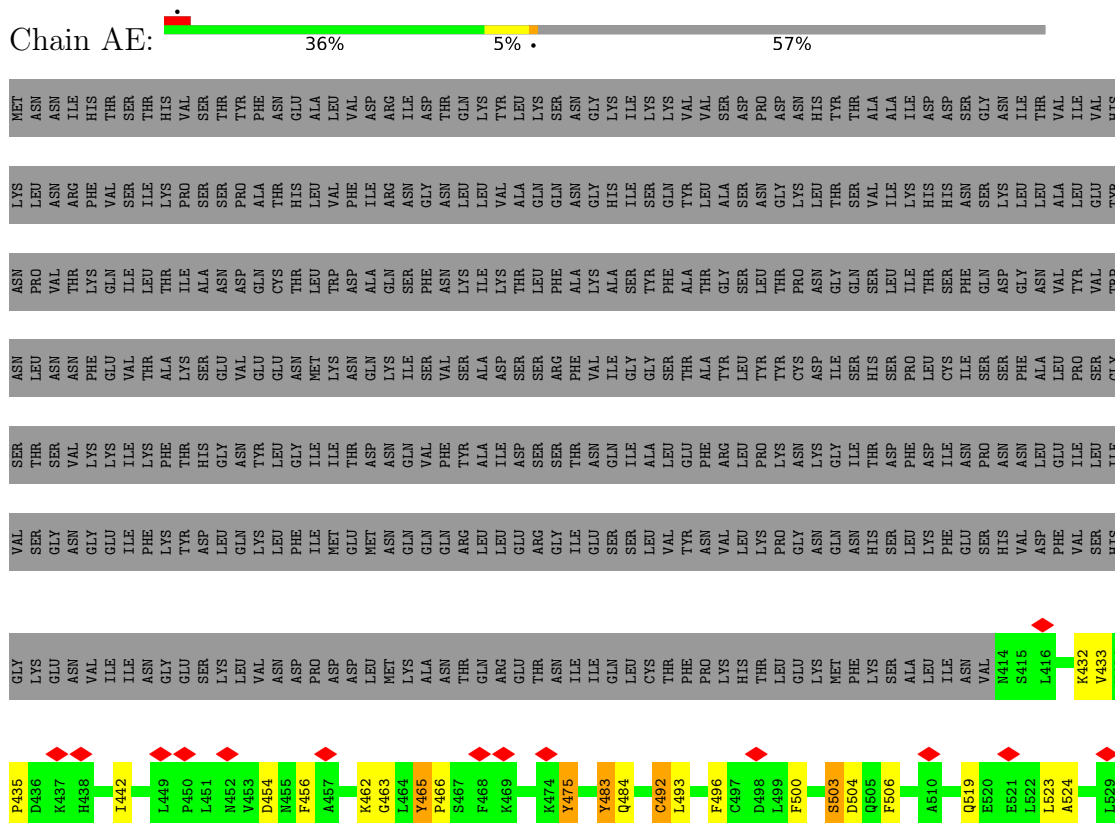
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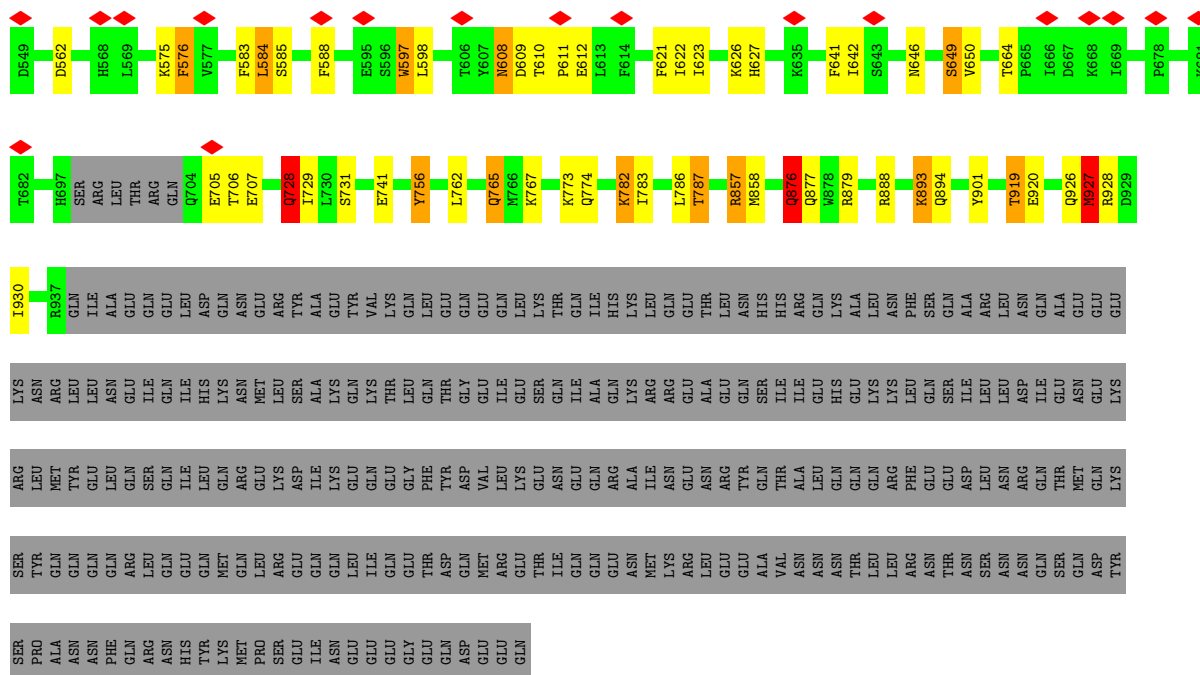
- Molecule 5: TBC1 domain family member 31



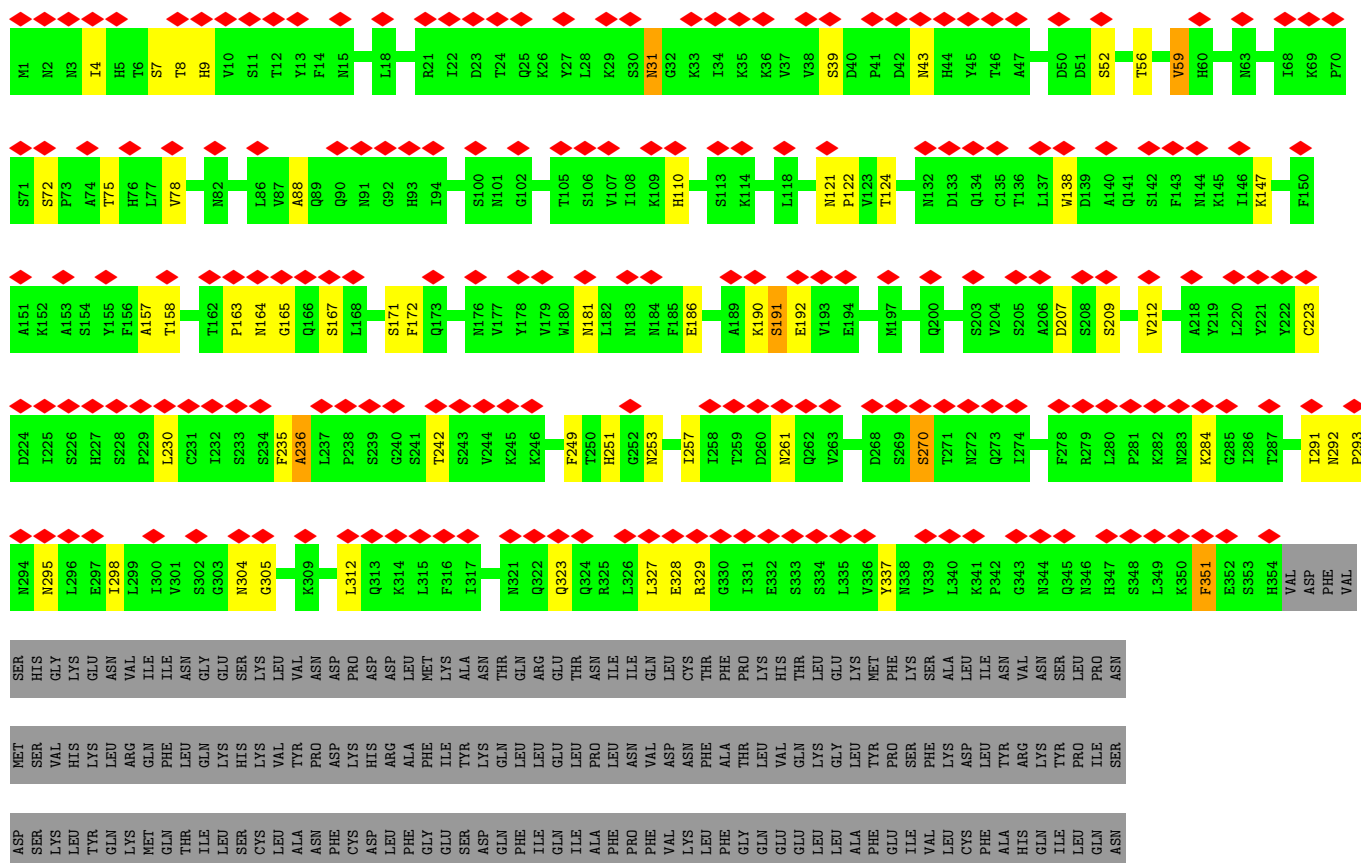
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- Molecule 5: TBC1 domain family member 31



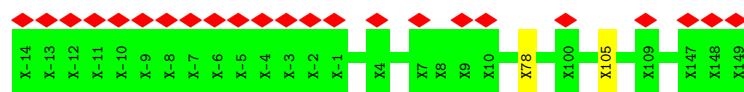


• Molecule 5: TBC1 domain family member 31

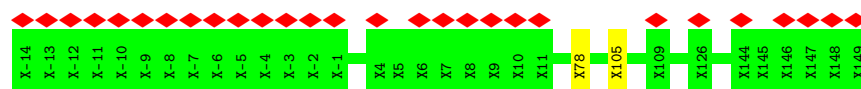




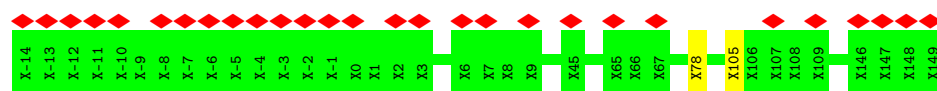




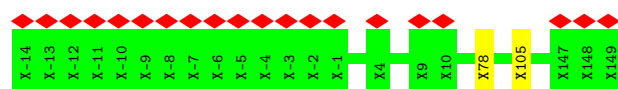
• Molecule 6: Unknown Protein Chain



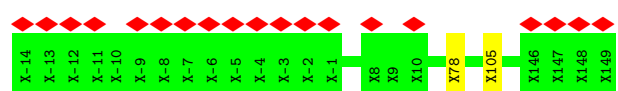
• Molecule 6: Unknown Protein Chain



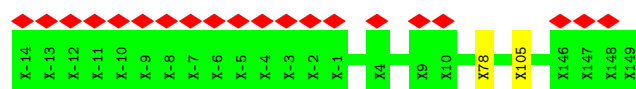
• Molecule 6: Unknown Protein Chain



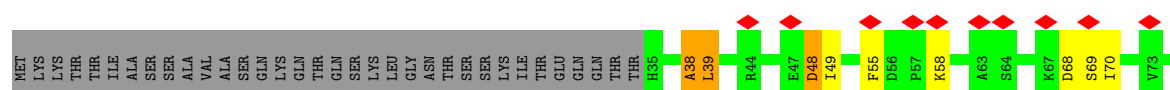
• Molecule 6: Unknown Protein Chain

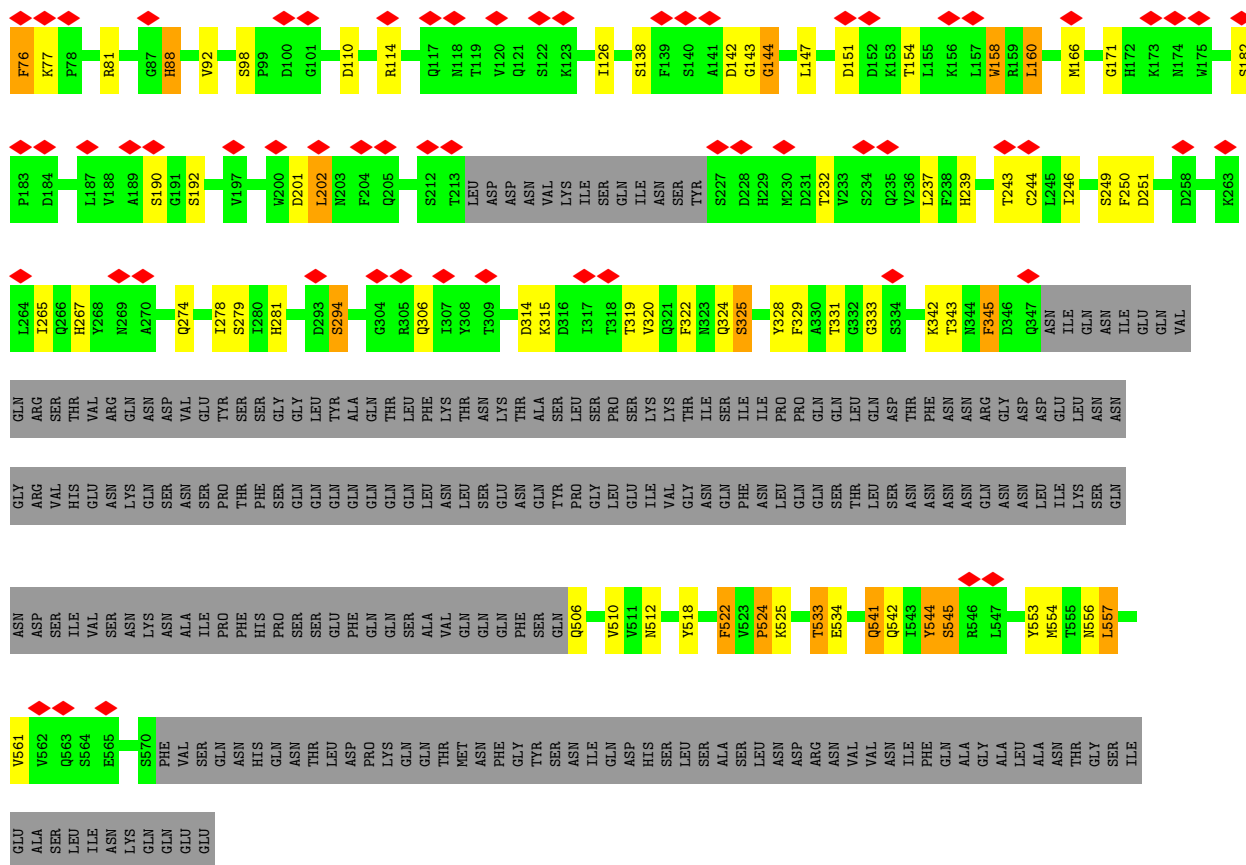


• Molecule 6: Unknown Protein Chain



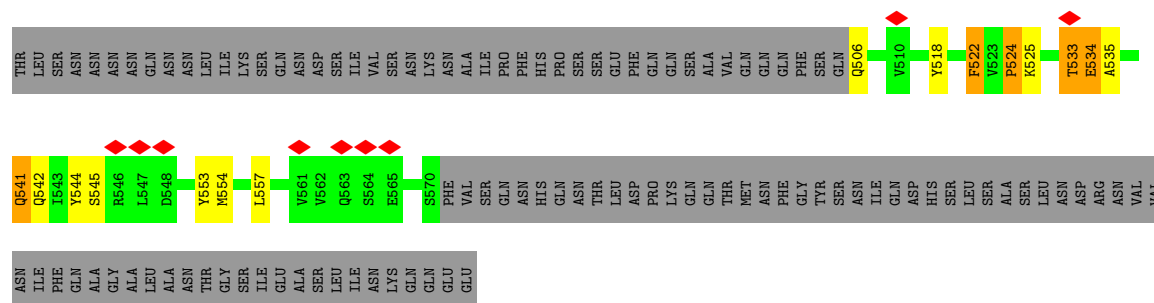
• Molecule 7: POC1 centriolar protein homolog



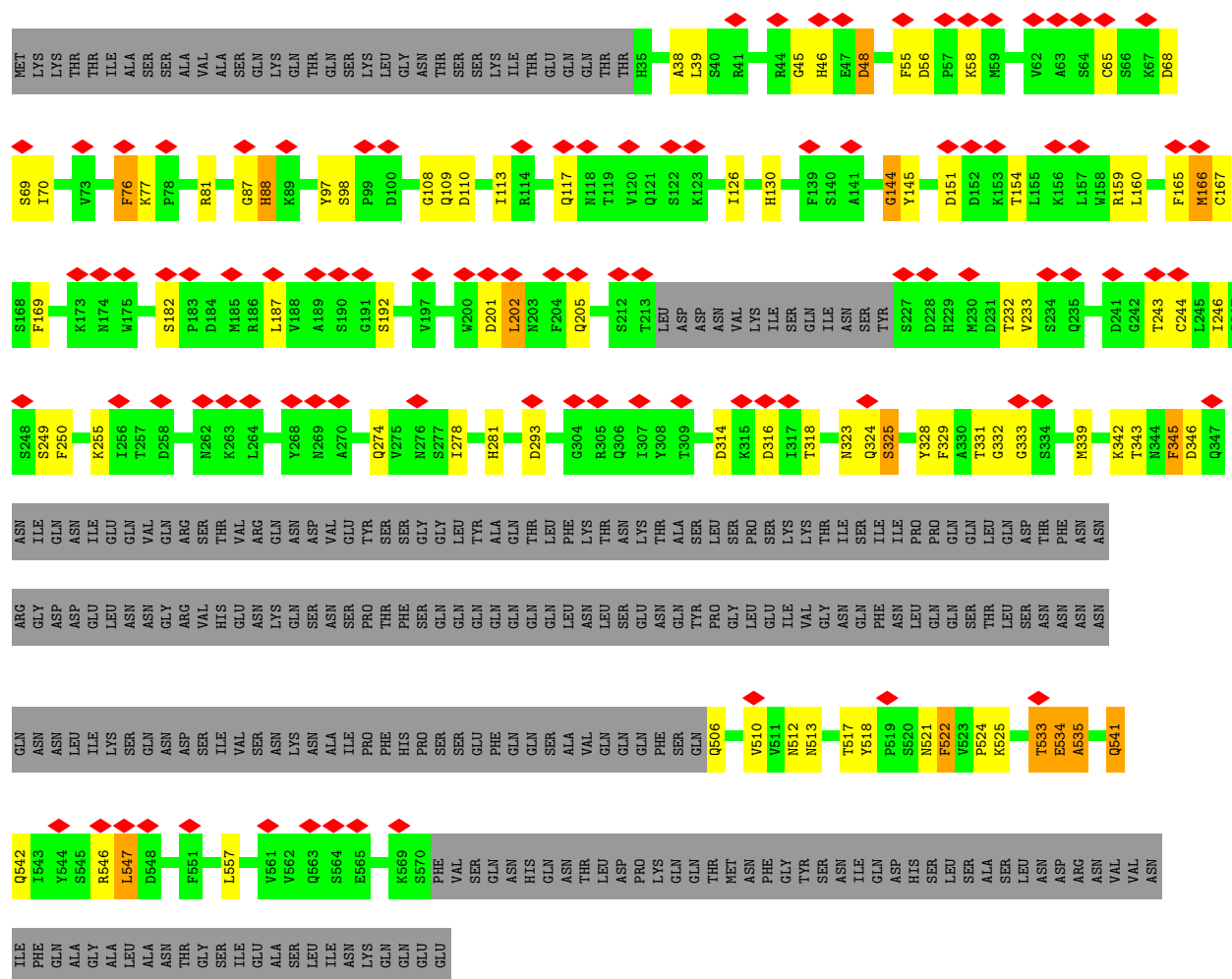
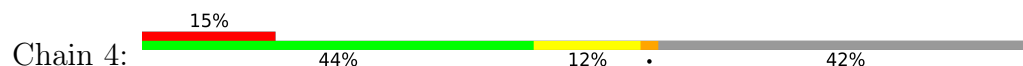


• Molecule 7: POC1 centriolar protein homolog

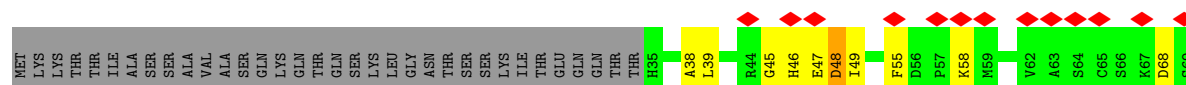
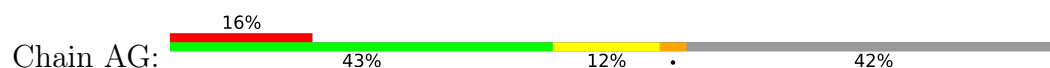


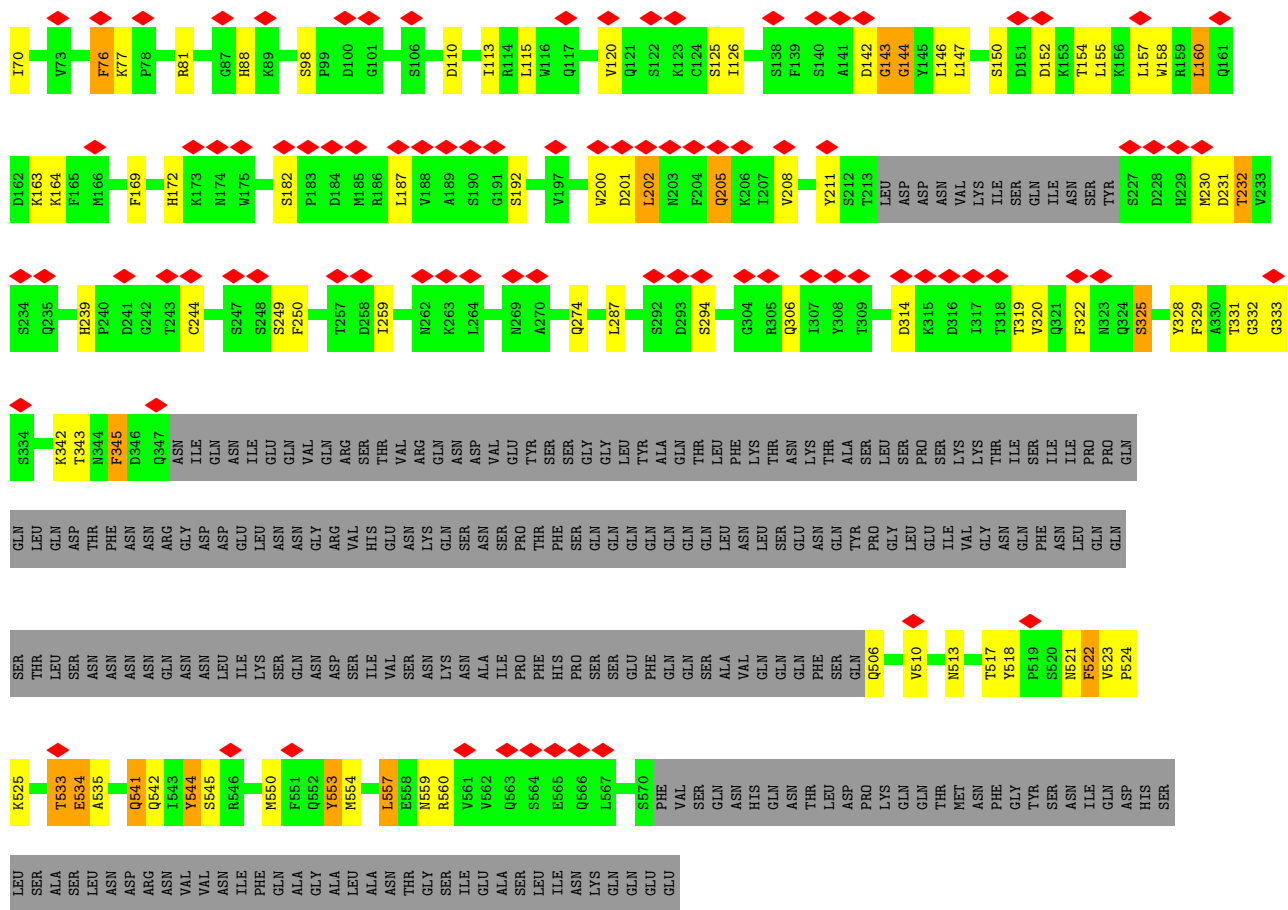


- Molecule 7: POC1 centriolar protein homolog

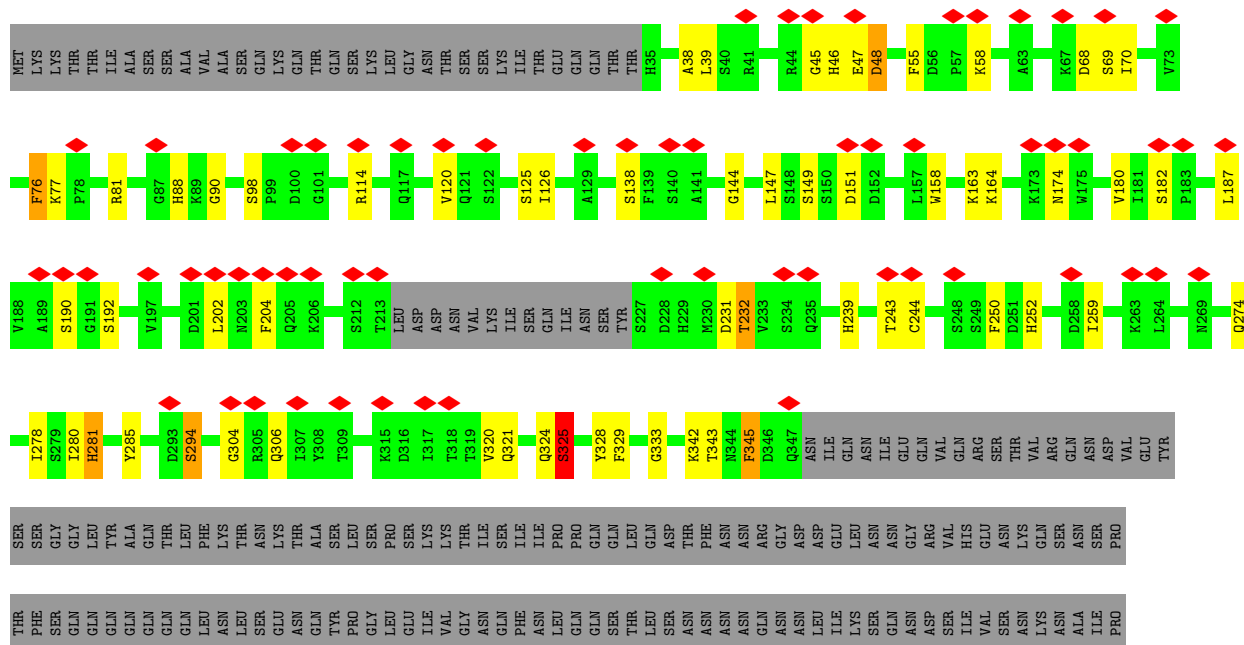


- Molecule 7: POC1 centriolar protein homolog

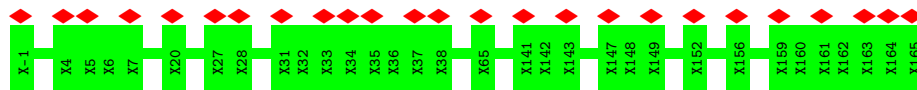




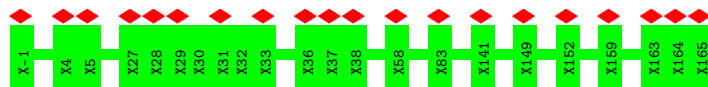
• Molecule 7: POC1 centriolar protein homolog



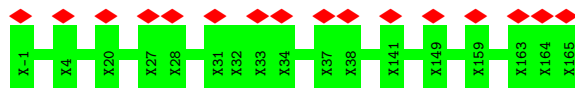
- Molecule 8: Unknown Protein Chain



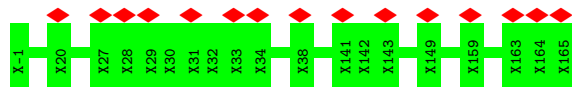
- Molecule 8: Unknown Protein Chain



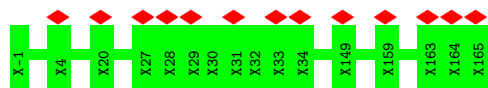
- Molecule 8: Unknown Protein Chain



- Molecule 8: Unknown Protein Chain



- Molecule 8: Unknown Protein Chain

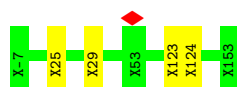


- Molecule 9: Unknown Protein Chain



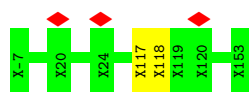
There are no outlier residues recorded for this chain.

- Molecule 9: Unknown Protein Chain



- Molecule 9: Unknown Protein Chain

Chain AC:  99%



- Molecule 9: Unknown Protein Chain

Chain Bj:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown Protein Chain

Chain Bu:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown Protein Chain

Chain CH:  100%

There are no outlier residues recorded for this chain.

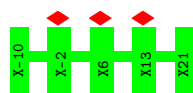
- Molecule 10: Unknown Protein Chain

Chain P:  100%



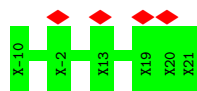
- Molecule 10: Unknown Protein Chain

Chain U:  9% 100%



- Molecule 10: Unknown Protein Chain

Chain AJ:  12% 100%



- Molecule 10: Unknown Protein Chain

Chain AW:  100%



- Molecule 10: Unknown Protein Chain

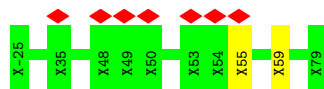


- Molecule 10: Unknown Protein Chain

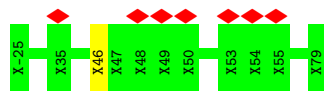


There are no outlier residues recorded for this chain.

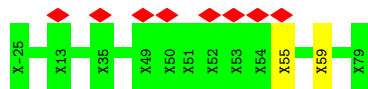
- Molecule 11: Unknown Protein Chain



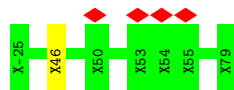
- Molecule 11: Unknown Protein Chain



- Molecule 11: Unknown Protein Chain

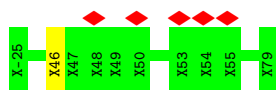


- Molecule 11: Unknown Protein Chain

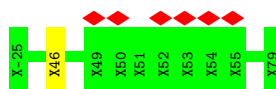


- Molecule 11: Unknown Protein Chain

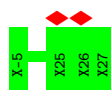




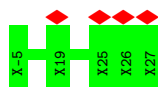
- Molecule 11: Unknown Protein Chain



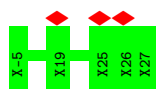
- Molecule 12: Unknown Protein Chain



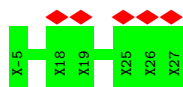
- Molecule 12: Unknown Protein Chain



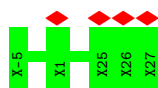
- Molecule 12: Unknown Protein Chain



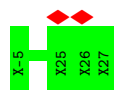
- Molecule 12: Unknown Protein Chain



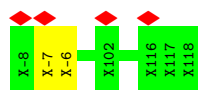
- Molecule 12: Unknown Protein Chain



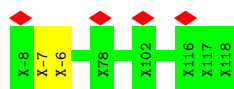
- Molecule 12: Unknown Protein Chain



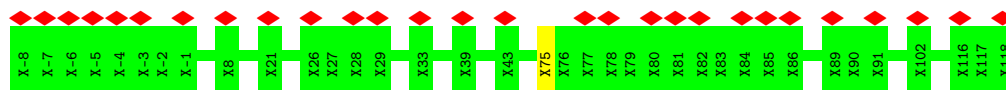
- Molecule 13: Unknown Protein Chain



- Molecule 13: Unknown Protein Chain



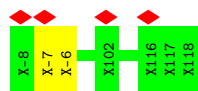
- Molecule 13: Unknown Protein Chain



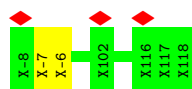
- Molecule 13: Unknown Protein Chain



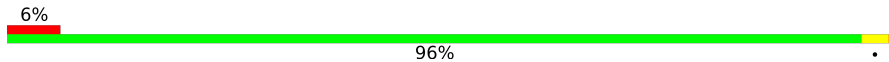
- Molecule 13: Unknown Protein Chain

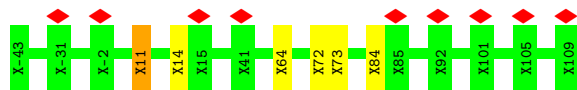


- Molecule 13: Unknown Protein Chain

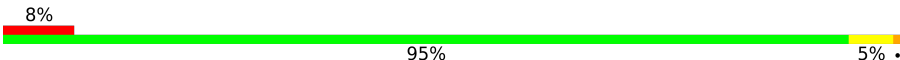


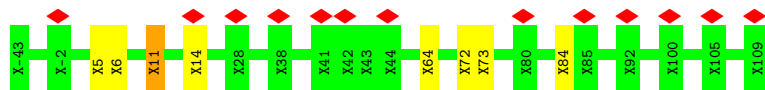
• Molecule 14: Unknown Protein Chain

Chain V:  6% 96%

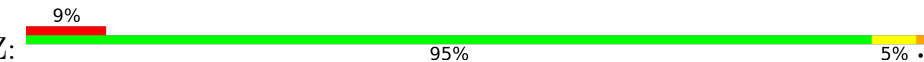


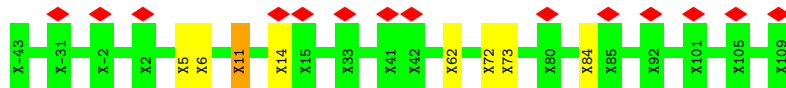
• Molecule 14: Unknown Protein Chain

Chain a:  8% 95% 5%

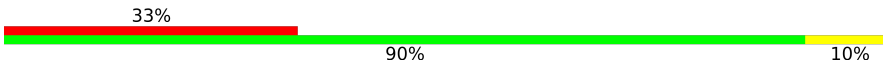


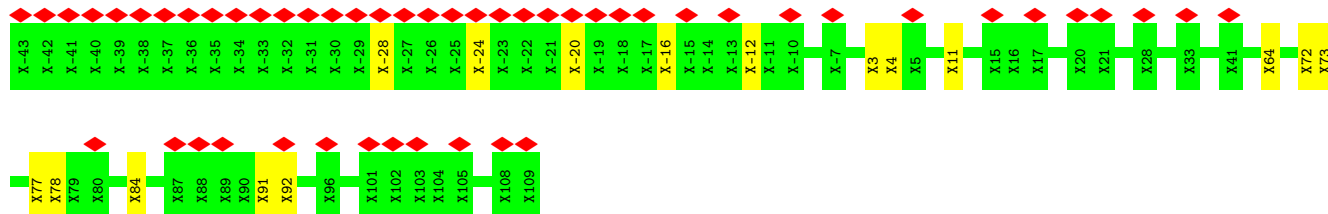
• Molecule 14: Unknown Protein Chain

Chain AZ:  9% 95% 5%

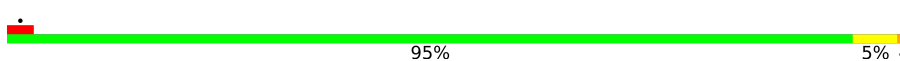


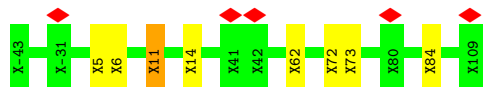
• Molecule 14: Unknown Protein Chain

Chain Am:  33% 90% 10%

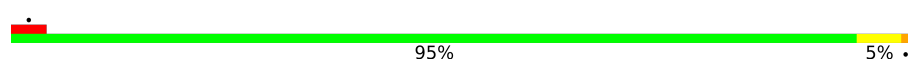


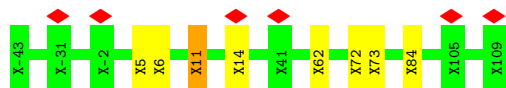
• Molecule 14: Unknown Protein Chain

Chain As:  1% 95% 5%

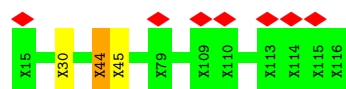


• Molecule 14: Unknown Protein Chain

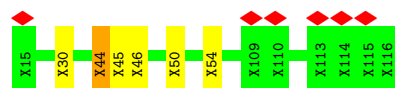
Chain CE:  1% 95% 5%



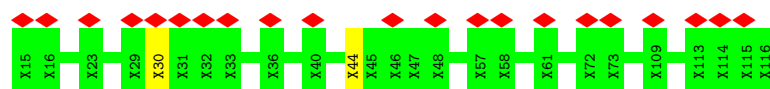
• Molecule 15: Unknown Protein Chain



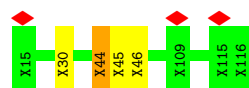
- Molecule 15: Unknown Protein Chain



- Molecule 15: Unknown Protein Chain



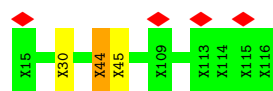
- Molecule 15: Unknown Protein Chain



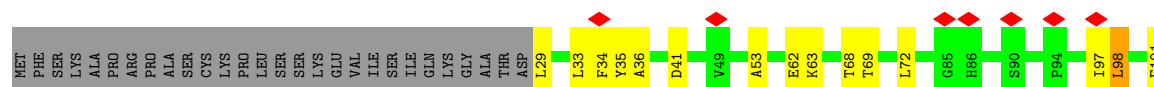
- Molecule 15: Unknown Protein Chain

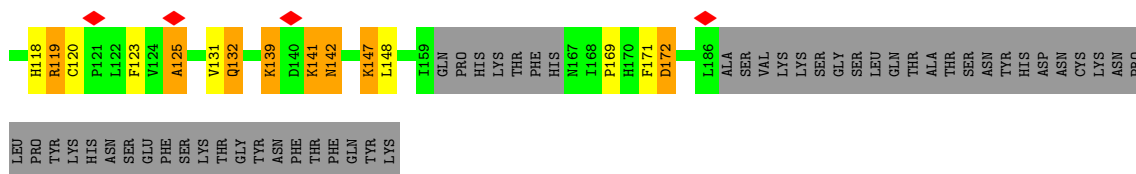


- Molecule 15: Unknown Protein Chain

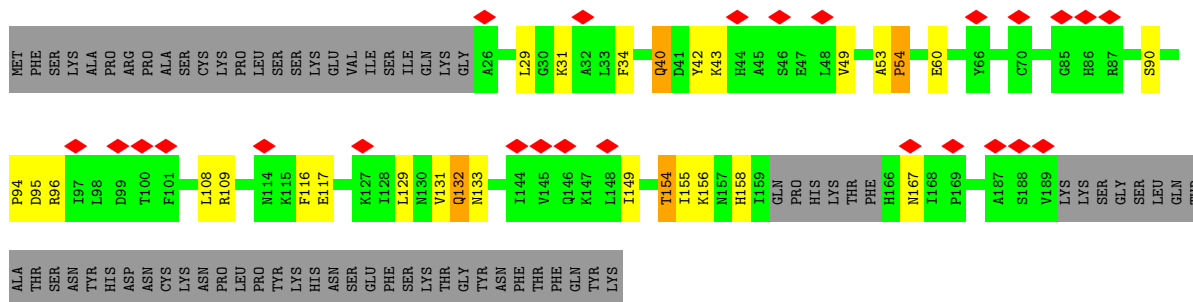


- Molecule 16: SWIM-type domain-containing protein

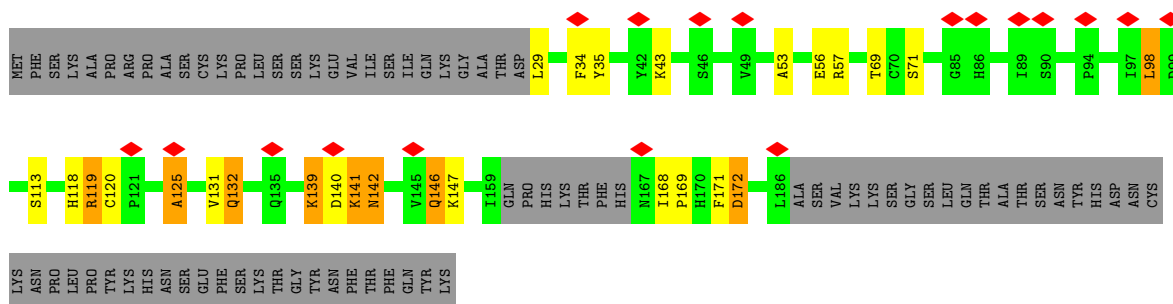




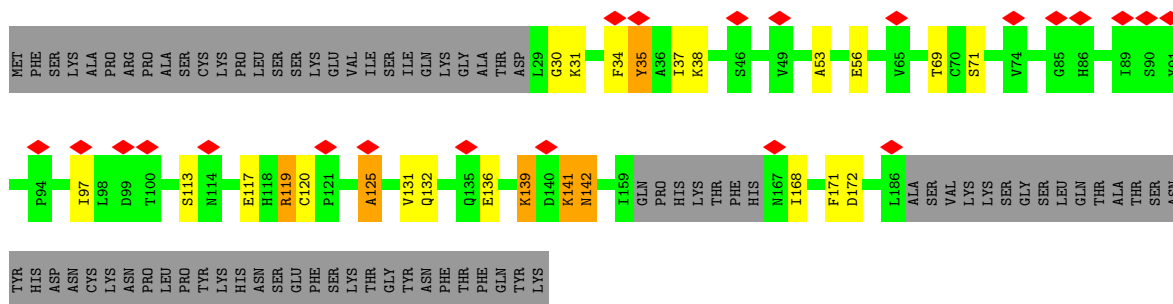
- Molecule 16: SWIM-type domain-containing protein



- Molecule 16: SWIM-type domain-containing protein

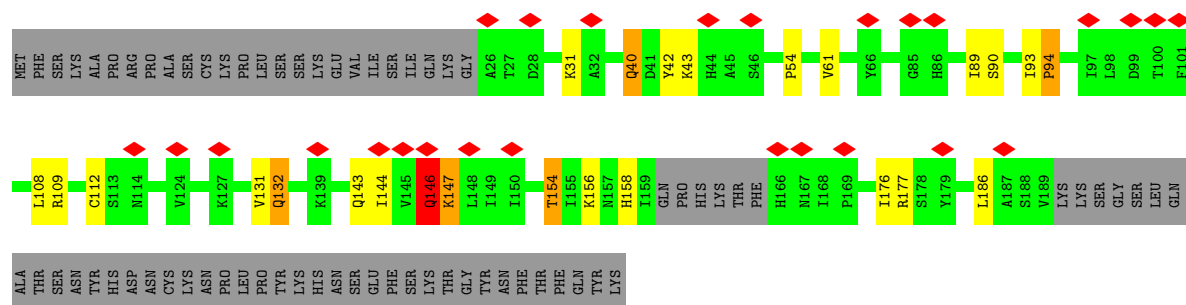


- Molecule 16: SWIM-type domain-containing protein

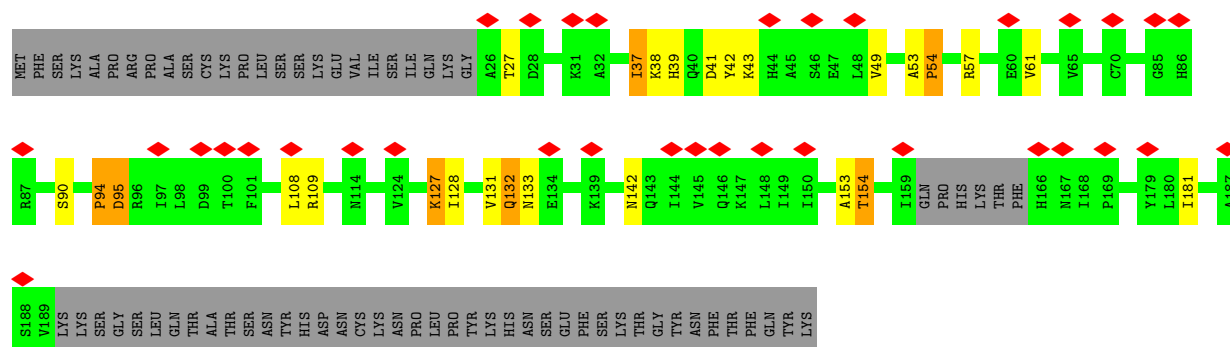


- Molecule 16: SWIM-type domain-containing protein

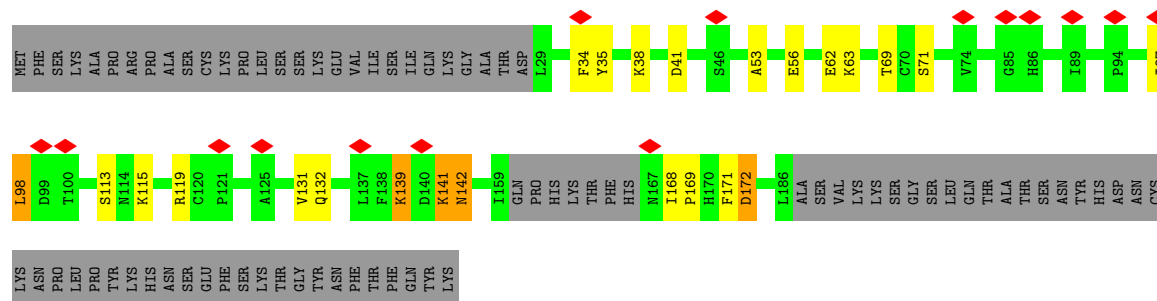




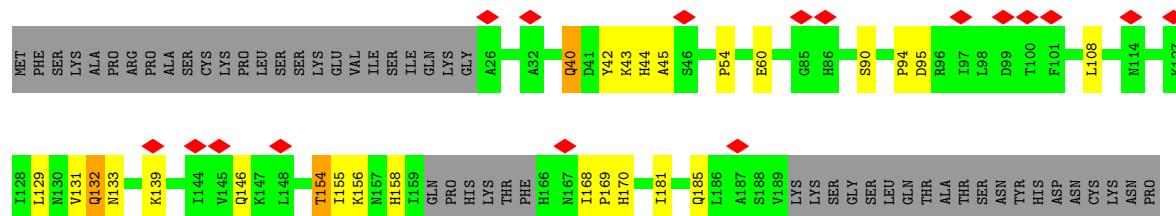
• Molecule 16: SWIM-type domain-containing protein



• Molecule 16: SWIM-type domain-containing protein



• Molecule 16: SWIM-type domain-containing protein



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- Molecule 16: SWIM-type domain-containing protein



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- Molecule 16: SWIM-type domain-containing protein



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- Molecule 16: SWIM-type domain-containing protein



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- Molecule 16: SWIM-type domain-containing protein



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S90
I93
P94
I97



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155485	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	13.599	Depositor
Minimum map value	0.000	Depositor
Average map value	0.223	Depositor
Map value standard deviation	1.035	Depositor
Recommended contour level	5	Depositor
Map size (Å)	631.2, 631.2, 631.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.315, 1.315, 1.315	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	1.44	3/2127 (0.1%)	1.93	50/2965 (1.7%)
1	BD	1.53	4/2127 (0.2%)	1.91	42/2965 (1.4%)
1	C	1.50	1/2127 (0.0%)	1.87	48/2965 (1.6%)
1	CP	1.55	2/2127 (0.1%)	1.99	53/2965 (1.8%)
1	Ca	1.51	2/2127 (0.1%)	1.96	51/2965 (1.7%)
1	i	1.59	4/2127 (0.2%)	1.88	38/2965 (1.3%)
2	BK	1.32	1/1412 (0.1%)	1.71	33/1969 (1.7%)
2	BR	1.38	0/1285	2.08	43/1793 (2.4%)
2	CW	1.39	4/1412 (0.3%)	1.89	37/1969 (1.9%)
2	Cd	1.45	1/1285 (0.1%)	1.90	47/1793 (2.6%)
2	Ch	1.31	3/1412 (0.2%)	1.74	34/1969 (1.7%)
2	D	1.28	2/1412 (0.1%)	1.74	34/1969 (1.7%)
2	f	1.34	2/1285 (0.2%)	1.92	42/1793 (2.3%)
2	k	1.35	3/1412 (0.2%)	1.90	52/1969 (2.6%)
2	q	1.30	0/1412	1.65	21/1969 (1.1%)
2	s	1.31	0/1285	1.77	39/1793 (2.2%)
2	y	1.42	0/1285	2.07	44/1793 (2.5%)
2	z	1.42	0/1285	2.07	44/1793 (2.5%)
3	1	1.32	1/3079 (0.0%)	1.91	97/4292 (2.3%)
3	7	1.34	6/4036 (0.1%)	1.84	112/5629 (2.0%)
3	BY	1.36	5/3838 (0.1%)	1.93	109/5354 (2.0%)
3	E	1.38	4/3594 (0.1%)	1.91	101/5013 (2.0%)
3	I	1.25	4/4036 (0.1%)	1.88	103/5629 (1.8%)
3	n	1.36	6/3299 (0.2%)	2.00	111/4600 (2.4%)
5	9	1.36	1/1508 (0.1%)	2.02	65/2105 (3.1%)
5	AB	1.40	5/1751 (0.3%)	2.02	74/2439 (3.0%)
5	AE	1.33	1/2582 (0.0%)	1.91	82/3608 (2.3%)
5	AO	1.34	1/1751 (0.1%)	1.94	64/2439 (2.6%)
5	AU	1.38	9/1751 (0.5%)	1.99	70/2439 (2.9%)
5	Bf	1.33	0/2332	1.87	71/3258 (2.2%)
5	Bt	1.40	4/1751 (0.2%)	2.07	69/2439 (2.8%)
5	G	1.38	2/2062 (0.1%)	1.96	75/2880 (2.6%)
5	L	1.24	0/2582	1.88	91/3608 (2.5%)
5	M	1.39	6/1751 (0.3%)	2.00	64/2439 (2.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	R	1.29	1/1751 (0.1%)	1.94	55/2439 (2.3%)
5	v	1.35	0/1788	2.04	68/2497 (2.7%)
7	4	1.55	8/1803 (0.4%)	2.06	81/2508 (3.2%)
7	AG	1.55	12/1803 (0.7%)	2.10	90/2508 (3.6%)
7	AM	1.55	2/1803 (0.1%)	2.05	74/2508 (3.0%)
7	Bm	1.51	5/1803 (0.3%)	2.08	84/2508 (3.3%)
7	J	1.52	11/1803 (0.6%)	2.09	80/2508 (3.2%)
7	O	1.44	5/1803 (0.3%)	1.91	53/2508 (2.1%)
16	A7	1.49	1/781 (0.1%)	2.03	26/1086 (2.4%)
16	Ai	1.38	0/746	2.02	35/1037 (3.4%)
16	An	1.36	0/746	1.94	26/1037 (2.5%)
16	Aq	1.48	1/781 (0.1%)	2.07	27/1086 (2.5%)
16	Av	1.52	2/781 (0.3%)	2.00	23/1086 (2.1%)
16	Az	1.35	0/746	2.02	25/1037 (2.4%)
16	CB	1.39	1/746 (0.1%)	2.01	28/1037 (2.7%)
16	CI	1.51	1/781 (0.1%)	2.05	29/1086 (2.7%)
16	CM	1.38	0/746	2.09	34/1037 (3.3%)
16	CT	1.54	1/781 (0.1%)	1.99	23/1086 (2.1%)
16	Z	1.39	1/746 (0.1%)	2.16	34/1037 (3.3%)
16	c	1.52	1/781 (0.1%)	1.96	22/1086 (2.0%)
All	All	1.40	140/94166 (0.1%)	1.95	3027/131255 (2.3%)

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	7
1	BD	0	7
1	C	0	5
1	CP	0	7
1	Ca	0	8
1	i	0	6
2	BK	0	9
2	BR	0	10
2	CW	0	11
2	Cd	0	15
2	Ch	0	11
2	D	0	8
2	f	0	11
2	k	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	q	0	7
2	s	0	10
2	y	0	11
2	z	0	11
3	1	0	10
3	7	0	18
3	BY	0	18
3	E	0	17
3	I	0	18
3	n	0	12
4	BO	0	1
4	BZ	0	1
4	Bw	0	1
4	F	0	1
4	d	0	1
4	o	0	1
5	9	0	9
5	AB	0	9
5	AE	0	18
5	AO	0	9
5	AU	0	9
5	Bf	0	11
5	Bt	0	8
5	G	0	12
5	L	0	17
5	M	0	9
5	R	0	11
5	v	0	10
6	B4	0	3
6	BV	0	3
6	Bg	0	3
6	H	0	3
6	l	0	3
6	w	0	3
7	4	0	13
7	AG	0	10
7	AM	0	13
7	Bm	0	13
7	J	0	10
7	O	0	12
11	0	0	1
11	B2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	Bq	0	1
11	CO	0	1
13	AS	0	1
14	AZ	0	3
14	Am	0	3
14	As	0	3
14	CE	0	3
14	V	0	3
14	a	0	3
15	AP	0	2
15	Aa	0	2
15	B5	0	2
15	CF	0	2
15	Cc	0	2
15	W	0	2
16	A7	0	5
16	Ai	0	5
16	An	0	5
16	Aq	0	6
16	Av	0	6
16	Az	0	3
16	CB	0	5
16	CI	0	5
16	CM	0	4
16	CT	0	5
16	Z	0	5
16	c	0	5
All	All	0	579

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	n	752	LYS	CA-C	9.79	1.57	1.52
7	4	144	GLY	CA-C	-7.76	1.43	1.52
5	Bt	283	ASN	CA-C	-7.34	1.43	1.53
1	Ca	204	PHE	CA-C	-7.05	1.44	1.52
7	4	130	HIS	CA-C	-6.99	1.49	1.53
2	Cd	70	LEU	CA-C	-6.63	1.47	1.52
7	Bm	154	THR	CA-C	-6.55	1.44	1.53
2	D	34	LEU	CA-C	-6.45	1.44	1.52
7	4	154	THR	CA-C	-6.41	1.44	1.52
2	CW	325	ILE	N-CA	-6.34	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	88	ALA	CA-C	-6.32	1.45	1.52
7	AG	314	ASP	CA-C	-6.27	1.46	1.53
1	i	198	SER	CA-C	-6.23	1.45	1.52
5	AU	300	ILE	CA-C	-6.17	1.45	1.52
7	Bm	172	HIS	CA-C	-6.17	1.45	1.52
1	BD	198	SER	CA-C	-6.16	1.45	1.52
5	Bt	88	ALA	CA-C	-6.14	1.45	1.52
5	AB	47	ALA	CA-C	-6.10	1.45	1.52
5	AU	181	ASN	CA-CB	-6.10	1.45	1.52
7	4	145	TYR	N-CA	-6.07	1.38	1.46
7	AG	154	THR	CA-C	-6.05	1.44	1.52
5	AB	130	ILE	CA-C	-6.01	1.45	1.52
1	CP	198	SER	CA-C	-5.98	1.45	1.52
7	O	115	LEU	CA-C	-5.97	1.45	1.53
3	E	113	LEU	CA-C	-5.96	1.45	1.52
3	n	773	MET	CA-CB	-5.91	1.43	1.53
5	G	616	PHE	CA-C	-5.87	1.45	1.52
5	AU	301	VAL	CA-C	-5.87	1.45	1.52
5	M	284	LYS	N-CA	-5.85	1.40	1.46
1	C	198	SER	CA-C	-5.84	1.45	1.52
5	AU	295	ASN	CA-C	-5.83	1.45	1.52
5	M	234	SER	CA-CB	-5.83	1.43	1.53
16	Z	132	GLN	CA-C	-5.83	1.47	1.52
7	AG	211	TYR	CA-C	-5.82	1.45	1.52
2	k	26	PRO	CA-C	5.80	1.58	1.53
5	AU	88	ALA	CA-C	-5.75	1.45	1.52
3	7	598	VAL	CA-C	5.75	1.60	1.52
7	J	154	THR	CA-C	-5.74	1.45	1.53
7	AG	172	HIS	CA-C	-5.72	1.45	1.52
5	G	617	ILE	N-CA	-5.71	1.39	1.46
5	R	88	ALA	CA-C	-5.71	1.45	1.52
7	AM	192	SER	CA-CB	-5.70	1.44	1.53
3	1	598	VAL	CA-C	5.65	1.60	1.52
7	J	279	SER	CA-CB	-5.62	1.44	1.53
3	7	272	LEU	CA-C	-5.61	1.45	1.52
5	Bt	300	ILE	CA-C	-5.61	1.46	1.52
16	CB	35	TYR	N-CA	-5.61	1.41	1.46
2	Ch	318	ILE	N-CA	-5.60	1.39	1.46
16	Av	181	ILE	CA-C	-5.60	1.45	1.52
7	J	237	LEU	CA-C	-5.59	1.46	1.52
3	7	234	LEU	CA-C	-5.58	1.46	1.52
7	AG	144	GLY	CA-C	-5.58	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CW	34	LEU	CA-C	-5.57	1.45	1.52
2	Ch	325	ILE	N-CA	-5.57	1.41	1.46
3	n	272	LEU	CA-C	-5.56	1.45	1.52
5	M	88	ALA	CA-CB	-5.49	1.46	1.53
7	AG	115	LEU	CA-C	-5.49	1.45	1.53
2	f	333	LYS	CA-C	-5.44	1.45	1.52
1	Ca	198	SER	CA-C	-5.43	1.46	1.52
5	Bt	234	SER	CA-CB	-5.43	1.44	1.53
3	BY	223	TYR	CA-C	-5.42	1.46	1.52
7	O	43	PHE	CA-C	-5.41	1.46	1.52
3	E	598	VAL	CA-C	5.41	1.59	1.52
1	A	238	VAL	CA-C	-5.38	1.46	1.52
7	J	557	LEU	CA-C	-5.37	1.45	1.52
7	O	506	GLN	C-N	5.37	1.40	1.33
7	AG	287	LEU	CA-C	-5.37	1.46	1.52
3	7	113	LEU	CA-C	-5.37	1.46	1.52
7	Bm	189	ALA	CA-CB	-5.36	1.44	1.53
3	BY	272	LEU	CA-C	-5.34	1.46	1.52
5	AU	301	VAL	CA-CB	-5.34	1.47	1.54
7	4	97	TYR	CA-C	-5.33	1.46	1.52
2	CW	281	ASN	N-CA	-5.32	1.39	1.46
3	BY	598	VAL	CA-C	5.32	1.58	1.52
7	J	518	TYR	N-CA	-5.31	1.42	1.46
1	A	198	SER	CA-C	-5.30	1.46	1.52
2	CW	83	GLU	CA-C	-5.30	1.45	1.52
5	AB	131	ALA	CA-CB	-5.30	1.45	1.53
1	BD	377	ILE	CA-C	-5.30	1.46	1.52
7	4	165	PHE	CA-C	-5.27	1.46	1.52
1	A	377	ILE	CA-C	-5.27	1.46	1.52
1	i	195	VAL	CA-CB	-5.26	1.48	1.54
2	D	83	GLU	CA-C	-5.25	1.45	1.52
7	AG	211	TYR	N-CA	-5.23	1.39	1.46
7	J	319	THR	CA-C	-5.22	1.46	1.52
7	AG	155	LEU	N-CA	-5.22	1.40	1.46
7	AG	147	LEU	CA-C	-5.22	1.45	1.52
3	7	610	LEU	CA-C	-5.22	1.45	1.52
7	AG	319	THR	CA-C	-5.21	1.46	1.52
7	AM	149	SER	CA-CB	-5.21	1.46	1.52
7	O	279	SER	CA-CB	-5.21	1.44	1.53
7	O	518	TYR	N-CA	-5.21	1.42	1.46
16	Aq	54	PRO	CA-C	-5.21	1.46	1.52
3	I	113	LEU	CA-C	-5.20	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BD	154	ARG	CA-C	-5.20	1.46	1.52
3	n	764	ARG	N-CA	-5.18	1.39	1.46
16	A7	181	ILE	CA-C	-5.18	1.46	1.52
3	E	97	TYR	CA-C	-5.17	1.48	1.53
2	k	7	ASN	N-CA	-5.17	1.40	1.46
7	4	323	ASN	CA-C	-5.17	1.46	1.52
5	AU	181	ASN	N-CA	-5.16	1.40	1.46
7	Bm	154	THR	N-CA	-5.16	1.39	1.45
2	Ch	318	ILE	CA-C	-5.16	1.46	1.52
1	CP	238	VAL	CA-C	-5.16	1.46	1.52
7	J	144	GLY	CA-C	-5.15	1.44	1.51
1	i	204	PHE	CA-C	-5.15	1.46	1.52
16	Av	41	ASP	CA-C	-5.14	1.47	1.53
7	AG	320	VAL	N-CA	-5.13	1.40	1.46
3	BY	249	TYR	CA-C	-5.13	1.46	1.52
2	BK	34	LEU	CA-C	-5.12	1.46	1.52
7	J	237	LEU	CA-CB	-5.12	1.45	1.53
3	n	598	VAL	CA-C	5.12	1.59	1.52
5	AE	500	PHE	CA-C	-5.12	1.46	1.52
7	Bm	149	SER	CA-CB	-5.11	1.46	1.52
5	AB	234	SER	CA-CB	-5.10	1.44	1.53
3	7	223	TYR	CA-C	-5.10	1.46	1.52
1	BD	238	VAL	CA-C	-5.10	1.46	1.52
5	M	47	ALA	CA-C	-5.09	1.46	1.52
5	AU	155	TYR	CA-C	-5.09	1.46	1.52
16	c	34	PHE	CA-C	-5.09	1.45	1.52
3	I	806	ILE	N-CA	-5.09	1.40	1.46
7	J	320	VAL	N-CA	-5.09	1.40	1.46
3	I	272	LEU	CA-C	-5.09	1.46	1.52
5	AU	301	VAL	N-CA	-5.09	1.40	1.46
7	4	192	SER	CA-CB	-5.09	1.46	1.53
3	E	272	LEU	CA-C	-5.08	1.46	1.52
7	J	192	SER	CA-CB	-5.08	1.45	1.53
3	n	98	LEU	CA-C	-5.07	1.46	1.52
7	J	92	VAL	CA-CB	-5.06	1.48	1.54
2	f	70	LEU	CA-C	-5.06	1.48	1.52
5	AB	131	ALA	CA-C	-5.05	1.46	1.52
5	9	610	THR	N-CA	-5.05	1.42	1.46
3	I	598	VAL	CA-C	5.05	1.59	1.52
1	i	7	ILE	CA-C	-5.04	1.47	1.52
5	M	242	THR	CA-C	-5.04	1.49	1.52
5	AO	88	ALA	CA-C	-5.04	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	CI	34	PHE	CA-CB	-5.03	1.45	1.53
2	k	32	ALA	CA-CB	-5.03	1.46	1.52
3	BY	168	ARG	CA-C	-5.03	1.48	1.53
16	CT	34	PHE	CA-CB	-5.02	1.45	1.53

All (3027) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	GLU	CA-C-O	-35.50	84.00	120.92
1	BD	301	GLU	CA-C-O	-35.40	84.11	120.92
1	i	301	GLU	CA-C-O	-33.51	84.04	121.58
1	CP	301	GLU	CA-C-O	-33.50	84.06	121.58
1	Ca	301	GLU	CA-C-O	-33.44	84.12	121.58
1	C	301	GLU	CA-C-O	-33.40	84.18	121.58
2	BR	294	GLN	CA-C-N	22.26	149.38	120.44
2	BR	294	GLN	C-N-CA	22.26	149.38	120.44
3	BY	773	MET	CA-C-N	22.12	150.52	120.44
3	BY	773	MET	C-N-CA	22.12	150.52	120.44
2	CW	280	ILE	CA-C-N	20.91	161.48	121.54
2	CW	280	ILE	C-N-CA	20.91	161.48	121.54
2	f	294	GLN	CA-C-N	20.81	148.74	120.44
2	f	294	GLN	C-N-CA	20.81	148.74	120.44
1	CP	68	SER	CA-C-N	20.58	151.59	120.31
1	CP	68	SER	C-N-CA	20.58	151.59	120.31
3	I	773	MET	CA-C-N	20.44	149.31	120.29
3	I	773	MET	C-N-CA	20.44	149.31	120.29
3	n	584	PRO	CA-C-N	19.70	146.68	120.28
3	n	584	PRO	C-N-CA	19.70	146.68	120.28
2	z	294	GLN	CA-C-N	19.43	146.86	120.44
2	z	294	GLN	C-N-CA	19.43	146.86	120.44
2	y	294	GLN	CA-C-N	19.38	146.80	120.44
2	y	294	GLN	C-N-CA	19.38	146.80	120.44
3	E	773	MET	CA-C-N	19.11	147.43	120.29
3	E	773	MET	C-N-CA	19.11	147.43	120.29
2	y	29	ILE	CA-C-N	18.04	153.47	122.26
2	y	29	ILE	C-N-CA	18.04	153.47	122.26
2	z	29	ILE	CA-C-N	18.04	153.47	122.26
2	z	29	ILE	C-N-CA	18.04	153.47	122.26
5	v	433	VAL	N-CA-C	17.07	127.53	111.48
16	Az	35	TYR	CA-C-N	16.92	153.86	121.54
16	Az	35	TYR	C-N-CA	16.92	153.86	121.54
7	J	557	LEU	N-CA-C	-16.38	85.03	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Ai	35	TYR	CA-C-N	16.21	152.49	121.54
16	Ai	35	TYR	C-N-CA	16.21	152.49	121.54
16	Z	35	TYR	CA-C-N	16.15	152.38	121.54
16	Z	35	TYR	C-N-CA	16.15	152.38	121.54
16	CM	35	TYR	CA-C-N	15.73	151.59	121.54
16	CM	35	TYR	C-N-CA	15.73	151.59	121.54
3	n	773	MET	CA-C-N	15.41	151.57	122.60
3	n	773	MET	C-N-CA	15.41	151.57	122.60
16	CB	35	TYR	CA-C-N	15.32	150.81	121.54
16	CB	35	TYR	C-N-CA	15.32	150.81	121.54
2	s	29	ILE	N-CA-C	15.21	125.59	111.45
2	BR	29	ILE	N-CA-C	15.11	124.73	110.53
16	Aq	131	VAL	N-CA-C	-14.65	98.68	113.47
5	G	433	VAL	N-CA-C	14.54	123.67	111.90
3	BY	785	VAL	N-CA-C	-14.02	99.50	113.10
5	v	557	ILE	N-CA-C	-13.99	94.39	110.21
5	AE	641	PHE	N-CA-C	13.62	126.20	111.36
7	AG	144	GLY	N-CA-C	-13.52	96.81	112.50
5	Bf	433	VAL	N-CA-C	13.45	124.45	111.67
3	BY	598	VAL	N-CA-C	13.41	122.76	111.90
3	1	559	SER	N-CA-C	13.38	129.38	112.92
1	A	68	SER	CA-C-N	13.29	147.49	121.58
1	A	68	SER	C-N-CA	13.29	147.49	121.58
5	v	622	ILE	N-CA-C	-13.29	95.57	110.05
3	BY	556	PRO	N-CA-C	-13.26	94.53	110.70
3	1	598	VAL	N-CA-C	13.10	122.83	111.56
5	G	653	ILE	N-CA-C	-12.98	97.82	111.58
16	A7	131	VAL	N-CA-C	-12.82	99.45	113.43
3	I	238	LEU	N-CA-C	12.79	128.20	112.59
3	I	559	SER	CA-C-N	12.76	144.67	121.70
3	I	559	SER	C-N-CA	12.76	144.67	121.70
16	CT	131	VAL	N-CA-C	-12.76	99.53	113.43
3	7	559	SER	N-CA-C	12.59	128.65	113.28
2	D	280	ILE	CA-C-N	12.58	144.35	121.70
2	D	280	ILE	C-N-CA	12.58	144.35	121.70
3	E	559	SER	N-CA-C	12.57	128.74	113.16
3	I	598	VAL	N-CA-C	12.56	122.36	111.56
3	n	559	SER	N-CA-C	12.47	128.62	112.41
2	Ch	297	LYS	N-CA-C	-12.47	94.45	110.53
2	BR	329	GLN	CA-C-N	12.45	144.11	121.70
2	BR	329	GLN	C-N-CA	12.45	144.11	121.70
5	Bt	39	SER	N-CA-C	12.44	127.50	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BY	238	LEU	N-CA-C	12.37	127.68	112.59
16	c	131	VAL	N-CA-C	-12.27	100.06	113.43
16	CI	131	VAL	N-CA-C	-12.24	100.09	113.43
1	BD	234	THR	N-CA-C	-12.23	96.07	110.13
3	E	238	LEU	N-CA-C	12.20	127.47	112.59
5	L	433	VAL	N-CA-C	12.06	121.93	111.56
5	AE	433	VAL	N-CA-C	11.98	121.86	111.56
3	n	238	LEU	N-CA-C	11.98	127.20	112.59
3	7	238	LEU	N-CA-C	11.97	127.19	112.59
1	BD	431	TYR	CA-C-N	11.93	132.67	120.38
1	BD	431	TYR	C-N-CA	11.93	132.67	120.38
3	E	559	SER	CA-C-N	11.87	143.06	121.70
3	E	559	SER	C-N-CA	11.87	143.06	121.70
3	7	559	SER	CA-C-N	11.85	143.04	121.70
3	7	559	SER	C-N-CA	11.85	143.04	121.70
5	9	434	TYR	N-CA-C	11.81	118.85	108.22
2	D	269	ASN	N-CA-C	11.79	128.16	111.30
3	I	556	PRO	N-CA-C	-11.73	99.21	110.47
3	I	559	SER	N-CA-C	11.71	126.83	112.54
3	n	598	VAL	N-CA-C	11.65	121.58	111.56
7	J	250	PHE	N-CA-C	-11.62	98.61	113.72
3	n	479	LEU	CA-C-N	11.59	142.55	121.70
3	n	479	LEU	C-N-CA	11.59	142.55	121.70
16	Av	131	VAL	N-CA-C	-11.54	100.85	113.43
3	7	512	GLN	N-CA-C	11.54	127.70	113.50
1	CP	234	THR	N-CA-C	-11.46	96.96	110.13
7	J	58	LYS	N-CA-C	-11.42	99.35	113.97
3	1	559	SER	CA-C-N	11.41	142.25	121.70
3	1	559	SER	C-N-CA	11.41	142.25	121.70
16	Av	90	SER	CA-C-N	11.41	142.23	121.70
16	Av	90	SER	C-N-CA	11.41	142.23	121.70
16	CM	141	LYS	CA-C-N	11.40	142.21	121.70
16	CM	141	LYS	C-N-CA	11.40	142.21	121.70
3	n	512	GLN	N-CA-C	11.39	127.51	113.50
7	AG	58	LYS	N-CA-C	-11.33	99.46	113.97
5	9	433	VAL	N-CA-C	11.33	121.08	111.90
3	I	479	LEU	CA-C-N	11.27	141.98	121.70
3	I	479	LEU	C-N-CA	11.27	141.98	121.70
16	CI	90	SER	CA-C-N	11.25	141.95	121.70
16	CI	90	SER	C-N-CA	11.25	141.95	121.70
3	E	479	LEU	CA-C-N	11.24	141.93	121.70
3	E	479	LEU	C-N-CA	11.24	141.93	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Z	141	LYS	CA-C-N	11.20	141.85	121.70
16	Z	141	LYS	C-N-CA	11.20	141.85	121.70
3	BY	601	THR	N-CA-C	-11.17	100.19	114.04
3	BY	479	LEU	CA-C-N	11.16	141.79	121.70
3	BY	479	LEU	C-N-CA	11.16	141.79	121.70
2	k	332	VAL	N-CA-C	-11.16	98.83	111.00
3	7	479	LEU	CA-C-N	11.16	141.78	121.70
3	7	479	LEU	C-N-CA	11.16	141.78	121.70
3	1	479	LEU	CA-C-N	11.13	141.73	121.70
3	1	479	LEU	C-N-CA	11.13	141.73	121.70
3	BY	512	GLN	N-CA-C	11.12	127.06	113.38
16	A7	90	SER	CA-C-N	11.10	141.69	121.70
16	A7	90	SER	C-N-CA	11.10	141.69	121.70
7	Bm	58	LYS	N-CA-C	-11.07	99.80	113.97
5	v	432	LYS	CA-C-N	-11.06	112.13	122.97
5	v	432	LYS	C-N-CA	-11.06	112.13	122.97
7	AM	58	LYS	N-CA-C	-11.06	99.82	113.97
5	M	280	LEU	CA-C-N	10.99	130.91	120.03
5	M	280	LEU	C-N-CA	10.99	130.91	120.03
3	1	238	LEU	N-CA-C	10.98	126.68	112.41
16	Az	141	LYS	CA-C-N	10.96	141.43	121.70
16	Az	141	LYS	C-N-CA	10.96	141.43	121.70
16	An	141	LYS	CA-C-N	10.96	141.42	121.70
16	An	141	LYS	C-N-CA	10.96	141.42	121.70
16	Aq	154	THR	N-CA-C	-10.90	96.46	110.53
3	E	792	GLN	N-CA-C	-10.86	98.67	112.90
16	CT	90	SER	CA-C-N	10.86	141.24	121.70
16	CT	90	SER	C-N-CA	10.86	141.24	121.70
16	CT	94	PRO	N-CA-C	-10.79	94.05	111.21
3	E	785	VAL	CA-C-O	-10.75	109.21	120.71
5	Bt	283	ASN	N-CA-C	-10.75	93.70	110.36
2	k	34	LEU	N-CA-C	10.73	126.50	113.41
1	C	431	TYR	CA-C-N	10.71	131.41	120.38
1	C	431	TYR	C-N-CA	10.71	131.41	120.38
16	c	90	SER	CA-C-N	10.70	140.96	121.70
16	c	90	SER	C-N-CA	10.70	140.96	121.70
3	E	512	GLN	N-CA-C	10.68	126.47	113.23
3	I	512	GLN	N-CA-C	10.64	126.59	113.50
16	CB	141	LYS	CA-C-N	10.64	140.85	121.70
16	CB	141	LYS	C-N-CA	10.64	140.85	121.70
7	4	58	LYS	N-CA-C	-10.64	100.36	113.97
16	Aq	94	PRO	N-CA-C	-10.58	94.38	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4	535	ALA	N-CA-C	-10.51	96.66	110.53
16	CT	154	THR	N-CA-C	-10.45	97.05	110.53
2	BK	269	ASN	N-CA-C	10.43	126.22	111.30
16	CI	94	PRO	N-CA-C	-10.36	94.74	111.21
3	n	556	PRO	N-CA-C	-10.33	98.10	110.70
2	Ch	280	ILE	CA-C-N	10.28	140.20	121.70
2	Ch	280	ILE	C-N-CA	10.28	140.20	121.70
2	BK	332	VAL	N-CA-C	-10.25	100.72	111.58
2	Ch	332	VAL	N-CA-C	-10.24	99.83	111.00
3	BY	556	PRO	CA-C-N	10.22	132.62	119.84
3	BY	556	PRO	C-N-CA	10.22	132.62	119.84
1	A	431	TYR	CA-C-N	10.22	130.90	120.38
1	A	431	TYR	C-N-CA	10.22	130.90	120.38
1	i	431	TYR	CA-C-N	10.18	130.87	120.38
1	i	431	TYR	C-N-CA	10.18	130.87	120.38
7	4	328	TYR	N-CA-C	10.18	122.79	108.74
3	1	512	GLN	N-CA-C	10.16	126.21	112.90
3	n	574	GLN	N-CA-C	-10.14	103.06	114.62
16	Aq	90	SER	CA-C-N	10.12	139.91	121.70
16	Aq	90	SER	C-N-CA	10.12	139.91	121.70
3	BY	786	ARG	N-CA-C	-10.05	99.56	112.23
5	Bf	545	HIS	CA-C-N	10.05	130.73	120.38
5	Bf	545	HIS	C-N-CA	10.05	130.73	120.38
1	Ca	431	TYR	CA-C-N	10.02	130.71	120.38
1	Ca	431	TYR	C-N-CA	10.02	130.71	120.38
2	k	280	ILE	CA-C-N	10.00	139.69	121.70
2	k	280	ILE	C-N-CA	10.00	139.69	121.70
5	AE	545	HIS	CA-C-N	9.98	130.66	120.38
5	AE	545	HIS	C-N-CA	9.98	130.66	120.38
16	Av	94	PRO	N-CA-C	-9.97	95.59	111.14
5	AU	39	SER	N-CA-C	9.91	123.95	108.79
7	Bm	328	TYR	N-CA-C	9.89	122.39	108.74
5	9	545	HIS	CA-C-N	9.88	130.56	120.38
5	9	545	HIS	C-N-CA	9.88	130.56	120.38
3	E	112	ILE	N-CA-C	-9.85	104.35	113.71
16	c	156	LYS	N-CA-C	-9.85	95.90	110.48
3	1	601	THR	N-CA-C	-9.83	101.39	113.97
3	1	112	ILE	N-CA-C	-9.81	104.39	113.71
2	D	332	VAL	N-CA-C	-9.78	100.34	111.00
1	CP	257	ILE	CA-C-N	9.79	139.31	121.70
1	CP	257	ILE	C-N-CA	9.79	139.31	121.70
5	Bf	519	GLN	CA-C-N	9.77	139.29	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Bf	519	GLN	C-N-CA	9.77	139.29	121.70
16	A7	154	THR	N-CA-C	-9.77	97.93	110.53
16	CI	154	THR	CA-C-O	-9.75	111.78	122.01
3	n	559	SER	CA-C-N	9.74	139.23	121.70
3	n	559	SER	C-N-CA	9.74	139.23	121.70
5	Bt	280	LEU	CA-C-N	9.73	129.55	120.21
5	Bt	280	LEU	C-N-CA	9.73	129.55	120.21
16	Av	154	THR	CA-C-O	-9.72	110.99	121.98
3	I	112	ILE	N-CA-C	-9.71	104.48	113.71
2	CW	332	VAL	N-CA-C	-9.71	100.42	111.00
16	c	154	THR	CA-C-O	-9.64	111.88	122.01
16	CI	179	TYR	N-CA-C	-9.64	97.05	110.35
1	CP	431	TYR	CA-C-N	9.63	130.30	120.38
1	CP	431	TYR	C-N-CA	9.63	130.30	120.38
16	CM	113	SER	N-CA-C	-9.62	97.56	110.55
16	CT	154	THR	CA-C-O	-9.61	110.89	121.94
5	AU	321	ASN	N-CA-C	-9.61	97.09	110.35
7	4	77	LYS	CA-C-N	9.58	129.33	119.56
7	4	77	LYS	C-N-CA	9.58	129.33	119.56
2	BR	90	GLU	N-CA-C	-9.57	97.14	110.35
3	7	112	ILE	N-CA-C	-9.56	104.62	113.71
1	Ca	288	HIS	N-CA-C	9.56	116.62	108.78
16	c	94	PRO	N-CA-C	-9.55	96.24	111.14
2	Ch	269	ASN	N-CA-C	9.55	122.63	109.54
16	Aq	154	THR	CA-C-O	-9.54	110.97	121.94
5	G	427	PHE	N-CA-C	-9.54	100.96	111.36
7	J	151	ASP	N-CA-C	9.53	124.17	112.54
3	BY	556	PRO	CB-CA-C	9.53	122.55	110.92
5	R	39	SER	N-CA-C	9.53	123.55	109.07
3	1	475	HIS	CA-C-N	9.52	129.27	119.56
3	1	475	HIS	C-N-CA	9.52	129.27	119.56
16	Av	54	PRO	N-CA-C	-9.52	96.38	111.03
7	AM	328	TYR	N-CA-C	9.47	122.21	108.86
7	4	144	GLY	N-CA-C	-9.45	101.54	112.50
16	A7	156	LYS	N-CA-C	-9.41	96.60	110.52
3	n	112	ILE	N-CA-C	-9.25	104.92	113.71
5	AU	329	ARG	N-CA-C	-9.25	102.50	113.88
7	Bm	281	HIS	CA-C-N	9.25	130.20	119.47
7	Bm	281	HIS	C-N-CA	9.25	130.20	119.47
3	n	601	THR	N-CA-C	-9.24	102.39	114.31
2	D	87	LEU	N-CA-C	-9.24	101.57	113.12
16	c	54	PRO	N-CA-C	-9.22	96.83	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	v	519	GLN	CA-C-N	9.21	138.28	121.70
5	v	519	GLN	C-N-CA	9.21	138.28	121.70
1	CP	257	ILE	N-CA-C	-9.20	96.75	108.89
5	G	762	LEU	N-CA-C	-9.20	101.34	111.36
5	9	519	GLN	CA-C-N	9.19	138.23	121.70
5	9	519	GLN	C-N-CA	9.19	138.23	121.70
2	k	351	ILE	N-CA-C	9.18	128.43	109.34
2	y	354	GLU	CA-C-O	-9.18	112.37	122.01
2	q	115	GLU	N-CA-C	-9.16	100.23	111.40
1	BD	288	HIS	N-CA-C	9.16	116.29	108.78
3	E	558	VAL	N-CA-C	9.15	119.95	110.62
5	R	292	ASN	CA-C-N	9.14	130.08	119.47
5	R	292	ASN	C-N-CA	9.14	130.08	119.47
2	z	354	GLU	CA-C-O	-9.14	112.42	122.01
5	L	432	LYS	CA-C-N	-9.14	113.85	123.08
5	L	432	LYS	C-N-CA	-9.14	113.85	123.08
5	AE	622	ILE	N-CA-C	-9.12	97.40	108.53
5	L	519	GLN	CA-C-N	9.09	138.07	121.70
5	L	519	GLN	C-N-CA	9.09	138.07	121.70
16	CI	154	THR	N-CA-C	-9.09	98.92	110.19
5	M	235	PHE	N-CA-C	9.05	122.64	108.79
16	CB	113	SER	N-CA-C	-9.05	98.33	110.55
5	AO	329	ARG	N-CA-C	-9.05	102.75	113.88
1	C	234	THR	N-CA-C	-9.04	95.59	109.41
1	i	398	LEU	CA-C-N	9.03	128.88	120.21
1	i	398	LEU	C-N-CA	9.03	128.88	120.21
5	AO	191	SER	CA-C-O	-9.02	111.59	121.33
2	CW	120	LYS	N-CA-C	-9.02	100.60	111.69
7	O	58	LYS	N-CA-C	-9.01	102.69	114.31
5	L	928	ARG	N-CA-C	-8.99	100.90	112.23
3	7	206	ILE	N-CA-C	-8.99	103.09	111.45
5	Bf	622	ILE	N-CA-C	-8.99	95.68	108.80
7	AM	328	TYR	CA-C-N	8.98	137.32	120.97
7	AM	328	TYR	C-N-CA	8.98	137.32	120.97
5	G	519	GLN	CA-C-N	8.98	137.87	121.70
5	G	519	GLN	C-N-CA	8.98	137.87	121.70
16	A7	154	THR	CA-C-O	-8.98	111.61	121.94
3	1	660	ILE	N-CA-C	-8.98	95.16	108.45
5	v	545	HIS	CA-C-N	8.96	129.61	120.38
5	v	545	HIS	C-N-CA	8.96	129.61	120.38
3	7	527	LEU	N-CA-C	-8.96	101.88	113.17
3	BY	660	ILE	N-CA-C	-8.93	95.23	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	An	113	SER	N-CA-C	-8.92	98.51	110.55
2	k	269	ASN	CA-C-N	8.92	137.75	121.70
2	k	269	ASN	C-N-CA	8.92	137.75	121.70
16	CI	54	PRO	N-CA-C	-8.88	97.35	111.03
3	E	601	THR	N-CA-C	-8.88	102.86	114.31
7	J	48	ASP	CA-C-O	-8.87	111.82	121.31
2	CW	269	ASN	CA-C-N	8.85	137.63	121.70
2	CW	269	ASN	C-N-CA	8.85	137.63	121.70
2	CW	269	ASN	N-CA-C	8.84	121.65	109.54
2	Ch	269	ASN	CA-C-N	8.84	137.60	121.70
2	Ch	269	ASN	C-N-CA	8.84	137.60	121.70
2	Cd	54	ASN	N-CA-C	-8.83	101.33	112.90
5	AE	519	GLN	CA-C-N	8.83	137.59	121.70
5	AE	519	GLN	C-N-CA	8.83	137.59	121.70
16	CT	156	LYS	N-CA-C	-8.82	97.46	110.52
3	1	558	VAL	N-CA-C	8.82	119.61	110.62
5	G	484	GLN	N-CA-C	-8.81	101.13	112.23
16	Z	131	VAL	N-CA-C	-8.81	98.29	109.30
3	E	512	GLN	CA-C-N	8.81	137.55	121.70
3	E	512	GLN	C-N-CA	8.81	137.55	121.70
5	M	282	LYS	N-CA-C	8.80	122.71	108.63
5	Bf	484	GLN	N-CA-C	-8.80	101.14	112.23
3	BY	881	ASP	N-CA-C	-8.80	101.38	112.90
5	Bt	72	SER	CA-C-N	8.79	128.74	120.03
5	Bt	72	SER	C-N-CA	8.79	128.74	120.03
3	1	256	GLN	N-CA-C	-8.79	103.14	114.04
7	Bm	328	TYR	CA-C-N	8.79	136.97	120.97
7	Bm	328	TYR	C-N-CA	8.79	136.97	120.97
5	v	562	ASP	CA-C-N	8.78	128.43	119.82
5	v	562	ASP	C-N-CA	8.78	128.43	119.82
16	c	154	THR	N-CA-C	-8.77	99.31	110.19
3	E	475	HIS	CA-C-N	8.76	128.49	119.56
3	E	475	HIS	C-N-CA	8.76	128.49	119.56
3	1	507	CYS	CA-C-N	8.76	128.40	119.82
3	1	507	CYS	C-N-CA	8.76	128.40	119.82
2	BR	314	GLU	N-CA-C	-8.76	101.43	112.90
5	G	622	ILE	N-CA-C	-8.75	94.52	108.95
5	AE	641	PHE	CA-C-N	8.75	137.45	121.70
5	AE	641	PHE	C-N-CA	8.75	137.45	121.70
5	v	576	PHE	N-CA-C	-8.74	98.98	110.43
3	BY	256	GLN	N-CA-C	-8.73	103.21	114.04
5	L	750	ARG	N-CA-C	-8.73	102.41	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4	48	ASP	CA-C-O	-8.73	111.97	121.31
7	AG	208	VAL	N-CA-C	-8.72	101.49	111.00
5	Bt	134	GLN	N-CA-C	8.71	120.75	108.74
5	AO	158	THR	N-CA-C	8.70	119.41	108.45
2	f	295	ASN	N-CA-C	-8.68	101.76	111.14
7	AG	48	ASP	CA-C-O	-8.67	112.03	121.31
3	I	601	THR	N-CA-C	-8.67	103.13	114.31
5	AE	622	ILE	CB-CA-C	8.67	123.57	110.91
2	BR	29	ILE	CA-C-O	-8.66	111.43	121.05
3	1	512	GLN	CA-C-N	8.66	137.29	121.70
3	1	512	GLN	C-N-CA	8.66	137.29	121.70
1	A	288	HIS	N-CA-C	8.65	115.87	108.78
1	Ca	234	THR	N-CA-C	-8.64	97.46	110.07
7	4	328	TYR	CA-C-N	8.63	136.68	120.97
7	4	328	TYR	C-N-CA	8.63	136.68	120.97
3	BY	559	SER	CA-C-N	8.63	137.23	121.70
3	BY	559	SER	C-N-CA	8.63	137.23	121.70
5	Bf	749	ILE	CA-C-O	-8.62	111.16	120.47
7	O	48	ASP	CA-C-O	-8.61	112.02	121.23
5	AU	292	ASN	CA-C-N	8.61	129.46	119.47
5	AU	292	ASN	C-N-CA	8.61	129.46	119.47
3	7	558	VAL	N-CA-C	8.60	119.41	110.72
2	k	103	ASN	N-CA-C	-8.58	102.01	111.36
2	BK	120	LYS	N-CA-C	-8.57	101.14	111.69
3	I	527	LEU	N-CA-C	-8.56	102.39	112.92
5	AE	646	ASN	CA-C-N	8.56	128.21	119.56
5	AE	646	ASN	C-N-CA	8.56	128.21	119.56
7	AG	211	TYR	N-CA-C	-8.56	95.35	108.96
3	BY	746	GLU	N-CA-C	-8.55	98.55	110.35
2	k	39	LEU	N-CA-C	-8.54	101.97	111.28
5	AE	762	LEU	N-CA-C	-8.54	102.05	111.36
5	AE	877	GLN	N-CA-C	-8.54	101.47	112.23
2	BR	54	ASN	N-CA-C	-8.54	101.71	112.90
2	BR	118	ASP	N-CA-C	-8.54	101.47	112.23
5	M	163	PRO	N-CA-C	8.54	124.53	113.86
2	Cd	87	LEU	N-CA-C	-8.54	101.47	112.23
16	Az	113	SER	N-CA-C	-8.53	99.03	110.55
7	Bm	151	ASP	N-CA-C	8.53	123.24	113.01
3	7	703	TYR	CA-C-N	8.52	130.49	119.84
3	7	703	TYR	C-N-CA	8.52	130.49	119.84
16	Z	123	PHE	N-CA-C	-8.52	101.01	111.40
5	L	562	ASP	CA-C-N	8.51	128.24	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	562	ASP	C-N-CA	8.51	128.24	119.56
3	BY	175	THR	CA-C-N	8.50	128.23	119.56
3	BY	175	THR	C-N-CA	8.50	128.23	119.56
5	v	484	GLN	N-CA-C	-8.50	101.53	112.23
5	L	653	ILE	N-CA-C	-8.49	102.58	111.58
3	n	475	HIS	CA-C-N	8.49	128.22	119.56
3	n	475	HIS	C-N-CA	8.49	128.22	119.56
5	L	546	PRO	N-CA-C	8.49	121.06	110.70
2	Ch	120	LYS	N-CA-C	-8.47	101.56	112.23
2	q	269	ASN	CA-C-N	8.46	136.92	121.70
2	q	269	ASN	C-N-CA	8.46	136.92	121.70
3	7	205	GLU	N-CA-C	8.46	120.41	108.74
3	E	574	GLN	N-CA-C	-8.45	101.94	113.18
5	M	72	SER	CA-C-N	8.44	128.39	120.03
5	M	72	SER	C-N-CA	8.44	128.39	120.03
16	An	168	ILE	CB-CA-C	-8.43	103.07	111.08
5	AU	298	ILE	N-CA-C	8.42	119.90	108.11
3	I	475	HIS	CA-C-N	8.41	128.14	119.56
3	I	475	HIS	C-N-CA	8.41	128.14	119.56
2	D	269	ASN	CA-C-N	8.41	136.83	121.70
2	D	269	ASN	C-N-CA	8.41	136.83	121.70
3	E	53	LYS	N-CA-C	-8.39	102.48	112.89
3	I	660	ILE	CA-C-N	8.39	136.80	121.70
3	I	660	ILE	C-N-CA	8.39	136.80	121.70
16	Z	139	LYS	CA-C-N	-8.38	108.79	122.11
16	Z	139	LYS	C-N-CA	-8.38	108.79	122.11
5	AU	158	THR	N-CA-C	8.38	119.30	108.24
3	7	175	THR	CA-C-N	8.37	128.10	119.56
3	7	175	THR	C-N-CA	8.37	128.10	119.56
16	CI	40	GLN	CA-C-O	-8.37	112.21	121.00
5	G	611	PRO	N-CA-C	8.37	124.78	113.98
5	v	503	SER	CA-C-O	-8.36	112.45	121.56
5	M	329	ARG	N-CA-C	-8.36	103.60	113.88
7	4	192	SER	N-CA-C	8.35	119.27	108.24
16	CT	49	VAL	N-CA-C	-8.35	102.29	110.72
3	1	667	GLN	N-CA-C	-8.34	101.97	112.90
5	9	484	GLN	N-CA-C	-8.34	102.14	111.82
5	Bt	253	ASN	CA-C-N	-8.34	109.22	122.73
5	Bt	253	ASN	C-N-CA	-8.34	109.22	122.73
5	M	292	ASN	CA-C-N	8.34	129.14	119.47
5	M	292	ASN	C-N-CA	8.34	129.14	119.47
2	Ch	13	LEU	N-CA-C	-8.33	101.99	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BY	512	GLN	CA-C-N	8.33	136.69	121.70
3	BY	512	GLN	C-N-CA	8.33	136.69	121.70
5	AE	484	GLN	N-CA-C	-8.32	101.74	112.23
16	CM	127	LYS	N-CA-C	-8.32	99.31	110.55
3	BY	475	HIS	CA-C-N	8.32	128.05	119.56
3	BY	475	HIS	C-N-CA	8.32	128.05	119.56
3	1	479	LEU	N-CA-C	8.30	122.69	112.23
3	1	622	LYS	CA-C-N	8.29	128.02	119.56
3	1	622	LYS	C-N-CA	8.29	128.02	119.56
5	AO	191	SER	N-CA-C	-8.29	96.47	109.07
2	CW	246	GLN	CA-C-N	8.29	136.62	121.70
2	CW	246	GLN	C-N-CA	8.29	136.62	121.70
2	y	43	LEU	N-CA-C	-8.28	103.30	113.41
16	CI	61	VAL	N-CA-C	-8.28	105.84	113.71
7	4	329	PHE	N-CA-C	8.28	121.46	110.53
2	Cd	331	ASN	N-CA-C	-8.28	102.62	114.12
2	z	43	LEU	N-CA-C	-8.27	103.32	113.41
7	J	328	TYR	CA-C-N	8.26	137.53	121.66
7	J	328	TYR	C-N-CA	8.26	137.53	121.66
3	n	175	THR	CA-C-N	8.26	127.98	119.56
3	n	175	THR	C-N-CA	8.26	127.98	119.56
5	Bt	310	TYR	N-CA-C	-8.26	96.66	108.96
16	c	49	VAL	N-CA-C	-8.25	102.38	110.72
2	D	103	ASN	N-CA-C	-8.25	102.37	111.36
2	f	46	SER	CA-C-N	8.24	132.42	120.38
2	f	46	SER	C-N-CA	8.24	132.42	120.38
2	z	290	ASN	CA-C-N	8.23	136.51	121.70
2	z	290	ASN	C-N-CA	8.23	136.51	121.70
7	J	143	GLY	N-CA-C	-8.23	103.63	115.64
5	L	484	GLN	N-CA-C	-8.23	101.86	112.23
5	v	442	ILE	N-CA-C	-8.23	104.48	111.56
2	y	290	ASN	CA-C-N	8.22	136.50	121.70
2	y	290	ASN	C-N-CA	8.22	136.50	121.70
2	CW	87	LEU	N-CA-C	-8.22	101.02	112.45
2	Cd	329	GLN	CA-C-N	8.21	137.22	121.54
2	Cd	329	GLN	C-N-CA	8.21	137.22	121.54
2	D	246	GLN	CA-C-N	8.20	136.46	121.70
2	D	246	GLN	C-N-CA	8.20	136.46	121.70
3	I	512	GLN	CA-C-N	8.20	136.46	121.70
3	I	512	GLN	C-N-CA	8.20	136.46	121.70
5	G	610	THR	CA-C-N	8.20	127.86	119.82
5	G	610	THR	C-N-CA	8.20	127.86	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Aq	146	GLN	CA-C-N	-8.20	106.75	120.68
16	Aq	146	GLN	C-N-CA	-8.20	106.75	120.68
2	CW	318	ILE	CA-C-O	-8.19	110.54	120.78
2	Cd	348	THR	N-CA-C	-8.18	101.92	112.23
3	7	475	HIS	CA-C-N	8.18	127.90	119.56
3	7	475	HIS	C-N-CA	8.18	127.90	119.56
5	Bt	261	ASN	N-CA-C	-8.18	100.27	113.19
5	Bt	289	PHE	N-CA-C	8.17	121.29	108.79
16	CB	168	ILE	CB-CA-C	-8.16	103.32	111.08
3	I	826	ARG	CA-C-O	-8.16	111.77	120.42
3	BY	792	GLN	CA-C-O	-8.16	110.59	119.97
2	CW	267	GLU	N-CA-C	-8.16	103.92	114.04
16	Aq	158	HIS	N-CA-C	-8.16	98.41	110.48
2	f	54	ASN	N-CA-C	-8.16	102.22	112.90
2	BK	269	ASN	CA-C-N	8.14	136.35	121.70
2	BK	269	ASN	C-N-CA	8.14	136.35	121.70
3	n	256	GLN	N-CA-C	-8.14	103.95	114.04
3	1	660	ILE	CA-C-N	8.13	136.34	121.70
3	1	660	ILE	C-N-CA	8.13	136.34	121.70
2	z	87	LEU	N-CA-C	-8.13	103.50	113.50
2	y	87	LEU	N-CA-C	-8.12	103.51	113.50
2	k	350	GLU	CA-C-N	8.12	136.59	121.97
2	k	350	GLU	C-N-CA	8.12	136.59	121.97
3	7	808	GLU	CA-C-O	-8.12	111.94	120.55
7	Bm	278	ILE	N-CA-C	8.12	119.08	107.88
5	v	653	ILE	N-CA-C	-8.11	102.98	111.58
5	AB	162	THR	CA-C-N	8.10	129.97	119.84
5	AB	162	THR	C-N-CA	8.10	129.97	119.84
3	E	507	CYS	CA-C-N	8.10	127.82	119.56
3	E	507	CYS	C-N-CA	8.10	127.82	119.56
16	Z	34	PHE	N-CA-C	-8.09	102.46	111.28
5	G	597	TRP	CA-C-O	-8.08	110.67	119.97
7	J	192	SER	N-CA-C	8.08	119.27	107.88
2	k	13	LEU	N-CA-C	-8.07	102.32	112.90
5	Bf	562	ASP	CA-C-N	8.07	127.80	119.56
5	Bf	562	ASP	C-N-CA	8.07	127.80	119.56
3	7	793	MET	N-CA-C	-8.07	102.06	112.23
7	4	534	GLU	N-CA-C	-8.07	103.26	113.43
2	k	26	PRO	N-CA-C	8.06	123.87	112.26
2	z	295	ASN	N-CA-C	-8.06	102.43	111.14
5	M	39	SER	N-CA-C	8.06	121.32	109.07
2	Ch	246	GLN	CA-C-N	8.05	136.19	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Ch	246	GLN	C-N-CA	8.05	136.19	121.70
2	q	103	ASN	N-CA-C	-8.05	102.58	111.36
1	Ca	398	LEU	CA-C-N	8.05	127.94	120.21
1	Ca	398	LEU	C-N-CA	8.05	127.94	120.21
5	v	433	VAL	N-CA-CB	-8.05	103.60	111.57
5	L	893	LYS	CA-C-O	-8.04	112.03	120.55
1	i	349	VAL	CA-C-O	-8.04	112.15	120.27
2	y	54	ASN	N-CA-C	-8.04	102.37	112.90
2	y	295	ASN	N-CA-C	-8.04	102.46	111.14
5	AE	928	ARG	N-CA-C	-8.04	102.10	112.23
2	BR	265	ASP	CA-C-O	-8.04	112.03	120.55
5	AB	312	LEU	N-CA-C	-8.03	102.11	112.23
3	E	264	ILE	N-CA-C	8.01	119.33	108.11
5	M	308	PHE	CA-C-N	8.01	136.12	121.70
5	M	308	PHE	C-N-CA	8.01	136.12	121.70
2	q	120	LYS	N-CA-C	-8.01	101.84	111.69
5	AE	728	GLN	CA-C-O	-8.01	111.93	120.42
16	Ai	131	VAL	N-CA-C	-8.01	99.29	109.30
5	9	622	ILE	N-CA-C	-8.01	97.11	108.80
7	O	77	LYS	CA-C-N	8.00	129.84	119.84
7	O	77	LYS	C-N-CA	8.00	129.84	119.84
2	BK	85	ASN	N-CA-C	-8.00	102.15	112.23
16	CI	156	LYS	N-CA-C	-8.00	97.56	110.20
2	z	54	ASN	N-CA-C	-8.00	102.43	112.90
7	J	202	LEU	N-CA-C	7.99	121.09	111.82
2	z	266	GLY	N-CA-C	-7.99	101.87	113.86
5	AO	292	ASN	CA-C-N	7.99	128.74	119.47
5	AO	292	ASN	C-N-CA	7.99	128.74	119.47
2	k	120	LYS	N-CA-C	-7.99	101.87	111.69
3	I	205	GLU	N-CA-C	7.98	120.25	108.60
7	O	70	ILE	N-CA-C	7.98	120.26	108.45
3	n	512	GLN	CA-C-N	7.98	136.06	121.70
3	n	512	GLN	C-N-CA	7.98	136.06	121.70
5	G	562	ASP	CA-C-N	7.97	128.72	119.47
5	G	562	ASP	C-N-CA	7.97	128.72	119.47
2	y	266	GLY	N-CA-C	-7.97	101.91	113.86
5	AE	893	LYS	CA-C-O	-7.97	112.11	120.55
5	L	475	TYR	CA-C-N	7.96	129.34	120.66
5	L	475	TYR	C-N-CA	7.96	129.34	120.66
5	L	920	GLU	N-CA-C	-7.96	102.20	112.23
7	J	328	TYR	N-CA-C	7.96	120.08	108.86
3	BY	660	ILE	CA-C-N	7.96	136.03	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BY	660	ILE	C-N-CA	7.96	136.03	121.70
3	n	622	LYS	CA-C-N	7.96	129.79	119.84
3	n	622	LYS	C-N-CA	7.96	129.79	119.84
5	Bf	859	ASP	N-CA-C	-7.96	102.21	112.23
2	z	33	GLU	N-CA-C	-7.96	102.20	112.23
16	Av	61	VAL	N-CA-C	-7.96	106.15	113.71
2	y	33	GLU	N-CA-C	-7.95	102.21	112.23
3	BY	631	VAL	CA-C-O	-7.93	112.44	120.85
3	7	601	THR	N-CA-C	-7.93	104.08	114.31
1	BD	349	VAL	CA-C-O	-7.93	112.27	120.27
3	BY	745	LEU	N-CA-C	-7.92	101.74	111.40
16	CM	139	LYS	CA-C-N	-7.91	109.53	122.11
16	CM	139	LYS	C-N-CA	-7.91	109.53	122.11
5	L	622	ILE	CB-CA-C	7.91	122.42	111.34
5	M	321	ASN	N-CA-C	-7.91	102.27	112.23
2	Cd	290	ASN	CA-C-N	7.90	135.93	121.70
2	Cd	290	ASN	C-N-CA	7.90	135.93	121.70
1	A	349	VAL	CA-C-O	-7.90	112.18	120.39
3	1	85	SER	N-CA-C	7.90	121.21	110.55
3	BY	805	GLN	N-CA-C	-7.89	103.11	112.89
5	R	329	ARG	N-CA-C	-7.88	104.19	113.88
7	O	151	ASP	N-CA-C	7.87	122.45	113.01
5	AE	475	TYR	CA-C-N	7.87	129.24	120.66
5	AE	475	TYR	C-N-CA	7.87	129.24	120.66
16	An	139	LYS	CA-C-N	-7.87	109.60	122.11
16	An	139	LYS	C-N-CA	-7.87	109.60	122.11
3	BY	206	ILE	N-CA-C	-7.87	105.04	111.81
5	L	909	LYS	N-CA-C	-7.87	102.31	112.23
5	AB	39	SER	CA-C-N	7.87	133.91	121.17
5	AB	39	SER	C-N-CA	7.87	133.91	121.17
5	G	432	LYS	CA-C-N	-7.86	115.03	122.66
5	G	432	LYS	C-N-CA	-7.86	115.03	122.66
5	Bf	462	LYS	CA-C-N	-7.86	109.10	120.97
5	Bf	462	LYS	C-N-CA	-7.86	109.10	120.97
3	n	507	CYS	CA-C-N	7.86	127.58	119.56
3	n	507	CYS	C-N-CA	7.86	127.58	119.56
2	q	269	ASN	N-CA-C	7.86	120.31	109.54
7	AM	522	PHE	CA-C-O	-7.86	112.57	120.82
5	AU	4	ILE	N-CA-C	7.86	119.60	108.36
3	1	264	ILE	N-CA-C	7.86	119.11	108.11
5	L	875	ILE	N-CA-C	-7.86	103.14	110.53
7	AG	77	LYS	CA-C-N	7.86	129.66	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AG	77	LYS	C-N-CA	7.86	129.66	119.84
2	BR	29	ILE	O-C-N	-7.86	113.73	121.90
5	L	859	ASP	N-CA-C	-7.85	102.61	112.90
3	I	558	VAL	N-CA-C	7.85	118.62	110.62
5	Bf	475	TYR	CA-C-N	7.84	129.21	120.66
5	Bf	475	TYR	C-N-CA	7.84	129.21	120.66
5	9	492	CYS	CA-C-O	-7.84	112.24	120.55
1	Ca	382	SER	N-CA-C	7.83	122.94	113.23
16	Ai	141	LYS	CA-C-N	7.83	135.79	121.70
16	Ai	141	LYS	C-N-CA	7.83	135.79	121.70
5	M	320	MET	CA-C-O	-7.83	110.97	119.97
1	C	349	VAL	CA-C-O	-7.82	112.37	120.27
3	7	454	ASN	N-CA-C	-7.81	102.38	112.23
2	BR	92	ILE	N-CA-C	-7.81	102.66	110.62
5	9	475	TYR	CA-C-N	7.80	129.17	120.66
5	9	475	TYR	C-N-CA	7.80	129.17	120.66
2	f	136	GLU	CA-C-O	-7.80	112.28	120.55
3	7	264	ILE	N-CA-C	7.80	119.03	108.11
7	AG	274	GLN	N-CA-C	-7.80	102.78	111.28
3	I	264	ILE	N-CA-C	7.79	119.02	108.11
3	E	660	ILE	N-CA-C	-7.79	96.91	108.12
5	AE	767	LYS	N-CA-C	-7.78	102.80	111.28
7	4	202	LEU	N-CA-C	7.78	122.88	113.23
3	1	631	VAL	CA-C-O	-7.78	112.86	120.95
5	Bf	503	SER	CA-C-O	-7.77	112.53	121.47
3	n	766	ILE	CA-C-N	7.77	133.92	121.34
3	n	766	ILE	C-N-CA	7.77	133.92	121.34
3	7	512	GLN	CA-C-N	7.76	135.67	121.70
3	7	512	GLN	C-N-CA	7.76	135.67	121.70
3	n	660	ILE	CA-C-N	7.75	135.66	121.70
3	n	660	ILE	C-N-CA	7.75	135.66	121.70
5	AU	308	PHE	CA-C-N	7.75	135.66	121.70
5	AU	308	PHE	C-N-CA	7.75	135.66	121.70
5	L	462	LYS	CA-C-N	-7.75	109.27	120.97
5	L	462	LYS	C-N-CA	-7.75	109.27	120.97
2	k	246	GLN	CA-C-N	7.75	135.65	121.70
2	k	246	GLN	C-N-CA	7.75	135.65	121.70
5	G	734	GLN	N-CA-C	-7.75	103.63	113.23
5	AE	876	GLN	CA-C-O	-7.75	112.21	120.42
2	Ch	238	GLU	N-CA-C	-7.74	102.17	111.69
5	9	653	ILE	N-CA-C	-7.74	103.37	111.58
3	E	85	SER	N-CA-C	7.73	120.99	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Cd	136	GLU	CA-C-O	-7.73	112.35	120.55
1	Ca	349	VAL	CA-C-O	-7.73	112.46	120.27
7	AG	328	TYR	CA-C-N	7.73	136.50	121.66
7	AG	328	TYR	C-N-CA	7.73	136.50	121.66
5	AE	432	LYS	CA-C-N	-7.72	115.28	123.08
5	AE	432	LYS	C-N-CA	-7.72	115.28	123.08
5	AE	562	ASP	CA-C-N	7.72	127.44	119.56
5	AE	562	ASP	C-N-CA	7.72	127.44	119.56
3	7	441	PHE	N-CA-C	-7.72	102.80	111.14
7	AM	553	TYR	N-CA-C	-7.72	103.47	113.12
16	Aq	61	VAL	N-CA-C	-7.72	106.38	113.71
3	n	631	VAL	CA-C-O	-7.71	112.67	120.85
3	1	175	THR	CA-C-N	7.71	127.43	119.56
3	1	175	THR	C-N-CA	7.71	127.43	119.56
5	AO	52	SER	N-CA-C	-7.71	102.81	112.90
2	f	348	THR	N-CA-C	-7.70	103.68	113.23
2	q	318	ILE	CA-C-O	-7.70	111.85	120.32
2	z	347	LYS	N-CA-C	-7.70	102.81	112.90
7	AM	542	GLN	N-CA-C	-7.70	103.89	113.28
3	I	685	VAL	N-CA-C	-7.69	98.74	108.89
5	M	158	THR	N-CA-C	7.69	118.39	108.24
3	I	175	THR	CA-C-N	7.68	127.40	119.56
3	I	175	THR	C-N-CA	7.68	127.40	119.56
2	BR	241	ARG	N-CA-C	-7.68	101.77	112.45
16	CT	61	VAL	N-CA-C	-7.68	106.41	113.71
7	J	322	PHE	N-CA-C	7.68	121.84	110.48
2	y	347	LYS	N-CA-C	-7.68	102.84	112.90
16	Az	139	LYS	CA-C-N	-7.67	110.18	122.53
16	Az	139	LYS	C-N-CA	-7.67	110.18	122.53
7	J	77	LYS	CA-C-N	7.67	129.43	119.84
7	J	77	LYS	C-N-CA	7.67	129.43	119.84
5	AE	783	ILE	N-CA-C	-7.66	101.55	112.35
2	BR	295	ASN	N-CA-C	-7.66	102.88	111.07
3	7	868	SER	N-CA-C	-7.66	99.70	110.50
3	BY	264	ILE	N-CA-C	7.66	118.83	108.11
2	q	12	LEU	CA-C-O	-7.65	112.44	120.55
2	BK	280	ILE	CA-C-N	7.65	135.46	121.70
2	BK	280	ILE	C-N-CA	7.65	135.46	121.70
7	J	274	GLN	N-CA-C	-7.64	102.95	111.28
5	Bf	653	ILE	N-CA-C	-7.64	103.48	111.58
2	s	240	LEU	N-CA-C	-7.63	101.84	112.45
5	9	462	LYS	CA-C-N	-7.63	109.45	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	9	462	LYS	C-N-CA	-7.63	109.45	120.97
5	AO	251	HIS	N-CA-C	7.63	119.59	111.28
3	E	803	ALA	N-CA-C	-7.63	103.56	113.17
2	k	32	ALA	N-CA-C	7.62	121.51	109.39
7	Bm	98	SER	CA-C-N	7.61	127.24	119.56
7	Bm	98	SER	C-N-CA	7.61	127.24	119.56
7	AM	274	GLN	N-CA-C	-7.61	102.99	111.28
5	AO	72	SER	CA-C-N	7.60	127.76	120.31
5	AO	72	SER	C-N-CA	7.60	127.76	120.31
2	Cd	330	ALA	N-CA-C	-7.59	94.63	110.80
3	E	36	LYS	CA-C-O	-7.59	112.51	120.55
5	AU	253	ASN	CA-C-O	-7.59	112.84	122.63
5	M	253	ASN	CA-C-O	-7.58	112.84	122.63
3	I	833	ILE	CA-C-O	-7.58	113.38	121.27
3	n	527	LEU	N-CA-C	-7.58	103.83	113.23
5	AO	190	LYS	N-CA-C	7.57	120.67	109.24
7	Bm	145	TYR	N-CA-C	7.57	121.25	109.52
16	Ai	147	LYS	N-CA-C	-7.57	104.05	113.28
3	E	205	GLU	N-CA-C	7.56	119.64	108.60
3	E	175	THR	CA-C-N	7.56	127.27	119.56
3	E	175	THR	C-N-CA	7.56	127.27	119.56
5	L	527	ILE	N-CA-C	-7.56	103.09	110.72
16	Ai	43	LYS	N-CA-C	-7.56	102.98	111.14
2	Cd	25	GLN	CA-C-N	7.55	127.51	120.03
2	Cd	25	GLN	C-N-CA	7.55	127.51	120.03
3	n	251	LEU	CA-C-N	7.55	127.51	120.03
3	n	251	LEU	C-N-CA	7.55	127.51	120.03
3	BY	36	LYS	CA-C-O	-7.55	112.55	120.55
2	Cd	265	ASP	CA-C-O	-7.54	112.55	120.55
7	J	142	ASP	N-CA-C	-7.54	103.14	111.36
3	BY	445	PRO	CA-C-O	-7.54	112.47	121.67
5	v	462	LYS	CA-C-N	-7.54	109.59	120.97
5	v	462	LYS	C-N-CA	-7.54	109.59	120.97
2	f	38	LEU	N-CA-C	-7.53	103.03	112.90
7	O	46	HIS	N-CA-C	-7.53	102.10	110.91
3	I	622	LYS	CA-C-N	7.53	128.20	119.47
3	I	622	LYS	C-N-CA	7.53	128.20	119.47
2	f	316	ASP	N-CA-C	-7.52	103.16	111.36
2	D	12	LEU	CA-C-O	-7.51	112.45	120.42
5	v	749	ILE	CA-C-O	-7.51	112.88	120.85
5	AE	857	ARG	CA-C-O	-7.51	111.61	120.10
7	O	328	TYR	N-CA-C	7.51	121.18	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	453	TRP	CA-C-O	-7.51	111.34	119.97
2	BK	246	GLN	CA-C-N	7.51	135.21	121.70
2	BK	246	GLN	C-N-CA	7.51	135.21	121.70
3	7	622	LYS	CA-C-N	7.50	128.18	119.47
3	7	622	LYS	C-N-CA	7.50	128.18	119.47
1	CP	349	VAL	CA-C-O	-7.50	112.58	120.39
16	CM	34	PHE	N-CA-C	-7.50	103.12	111.82
2	D	120	LYS	N-CA-C	-7.50	102.47	111.69
16	Aq	156	LYS	N-CA-C	-7.50	97.90	109.52
2	BR	136	GLU	CA-C-O	-7.50	112.47	120.42
5	G	642	ILE	N-CA-C	7.49	118.29	110.72
7	AM	250	PHE	N-CA-C	-7.49	103.94	113.23
3	BY	133	VAL	N-CA-C	7.49	118.91	108.12
3	E	746	GLU	N-CA-C	-7.49	100.91	110.19
7	AM	329	PHE	N-CA-C	7.48	120.40	110.53
3	1	527	LEU	N-CA-C	-7.47	103.11	112.90
7	AG	70	ILE	N-CA-C	7.47	118.21	108.35
3	I	663	GLN	N-CA-C	-7.47	102.82	112.23
3	7	524	VAL	N-CA-C	-7.47	103.00	110.62
5	AE	462	LYS	CA-C-N	-7.47	109.69	120.97
5	AE	462	LYS	C-N-CA	-7.47	109.69	120.97
7	AG	294	SER	CA-C-N	7.47	135.14	121.70
7	AG	294	SER	C-N-CA	7.47	135.14	121.70
5	9	442	ILE	N-CA-C	-7.46	104.58	111.67
2	Cd	32	ALA	CA-C-O	-7.46	112.57	120.63
5	AB	280	LEU	CA-C-N	7.46	129.16	119.84
5	AB	280	LEU	C-N-CA	7.46	129.16	119.84
3	7	85	SER	N-CA-C	7.45	120.61	110.55
7	AM	70	ILE	N-CA-C	7.45	119.48	108.45
16	CB	176	ILE	N-CA-C	-7.45	101.45	111.44
5	AU	236	ALA	CA-C-O	-7.45	112.93	121.72
5	G	462	LYS	CA-C-N	-7.44	109.73	120.97
5	G	462	LYS	C-N-CA	-7.44	109.73	120.97
7	Bm	274	GLN	N-CA-C	-7.44	103.17	111.28
2	D	268	ILE	N-CA-C	7.44	118.23	110.72
7	4	187	LEU	N-CA-C	7.44	121.78	109.95
5	AB	292	ASN	CA-C-N	7.44	129.14	119.84
5	AB	292	ASN	C-N-CA	7.44	129.14	119.84
2	k	115	GLU	N-CA-C	-7.43	103.11	111.14
16	CB	35	TYR	CA-C-O	7.43	123.01	118.33
5	v	597	TRP	CA-C-O	-7.43	113.02	120.82
5	L	749	ILE	CA-C-O	-7.42	112.45	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Cd	38	LEU	N-CA-C	-7.42	104.03	113.23
3	I	36	LYS	CA-C-O	-7.42	112.56	120.42
3	BY	610	LEU	N-CA-C	-7.42	103.69	112.89
3	I	631	VAL	CA-C-O	-7.42	113.24	120.95
16	Az	171	PHE	CA-C-N	7.41	135.04	121.70
16	Az	171	PHE	C-N-CA	7.41	135.04	121.70
7	4	151	ASP	N-CA-C	7.41	122.14	113.18
5	L	622	ILE	N-CA-C	-7.40	99.79	108.82
5	v	492	CYS	CA-C-O	-7.40	112.71	120.55
3	1	205	GLU	N-CA-C	7.40	119.40	108.60
3	7	36	LYS	CA-C-O	-7.40	112.70	120.55
5	AE	503	SER	CA-C-O	-7.40	112.80	121.16
3	E	622	LYS	CA-C-N	7.40	128.05	119.47
3	E	622	LYS	C-N-CA	7.40	128.05	119.47
1	CP	259	THR	N-CA-C	7.40	119.81	108.42
7	AM	77	LYS	CA-C-N	7.39	129.08	119.84
7	AM	77	LYS	C-N-CA	7.39	129.08	119.84
3	I	786	ARG	N-CA-C	-7.38	102.61	111.69
3	n	36	LYS	CA-C-O	-7.38	112.72	120.55
2	BR	290	ASN	CA-C-N	7.38	134.99	121.70
2	BR	290	ASN	C-N-CA	7.38	134.99	121.70
5	G	749	ILE	CA-C-O	-7.38	112.81	120.71
5	AE	492	CYS	CA-C-O	-7.38	112.73	120.55
5	G	492	CYS	CA-C-O	-7.38	112.73	120.55
3	n	85	SER	N-CA-C	7.38	120.51	110.55
5	AU	142	SER	N-CA-C	7.38	121.70	111.74
5	M	40	ASP	N-CA-C	7.37	122.47	109.58
16	CM	169	PRO	N-CA-C	-7.35	99.64	111.19
3	I	785	VAL	CA-C-O	-7.35	112.79	120.14
5	L	762	LEU	N-CA-C	-7.35	103.35	111.36
5	Bf	642	ILE	N-CA-C	7.35	119.37	111.58
2	k	267	GLU	N-CA-C	-7.34	104.85	113.88
2	BK	12	LEU	CA-C-O	-7.34	112.77	120.55
2	CW	124	GLN	N-CA-C	-7.33	103.30	112.90
5	G	503	SER	CA-C-O	-7.33	112.70	121.05
2	CW	317	SER	N-CA-C	-7.32	100.39	110.35
16	CM	125	ALA	CA-C-O	-7.32	112.66	120.42
1	i	288	HIS	N-CA-C	7.32	115.78	108.75
3	7	445	PRO	CA-C-O	-7.32	113.05	122.12
2	Ch	343	GLU	N-CA-C	-7.32	102.69	111.69
5	AU	72	SER	CA-C-N	7.31	127.47	120.31
5	AU	72	SER	C-N-CA	7.31	127.47	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Bm	77	LYS	CA-C-N	7.31	128.98	119.84
7	Bm	77	LYS	C-N-CA	7.31	128.98	119.84
3	BY	733	LYS	N-CA-C	-7.31	104.39	112.72
2	z	348	THR	N-CA-C	-7.31	103.33	112.90
3	I	85	SER	N-CA-C	7.30	120.41	110.55
2	f	265	ASP	CA-C-O	-7.30	111.85	120.10
7	Bm	329	PHE	N-CA-C	7.30	120.17	110.53
2	y	348	THR	N-CA-C	-7.30	103.34	112.90
3	E	527	LEU	N-CA-C	-7.30	104.38	113.28
1	i	100	ALA	CA-C-N	7.30	128.96	119.84
1	i	100	ALA	C-N-CA	7.30	128.96	119.84
7	Bm	533	THR	CA-C-N	-7.29	109.81	122.79
7	Bm	533	THR	C-N-CA	-7.29	109.81	122.79
2	y	83	GLU	N-CA-C	-7.29	103.34	111.28
7	Bm	154	THR	N-CA-C	-7.28	99.69	110.46
2	z	83	GLU	N-CA-C	-7.28	103.34	111.28
7	4	541	GLN	CA-C-N	-7.28	110.53	122.54
7	4	541	GLN	C-N-CA	-7.28	110.53	122.54
7	4	182	SER	CA-C-N	7.27	127.20	119.85
7	4	182	SER	C-N-CA	7.27	127.20	119.85
2	s	29	ILE	CA-C-O	-7.27	111.96	120.83
2	Ch	12	LEU	CA-C-O	-7.27	112.85	120.55
5	L	919	THR	CA-C-O	-7.26	112.85	120.55
2	Cd	86	ASN	CA-C-O	-7.26	112.18	120.24
16	Av	38	LYS	N-CA-C	-7.26	103.08	112.23
5	AU	283	ASN	CA-C-N	7.26	134.77	121.70
5	AU	283	ASN	C-N-CA	7.26	134.77	121.70
16	CB	175	GLY	CA-C-O	-7.26	112.96	120.66
3	BY	622	LYS	CA-C-N	7.25	127.88	119.47
3	BY	622	LYS	C-N-CA	7.25	127.88	119.47
3	E	206	ILE	N-CA-C	-7.25	104.71	111.45
3	I	125	THR	N-CA-C	-7.25	98.39	109.41
5	AE	919	THR	CA-C-O	-7.25	112.86	120.55
5	Bt	158	THR	N-CA-C	7.25	117.44	107.73
7	AG	76	PHE	CA-C-O	-7.24	112.86	120.89
16	Aq	90	SER	N-CA-C	7.24	126.21	110.80
3	n	205	GLU	N-CA-C	7.24	119.16	108.60
2	BK	83	GLU	N-CA-C	-7.24	103.42	112.90
3	1	441	PHE	N-CA-C	-7.23	103.33	111.14
16	Ai	171	PHE	CA-C-N	7.23	134.71	121.70
16	Ai	171	PHE	C-N-CA	7.23	134.71	121.70
3	I	803	ALA	N-CA-C	-7.21	104.45	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	266	GLY	N-CA-C	-7.21	103.05	113.86
2	q	86	ASN	N-CA-C	-7.21	102.43	112.45
7	AG	328	TYR	N-CA-C	7.21	119.42	109.18
16	Aq	146	GLN	CA-C-O	-7.21	112.78	120.42
3	E	703	TYR	CA-C-N	7.21	128.85	119.84
3	E	703	TYR	C-N-CA	7.21	128.85	119.84
5	M	289	PHE	N-CA-C	7.20	119.80	108.79
2	s	266	GLY	N-CA-C	-7.19	103.08	113.86
5	Bf	432	LYS	CA-C-N	-7.18	114.08	122.63
5	Bf	432	LYS	C-N-CA	-7.18	114.08	122.63
5	v	475	TYR	CA-C-N	7.18	128.49	120.66
5	v	475	TYR	C-N-CA	7.18	128.49	120.66
5	AB	236	ALA	CA-C-O	-7.18	113.25	121.72
16	Ai	34	PHE	N-CA-C	-7.18	103.45	111.71
1	BD	401	TYR	N-CA-C	-7.18	99.04	109.59
5	L	597	TRP	CA-C-O	-7.17	111.73	119.97
2	CW	13	LEU	N-CA-C	-7.17	103.55	111.36
2	s	136	GLU	CA-C-O	-7.17	112.95	120.55
3	7	251	LEU	CA-C-N	7.17	127.12	120.03
3	7	251	LEU	C-N-CA	7.17	127.12	120.03
7	AM	76	PHE	CA-C-O	-7.16	112.94	120.89
2	y	89	SER	N-CA-C	-7.16	103.56	111.36
5	M	236	ALA	CA-C-O	-7.16	113.28	121.72
5	R	42	ASP	N-CA-C	-7.16	104.43	113.02
5	AO	236	ALA	CA-C-O	-7.16	113.37	121.81
2	z	89	SER	N-CA-C	-7.15	103.56	111.36
3	E	445	PRO	CA-C-O	-7.15	112.94	121.67
5	R	308	PHE	CA-C-N	7.15	134.58	121.70
5	R	308	PHE	C-N-CA	7.15	134.58	121.70
5	AE	920	GLU	N-CA-C	-7.15	103.57	111.36
1	A	100	ALA	CA-C-N	7.15	128.77	119.84
1	A	100	ALA	C-N-CA	7.15	128.77	119.84
2	CW	123	LEU	CA-C-O	-7.15	112.97	120.55
3	1	676	THR	CA-C-N	7.14	124.80	119.66
3	1	676	THR	C-N-CA	7.14	124.80	119.66
2	Ch	342	LEU	CA-C-O	-7.13	111.77	119.97
2	q	357	ARG	CA-C-O	-7.13	111.76	122.38
2	k	269	ASN	N-CA-C	7.12	119.30	109.54
3	BY	533	PHE	CA-C-O	-7.12	113.34	120.82
5	G	475	TYR	CA-C-N	7.12	128.42	120.66
5	G	475	TYR	C-N-CA	7.12	128.42	120.66
3	I	660	ILE	N-CA-C	-7.12	97.91	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	LEU	N-CA-C	-7.11	101.15	110.39
5	G	609	ASP	N-CA-C	-7.10	101.86	111.87
1	A	155	ASP	CA-C-O	-7.09	113.31	121.54
3	E	125	THR	N-CA-C	-7.09	98.63	109.41
3	BY	85	SER	N-CA-C	7.09	120.12	110.55
2	k	29	ILE	N-CA-C	7.09	118.09	108.17
7	O	506	GLN	CA-C-N	7.09	126.79	119.56
7	O	506	GLN	C-N-CA	7.09	126.79	119.56
5	AB	114	LYS	N-CA-C	-7.09	104.26	113.12
5	AE	546	PRO	CA-C-N	7.09	128.70	119.84
5	AE	546	PRO	C-N-CA	7.09	128.70	119.84
2	Ch	280	ILE	CB-CA-C	7.09	122.91	111.29
2	BR	89	SER	N-CA-C	-7.08	103.64	111.36
1	BD	398	LEU	CA-C-N	7.08	128.69	119.84
1	BD	398	LEU	C-N-CA	7.08	128.69	119.84
16	CB	139	LYS	CA-C-N	-7.08	110.86	122.11
16	CB	139	LYS	C-N-CA	-7.08	110.86	122.11
7	O	110	ASP	N-CA-C	7.08	122.04	113.41
5	v	611	PRO	CA-C-N	7.08	134.44	121.70
5	v	611	PRO	C-N-CA	7.08	134.44	121.70
7	4	522	PHE	CA-C-O	-7.08	113.39	120.82
2	CW	102	TYR	N-CA-C	-7.07	103.63	112.90
2	Cd	354	GLU	CA-C-O	-7.07	114.24	122.37
16	An	34	PHE	N-CA-C	-7.07	103.58	111.71
3	7	803	ALA	N-CA-C	-7.06	104.27	113.17
7	AM	98	SER	CA-C-N	7.06	126.74	119.82
7	AM	98	SER	C-N-CA	7.06	126.74	119.82
16	Z	171	PHE	CA-C-N	7.06	134.40	121.70
16	Z	171	PHE	C-N-CA	7.06	134.40	121.70
1	Ca	131	ASN	CA-C-N	7.06	127.47	119.92
1	Ca	131	ASN	C-N-CA	7.06	127.47	119.92
2	k	85	ASN	N-CA-C	-7.06	103.34	112.23
5	9	562	ASP	CA-C-N	7.05	127.20	119.87
5	9	562	ASP	C-N-CA	7.05	127.20	119.87
7	AG	182	SER	CA-C-N	7.05	126.97	119.85
7	AG	182	SER	C-N-CA	7.05	126.97	119.85
2	BR	29	ILE	CA-C-N	7.05	135.00	121.54
2	BR	29	ILE	C-N-CA	7.05	135.00	121.54
2	s	314	GLU	CA-C-O	-7.04	113.08	120.55
2	Cd	322	LYS	CA-C-N	7.04	126.72	119.82
2	Cd	322	LYS	C-N-CA	7.04	126.72	119.82
7	AM	333	GLY	CA-C-N	7.04	131.01	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AM	333	GLY	C-N-CA	7.04	131.01	120.31
1	i	155	ASP	CA-C-O	-7.03	113.38	121.54
3	n	677	PRO	CA-C-N	7.03	127.18	119.87
3	n	677	PRO	C-N-CA	7.03	127.18	119.87
5	AB	284	LYS	CA-C-N	7.03	131.59	121.54
5	AB	284	LYS	C-N-CA	7.03	131.59	121.54
2	k	280	ILE	CB-CA-C	7.03	122.81	111.29
2	CW	12	LEU	CA-C-O	-7.03	112.16	120.10
5	Bt	236	ALA	CA-C-O	-7.02	113.52	121.81
2	k	99	GLN	N-CA-C	-7.02	103.38	112.23
1	Ca	155	ASP	CA-C-O	-7.02	113.40	121.54
1	Ca	349	VAL	O-C-N	-7.02	115.88	123.18
5	v	467	SER	N-CA-C	-7.02	103.78	114.16
5	Bt	308	PHE	CA-C-N	7.01	134.32	121.70
5	Bt	308	PHE	C-N-CA	7.01	134.32	121.70
3	I	827	ALA	N-CA-C	-7.01	103.39	112.23
3	n	264	ILE	N-CA-C	7.01	117.93	108.11
5	G	545	HIS	CA-C-N	7.00	127.59	120.38
5	G	545	HIS	C-N-CA	7.00	127.59	120.38
7	J	294	SER	CA-C-O	-7.00	111.94	122.38
5	v	646	ASN	CA-C-N	7.00	126.70	119.56
5	v	646	ASN	C-N-CA	7.00	126.70	119.56
5	v	588	PHE	N-CA-C	7.00	125.71	110.80
2	f	321	SER	N-CA-C	7.00	118.70	111.14
2	k	355	TYR	CA-C-O	-7.00	111.17	119.15
5	Bt	292	ASN	CA-C-N	7.00	126.70	119.56
5	Bt	292	ASN	C-N-CA	7.00	126.70	119.56
7	4	250	PHE	N-CA-C	-7.00	103.70	111.82
3	7	881	ASP	N-CA-C	-7.00	102.72	112.45
5	9	642	ILE	N-CA-C	7.00	118.63	111.00
7	AG	553	TYR	N-CA-C	-7.00	104.38	113.12
16	A7	54	PRO	N-CA-C	-6.99	100.23	111.14
1	i	349	VAL	O-C-N	-6.99	115.91	123.18
5	L	599	GLN	CA-C-N	6.99	130.34	120.28
5	L	599	GLN	C-N-CA	6.99	130.34	120.28
7	O	194	ASP	N-CA-C	-6.99	102.61	113.02
2	Ch	296	ASP	N-CA-C	-6.99	103.75	112.90
1	A	398	LEU	CA-C-N	6.98	126.91	120.21
1	A	398	LEU	C-N-CA	6.98	126.91	120.21
3	7	864	GLN	N-CA-C	-6.97	104.90	113.41
7	AM	204	PHE	N-CA-C	-6.97	105.40	114.04
2	Ch	65	ILE	N-CA-C	-6.97	103.68	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	295	ASN	N-CA-C	-6.96	103.30	114.09
2	BK	103	ASN	N-CA-C	-6.96	103.77	111.36
2	Ch	82	ARG	CA-C-O	-6.96	111.50	120.00
5	AB	351	PHE	N-CA-C	6.96	119.82	108.26
7	AG	522	PHE	CA-C-O	-6.96	113.51	120.82
5	R	163	PRO	N-CA-C	6.96	122.89	113.84
2	y	53	LYS	CA-C-O	-6.96	113.17	120.55
5	AE	576	PHE	N-CA-C	-6.96	101.36	110.33
1	CP	349	VAL	O-C-N	-6.96	115.82	123.20
7	O	250	PHE	N-CA-C	-6.96	104.80	113.28
3	7	238	LEU	CA-C-N	6.95	134.22	121.70
3	7	238	LEU	C-N-CA	6.95	134.22	121.70
5	9	609	ASP	N-CA-C	-6.94	101.98	111.56
7	AG	68	ASP	N-CA-C	6.94	118.82	107.23
3	E	791	GLN	CA-C-O	-6.94	112.26	120.10
3	1	703	TYR	CA-C-N	6.94	128.51	119.84
3	1	703	TYR	C-N-CA	6.94	128.51	119.84
7	AG	250	PHE	N-CA-C	-6.94	103.77	111.82
5	AU	40	ASP	CA-C-N	6.94	126.64	119.56
5	AU	40	ASP	C-N-CA	6.94	126.64	119.56
5	R	158	THR	N-CA-C	6.93	117.39	108.24
2	z	53	LYS	CA-C-O	-6.93	113.20	120.55
3	n	660	ILE	N-CA-C	-6.93	98.20	108.45
2	Cd	266	GLY	N-CA-C	-6.93	103.47	113.86
2	f	86	ASN	CA-C-O	-6.92	112.56	120.24
7	J	553	TYR	N-CA-C	-6.92	104.97	113.41
1	Ca	100	ALA	CA-C-N	6.92	128.49	119.84
1	Ca	100	ALA	C-N-CA	6.92	128.49	119.84
2	Ch	319	LEU	N-CA-C	-6.92	104.99	113.50
2	s	265	ASP	CA-C-O	-6.92	113.22	120.55
3	BY	785	VAL	CA-C-O	-6.92	113.36	119.38
3	BY	793	MET	N-CA-C	-6.91	103.53	112.23
7	Bm	522	PHE	CA-C-O	-6.90	113.58	120.82
2	BR	117	GLN	CA-C-O	-6.89	111.65	119.79
3	E	441	PHE	N-CA-C	-6.89	103.70	111.14
3	E	785	VAL	N-CA-C	-6.89	103.49	111.00
1	BD	264	LYS	CB-CA-C	-6.89	108.62	116.54
5	L	927	MET	CA-C-O	-6.88	111.67	119.79
5	L	646	ASN	CA-C-N	6.88	126.58	119.56
5	L	646	ASN	C-N-CA	6.88	126.58	119.56
5	R	59	VAL	O-C-N	-6.88	115.91	123.20
3	7	792	GLN	CA-C-O	-6.87	112.07	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Bf	483	TYR	CA-C-O	-6.87	113.82	120.90
2	k	350	GLU	CB-CA-C	-6.87	102.34	111.82
7	O	174	ASN	N-CA-C	6.87	124.32	114.16
2	BR	266	GLY	N-CA-C	-6.86	103.57	113.86
7	AG	154	THR	N-CA-C	6.86	118.92	109.18
3	I	441	PHE	N-CA-C	-6.85	103.74	111.14
1	BD	349	VAL	O-C-N	-6.85	116.05	123.18
1	A	349	VAL	O-C-N	-6.84	115.94	123.20
1	C	38	GLU	N-CA-C	-6.84	100.18	110.24
3	E	238	LEU	CA-C-N	6.84	134.02	121.70
3	E	238	LEU	C-N-CA	6.84	134.02	121.70
2	s	40	ASN	N-CA-C	-6.84	103.61	112.23
1	C	349	VAL	O-C-N	-6.84	116.06	123.18
3	n	155	THR	N-CA-C	-6.84	104.61	114.12
16	An	131	VAL	N-CA-C	-6.84	100.75	109.30
16	An	35	TYR	CA-C-N	6.83	133.99	121.70
16	An	35	TYR	C-N-CA	6.83	133.99	121.70
3	BY	559	SER	N-CA-C	6.82	122.13	109.24
3	I	537	VAL	N-CA-C	-6.81	103.84	110.72
2	Cd	53	LYS	CA-C-O	-6.81	113.33	120.55
3	1	610	LEU	N-CA-C	-6.81	104.23	112.54
5	AB	308	PHE	CA-C-N	6.81	133.96	121.70
5	AB	308	PHE	C-N-CA	6.81	133.96	121.70
3	1	238	LEU	CA-C-N	6.81	133.95	121.70
3	1	238	LEU	C-N-CA	6.81	133.95	121.70
3	BY	238	LEU	CA-C-N	6.80	133.95	121.70
3	BY	238	LEU	C-N-CA	6.80	133.95	121.70
5	G	519	GLN	N-CA-C	6.80	121.75	113.38
3	n	768	THR	CA-C-N	6.80	130.07	120.28
3	n	768	THR	C-N-CA	6.80	130.07	120.28
16	Az	71	SER	N-CA-C	-6.80	103.95	111.36
3	E	631	VAL	CA-C-O	-6.80	113.88	120.95
16	CM	174	GLU	N-CA-C	-6.79	91.97	111.00
5	Bt	252	GLY	N-CA-C	-6.79	100.59	112.55
2	k	83	GLU	N-CA-C	-6.79	104.01	112.90
1	A	128	LEU	N-CA-C	6.79	120.30	109.24
3	BY	880	LEU	CA-C-O	-6.79	113.23	120.42
5	AE	463	GLY	N-CA-C	6.79	120.66	110.75
7	4	246	ILE	N-CA-CB	-6.78	102.05	111.41
5	AB	39	SER	N-CA-C	6.78	119.48	109.24
5	R	72	SER	CA-C-N	6.78	126.70	119.85
5	R	72	SER	C-N-CA	6.78	126.70	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Bt	61	LYS	N-CA-C	-6.78	105.95	114.56
5	G	483	TYR	CA-C-O	-6.78	113.92	120.90
5	9	687	PHE	N-CA-C	-6.78	100.00	110.10
2	Ch	267	GLU	N-CA-C	-6.78	104.89	113.43
3	E	51	ASP	N-CA-C	6.78	119.70	110.55
1	C	26	ASN	N-CA-C	-6.77	99.64	110.14
5	L	858	MET	CA-C-O	-6.77	112.18	119.97
1	BD	100	ALA	CA-C-N	6.77	128.30	119.84
1	BD	100	ALA	C-N-CA	6.77	128.30	119.84
3	n	206	ILE	N-CA-C	-6.77	105.16	111.45
3	BY	677	PRO	CA-C-N	6.76	126.91	119.87
3	BY	677	PRO	C-N-CA	6.76	126.91	119.87
5	Bt	31	ASN	CA-C-O	-6.76	114.60	122.37
2	s	29	ILE	CA-C-N	6.76	133.86	121.70
2	s	29	ILE	C-N-CA	6.76	133.86	121.70
3	7	453	TRP	CA-C-N	-6.76	109.19	120.68
3	7	453	TRP	C-N-CA	-6.76	109.19	120.68
3	BY	428	PHE	CA-C-N	6.76	130.46	120.87
3	BY	428	PHE	C-N-CA	6.76	130.46	120.87
5	Bf	609	ASP	N-CA-C	-6.76	103.63	112.41
3	E	660	ILE	CA-C-N	6.75	133.86	121.70
3	E	660	ILE	C-N-CA	6.75	133.86	121.70
2	s	322	LYS	CA-C-N	6.75	126.43	119.82
2	s	322	LYS	C-N-CA	6.75	126.43	119.82
5	AU	175	GLY	N-CA-C	-6.75	106.01	115.32
5	Bt	337	TYR	CA-C-O	-6.75	112.21	119.97
7	Bm	182	SER	CA-C-N	6.75	126.66	119.85
7	Bm	182	SER	C-N-CA	6.75	126.66	119.85
1	C	100	ALA	CA-C-N	6.74	128.27	119.84
1	C	100	ALA	C-N-CA	6.74	128.27	119.84
7	Bm	166	MET	N-CA-CB	-6.74	100.63	110.47
2	BR	38	LEU	N-CA-C	-6.74	103.74	112.23
2	D	65	ILE	N-CA-C	-6.73	103.66	111.00
5	G	575	LYS	N-CA-C	6.73	120.11	109.81
7	O	90	GLY	N-CA-C	-6.73	102.86	112.55
2	BK	331	ASN	CA-C-O	-6.73	111.10	119.38
5	Bf	492	CYS	CA-C-O	-6.73	113.29	120.42
16	c	158	HIS	N-CA-C	-6.73	101.02	110.50
3	I	238	LEU	CA-C-N	6.72	133.80	121.70
3	I	238	LEU	C-N-CA	6.72	133.80	121.70
5	L	545	HIS	CA-C-N	6.71	127.30	120.38
5	L	545	HIS	C-N-CA	6.71	127.30	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AE	782	LYS	CA-C-O	-6.71	111.65	119.24
3	E	444	PHE	CA-C-N	6.71	126.63	119.85
3	E	444	PHE	C-N-CA	6.71	126.63	119.85
3	1	444	PHE	CA-C-N	6.71	126.67	120.03
3	1	444	PHE	C-N-CA	6.71	126.67	120.03
7	AG	322	PHE	N-CA-C	6.71	119.96	110.50
16	Aq	54	PRO	N-CA-C	-6.71	100.54	111.21
5	L	875	ILE	CA-C-O	-6.71	113.60	121.05
16	Z	148	LEU	N-CA-C	-6.71	103.78	112.23
16	CB	171	PHE	CA-C-N	6.70	133.77	121.70
16	CB	171	PHE	C-N-CA	6.70	133.77	121.70
3	I	471	ARG	CA-C-O	-6.70	112.20	122.32
3	I	805	GLN	N-CA-C	-6.70	104.97	113.01
5	M	351	PHE	N-CA-C	6.70	119.38	108.26
5	AU	351	PHE	N-CA-C	6.69	119.37	108.26
1	Ca	132	PRO	CA-C-O	-6.69	113.58	121.95
3	n	238	LEU	CA-C-N	6.69	133.74	121.70
3	n	238	LEU	C-N-CA	6.69	133.74	121.70
3	BY	441	PHE	N-CA-C	-6.69	103.91	111.14
1	Ca	214	ILE	N-CA-C	-6.69	105.32	111.67
5	AO	31	ASN	CA-C-O	-6.68	114.68	122.37
3	I	921	LYS	CA-C-O	-6.68	113.81	120.82
7	J	38	ALA	N-CA-C	6.67	120.45	111.24
16	c	90	SER	N-CA-C	6.67	125.00	110.80
2	BR	37	LYS	CA-C-O	-6.67	113.48	120.55
5	Bt	146	ILE	N-CA-C	-6.66	105.25	111.45
5	L	585	SER	N-CA-C	-6.66	104.98	113.23
1	CP	398	LEU	CA-C-N	6.65	128.16	119.84
1	CP	398	LEU	C-N-CA	6.65	128.16	119.84
7	J	126	ILE	N-CA-C	6.65	118.41	108.23
16	CB	53	ALA	CA-C-N	6.65	126.57	119.85
16	CB	53	ALA	C-N-CA	6.65	126.57	119.85
5	L	492	CYS	CA-C-O	-6.65	113.50	120.55
3	I	733	LYS	N-CA-C	-6.65	105.16	113.20
5	AU	213	ILE	N-CA-C	6.65	117.47	108.17
5	v	463	GLY	N-CA-C	6.64	120.45	110.75
5	R	236	ALA	CA-C-O	-6.64	113.69	121.46
16	Ai	125	ALA	CA-C-O	-6.64	113.51	120.55
5	L	483	TYR	CA-C-O	-6.63	114.07	120.90
3	7	312	TYR	N-CA-C	6.63	119.75	109.07
16	Av	127	LYS	CA-C-O	-6.63	113.98	121.81
7	O	206	LYS	N-CA-C	6.63	119.26	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Bf	621	PHE	CA-C-N	6.63	132.47	122.92
5	Bf	621	PHE	C-N-CA	6.63	132.47	122.92
2	f	32	ALA	CA-C-O	-6.63	113.47	120.63
7	AM	39	LEU	N-CA-C	-6.63	100.22	110.10
7	AM	81	ARG	CA-C-N	6.63	126.54	119.85
7	AM	81	ARG	C-N-CA	6.63	126.54	119.85
5	R	253	ASN	CA-C-O	-6.62	112.51	122.38
3	n	662	ILE	CA-C-O	-6.62	113.83	120.85
5	Bt	150	PHE	N-CA-C	6.62	120.31	109.72
5	Bf	576	PHE	N-CA-C	-6.61	101.99	110.19
5	L	463	GLY	N-CA-C	6.61	120.40	110.75
7	AG	533	THR	CA-C-N	-6.61	110.73	122.42
7	AG	533	THR	C-N-CA	-6.61	110.73	122.42
7	J	533	THR	CA-C-N	-6.60	111.01	122.36
7	J	533	THR	C-N-CA	-6.60	111.01	122.36
2	f	91	ILE	N-CA-C	-6.60	104.06	110.72
5	L	642	ILE	N-CA-C	6.59	118.19	111.00
5	AE	585	SER	N-CA-C	-6.59	105.05	113.23
5	Bf	646	ASN	CA-C-N	6.59	126.22	119.56
5	Bf	646	ASN	C-N-CA	6.59	126.22	119.56
3	I	459	LEU	CA-C-N	6.58	126.29	119.64
3	I	459	LEU	C-N-CA	6.58	126.29	119.64
1	CP	155	ASP	CA-C-O	-6.58	113.90	121.54
16	Ai	57	ARG	N-CA-C	6.58	120.25	109.72
1	BD	417	LYS	N-CA-C	-6.58	105.88	114.04
2	q	82	ARG	CA-C-O	-6.58	111.97	120.00
3	BY	459	LEU	CA-C-N	6.58	127.14	120.04
3	BY	459	LEU	C-N-CA	6.58	127.14	120.04
3	n	663	GLN	N-CA-C	-6.58	103.94	112.23
5	9	463	GLY	N-CA-C	6.57	120.35	110.75
7	Bm	238	PHE	N-CA-C	6.57	120.23	109.72
7	Bm	541	GLN	CA-C-N	-6.57	111.70	122.54
7	Bm	541	GLN	C-N-CA	-6.57	111.70	122.54
2	BR	53	LYS	CA-C-O	-6.57	113.54	120.63
7	AM	533	THR	CA-C-N	-6.56	110.81	122.42
7	AM	533	THR	C-N-CA	-6.56	110.81	122.42
7	Bm	187	LEU	N-CA-C	6.56	120.21	109.72
2	f	53	LYS	CA-C-O	-6.55	113.60	120.55
5	v	483	TYR	CA-C-O	-6.55	114.15	120.90
1	i	415	ASN	N-CA-C	-6.55	96.96	108.23
2	s	37	LYS	CA-C-O	-6.55	112.14	119.67
7	4	126	ILE	N-CA-C	6.55	117.56	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AO	39	SER	N-CA-C	6.55	119.18	110.53
5	AE	483	TYR	CA-C-O	-6.55	114.16	120.90
16	Az	56	GLU	N-CA-C	6.55	120.53	112.54
5	9	585	SER	N-CA-C	-6.54	105.45	113.50
2	Ch	237	GLN	CA-C-O	-6.54	112.45	119.97
5	G	493	LEU	N-CA-C	-6.53	104.00	112.23
5	L	493	LEU	N-CA-C	-6.53	104.00	112.23
1	i	214	ILE	N-CA-C	-6.53	105.46	111.67
7	4	130	HIS	N-CA-C	6.53	115.02	108.75
7	AG	55	PHE	N-CA-C	6.53	120.15	109.24
16	Ai	119	ARG	N-CA-C	-6.53	104.92	114.39
5	9	611	PRO	N-CA-C	6.53	123.89	113.12
7	AM	190	SER	N-CA-C	6.53	118.99	109.07
16	CI	39	HIS	N-CA-C	-6.53	97.88	108.52
7	J	522	PHE	CA-C-O	-6.53	113.00	120.24
7	Bm	202	LEU	CA-C-N	-6.53	110.41	122.09
7	Bm	202	LEU	C-N-CA	-6.53	110.41	122.09
5	AO	304	ASN	N-CA-C	-6.52	104.58	112.54
5	9	465	TYR	CA-C-N	6.52	126.21	119.82
5	9	465	TYR	C-N-CA	6.52	126.21	119.82
1	Ca	240	ILE	CB-CA-C	-6.52	102.05	110.98
7	Bm	113	ILE	CA-C-N	-6.52	113.00	122.19
7	Bm	113	ILE	C-N-CA	-6.52	113.00	122.19
16	CB	131	VAL	N-CA-C	-6.52	101.16	109.30
5	AO	293	PRO	N-CA-C	6.51	123.25	113.81
5	9	432	LYS	CA-C-N	-6.51	116.35	122.66
5	9	432	LYS	C-N-CA	-6.51	116.35	122.66
16	Az	172	ASP	CA-C-N	6.51	131.29	120.62
16	Az	172	ASP	C-N-CA	6.51	131.29	120.62
3	I	112	ILE	CB-CA-C	-6.50	104.52	110.63
16	Ai	56	GLU	N-CA-C	6.50	120.47	112.54
16	An	56	GLU	N-CA-C	6.50	118.45	111.36
7	Bm	47	GLU	N-CA-C	6.50	119.36	111.82
5	G	669	ILE	N-CA-C	6.50	117.27	108.17
5	AU	261	ASN	N-CA-C	-6.50	104.92	112.92
5	Bf	767	LYS	N-CA-C	-6.50	104.23	111.71
5	G	767	LYS	N-CA-C	-6.50	104.24	111.71
5	L	927	MET	N-CA-C	-6.50	104.04	112.23
3	I	703	TYR	CA-C-N	6.50	127.96	119.84
3	I	703	TYR	C-N-CA	6.50	127.96	119.84
2	z	239	GLN	CA-C-O	-6.49	112.76	120.10
7	J	182	SER	CA-C-N	6.49	126.41	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	182	SER	C-N-CA	6.49	126.41	119.85
2	f	137	ASN	N-CA-C	-6.49	104.29	111.36
7	4	98	SER	CA-C-N	6.49	127.95	119.84
7	4	98	SER	C-N-CA	6.49	127.95	119.84
2	BR	95	SER	N-CA-C	-6.48	104.06	112.23
5	9	503	SER	CA-C-O	-6.48	113.90	121.16
2	BR	239	GLN	CA-C-O	-6.48	112.78	120.10
2	k	318	ILE	CA-C-O	-6.48	113.25	120.96
3	n	709	ASP	N-CA-C	6.48	124.60	110.80
1	i	126	GLN	N-CA-C	6.48	119.69	109.39
2	y	239	GLN	CA-C-O	-6.48	112.78	120.10
5	v	504	ASP	N-CA-C	-6.47	104.42	112.90
3	7	236	GLY	N-CA-C	-6.47	101.31	112.06
5	AU	293	PRO	N-CA-C	6.47	123.20	113.81
5	Bf	584	LEU	CA-C-O	-6.47	114.09	120.89
2	BR	137	ASN	N-CA-C	-6.47	103.73	111.69
3	n	632	ALA	N-CA-C	-6.47	104.31	111.82
5	AB	121	ASN	CA-C-N	6.47	126.60	119.87
5	AB	121	ASN	C-N-CA	6.47	126.60	119.87
3	BY	114	SER	N-CA-C	-6.47	104.53	112.88
5	R	351	PHE	N-CA-C	6.47	118.99	108.26
5	L	611	PRO	CA-C-O	-6.46	116.40	121.38
5	9	519	GLN	N-CA-C	6.46	121.31	113.17
5	AU	121	ASN	CA-C-N	6.46	126.59	119.87
5	AU	121	ASN	C-N-CA	6.46	126.59	119.87
5	Bt	4	ILE	N-CA-C	6.46	116.93	107.37
16	An	35	TYR	CA-C-O	-6.46	111.27	120.51
2	BK	73	LEU	N-CA-C	-6.46	104.09	112.23
7	4	542	GLN	N-CA-C	-6.46	105.03	113.17
16	A7	108	LEU	CB-CA-C	-6.46	102.09	111.91
5	L	876	GLN	N-CA-C	-6.46	104.44	112.90
2	k	34	LEU	N-CA-CB	-6.45	101.06	110.47
5	Bf	463	GLY	N-CA-C	6.45	120.16	110.75
16	CT	90	SER	N-CA-C	6.44	124.53	110.80
5	M	274	ILE	N-CA-C	6.44	118.07	108.54
5	Bt	267	ILE	N-CA-C	6.44	117.12	108.11
7	AM	278	ILE	N-CA-C	6.43	118.41	108.44
5	Bt	59	VAL	O-C-N	-6.43	116.38	123.20
5	L	455	ASN	N-CA-C	6.43	119.28	111.82
7	AM	68	ASP	N-CA-C	6.43	118.13	107.20
16	Av	90	SER	N-CA-C	6.43	124.49	110.80
5	M	346	ASN	N-CA-C	6.43	120.22	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AB	124	THR	CA-C-O	-6.43	111.83	118.90
16	A7	155	ILE	N-CA-C	6.42	118.64	108.87
5	Bt	351	PHE	N-CA-C	6.42	118.92	108.26
7	O	39	LEU	N-CA-C	-6.42	100.53	110.10
7	O	541	GLN	CA-C-N	-6.42	111.95	122.54
7	O	541	GLN	C-N-CA	-6.42	111.95	122.54
1	CP	398	LEU	N-CA-C	-6.42	102.05	110.39
3	I	662	ILE	CA-C-O	-6.41	114.05	120.85
5	L	761	LYS	N-CA-C	-6.41	105.42	113.18
3	1	51	ASP	N-CA-C	6.41	119.20	110.55
5	G	733	GLU	CA-C-O	-6.41	113.76	120.55
3	I	445	PRO	CA-C-O	-6.41	113.85	121.67
5	G	434	TYR	CA-C-N	6.41	126.75	119.83
5	G	434	TYR	C-N-CA	6.41	126.75	119.83
5	M	316	PHE	N-CA-C	-6.41	104.22	111.14
5	v	551	LEU	N-CA-C	-6.40	104.30	111.28
3	1	36	LYS	CA-C-O	-6.40	112.61	119.97
7	Bm	553	TYR	N-CA-C	-6.40	105.12	113.12
5	AE	927	MET	CA-C-O	-6.40	111.51	119.38
5	AO	223	CYS	N-CA-C	6.40	120.47	110.17
5	AO	4	ILE	N-CA-C	6.39	117.32	107.99
2	q	13	LEU	N-CA-C	-6.39	104.18	112.23
16	CI	31	LYS	N-CA-C	-6.39	106.02	113.88
5	L	690	TYR	N-CA-C	6.39	121.95	112.94
16	Av	127	LYS	O-C-N	-6.39	115.57	122.85
1	CP	100	ALA	CA-C-N	6.39	127.83	119.84
1	CP	100	ALA	C-N-CA	6.39	127.83	119.84
5	AB	31	ASN	CA-C-O	-6.39	115.03	122.37
5	Bt	40	ASP	CA-C-N	6.39	126.07	119.56
5	Bt	40	ASP	C-N-CA	6.39	126.07	119.56
1	CP	218	GLN	CA-C-N	6.38	126.57	120.31
1	CP	218	GLN	C-N-CA	6.38	126.57	120.31
3	I	331	ILE	CB-CA-C	-6.38	103.80	111.97
5	AB	163	PRO	N-CA-C	6.38	125.62	112.47
16	CT	54	PRO	N-CA-C	-6.38	100.86	111.26
5	v	664	THR	CA-C-N	6.38	126.35	119.78
5	v	664	THR	C-N-CA	6.38	126.35	119.78
1	Ca	70	SER	N-CA-C	-6.38	104.94	114.64
5	Bf	858	MET	CA-C-O	-6.38	112.27	119.79
2	Cd	37	LYS	CA-C-O	-6.38	113.66	120.42
5	AE	858	MET	N-CA-C	-6.37	104.20	112.23
5	Bt	253	ASN	CA-C-O	-6.37	112.88	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	598	VAL	N-CA-C	6.37	122.59	109.34
7	O	294	SER	CA-C-O	-6.37	112.89	122.38
16	c	155	ILE	N-CA-C	6.37	117.09	108.17
5	AO	328	GLU	N-CA-C	-6.37	105.47	113.18
16	Ai	139	LYS	CA-C-N	-6.37	113.21	122.44
16	Ai	139	LYS	C-N-CA	-6.37	113.21	122.44
5	M	59	VAL	O-C-N	-6.36	116.46	123.20
7	AM	120	VAL	N-CA-C	6.36	117.98	108.96
2	z	91	ILE	N-CA-C	-6.36	104.30	110.72
5	G	465	TYR	CA-C-N	6.35	126.04	119.56
5	G	465	TYR	C-N-CA	6.35	126.04	119.56
16	Z	125	ALA	CA-C-O	-6.35	113.81	120.55
16	CB	125	ALA	CA-C-O	-6.35	113.82	120.55
3	n	125	THR	N-CA-C	-6.35	99.76	109.41
7	4	70	ILE	N-CA-C	6.35	117.92	108.46
2	y	91	ILE	N-CA-C	-6.35	104.31	110.72
7	AM	306	GLN	N-CA-C	-6.35	100.44	109.96
2	D	85	ASN	N-CA-C	-6.35	105.02	112.89
5	9	483	TYR	CA-C-O	-6.34	114.14	120.80
3	BY	507	CYS	CA-C-N	6.34	127.77	119.84
3	BY	507	CYS	C-N-CA	6.34	127.77	119.84
2	q	34	LEU	N-CA-C	-6.34	104.29	111.14
16	An	71	SER	N-CA-C	-6.34	104.45	111.36
16	Az	53	ALA	CA-C-N	6.34	126.30	120.03
16	Az	53	ALA	C-N-CA	6.34	126.30	120.03
3	7	112	ILE	CB-CA-C	-6.33	104.68	110.63
3	n	327	PHE	N-CA-C	-6.33	103.65	112.45
7	AG	187	LEU	N-CA-C	6.33	120.02	109.95
16	CB	55	ILE	N-CA-C	6.33	119.87	113.47
1	Ca	264	LYS	CB-CA-C	-6.33	109.26	116.54
5	M	280	LEU	N-CA-C	6.33	120.45	109.82
5	AU	320	MET	N-CA-C	-6.33	97.32	110.80
16	Ai	146	GLN	CA-C-O	-6.33	113.80	120.63
3	7	507	CYS	CA-C-N	6.32	127.74	119.84
3	7	507	CYS	C-N-CA	6.32	127.74	119.84
1	C	415	ASN	N-CA-C	-6.32	97.36	108.23
3	1	459	LEU	CA-C-N	6.32	126.02	119.64
3	1	459	LEU	C-N-CA	6.32	126.02	119.64
5	AU	31	ASN	CA-C-O	-6.32	115.11	122.37
5	Bf	750	ARG	N-CA-C	-6.32	104.62	112.90
5	Bt	274	ILE	N-CA-C	6.32	116.34	107.37
16	An	125	ALA	CA-C-O	-6.31	113.86	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	666	LEU	CA-C-O	-6.31	113.73	120.42
2	BK	298	ILE	N-CA-C	-6.31	104.35	110.72
7	AG	81	ARG	CA-C-N	6.31	126.22	119.85
7	AG	81	ARG	C-N-CA	6.31	126.22	119.85
5	M	328	GLU	N-CA-C	-6.30	105.56	113.18
5	M	337	TYR	CA-C-O	-6.30	112.36	119.79
7	4	506	GLN	CA-C-N	6.30	126.78	119.47
7	4	506	GLN	C-N-CA	6.30	126.78	119.47
7	AG	120	VAL	N-CA-C	6.30	117.90	108.96
5	AU	162	THR	CA-C-N	6.30	127.71	119.84
5	AU	162	THR	C-N-CA	6.30	127.71	119.84
7	J	81	ARG	CA-C-N	6.29	126.21	119.85
7	J	81	ARG	C-N-CA	6.29	126.21	119.85
16	Ai	168	ILE	CB-CA-C	-6.29	105.10	111.08
5	G	576	PHE	CB-CA-C	-6.29	97.90	110.42
5	M	40	ASP	CA-C-N	6.29	125.98	119.56
5	M	40	ASP	C-N-CA	6.29	125.98	119.56
2	BK	25	GLN	N-CA-C	6.29	118.67	109.30
3	I	922	GLN	N-CA-C	-6.29	104.67	112.90
5	L	611	PRO	N-CA-C	6.29	123.49	113.12
5	AU	274	ILE	N-CA-C	6.29	117.85	108.23
1	i	218	GLN	CA-C-N	6.28	126.47	120.31
1	i	218	GLN	C-N-CA	6.28	126.47	120.31
3	1	529	THR	N-CA-C	-6.28	104.49	111.71
5	AU	212	VAL	N-CA-C	6.28	117.81	108.46
2	z	73	LEU	N-CA-C	-6.28	104.68	112.90
3	7	809	ASN	N-CA-C	-6.27	104.68	112.90
7	Bm	68	ASP	N-CA-C	6.27	117.86	107.20
7	AG	192	SER	N-CA-C	6.27	117.75	108.60
3	7	805	GLN	N-CA-C	-6.26	104.90	112.54
7	Bm	70	ILE	N-CA-C	6.26	117.72	108.45
16	An	35	TYR	O-C-N	-6.26	114.26	122.59
5	AE	519	GLN	N-CA-C	6.26	121.08	113.38
5	M	75	THR	N-CA-C	-6.25	104.71	112.90
7	4	81	ARG	CA-C-N	6.25	126.17	119.85
7	4	81	ARG	C-N-CA	6.25	126.17	119.85
2	y	73	LEU	N-CA-C	-6.25	104.71	112.90
2	y	258	LYS	N-CA-C	-6.25	104.47	111.28
5	AO	171	SER	N-CA-C	6.25	119.44	108.75
1	BD	95	LEU	N-CA-C	-6.25	104.55	111.36
3	1	445	PRO	CA-C-O	-6.25	114.08	122.08
5	AU	75	THR	N-CA-C	-6.25	103.77	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AG	38	ALA	N-CA-C	6.25	119.86	111.24
5	R	31	ASN	CA-C-O	-6.24	115.19	122.37
7	J	68	ASP	N-CA-C	6.24	117.65	107.23
3	1	236	GLY	N-CA-C	-6.24	101.71	112.06
5	v	609	ASP	N-CA-C	-6.24	104.30	112.41
5	Bt	163	PRO	N-CA-C	6.24	121.65	113.86
3	n	445	PRO	CA-C-O	-6.23	113.52	122.31
7	AG	98	SER	CA-C-N	6.23	125.92	119.56
7	AG	98	SER	C-N-CA	6.23	125.92	119.56
7	AG	306	GLN	N-CA-C	-6.23	101.71	110.50
5	AE	609	ASP	N-CA-C	-6.23	103.08	111.87
7	AM	144	GLY	N-CA-C	-6.23	105.08	113.24
1	BD	203	LYS	N-CA-C	6.23	118.89	109.23
5	R	44	HIS	N-CA-C	6.23	118.15	111.36
16	An	171	PHE	CA-C-N	6.23	132.91	121.70
16	An	171	PHE	C-N-CA	6.23	132.91	121.70
5	Bt	327	LEU	N-CA-C	-6.23	104.38	112.23
1	C	218	GLN	CA-C-N	6.22	126.41	120.31
1	C	218	GLN	C-N-CA	6.22	126.41	120.31
3	I	680	ILE	N-CA-C	6.22	114.05	107.76
7	Bm	143	GLY	N-CA-C	6.22	124.81	114.48
2	k	12	LEU	CA-C-O	-6.22	113.95	120.55
5	AU	59	VAL	CA-C-O	-6.22	113.87	120.53
5	M	252	GLY	CA-C-N	-6.22	112.85	122.05
5	M	252	GLY	C-N-CA	-6.22	112.85	122.05
3	n	703	TYR	CA-C-N	6.22	127.61	119.84
3	n	703	TYR	C-N-CA	6.22	127.61	119.84
7	AM	182	SER	CA-C-N	6.22	126.13	119.85
7	AM	182	SER	C-N-CA	6.22	126.13	119.85
2	z	258	LYS	N-CA-C	-6.21	104.51	111.28
7	O	524	PRO	N-CA-C	-6.21	101.71	111.34
3	n	459	LEU	CA-C-N	6.21	126.75	120.04
3	n	459	LEU	C-N-CA	6.21	126.75	120.04
3	I	327	PHE	N-CA-C	-6.21	103.81	112.45
7	J	39	LEU	N-CA-C	-6.21	100.84	110.10
7	J	70	ILE	N-CA-C	6.21	117.64	108.45
3	1	291	LEU	N-CA-C	6.21	119.36	108.75
5	L	506	PHE	N-CA-C	-6.20	105.85	113.41
7	4	533	THR	CA-C-O	-6.20	114.52	120.90
3	n	114	SER	N-CA-C	-6.20	104.89	112.88
5	AO	147	LYS	N-CA-C	6.20	117.96	108.42
3	E	610	LEU	N-CA-C	-6.19	104.99	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	503	SER	CA-C-O	-6.19	114.16	121.16
3	1	609	TRP	CA-C-O	-6.18	111.01	119.05
1	BD	126	GLN	N-CA-C	6.18	119.28	108.52
5	Bf	611	PRO	N-CA-C	6.18	125.21	112.47
5	Bt	286	ILE	N-CA-CB	6.18	118.42	110.13
1	Ca	95	LEU	N-CA-C	-6.18	104.62	111.36
1	BD	218	GLN	CA-C-N	6.18	126.37	120.31
1	BD	218	GLN	C-N-CA	6.18	126.37	120.31
3	E	327	PHE	N-CA-C	-6.17	103.87	112.45
5	M	31	ASN	CA-C-O	-6.17	115.27	122.37
3	7	697	TYR	CA-C-N	6.17	126.14	120.03
3	7	697	TYR	C-N-CA	6.17	126.14	120.03
1	BD	288	HIS	CA-C-O	6.17	121.52	117.94
2	y	25	GLN	CA-C-N	6.17	126.08	119.85
2	y	25	GLN	C-N-CA	6.17	126.08	119.85
3	1	680	ILE	N-CA-C	6.17	113.99	107.76
3	BY	117	LEU	N-CA-C	-6.17	97.13	107.99
16	Ai	142	ASN	N-CA-CB	6.17	120.98	110.50
2	z	25	GLN	CA-C-N	6.17	126.08	119.85
2	z	25	GLN	C-N-CA	6.17	126.08	119.85
5	AU	134	GLN	N-CA-C	6.17	118.55	109.24
5	AU	303	GLY	N-CA-C	-6.17	107.24	115.32
16	CM	61	VAL	CB-CA-C	-6.17	104.53	111.80
3	7	152	ASN	CA-C-N	6.16	128.90	120.46
3	7	152	ASN	C-N-CA	6.16	128.90	120.46
2	k	82	ARG	CA-C-O	-6.16	112.28	119.24
5	Bf	762	LEU	N-CA-C	-6.16	105.25	112.89
3	7	880	LEU	CA-C-O	-6.16	113.89	120.42
5	AO	75	THR	N-CA-C	-6.16	104.12	111.69
1	CP	203	LYS	N-CA-C	6.16	119.23	109.50
7	4	255	LYS	CA-C-N	-6.16	115.11	123.12
7	4	255	LYS	C-N-CA	-6.16	115.11	123.12
3	BY	837	MET	CA-C-O	-6.16	114.69	121.28
3	n	93	LYS	CA-C-N	6.15	125.84	119.56
3	n	93	LYS	C-N-CA	6.15	125.84	119.56
5	G	577	VAL	CA-C-N	6.15	128.84	120.54
5	G	577	VAL	C-N-CA	6.15	128.84	120.54
7	J	541	GLN	CA-C-N	-6.15	112.39	122.54
7	J	541	GLN	C-N-CA	-6.15	112.39	122.54
2	s	315	MET	N-CA-C	-6.15	105.60	113.23
2	s	32	ALA	CA-C-O	-6.15	113.99	120.63
7	4	169	PHE	N-CA-C	6.15	118.51	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AO	298	ILE	N-CA-C	6.15	116.72	108.11
7	AG	150	SER	N-CA-C	6.15	119.62	110.52
16	CM	71	SER	N-CA-C	-6.15	104.66	111.36
2	q	246	GLN	CA-C-N	6.14	132.76	121.70
2	q	246	GLN	C-N-CA	6.14	132.76	121.70
5	9	456	PHE	N-CA-C	-6.14	104.67	111.36
2	s	83	GLU	N-CA-C	-6.14	104.59	111.28
3	7	133	VAL	N-CA-C	6.14	116.96	108.12
3	7	64	GLY	N-CA-C	-6.14	106.85	115.32
2	s	310	LYS	N-CA-C	-6.13	105.08	113.30
2	BK	13	LEU	N-CA-C	-6.13	105.62	113.23
5	Bt	295	ASN	N-CA-C	-6.13	105.08	114.16
7	J	98	SER	N-CA-C	-6.13	101.32	109.84
7	AM	47	GLU	N-CA-C	6.13	117.96	111.28
16	CB	119	ARG	N-CA-C	-6.13	105.50	114.39
16	CT	155	ILE	N-CA-C	6.13	118.19	108.87
1	A	371	HIS	N-CA-C	-6.12	101.87	110.50
7	J	202	LEU	CA-C-O	-6.12	112.93	119.97
1	Ca	218	GLN	CA-C-N	6.12	126.31	120.31
1	Ca	218	GLN	C-N-CA	6.12	126.31	120.31
5	AO	164	ASN	CA-C-N	6.12	129.07	120.57
5	AO	164	ASN	C-N-CA	6.12	129.07	120.57
2	Ch	158	LYS	N-CA-C	-6.12	103.94	111.40
3	E	251	LEU	CA-C-N	6.11	126.08	120.03
3	E	251	LEU	C-N-CA	6.11	126.08	120.03
3	7	327	PHE	N-CA-C	-6.11	103.95	112.45
3	n	480	ASN	N-CA-CB	6.11	120.89	110.50
5	AB	59	VAL	O-C-N	-6.11	116.45	122.99
5	AO	257	ILE	N-CA-C	6.11	116.67	108.11
5	AB	102	GLY	N-CA-C	-6.11	104.34	114.48
5	Bf	503	SER	O-C-N	-6.11	116.06	122.96
3	n	444	PHE	CA-C-N	6.11	126.07	120.21
3	n	444	PHE	C-N-CA	6.11	126.07	120.21
5	G	597	TRP	N-CA-C	-6.10	104.74	111.82
5	AU	124	THR	CA-C-O	-6.10	112.19	118.90
16	CT	132	GLN	CA-C-O	-6.10	111.78	120.51
16	c	109	ARG	N-CA-C	6.10	118.69	109.23
3	n	676	THR	CA-C-N	6.10	124.05	119.66
3	n	676	THR	C-N-CA	6.10	124.05	119.66
3	1	152	ASN	CA-C-N	6.10	129.13	120.53
3	1	152	ASN	C-N-CA	6.10	129.13	120.53
7	4	510	VAL	N-CA-C	-6.10	105.12	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	834	ALA	N-CA-C	-6.10	104.55	112.23
2	k	274	ARG	N-CA-C	-6.10	104.75	111.82
2	f	290	ASN	CA-C-N	6.09	132.66	121.70
2	f	290	ASN	C-N-CA	6.09	132.66	121.70
2	s	38	LEU	N-CA-C	-6.09	105.68	113.23
16	An	119	ARG	N-CA-C	-6.09	105.56	114.39
7	Bm	285	TYR	CA-C-N	-6.09	113.36	122.74
7	Bm	285	TYR	C-N-CA	-6.09	113.36	122.74
1	Ca	415	ASN	N-CA-C	-6.09	96.91	108.17
2	Cd	347	LYS	CA-C-O	-6.09	114.10	120.55
2	f	89	SER	N-CA-C	-6.08	104.56	112.23
2	BR	25	GLN	CA-C-N	6.08	126.05	119.78
2	BR	25	GLN	C-N-CA	6.08	126.05	119.78
2	Cd	291	TYR	CA-C-N	-6.08	111.06	120.31
2	Cd	291	TYR	C-N-CA	-6.08	111.06	120.31
7	AM	510	VAL	N-CA-C	-6.08	105.13	111.58
1	BD	26	ASN	N-CA-C	-6.08	100.71	110.14
5	v	764	ARG	N-CA-C	-6.08	104.73	111.36
7	Bm	39	LEU	N-CA-C	-6.08	101.04	110.10
2	Ch	280	ILE	N-CA-C	-6.08	96.70	109.34
5	R	274	ILE	N-CA-C	6.08	116.86	107.99
5	L	858	MET	CA-C-N	-6.07	110.34	121.52
5	L	858	MET	C-N-CA	-6.07	110.34	121.52
2	f	347	LYS	CA-C-O	-6.07	114.11	120.55
16	Az	168	ILE	CB-CA-C	-6.07	105.31	111.08
2	f	333	LYS	N-CA-C	-6.07	104.75	111.36
3	BY	444	PHE	CA-C-N	6.07	125.98	119.85
3	BY	444	PHE	C-N-CA	6.07	125.98	119.85
7	4	166	MET	N-CA-CB	-6.07	101.51	110.49
3	7	53	LYS	N-CA-C	-6.07	105.37	112.89
3	BY	327	PHE	N-CA-C	-6.07	104.02	112.45
5	9	624	TYR	N-CA-C	-6.06	105.84	113.18
5	G	584	LEU	CA-C-O	-6.06	114.53	120.89
3	1	481	LEU	N-CA-C	6.06	118.68	111.71
3	BY	527	LEU	N-CA-C	-6.06	105.89	113.28
5	Bf	749	ILE	CA-C-N	-6.06	110.37	121.52
5	Bf	749	ILE	C-N-CA	-6.06	110.37	121.52
7	Bm	212	SER	N-CA-C	6.06	117.35	108.14
1	BD	208	HIS	N-CA-C	-6.06	102.42	109.93
5	AE	496	PHE	N-CA-C	-6.05	104.01	111.40
5	Bt	38	VAL	CB-CA-C	6.05	119.85	110.83
7	4	68	ASP	N-CA-C	6.05	117.34	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AM	55	PHE	N-CA-C	6.05	118.61	109.23
7	4	39	LEU	N-CA-C	-6.05	101.09	110.10
5	AE	894	GLN	N-CA-C	-6.05	104.61	112.23
1	BD	401	TYR	CB-CA-C	-6.05	101.19	110.26
7	J	190	SER	N-CA-C	6.05	118.26	109.07
2	s	272	LYS	CA-C-N	6.04	130.81	120.72
2	s	272	LYS	C-N-CA	6.04	130.81	120.72
3	7	51	ASP	N-CA-C	6.04	118.71	110.55
1	A	288	HIS	CA-C-O	6.04	121.44	117.94
16	Az	119	ARG	N-CA-C	-6.03	105.47	114.64
3	BY	480	ASN	N-CA-CB	6.03	120.75	110.50
3	BY	534	CYS	N-CA-C	-6.03	104.63	112.23
16	CM	119	ARG	N-CA-C	-6.03	105.65	114.39
3	I	479	LEU	N-CA-C	6.03	120.76	113.41
1	i	371	HIS	N-CA-C	-6.02	101.56	110.48
7	J	329	PHE	CB-CA-C	-6.02	98.28	111.71
16	Az	34	PHE	N-CA-C	-6.02	104.83	111.82
3	1	526	LEU	CA-C-O	-6.02	114.09	120.71
5	AB	61	LYS	N-CA-C	-6.02	106.55	114.31
5	AU	325	ARG	N-CA-C	-6.02	104.28	111.69
16	Aq	31	LYS	N-CA-C	-6.02	106.07	113.41
7	O	265	ILE	N-CA-C	6.02	117.96	111.58
1	BD	155	ASP	CA-C-O	-6.02	113.56	121.08
3	1	64	GLY	N-CA-C	-6.01	107.02	115.32
5	AE	456	PHE	N-CA-C	-6.01	104.80	111.36
2	k	278	GLY	N-CA-C	6.01	119.91	111.19
5	AO	212	VAL	N-CA-C	6.01	118.65	108.86
3	1	327	PHE	N-CA-C	-6.01	104.10	112.45
7	AG	202	LEU	CA-C-N	-6.01	111.18	120.31
7	AG	202	LEU	C-N-CA	-6.01	111.18	120.31
1	BD	415	ASN	N-CA-C	-6.01	97.06	108.17
1	CP	415	ASN	N-CA-C	-6.01	97.06	108.17
3	I	235	ILE	N-CA-C	6.00	116.52	108.11
7	4	274	GLN	N-CA-C	-6.00	104.74	111.28
5	v	521	GLU	N-CA-C	6.00	117.62	111.14
5	Bf	581	TRP	N-CA-C	6.00	121.79	113.45
5	AO	172	PHE	N-CA-C	6.00	118.65	110.55
2	z	38	LEU	N-CA-C	-6.00	105.05	112.90
7	4	202	LEU	CA-C-N	-5.99	110.50	121.52
7	4	202	LEU	C-N-CA	-5.99	110.50	121.52
16	Z	53	ALA	CA-C-N	5.99	125.90	119.85
16	Z	53	ALA	C-N-CA	5.99	125.90	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	i	208	HIS	N-CA-C	-5.99	102.50	109.93
3	7	680	ILE	N-CA-C	5.99	115.12	108.05
2	Cd	137	ASN	N-CA-C	-5.99	104.32	111.69
3	I	53	LYS	N-CA-C	-5.99	105.47	112.89
2	y	240	LEU	N-CA-C	-5.99	104.13	112.45
7	AG	110	ASP	N-CA-C	5.99	120.60	113.12
5	G	576	PHE	N-CA-C	-5.99	98.05	110.80
5	9	464	LEU	CA-C-N	5.99	132.47	121.70
5	9	464	LEU	C-N-CA	5.99	132.47	121.70
7	O	38	ALA	N-CA-C	5.98	119.64	111.39
3	7	598	VAL	N-CA-C	5.98	121.78	109.34
16	Av	142	ASN	N-CA-C	-5.98	100.86	109.29
2	Cd	329	GLN	O-C-N	-5.98	114.64	122.59
2	z	240	LEU	N-CA-C	-5.98	104.14	112.45
3	E	774	ARG	N-CA-C	-5.98	104.85	111.36
2	y	38	LEU	N-CA-C	-5.98	105.07	112.90
5	G	463	GLY	N-CA-C	5.97	119.47	110.75
5	9	646	ASN	CA-C-N	5.97	126.08	119.87
5	9	646	ASN	C-N-CA	5.97	126.08	119.87
16	Ai	53	ALA	CA-C-N	5.97	125.94	120.03
16	Ai	53	ALA	C-N-CA	5.97	125.94	120.03
3	BY	748	LEU	N-CA-C	-5.97	104.89	111.82
5	R	121	ASN	CA-C-N	5.97	126.08	119.87
5	R	121	ASN	C-N-CA	5.97	126.08	119.87
2	f	291	TYR	N-CA-C	5.97	127.71	111.00
2	k	331	ASN	CA-C-O	-5.97	112.04	119.38
3	E	256	GLN	N-CA-C	-5.97	106.64	114.04
16	Aq	143	GLN	CA-C-N	-5.97	117.12	122.97
16	Aq	143	GLN	C-N-CA	-5.97	117.12	122.97
7	AG	47	GLU	N-CA-C	5.96	118.55	111.33
5	AO	270	SER	CA-C-O	-5.96	113.11	119.97
5	Bf	597	TRP	N-CA-C	-5.96	105.50	112.89
7	O	98	SER	CA-C-N	5.96	125.64	119.56
7	O	98	SER	C-N-CA	5.96	125.64	119.56
3	n	43	TRP	N-CA-C	5.96	117.59	108.12
3	7	863	ASP	CA-C-O	-5.96	113.37	120.10
5	AE	782	LYS	CA-C-N	-5.95	111.59	120.82
5	AE	782	LYS	C-N-CA	-5.95	111.59	120.82
3	BY	703	TYR	CA-C-N	5.95	127.28	119.84
3	BY	703	TYR	C-N-CA	5.95	127.28	119.84
1	Ca	371	HIS	N-CA-C	-5.95	102.11	110.50
3	7	707	SER	N-CA-C	5.95	119.95	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AG	169	PHE	N-CA-C	5.95	118.19	108.55
7	AG	202	LEU	N-CA-C	5.95	120.69	112.90
16	An	117	GLU	N-CA-C	5.95	119.63	111.54
16	CI	109	ARG	N-CA-C	5.95	118.45	109.23
3	I	737	THR	N-CA-C	-5.95	105.98	113.18
16	A7	94	PRO	CA-C-N	5.95	132.90	121.54
16	A7	94	PRO	C-N-CA	5.95	132.90	121.54
5	AB	312	LEU	N-CA-CB	5.95	119.45	110.30
5	AO	312	LEU	N-CA-CB	5.95	119.46	110.30
5	M	38	VAL	CA-C-N	-5.94	111.47	121.75
5	M	38	VAL	C-N-CA	-5.94	111.47	121.75
5	AB	42	ASP	N-CA-C	-5.94	105.89	113.02
5	L	749	ILE	CA-C-N	-5.94	111.20	121.66
5	L	749	ILE	C-N-CA	-5.94	111.20	121.66
16	c	132	GLN	N-CA-C	-5.94	98.15	110.80
7	AG	314	ASP	CB-CA-C	-5.94	103.44	112.11
1	Ca	288	HIS	CA-C-O	5.94	121.38	117.94
2	s	354	GLU	CA-C-O	-5.93	112.02	120.51
7	4	332	GLY	N-CA-C	-5.93	106.31	111.95
5	AB	253	ASN	CA-C-O	-5.93	113.54	122.38
16	CM	142	ASN	N-CA-CB	5.93	120.58	110.50
16	Z	169	PRO	N-CA-C	-5.93	101.91	111.03
2	CW	24	THR	CA-C-N	-5.93	116.01	122.59
2	CW	24	THR	C-N-CA	-5.93	116.01	122.59
2	D	83	GLU	N-CA-C	-5.92	104.40	111.69
3	n	301	ILE	N-CA-C	5.92	116.83	108.36
7	Bm	202	LEU	N-CA-C	5.92	120.51	113.16
16	Av	37	ILE	CA-C-O	-5.92	113.60	120.83
16	Z	147	LYS	CA-C-O	-5.92	114.27	120.55
5	v	597	TRP	N-CA-C	-5.92	104.73	111.07
3	7	256	GLN	N-CA-C	-5.92	106.70	114.04
5	AB	270	SER	CA-C-O	-5.92	113.16	119.97
1	A	95	LEU	N-CA-C	-5.92	104.77	112.23
5	R	40	ASP	CA-C-N	5.92	126.03	119.87
5	R	40	ASP	C-N-CA	5.92	126.03	119.87
7	4	278	ILE	N-CA-C	5.92	118.73	108.90
7	J	55	PHE	N-CA-C	5.92	119.12	109.24
7	J	278	ILE	N-CA-C	5.92	116.88	108.42
7	AG	541	GLN	CA-C-N	-5.92	112.78	122.54
7	AG	541	GLN	C-N-CA	-5.92	112.78	122.54
16	Az	115	LYS	N-CA-C	-5.91	107.88	114.62
3	I	256	GLN	N-CA-C	-5.91	106.71	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	281	HIS	CA-C-N	5.91	127.23	119.84
7	J	281	HIS	C-N-CA	5.91	127.23	119.84
16	Z	36	ALA	CA-C-N	5.91	131.24	121.54
16	Z	36	ALA	C-N-CA	5.91	131.24	121.54
3	7	480	ASN	N-CA-CB	5.91	120.55	110.50
5	9	551	LEU	N-CA-C	-5.91	104.96	111.82
5	L	502	GLU	N-CA-C	5.91	120.77	113.50
3	E	480	ASN	N-CA-CB	5.91	120.54	110.50
3	E	493	TYR	N-CA-C	-5.91	104.97	111.82
5	R	75	THR	N-CA-C	-5.91	105.16	112.90
7	AM	202	LEU	N-CA-C	5.91	119.74	112.54
16	A7	90	SER	N-CA-C	5.91	123.38	110.80
3	7	837	MET	O-C-N	-5.90	118.10	123.41
2	BR	329	GLN	CA-C-O	-5.90	115.02	122.63
16	CB	56	GLU	N-CA-C	5.90	120.55	113.23
1	C	288	HIS	N-CA-CB	-5.90	100.52	110.49
3	I	251	LEU	CA-C-N	5.90	125.87	120.03
3	I	251	LEU	C-N-CA	5.90	125.87	120.03
7	O	182	SER	CA-C-N	5.90	125.81	119.85
7	O	182	SER	C-N-CA	5.90	125.81	119.85
5	v	496	PHE	N-CA-C	-5.90	104.77	111.14
5	AU	286	ILE	CB-CA-C	-5.90	102.04	110.83
2	CW	101	LYS	CA-C-O	-5.90	113.43	120.10
2	z	304	GLN	N-CA-C	-5.90	104.93	111.36
5	AB	158	THR	N-CA-C	5.90	117.18	108.86
3	BY	526	LEU	CA-C-O	-5.90	114.70	120.89
7	J	561	VAL	N-CA-C	-5.90	104.76	110.72
7	4	281	HIS	CA-C-N	5.90	126.31	119.47
7	4	281	HIS	C-N-CA	5.90	126.31	119.47
1	A	234	THR	N-CA-C	-5.90	96.78	109.81
1	C	361	GLN	N-CA-C	-5.89	100.89	110.20
2	f	82	ARG	N-CA-C	-5.89	104.94	111.36
2	k	280	ILE	N-CA-C	-5.89	97.08	109.34
16	Aq	186	LEU	N-CA-C	-5.89	104.86	111.28
1	Ca	202	TYR	CA-C-N	-5.89	112.57	122.29
1	Ca	202	TYR	C-N-CA	-5.89	112.57	122.29
7	O	542	GLN	N-CA-C	-5.89	105.75	113.17
5	Bf	546	PRO	N-CA-C	5.89	117.89	110.70
5	M	270	SER	CA-C-O	-5.89	113.20	119.97
5	v	575	LYS	N-CA-C	5.89	118.36	109.41
2	f	83	GLU	N-CA-C	-5.88	104.87	111.28
5	Bt	207	ASP	N-CA-C	-5.88	96.03	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	42	ASP	CA-C-N	5.88	130.48	122.19
5	M	42	ASP	C-N-CA	5.88	130.48	122.19
3	BY	64	GLY	N-CA-C	-5.88	107.20	115.32
3	E	526	LEU	CA-C-O	-5.88	114.25	120.71
5	R	61	LYS	N-CA-C	-5.88	106.73	114.31
3	n	747	LYS	CB-CA-C	-5.88	98.73	110.42
5	AE	597	TRP	N-CA-C	-5.88	105.77	113.17
7	AG	329	PHE	CB-CA-C	-5.88	98.61	111.71
3	E	479	LEU	N-CA-C	5.87	120.59	112.90
5	AO	191	SER	CA-C-N	5.87	132.27	121.70
5	AO	191	SER	C-N-CA	5.87	132.27	121.70
5	Bt	270	SER	CA-C-O	-5.87	113.22	119.97
7	J	333	GLY	CA-C-N	5.87	130.52	120.72
7	J	333	GLY	C-N-CA	5.87	130.52	120.72
2	f	37	LYS	CA-C-O	-5.87	114.33	120.55
2	s	73	LEU	N-CA-C	-5.87	104.29	112.45
3	BY	558	VAL	N-CA-C	-5.87	107.15	111.90
1	C	3	PHE	N-CA-C	5.87	118.10	109.24
2	y	304	GLN	N-CA-C	-5.87	104.97	111.36
5	AO	261	ASN	N-CA-C	-5.87	105.89	113.16
2	BK	115	GLU	N-CA-C	-5.87	104.97	111.36
3	7	689	ASN	N-CA-C	-5.86	104.33	112.30
1	CP	6	ILE	N-CA-C	-5.86	99.26	108.23
5	L	609	ASP	CA-C-N	5.86	132.40	123.96
5	L	609	ASP	C-N-CA	5.86	132.40	123.96
5	Bt	75	THR	N-CA-C	-5.86	105.22	112.90
16	Z	118	HIS	N-CA-C	5.86	123.27	110.80
5	v	714	GLU	N-CA-C	-5.86	105.03	111.82
7	AM	90	GLY	N-CA-C	-5.86	104.12	112.55
7	Bm	266	GLN	CA-C-N	5.86	131.71	122.34
7	Bm	266	GLN	C-N-CA	5.86	131.71	122.34
3	1	469	LEU	N-CA-C	-5.85	104.32	112.45
2	BR	291	TYR	N-CA-C	5.85	127.38	111.00
5	AB	337	TYR	CA-C-O	-5.85	112.89	119.79
7	AG	205	GLN	N-CA-C	5.85	119.63	111.74
7	J	201	ASP	CA-C-N	5.85	129.20	120.31
7	J	201	ASP	C-N-CA	5.85	129.20	120.31
16	Z	101	PHE	CB-CA-C	-5.84	101.09	110.79
16	CI	90	SER	N-CA-C	5.84	123.24	110.80
1	CP	250	VAL	N-CA-C	5.84	116.29	108.11
7	Bm	76	PHE	CA-C-O	-5.84	113.08	120.84
7	Bm	200	TRP	CA-C-N	5.84	129.65	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Bm	200	TRP	C-N-CA	5.84	129.65	121.24
5	AU	186	GLU	CA-C-N	-5.84	115.07	122.37
5	AU	186	GLU	C-N-CA	-5.84	115.07	122.37
7	J	251	ASP	N-CA-C	-5.83	99.63	108.67
5	9	621	PHE	CA-C-N	5.83	131.32	122.92
5	9	621	PHE	C-N-CA	5.83	131.32	122.92
16	A7	158	HIS	N-CA-C	-5.83	101.65	110.28
1	CP	371	HIS	N-CA-C	-5.83	102.28	110.50
1	Ca	132	PRO	CA-C-N	-5.83	111.65	122.09
1	Ca	132	PRO	C-N-CA	-5.83	111.65	122.09
16	An	53	ALA	CA-C-N	5.83	125.74	119.85
16	An	53	ALA	C-N-CA	5.83	125.74	119.85
1	A	218	GLN	CA-C-N	5.83	126.02	120.31
1	A	218	GLN	C-N-CA	5.83	126.02	120.31
16	Az	131	VAL	N-CA-C	-5.83	102.02	109.30
3	BY	205	GLU	N-CA-C	5.83	117.11	108.60
5	9	493	LEU	N-CA-C	-5.82	104.89	112.23
7	4	55	PHE	N-CA-C	5.82	118.96	109.24
5	G	625	PHE	CA-C-O	-5.82	113.96	121.17
3	E	459	LEU	CA-C-N	5.82	126.32	120.04
3	E	459	LEU	C-N-CA	5.82	126.32	120.04
2	BK	280	ILE	N-CA-C	5.82	121.44	109.34
16	CM	57	ARG	N-CA-C	5.82	118.69	109.50
3	n	232	TYR	N-CA-C	5.81	118.24	109.23
16	CM	126	LEU	N-CA-C	-5.81	105.86	113.12
3	I	152	ASN	CA-C-N	5.81	128.41	120.46
3	I	152	ASN	C-N-CA	5.81	128.41	120.46
7	J	315	LYS	N-CA-C	5.81	119.39	107.37
2	s	321	SER	N-CA-C	5.81	120.43	113.23
5	AB	298	ILE	N-CA-C	5.81	116.24	108.11
5	9	597	TRP	CA-C-O	-5.81	112.11	119.31
5	L	456	PHE	N-CA-C	-5.80	104.87	111.14
5	M	212	VAL	N-CA-C	5.80	116.48	108.12
7	Bm	250	PHE	N-CA-C	-5.80	105.09	111.82
3	n	53	LYS	N-CA-C	-5.80	105.69	112.89
5	v	503	SER	O-C-N	-5.80	116.01	122.86
1	Ca	203	LYS	N-CA-C	5.80	118.22	109.23
1	C	131	ASN	CA-C-N	5.80	125.73	119.76
1	C	131	ASN	C-N-CA	5.80	125.73	119.76
5	v	622	ILE	CB-CA-C	5.80	117.97	111.59
5	AO	39	SER	CA-C-N	5.80	129.32	121.20
5	AO	39	SER	C-N-CA	5.80	129.32	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Bm	141	ALA	N-CA-C	5.80	117.60	111.28
7	O	171	GLY	N-CA-C	-5.80	105.71	115.80
3	n	598	VAL	O-C-N	-5.80	116.82	121.98
7	4	202	LEU	CA-C-O	-5.80	112.49	119.27
3	7	43	TRP	N-CA-C	5.80	117.34	108.12
3	7	610	LEU	N-CA-C	-5.80	105.70	112.89
7	AG	521	ASN	CA-C-N	5.80	127.97	120.44
7	AG	521	ASN	C-N-CA	5.80	127.97	120.44
5	R	285	GLY	CA-C-N	-5.79	114.89	122.37
5	R	285	GLY	C-N-CA	-5.79	114.89	122.37
3	n	155	THR	CA-C-N	5.79	130.40	122.34
3	n	155	THR	C-N-CA	5.79	130.40	122.34
3	n	526	LEU	CA-C-O	-5.79	114.34	120.71
7	4	547	LEU	N-CA-C	-5.79	104.32	111.33
16	Av	108	LEU	CB-CA-C	-5.79	103.11	111.91
5	AO	207	ASP	N-CA-C	-5.79	97.71	108.02
1	A	415	ASN	N-CA-C	-5.79	97.46	108.17
2	z	86	ASN	CA-C-O	-5.79	113.81	120.24
5	AE	621	PHE	CA-C-N	5.79	131.39	123.46
5	AE	621	PHE	C-N-CA	5.79	131.39	123.46
16	An	139	LYS	CA-C-O	-5.79	112.98	119.98
7	Bm	55	PHE	N-CA-C	5.79	118.20	109.23
5	Bt	310	TYR	CA-C-N	-5.79	113.22	122.53
5	Bt	310	TYR	C-N-CA	-5.79	113.22	122.53
1	i	26	ASN	N-CA-C	-5.78	101.17	110.14
7	Bm	81	ARG	CA-C-N	5.78	125.69	119.85
7	Bm	81	ARG	C-N-CA	5.78	125.69	119.85
1	C	144	ASP	N-CA-C	-5.78	105.33	112.90
7	O	522	PHE	N-CA-C	-5.78	104.42	112.45
5	L	908	GLU	CA-C-O	-5.78	112.27	119.38
1	C	37	GLN	N-CA-C	-5.78	100.57	109.52
2	k	15	ARG	N-CA-C	-5.78	105.12	111.82
16	Av	132	GLN	CA-C-O	-5.77	112.25	120.51
3	n	609	TRP	CA-C-O	-5.77	111.55	119.05
3	I	480	ASN	N-CA-CB	5.77	120.30	110.50
3	7	93	LYS	CA-C-N	5.77	125.44	119.56
3	7	93	LYS	C-N-CA	5.77	125.44	119.56
5	AU	252	GLY	CA-C-N	-5.77	113.52	122.05
5	AU	252	GLY	C-N-CA	-5.77	113.52	122.05
3	BY	471	ARG	CA-C-O	-5.77	112.50	120.52
7	O	274	GLN	N-CA-C	-5.76	104.90	111.07
2	BK	82	ARG	CA-C-O	-5.76	112.73	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	68	ASP	N-CA-C	5.76	116.86	107.23
2	D	267	GLU	N-CA-C	-5.76	106.79	113.88
5	v	499	LEU	CB-CA-C	-5.76	101.18	110.74
5	9	512	PRO	CA-C-N	-5.76	112.11	120.29
5	9	512	PRO	C-N-CA	-5.76	112.11	120.29
5	Bf	546	PRO	CA-C-N	5.76	127.04	119.84
5	Bf	546	PRO	C-N-CA	5.76	127.04	119.84
3	I	908	ARG	N-CA-C	-5.76	105.08	111.36
2	y	272	LYS	CA-C-N	5.76	129.06	120.31
2	y	272	LYS	C-N-CA	5.76	129.06	120.31
5	AO	163	PRO	N-CA-C	5.76	122.18	114.18
2	z	272	LYS	CA-C-N	5.76	129.06	120.31
2	z	272	LYS	C-N-CA	5.76	129.06	120.31
2	k	32	ALA	CB-CA-C	-5.75	102.73	112.00
16	CI	49	VAL	N-CA-C	-5.75	104.91	110.72
2	y	86	ASN	CA-C-O	-5.75	113.85	120.24
5	AB	257	ILE	N-CA-C	5.75	116.41	108.12
16	A7	168	ILE	CA-C-N	5.75	125.71	119.78
16	A7	168	ILE	C-N-CA	5.75	125.71	119.78
5	Bt	341	LYS	CA-C-N	5.75	125.69	119.76
5	Bt	341	LYS	C-N-CA	5.75	125.69	119.76
1	C	406	SER	N-CA-C	5.75	117.63	111.36
5	AB	69	LYS	N-CA-C	5.75	122.52	109.81
16	CI	108	LEU	CB-CA-C	-5.75	103.18	111.91
2	CW	123	LEU	CA-C-N	-5.75	110.95	121.52
2	CW	123	LEU	C-N-CA	-5.75	110.95	121.52
5	v	506	PHE	N-CA-C	-5.75	106.40	113.41
3	7	795	LYS	N-CA-C	-5.75	105.16	111.82
1	Ca	258	ILE	N-CA-C	-5.74	105.49	111.58
5	AU	52	SER	N-CA-C	-5.74	103.78	112.04
16	A7	132	GLN	CA-C-O	-5.74	112.30	120.51
3	I	291	LEU	N-CA-C	5.74	118.81	109.06
5	R	328	GLU	N-CA-C	-5.74	106.24	113.18
5	AO	138	TRP	N-CA-C	5.74	117.79	109.07
1	A	417	LYS	N-CA-C	-5.74	106.20	113.43
5	AU	194	GLU	CA-C-N	-5.74	113.98	122.41
5	AU	194	GLU	C-N-CA	-5.74	113.98	122.41
3	BY	816	ASP	N-CA-C	-5.74	105.17	111.82
7	J	545	SER	N-CA-C	-5.73	105.03	111.28
1	A	281	SER	N-CA-C	5.73	115.67	108.45
2	D	357	ARG	CA-C-O	-5.73	112.31	120.51
5	G	611	PRO	CA-C-N	5.73	132.01	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	611	PRO	C-N-CA	5.73	132.01	121.70
5	L	602	ASP	N-CA-C	-5.73	105.96	113.12
16	Z	142	ASN	N-CA-CB	5.73	120.24	110.50
2	z	265	ASP	CA-C-O	-5.73	113.38	119.97
7	AG	202	LEU	CA-C-O	-5.73	112.90	119.60
3	I	133	VAL	N-CA-C	5.72	116.36	108.12
7	AG	333	GLY	CA-C-N	5.72	130.28	120.72
7	AG	333	GLY	C-N-CA	5.72	130.28	120.72
16	CT	158	HIS	N-CA-C	-5.72	101.81	110.28
1	Ca	160	ILE	N-CA-C	5.72	116.09	107.80
16	Ai	140	ASP	N-CA-C	5.71	117.69	107.80
3	BY	488	GLN	N-CA-C	5.71	118.47	109.39
1	CP	131	ASN	CA-C-N	5.71	125.67	119.78
1	CP	131	ASN	C-N-CA	5.71	125.67	119.78
16	CT	73	LEU	CA-C-N	-5.71	112.63	120.46
16	CT	73	LEU	C-N-CA	-5.71	112.63	120.46
16	Z	97	ILE	N-CA-C	-5.71	105.28	110.82
3	7	481	LEU	N-CA-C	5.71	117.50	111.28
3	7	97	TYR	N-CA-C	-5.71	103.36	111.24
3	7	769	TYR	CB-CA-C	-5.71	100.97	110.68
7	AM	558	GLU	N-CA-C	-5.71	105.96	114.64
5	AO	351	PHE	N-CA-CB	-5.71	102.17	110.84
7	O	192	SER	N-CA-C	5.71	115.64	108.45
7	AM	281	HIS	CA-C-N	5.71	126.09	119.47
7	AM	281	HIS	C-N-CA	5.71	126.09	119.47
2	z	333	LYS	N-CA-C	-5.71	105.14	111.36
2	D	331	ASN	CA-C-N	-5.70	111.42	120.55
2	D	331	ASN	C-N-CA	-5.70	111.42	120.55
2	y	333	LYS	N-CA-C	-5.70	105.14	111.36
5	AE	664	THR	CA-C-N	5.70	125.65	119.78
5	AE	664	THR	C-N-CA	5.70	125.65	119.78
2	y	265	ASP	CA-C-O	-5.70	113.42	119.97
3	7	526	LEU	O-C-N	-5.70	115.50	122.11
16	Aq	112	CYS	N-CA-C	5.70	118.92	110.48
1	BD	281	SER	N-CA-C	5.70	115.63	108.45
7	Bm	295	LYS	N-CA-C	5.70	118.53	110.50
7	AG	39	LEU	N-CA-C	-5.69	101.62	110.10
7	AG	331	THR	N-CA-C	5.69	117.26	109.18
3	BY	291	LEU	N-CA-C	5.69	118.74	109.06
5	R	38	VAL	CA-C-N	-5.69	111.91	121.75
5	R	38	VAL	C-N-CA	-5.69	111.91	121.75
1	BD	250	VAL	N-CA-C	5.69	116.08	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CW	82	ARG	CA-C-O	-5.69	112.81	119.24
3	E	291	LEU	N-CA-C	5.69	118.47	108.75
2	k	25	GLN	CA-C-N	5.69	128.98	120.96
2	k	25	GLN	C-N-CA	5.69	128.98	120.96
5	v	584	LEU	CA-C-O	-5.69	114.46	120.71
2	BR	46	SER	CA-C-N	5.69	129.70	120.60
2	BR	46	SER	C-N-CA	5.69	129.70	120.60
5	AB	295	ASN	N-CA-C	-5.68	104.21	113.19
5	L	608	ASN	O-C-N	-5.68	115.24	122.34
3	BY	847	LEU	CA-C-O	-5.68	112.70	119.35
3	n	610	LEU	N-CA-C	-5.68	105.85	112.89
3	I	481	LEU	N-CA-C	5.68	118.24	111.71
5	AB	290	ASP	CB-CA-C	-5.68	102.33	110.62
3	l	153	ILE	CB-CA-C	-5.68	104.60	112.04
1	A	342	ASN	CA-C-N	-5.68	112.92	122.29
1	A	342	ASN	C-N-CA	-5.68	112.92	122.29
5	G	587	PHE	CA-C-N	5.68	128.67	120.38
5	G	587	PHE	C-N-CA	5.68	128.67	120.38
3	n	73	LYS	N-CA-C	-5.68	106.19	113.23
2	y	291	TYR	N-CA-C	5.68	126.89	111.00
16	A7	60	GLU	N-CA-C	5.68	118.92	110.52
3	BY	110	TYR	N-CA-CB	-5.67	101.29	110.71
1	CP	59	ASP	CA-C-N	5.67	130.19	122.19
1	CP	59	ASP	C-N-CA	5.67	130.19	122.19
7	AG	160	LEU	CA-C-N	5.67	129.27	121.33
7	AG	160	LEU	C-N-CA	5.67	129.27	121.33
16	CI	158	HIS	N-CA-C	-5.67	101.89	110.28
2	z	291	TYR	N-CA-C	5.67	126.88	111.00
3	n	110	TYR	N-CA-CB	-5.67	101.30	110.71
5	Bf	588	PHE	N-CA-C	5.67	119.81	113.01
5	Bf	597	TRP	CA-C-O	-5.67	112.29	119.31
7	J	324	GLN	CA-C-N	5.66	132.36	121.54
7	J	324	GLN	C-N-CA	5.66	132.36	121.54
3	7	125	THR	N-CA-C	-5.66	100.74	109.52
5	G	511	PHE	CA-C-N	5.66	125.28	119.56
5	G	511	PHE	C-N-CA	5.66	125.28	119.56
7	AM	48	ASP	CA-C-O	-5.66	112.41	120.51
5	G	765	GLN	CA-C-O	-5.66	111.86	119.11
3	I	496	THR	CA-C-N	5.66	127.86	120.28
3	I	496	THR	C-N-CA	5.66	127.86	120.28
3	n	64	GLY	N-CA-C	-5.66	107.51	115.32
2	s	239	GLN	CA-C-O	-5.66	113.46	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	CT	129	LEU	N-CA-C	5.66	117.53	111.36
16	Aq	108	LEU	CB-CA-C	-5.66	103.31	111.91
5	AE	623	ILE	CA-C-N	5.66	128.13	120.38
5	AE	623	ILE	C-N-CA	5.66	128.13	120.38
7	AG	513	ASN	N-CA-C	5.65	118.91	111.28
3	I	526	LEU	O-C-N	-5.65	115.82	122.32
7	J	265	ILE	N-CA-C	5.65	116.67	111.81
7	J	306	GLN	N-CA-C	-5.65	101.91	110.28
5	M	208	SER	N-CA-C	5.65	119.46	110.70
3	1	480	ASN	N-CA-CB	5.65	120.11	110.50
5	Bt	257	ILE	N-CA-C	5.65	116.08	108.17
5	M	181	ASN	N-CA-C	-5.65	98.04	107.99
3	1	73	LYS	N-CA-C	-5.65	106.22	113.23
2	BR	73	LEU	N-CA-C	-5.65	104.59	112.45
7	Bm	332	GLY	N-CA-C	-5.65	105.96	112.29
16	CT	167	ASN	N-CA-C	5.65	119.36	111.56
5	L	609	ASP	N-CA-C	-5.65	103.91	111.87
3	1	331	ILE	CB-CA-C	-5.65	104.74	111.97
7	4	113	ILE	CA-C-N	-5.65	115.26	122.77
7	4	113	ILE	C-N-CA	-5.65	115.26	122.77
5	Bt	121	ASN	CA-C-N	5.65	125.74	119.87
5	Bt	121	ASN	C-N-CA	5.65	125.74	119.87
1	i	179	MET	N-CA-C	-5.64	104.60	112.45
3	7	313	LEU	CA-C-N	-5.64	115.75	123.14
3	7	313	LEU	C-N-CA	-5.64	115.75	123.14
5	M	298	ILE	N-CA-C	5.64	116.01	108.11
5	AB	4	ILE	N-CA-C	5.64	116.89	108.54
5	AU	40	ASP	N-CA-C	5.64	119.45	109.58
1	C	371	HIS	N-CA-C	-5.64	102.55	110.50
5	v	493	LEU	N-CA-C	-5.64	104.75	111.69
5	AU	209	SER	N-CA-C	-5.64	106.24	113.23
5	AB	257	ILE	CA-C-N	-5.64	116.20	123.19
5	AB	257	ILE	C-N-CA	-5.64	116.20	123.19
1	A	258	ILE	N-CA-C	-5.63	106.21	111.45
1	C	318	GLN	N-CA-C	-5.63	100.95	109.85
3	I	555	ASN	N-CA-C	-5.63	100.79	109.41
7	J	544	TYR	N-CA-C	-5.63	106.57	113.50
2	Cd	82	ARG	N-CA-C	-5.63	104.76	111.69
3	I	491	LYS	N-CA-C	-5.63	106.95	113.88
7	O	522	PHE	CA-C-O	-5.63	113.13	120.00
2	s	313	THR	N-CA-C	-5.63	105.14	111.28
5	AB	118	LEU	N-CA-C	5.63	118.73	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AB	212	VAL	N-CA-C	5.63	115.78	108.35
7	AM	534	GLU	N-CA-C	-5.63	107.06	114.04
16	CB	40	GLN	N-CA-C	5.63	115.82	107.88
2	CW	85	ASN	N-CA-C	-5.63	105.91	112.89
3	I	780	ASP	N-CA-C	-5.63	105.22	111.36
2	s	137	ASN	N-CA-C	-5.63	104.77	111.69
7	J	510	VAL	N-CA-C	-5.63	105.62	111.58
5	L	543	PHE	N-CA-C	5.62	115.37	108.11
16	c	167	ASN	N-CA-C	5.62	119.80	111.87
7	4	38	ALA	N-CA-C	5.62	119.00	111.24
16	CM	53	ALA	CA-C-N	5.62	125.60	120.03
16	CM	53	ALA	C-N-CA	5.62	125.60	120.03
5	v	669	ILE	CA-C-N	5.62	127.75	120.44
5	v	669	ILE	C-N-CA	5.62	127.75	120.44
16	Ai	169	PRO	N-CA-C	-5.62	102.37	111.14
2	D	25	GLN	N-CA-C	5.62	118.83	108.94
2	Ch	331	ASN	CA-C-O	-5.62	112.46	119.38
3	I	153	ILE	N-CA-C	5.62	116.35	110.62
3	E	662	ILE	CA-C-O	-5.62	114.28	120.96
3	I	670	LEU	CA-C-N	-5.62	110.98	120.58
3	I	670	LEU	C-N-CA	-5.62	110.98	120.58
16	c	29	LEU	N-CA-C	-5.62	105.31	111.82
3	BY	155	THR	N-CA-C	-5.62	107.43	114.56
1	A	217	ILE	N-CA-C	-5.61	99.64	108.23
2	D	331	ASN	CA-C-O	-5.61	112.48	119.38
2	k	21	LEU	N-CA-C	-5.61	106.02	112.92
5	AE	888	ARG	N-CA-C	-5.61	105.16	111.28
1	BD	42	ARG	N-CA-C	-5.61	106.48	113.55
7	Bm	333	GLY	CA-C-N	5.61	130.09	120.72
7	Bm	333	GLY	C-N-CA	5.61	130.09	120.72
7	Bm	542	GLN	N-CA-C	-5.61	106.10	113.17
2	Cd	21	LEU	CA-C-N	5.61	130.10	122.19
2	Cd	21	LEU	C-N-CA	5.61	130.10	122.19
3	E	64	GLY	N-CA-C	-5.61	107.58	115.32
2	f	21	LEU	CA-C-N	5.61	130.10	122.19
2	f	21	LEU	C-N-CA	5.61	130.10	122.19
5	9	468	PHE	N-CA-C	5.61	118.79	108.58
5	AE	493	LEU	N-CA-C	-5.61	105.16	112.23
5	L	577	VAL	CB-CA-C	-5.61	102.09	111.29
3	BY	792	GLN	O-C-N	-5.61	115.38	122.27
7	O	202	LEU	CA-C-O	-5.60	113.11	119.78
2	k	11	TYR	N-CA-C	-5.60	105.17	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AG	314	ASP	CA-C-N	-5.60	114.67	123.13
7	AG	314	ASP	C-N-CA	-5.60	114.67	123.13
7	AM	126	ILE	N-CA-C	5.60	116.80	108.23
2	CW	331	ASN	CA-C-O	-5.60	112.49	119.38
5	AE	765	GLN	CA-C-O	-5.60	111.94	119.11
5	G	574	PHE	N-CA-C	-5.60	100.17	109.46
16	Z	72	LEU	CB-CA-C	-5.60	101.33	110.85
5	9	690	TYR	N-CA-C	5.60	122.03	113.19
16	CI	155	ILE	N-CA-C	5.60	116.01	108.17
16	CT	185	GLN	CA-C-N	-5.60	111.80	120.31
16	CT	185	GLN	C-N-CA	-5.60	111.80	120.31
2	D	278	GLY	N-CA-C	5.59	119.30	111.19
16	c	149	ILE	N-CA-C	-5.59	104.90	111.00
5	AO	165	GLY	N-CA-C	-5.59	102.47	111.59
16	Aq	147	LYS	N-CA-C	-5.59	105.18	112.23
5	AB	213	ILE	N-CA-C	5.59	116.00	108.17
7	AG	506	GLN	CA-C-N	5.59	125.26	119.56
7	AG	506	GLN	C-N-CA	5.59	125.26	119.56
5	Bf	493	LEU	N-CA-C	-5.59	104.81	111.69
3	I	660	ILE	CA-C-O	-5.59	114.62	120.76
3	1	110	TYR	N-CA-CB	-5.59	101.44	110.71
3	1	713	GLU	N-CA-C	-5.59	105.19	111.28
3	E	670	LEU	CA-C-N	-5.58	111.03	120.58
3	E	670	LEU	C-N-CA	-5.58	111.03	120.58
5	R	280	LEU	CA-C-N	5.58	125.78	120.31
5	R	280	LEU	C-N-CA	5.58	125.78	120.31
16	Aq	132	GLN	CA-C-O	-5.58	112.52	120.51
2	CW	158	LYS	N-CA-C	-5.58	104.00	112.04
5	M	162	THR	CA-C-N	5.58	125.20	119.56
5	M	162	THR	C-N-CA	5.58	125.20	119.56
1	i	250	VAL	N-CA-C	5.58	115.93	108.11
3	BY	709	ASP	N-CA-C	5.58	122.69	110.80
2	z	310	LYS	N-CA-C	-5.58	105.82	113.30
5	Bf	442	ILE	N-CA-C	-5.58	106.76	111.56
5	Bf	554	ILE	CA-C-N	-5.58	112.80	120.28
5	Bf	554	ILE	C-N-CA	-5.58	112.80	120.28
16	c	132	GLN	CA-C-O	-5.58	112.53	120.51
7	AG	510	VAL	N-CA-C	-5.58	105.67	111.58
5	AO	191	SER	O-C-N	-5.58	116.89	123.25
16	Ai	142	ASN	CB-CA-C	-5.58	99.50	110.10
2	Ch	318	ILE	CA-C-N	-5.58	112.28	121.92
2	Ch	318	ILE	C-N-CA	-5.58	112.28	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	q	267	GLU	N-CA-C	-5.57	107.02	113.88
3	n	441	PHE	N-CA-C	-5.57	104.61	111.40
2	y	310	LYS	N-CA-C	-5.57	105.84	113.30
1	A	203	LYS	N-CA-C	5.57	118.30	109.50
2	CW	83	GLU	N-CA-C	-5.57	104.84	111.69
3	BY	43	TRP	N-CA-C	5.57	116.97	108.12
5	Bt	278	PHE	N-CA-C	5.57	117.47	108.34
1	CP	202	TYR	CA-C-N	-5.57	113.94	122.62
1	CP	202	TYR	C-N-CA	-5.57	113.94	122.62
1	CP	69	ASN	N-CA-C	-5.56	105.36	111.82
7	AG	126	ILE	CB-CA-C	-5.56	104.23	110.96
7	AG	126	ILE	N-CA-C	5.56	116.74	108.23
3	1	133	VAL	N-CA-C	5.56	116.13	108.12
2	D	82	ARG	CA-C-O	-5.56	112.96	119.24
16	CM	131	VAL	N-CA-C	-5.56	102.35	109.30
16	Z	33	LEU	CB-CA-C	-5.55	101.42	110.85
5	M	281	PRO	N-CA-C	5.54	119.72	111.41
1	i	258	ILE	N-CA-C	-5.54	105.70	111.58
5	v	611	PRO	N-CA-C	5.54	123.89	112.47
3	7	832	PHE	N-CA-C	-5.54	105.32	111.36
5	L	586	GLY	CA-C-N	5.54	132.12	121.54
5	L	586	GLY	C-N-CA	5.54	132.12	121.54
5	M	209	SER	N-CA-C	-5.54	106.02	112.89
16	Z	119	ARG	N-CA-C	-5.54	106.36	114.39
3	7	894	GLN	N-CA-C	-5.54	105.32	111.36
2	Cd	326	ALA	N-CA-C	-5.54	105.24	111.28
5	R	316	PHE	N-CA-C	-5.54	105.14	111.07
5	AU	163	PRO	N-CA-C	5.54	123.88	112.47
5	G	496	PHE	N-CA-C	-5.54	105.16	111.14
1	Ca	318	GLN	N-CA-C	-5.54	100.93	109.52
3	E	112	ILE	CB-CA-C	-5.54	105.42	110.63
5	L	765	GLN	CA-C-O	-5.54	112.02	119.11
7	J	557	LEU	CA-C-O	-5.54	114.91	121.66
5	G	626	LYS	N-CA-C	-5.53	105.66	112.90
1	i	281	SER	N-CA-C	5.53	115.41	108.45
7	4	318	THR	N-CA-C	-5.53	106.90	113.97
5	AB	300	ILE	CA-C-N	-5.53	115.83	122.90
5	AB	300	ILE	C-N-CA	-5.53	115.83	122.90
5	AB	274	ILE	N-CA-C	5.52	116.32	107.98
1	A	6	ILE	N-CA-C	-5.52	99.78	108.23
5	AE	442	ILE	N-CA-C	-5.52	106.81	111.56
7	AM	174	ASN	N-CA-C	5.52	121.89	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AE	546	PRO	N-CA-C	5.52	117.43	110.70
5	M	252	GLY	N-CA-C	-5.51	103.54	112.31
2	f	322	LYS	CA-C-N	5.51	125.22	119.82
2	f	322	LYS	C-N-CA	5.51	125.22	119.82
2	z	56	ASN	N-CA-C	-5.51	105.42	111.82
3	E	31	ASP	CA-C-N	-5.51	115.92	123.14
3	E	31	ASP	C-N-CA	-5.51	115.92	123.14
2	y	56	ASN	N-CA-C	-5.51	105.42	111.82
1	i	95	LEU	N-CA-C	-5.51	105.28	112.23
16	Ai	113	SER	N-CA-C	-5.51	102.37	110.52
3	E	73	LYS	N-CA-C	-5.51	105.69	112.90
7	AG	550	MET	N-CA-C	5.51	117.36	111.36
2	q	358	ARG	N-CA-C	5.50	120.68	113.30
3	I	805	GLN	CA-C-N	5.50	128.00	120.46
3	I	805	GLN	C-N-CA	5.50	128.00	120.46
3	1	43	TRP	N-CA-C	5.50	116.87	108.12
5	AB	87	VAL	CB-CA-C	-5.50	102.96	110.77
2	q	277	VAL	N-CA-C	5.50	116.56	111.45
5	G	464	LEU	CA-C-N	5.50	131.60	121.70
5	G	464	LEU	C-N-CA	5.50	131.60	121.70
1	i	202	TYR	CA-C-N	-5.50	114.04	122.62
1	i	202	TYR	C-N-CA	-5.50	114.04	122.62
5	AU	16	GLU	N-CA-C	5.50	117.98	111.33
1	Ca	90	GLN	N-CA-C	5.50	119.99	113.28
1	i	203	LYS	N-CA-C	5.49	118.18	109.50
5	AB	87	VAL	N-CA-C	5.49	115.77	107.75
1	BD	214	ILE	N-CA-C	-5.49	106.45	111.67
2	Cd	329	GLN	CA-C-O	-5.49	112.65	120.51
3	E	110	TYR	N-CA-CB	-5.49	101.60	110.71
2	BK	318	ILE	CA-C-O	-5.49	114.43	120.96
1	CP	342	ASN	CA-C-N	-5.49	113.23	122.29
1	CP	342	ASN	C-N-CA	-5.49	113.23	122.29
7	Bm	98	SER	N-CA-C	-5.49	102.05	110.01
3	I	507	CYS	CA-C-N	5.49	126.70	119.84
3	I	507	CYS	C-N-CA	5.49	126.70	119.84
3	I	847	LEU	CA-C-O	-5.49	113.14	119.56
5	L	464	LEU	CA-C-N	5.48	131.57	121.70
5	L	464	LEU	C-N-CA	5.48	131.57	121.70
5	R	59	VAL	CA-C-O	-5.48	114.69	120.39
5	9	609	ASP	CA-C-N	5.48	131.86	123.96
5	9	609	ASP	C-N-CA	5.48	131.86	123.96
5	AO	284	LYS	N-CA-C	-5.48	104.84	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Az	142	ASN	N-CA-CB	5.48	119.82	110.50
1	A	202	TYR	CA-C-N	-5.48	114.07	122.62
1	A	202	TYR	C-N-CA	-5.48	114.07	122.62
5	v	434	TYR	N-CA-C	5.48	114.61	108.25
1	Ca	126	GLN	N-CA-C	5.48	118.11	109.39
3	7	588	LEU	N-CA-C	-5.48	104.95	111.69
3	7	538	ILE	CA-C-N	-5.48	112.94	120.28
3	7	538	ILE	C-N-CA	-5.48	112.94	120.28
3	E	609	TRP	CA-C-O	-5.48	111.93	119.05
5	R	293	PRO	N-CA-C	5.48	121.75	113.81
3	n	762	GLU	CB-CA-C	-5.48	101.70	110.79
7	4	65	CYS	N-CA-C	5.48	117.40	109.07
1	Ca	342	ASN	CA-C-N	-5.48	113.25	122.29
1	Ca	342	ASN	C-N-CA	-5.48	113.25	122.29
2	D	281	ASN	N-CA-C	5.47	126.33	111.00
5	R	207	ASP	N-CA-C	-5.47	96.68	107.69
16	Z	41	ASP	N-CA-C	5.47	117.31	110.91
1	CP	257	ILE	CA-C-O	-5.47	114.61	120.85
2	f	73	LEU	N-CA-C	-5.47	104.96	111.69
3	n	782	GLU	N-CA-C	-5.47	105.70	112.38
5	AO	78	VAL	N-CA-C	5.47	115.77	108.11
16	CM	68	THR	N-CA-C	5.47	118.53	110.59
5	AO	295	ASN	N-CA-C	-5.47	105.25	113.89
2	BK	158	LYS	N-CA-C	-5.47	105.32	111.28
3	E	155	THR	N-CA-C	-5.47	107.61	114.56
5	9	506	PHE	N-CA-C	-5.47	106.74	113.41
7	AG	523	VAL	N-CA-C	5.47	118.91	112.35
1	CP	42	ARG	N-CA-C	-5.47	106.66	113.55
7	J	110	ASP	N-CA-C	5.47	120.60	113.88
3	7	296	PRO	N-CA-C	-5.47	101.92	110.50
1	C	203	LYS	N-CA-C	5.46	118.14	109.50
7	AM	259	ILE	N-CA-C	5.46	115.97	107.99
5	M	106	SER	N-CA-C	5.46	117.40	108.55
3	BY	31	ASP	CA-C-N	-5.46	115.98	123.14
3	BY	31	ASP	C-N-CA	-5.46	115.98	123.14
5	Bf	611	PRO	CA-C-N	5.46	131.53	121.70
5	Bf	611	PRO	C-N-CA	5.46	131.53	121.70
3	1	602	ASP	N-CA-C	-5.46	104.17	112.04
1	Ca	434	ILE	CB-CA-C	-5.46	105.20	112.46
3	7	713	GLU	N-CA-C	-5.46	105.33	111.28
1	C	37	GLN	CA-C-N	-5.46	113.25	121.05
1	C	37	GLN	C-N-CA	-5.46	113.25	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	147	ILE	CB-CA-C	-5.46	104.98	111.97
2	s	37	LYS	CA-C-N	-5.46	112.05	121.66
2	s	37	LYS	C-N-CA	-5.46	112.05	121.66
5	9	554	ILE	CA-C-N	-5.46	112.42	120.28
5	9	554	ILE	C-N-CA	-5.46	112.42	120.28
5	AB	257	ILE	CB-CA-C	-5.46	102.36	110.33
3	7	733	LYS	N-CA-C	-5.46	107.19	112.97
5	AE	611	PRO	N-CA-C	5.46	123.71	112.47
7	AM	513	ASN	N-CA-C	5.46	118.77	111.24
5	AE	588	PHE	N-CA-C	5.46	119.68	113.19
5	AE	641	PHE	CA-C-O	-5.46	114.64	120.42
7	Bm	192	SER	N-CA-C	5.46	115.44	108.24
3	I	785	VAL	N-CA-C	-5.45	107.06	111.91
7	Bm	255	LYS	CA-C-N	-5.45	116.00	123.14
7	Bm	255	LYS	C-N-CA	-5.45	116.00	123.14
7	4	314	ASP	CB-CA-C	-5.45	104.15	112.11
16	Av	109	ARG	N-CA-C	5.45	117.70	109.41
7	O	76	PHE	CA-C-O	-5.45	113.59	120.84
7	4	345	PHE	N-CA-C	-5.45	106.63	113.28
1	BD	324	VAL	CA-C-N	-5.45	115.20	122.72
1	BD	324	VAL	C-N-CA	-5.45	115.20	122.72
5	Bf	741	GLU	N-CA-C	-5.45	105.42	111.36
7	Bm	506	GLN	CA-C-N	5.45	125.12	119.56
7	Bm	506	GLN	C-N-CA	5.45	125.12	119.56
3	7	609	TRP	CA-C-O	-5.45	111.97	119.05
5	Bt	16	GLU	N-CA-C	5.45	117.22	111.28
5	AB	59	VAL	CA-C-O	-5.45	114.49	120.48
2	Ch	280	ILE	CA-C-O	-5.45	113.97	120.78
5	AE	787	THR	N-CA-C	-5.44	105.35	111.28
1	C	202	TYR	CA-C-N	-5.44	114.13	122.62
1	C	202	TYR	C-N-CA	-5.44	114.13	122.62
3	7	672	TYR	N-CA-C	-5.44	105.77	112.90
7	J	542	GLN	N-CA-C	-5.44	106.31	113.17
16	Az	38	LYS	N-CA-C	-5.44	105.74	112.38
5	M	175	GLY	N-CA-C	-5.44	107.81	115.32
3	I	598	VAL	N-CA-CB	-5.44	105.43	111.41
3	n	31	ASP	CA-C-N	-5.44	116.02	123.14
3	n	31	ASP	C-N-CA	-5.44	116.02	123.14
7	AM	38	ALA	CA-C-N	-5.44	113.15	120.82
7	AM	38	ALA	C-N-CA	-5.44	113.15	120.82
5	AO	157	ALA	N-CA-C	5.44	120.28	113.43
5	Bf	602	ASP	N-CA-C	-5.44	105.00	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	280	ILE	O-C-N	-5.43	115.78	122.57
3	1	112	ILE	CB-CA-C	-5.43	105.52	110.63
5	Bt	10	VAL	N-CA-C	5.43	115.91	111.62
5	AB	300	ILE	N-CA-C	5.43	116.55	108.46
16	CM	171	PHE	CA-C-N	5.43	131.48	121.70
16	CM	171	PHE	C-N-CA	5.43	131.48	121.70
5	M	43	ASN	N-CA-C	5.43	119.07	111.74
1	i	358	ILE	N-CA-C	5.43	115.67	107.80
2	D	318	ILE	CA-C-O	-5.43	114.50	120.96
2	CW	93	LEU	CA-C-O	-5.43	112.16	119.11
16	An	38	LYS	N-CA-C	-5.43	104.76	111.33
3	E	662	ILE	CA-C-N	-5.43	112.06	120.31
3	E	662	ILE	C-N-CA	-5.43	112.06	120.31
16	An	142	ASN	N-CA-CB	5.43	119.72	110.50
2	f	136	GLU	CA-C-N	-5.42	112.59	120.29
2	f	136	GLU	C-N-CA	-5.42	112.59	120.29
5	9	584	LEU	CA-C-N	-5.42	112.54	121.92
5	9	584	LEU	C-N-CA	-5.42	112.54	121.92
5	AB	303	GLY	N-CA-C	-5.42	108.71	114.67
2	CW	22	HIS	N-CA-C	5.42	119.06	111.74
5	AB	293	PRO	N-CA-C	5.42	123.63	112.47
7	AM	38	ALA	N-CA-C	5.42	118.72	111.24
5	R	295	ASN	N-CA-C	-5.42	105.70	114.09
5	v	756	TYR	CA-C-O	-5.42	113.22	119.56
5	Bf	585	SER	N-CA-C	-5.42	106.84	113.50
2	CW	108	ARG	CA-C-N	-5.42	113.02	120.28
2	CW	108	ARG	C-N-CA	-5.42	113.02	120.28
3	I	894	GLN	N-CA-C	-5.41	105.46	111.36
7	J	345	PHE	N-CA-C	-5.41	106.68	113.28
3	n	526	LEU	O-C-N	-5.41	116.54	122.38
5	Bf	816	ASP	N-CA-C	-5.41	105.46	111.36
3	E	132	GLN	CA-C-N	-5.41	115.47	122.99
3	E	132	GLN	C-N-CA	-5.41	115.47	122.99
2	BK	93	LEU	CA-C-N	-5.41	112.41	122.09
2	BK	93	LEU	C-N-CA	-5.41	112.41	122.09
7	O	534	GLU	CA-C-N	-5.41	113.03	120.28
7	O	534	GLU	C-N-CA	-5.41	113.03	120.28
2	q	328	SER	N-CA-C	-5.41	107.33	114.31
3	1	31	ASP	CA-C-N	-5.41	116.06	123.14
3	1	31	ASP	C-N-CA	-5.41	116.06	123.14
5	L	894	GLN	N-CA-C	-5.41	105.47	111.36
7	O	244	CYS	CA-C-N	-5.41	112.42	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	244	CYS	C-N-CA	-5.41	112.42	121.39
2	Cd	89	SER	N-CA-C	-5.40	105.47	111.36
3	BY	682	GLN	CB-CA-C	-5.40	103.70	111.91
5	Bf	803	ASP	N-CA-C	5.40	118.33	111.69
16	CI	132	GLN	CA-C-O	-5.40	112.79	120.51
2	D	120	LYS	CA-C-N	5.40	127.78	120.44
2	D	120	LYS	C-N-CA	5.40	127.78	120.44
2	k	113	GLN	N-CA-C	-5.40	105.48	111.36
5	AE	597	TRP	CA-C-O	-5.40	113.03	119.35
5	AO	56	THR	CA-C-N	-5.40	115.49	122.99
5	AO	56	THR	C-N-CA	-5.40	115.49	122.99
7	J	88	HIS	CB-CA-C	-5.39	104.23	112.11
5	L	664	THR	CA-C-N	5.39	125.33	119.78
5	L	664	THR	C-N-CA	5.39	125.33	119.78
7	AM	114	ARG	CA-C-N	-5.39	115.16	123.14
7	AM	114	ARG	C-N-CA	-5.39	115.16	123.14
7	AG	332	GLY	N-CA-C	-5.39	106.25	112.29
7	AM	545	SER	N-CA-C	-5.39	105.40	111.28
5	Bt	59	VAL	CA-C-O	-5.39	114.79	120.39
2	f	290	ASN	N-CA-C	-5.39	99.33	110.80
3	7	493	TYR	N-CA-C	-5.39	105.57	111.82
7	AG	88	HIS	CB-CA-C	-5.39	104.25	112.11
7	Bm	110	ASP	N-CA-C	5.39	119.98	113.41
1	A	213	LEU	N-CA-C	5.38	118.03	110.23
5	AE	506	PHE	N-CA-C	-5.38	106.84	113.41
16	Av	153	ALA	CA-C-N	5.38	130.24	121.74
16	Av	153	ALA	C-N-CA	5.38	130.24	121.74
7	4	109	GLN	CA-C-N	5.38	129.82	120.68
7	4	109	GLN	C-N-CA	5.38	129.82	120.68
16	CT	27	THR	N-CA-C	5.38	116.45	108.86
2	Cd	30	GLU	N-CA-C	-5.38	106.39	113.17
7	J	331	THR	N-CA-C	5.38	116.82	109.18
5	9	584	LEU	CA-C-O	-5.38	115.24	120.89
5	AB	222	TYR	N-CA-C	5.38	117.67	108.90
7	Bm	38	ALA	N-CA-C	5.38	118.66	111.24
7	AM	151	ASP	N-CA-C	5.38	122.25	110.80
16	CI	37	ILE	N-CA-C	-5.38	106.56	111.67
5	L	584	LEU	CA-C-O	-5.37	112.83	120.51
5	AB	194	GLU	CA-C-N	-5.37	115.05	122.30
5	AB	194	GLU	C-N-CA	-5.37	115.05	122.30
3	n	752	LYS	N-CA-C	5.37	116.68	108.30
16	CI	40	GLN	N-CA-C	5.37	116.82	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	144	SER	N-CA-C	-5.37	102.25	110.14
5	AE	926	GLN	N-CA-C	-5.37	105.99	112.54
7	O	200	TRP	CA-C-N	5.37	129.50	121.72
7	O	200	TRP	C-N-CA	5.37	129.50	121.72
2	k	48	GLY	N-CA-C	-5.37	106.29	112.73
5	AE	503	SER	O-C-N	-5.37	116.40	123.16
16	A7	185	GLN	CA-C-N	-5.37	112.15	120.31
16	A7	185	GLN	C-N-CA	-5.37	112.15	120.31
16	c	31	LYS	N-CA-C	-5.36	107.28	113.88
2	Cd	53	LYS	N-CA-C	-5.36	105.43	111.28
7	4	76	PHE	CA-C-O	-5.36	112.84	120.51
3	7	866	ILE	N-CA-C	-5.36	105.16	111.00
2	BR	104	LEU	N-CA-C	-5.36	105.88	112.90
3	BY	516	MET	CA-C-N	5.36	125.03	119.56
3	BY	516	MET	C-N-CA	5.36	125.03	119.56
16	CT	109	ARG	N-CA-C	5.36	117.54	109.23
7	O	533	THR	CA-C-O	-5.36	115.27	120.89
5	9	597	TRP	N-CA-C	-5.36	106.25	112.89
7	Bm	147	LEU	N-CA-C	5.35	117.99	110.23
5	Bt	188	THR	N-CA-C	-5.35	107.12	113.97
7	J	506	GLN	CA-C-N	5.35	125.02	119.56
7	J	506	GLN	C-N-CA	5.35	125.02	119.56
5	Bt	261	ASN	CA-C-N	5.35	129.74	122.19
5	Bt	261	ASN	C-N-CA	5.35	129.74	122.19
5	L	539	TYR	N-CA-C	5.35	118.97	112.23
3	BY	599	VAL	N-CA-CB	-5.35	102.41	111.50
3	I	153	ILE	CB-CA-C	-5.35	104.92	112.14
5	AO	312	LEU	N-CA-C	-5.35	105.49	112.23
1	A	434	ILE	CB-CA-C	-5.34	105.35	112.46
16	CB	139	LYS	CA-C-O	-5.34	112.87	120.51
1	Ca	398	LEU	N-CA-C	-5.34	103.44	110.39
7	4	521	ASN	CA-C-N	5.34	127.39	120.44
7	4	521	ASN	C-N-CA	5.34	127.39	120.44
5	AE	465	TYR	CA-C-N	5.34	126.52	119.84
5	AE	465	TYR	C-N-CA	5.34	126.52	119.84
7	AG	542	GLN	N-CA-C	-5.34	106.44	113.17
5	AU	319	GLU	CA-C-N	5.34	131.74	121.54
5	AU	319	GLU	C-N-CA	5.34	131.74	121.54
16	Aq	144	ILE	CB-CA-C	-5.34	107.17	111.71
2	f	91	ILE	N-CA-CB	5.34	118.59	110.58
3	7	459	LEU	CA-C-N	5.34	125.03	119.64
3	7	459	LEU	C-N-CA	5.34	125.03	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AB	261	ASN	N-CA-C	-5.34	106.35	112.92
1	C	364	VAL	N-CA-C	5.34	119.51	112.04
5	M	1	MET	CA-C-N	5.34	131.31	121.70
5	M	1	MET	C-N-CA	5.34	131.31	121.70
5	L	638	LEU	N-CA-C	-5.34	105.13	111.69
5	AO	305	GLY	N-CA-C	-5.34	108.34	114.69
16	Av	39	HIS	N-CA-C	-5.34	98.68	108.02
5	Bf	765	GLN	CA-C-O	-5.33	112.28	119.11
5	G	646	ASN	CA-C-N	5.33	124.95	119.56
5	G	646	ASN	C-N-CA	5.33	124.95	119.56
3	n	451	VAL	CB-CA-C	-5.33	105.06	112.04
3	n	670	LEU	CA-C-O	-5.33	112.70	119.31
5	G	624	TYR	N-CA-C	-5.33	105.55	111.36
3	l	660	ILE	CA-C-O	-5.33	114.90	120.76
16	c	108	LEU	CB-CA-C	-5.33	103.81	111.91
1	CP	208	HIS	N-CA-C	-5.33	103.32	109.93
1	CP	214	ILE	N-CA-C	-5.33	107.23	111.81
16	Az	169	PRO	N-CA-C	-5.33	102.83	111.14
5	G	442	ILE	N-CA-C	-5.33	106.98	111.56
5	v	573	ASN	N-CA-C	5.33	118.93	111.74
5	AO	209	SER	N-CA-C	-5.33	106.63	113.23
2	s	27	LEU	N-CA-C	5.32	118.26	109.85
3	E	471	ARG	CA-C-O	-5.32	113.12	120.52
3	I	837	MET	CA-C-O	-5.32	114.89	121.06
5	AU	102	GLY	N-CA-C	-5.32	105.65	114.48
16	CB	35	TYR	N-CA-C	5.32	113.86	108.75
1	CP	126	GLN	N-CA-C	5.32	117.77	108.52
5	R	194	GLU	CA-C-N	-5.32	115.35	122.42
5	R	194	GLU	C-N-CA	-5.32	115.35	122.42
2	Ch	357	ARG	CA-C-O	-5.32	113.34	119.56
16	Z	147	LYS	CA-C-N	-5.32	111.64	120.68
16	Z	147	LYS	C-N-CA	-5.32	111.64	120.68
7	AG	152	ASP	CB-CA-C	-5.32	104.64	111.50
7	AG	239	HIS	CA-C-N	5.32	125.64	119.47
7	AG	239	HIS	C-N-CA	5.32	125.64	119.47
7	J	166	MET	N-CA-CB	-5.31	102.61	110.53
3	l	128	ILE	N-CA-C	-5.31	101.88	108.89
1	A	179	MET	N-CA-C	-5.31	104.39	112.04
2	BR	321	SER	N-CA-C	5.31	119.86	112.90
3	I	831	LYS	N-CA-C	-5.31	105.57	111.36
5	L	930	ILE	N-CA-C	-5.31	105.36	110.72
2	y	14	LEU	CA-C-N	5.31	127.39	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	y	14	LEU	C-N-CA	5.31	127.39	120.28
7	J	246	ILE	N-CA-CB	-5.31	104.74	111.64
2	s	91	ILE	N-CA-C	-5.31	105.36	110.72
16	CM	173	ILE	CA-C-N	5.31	131.25	121.70
16	CM	173	ILE	C-N-CA	5.31	131.25	121.70
2	Cd	48	GLY	N-CA-C	-5.31	106.29	113.24
1	C	388	TRP	N-CA-CB	5.30	117.00	110.53
5	R	256	GLY	N-CA-C	-5.30	104.94	112.37
2	f	265	ASP	CA-C-N	-5.30	113.66	120.34
2	f	265	ASP	C-N-CA	-5.30	113.66	120.34
2	k	280	ILE	CA-C-O	-5.30	114.15	120.78
7	AG	345	PHE	N-CA-C	-5.30	106.81	113.28
3	BY	755	ALA	CA-C-O	-5.30	114.80	120.42
16	CI	185	GLN	CA-C-N	-5.30	112.25	120.31
16	CI	185	GLN	C-N-CA	-5.30	112.25	120.31
7	4	233	VAL	N-CA-C	-5.30	102.21	109.37
3	n	558	VAL	N-CA-C	5.30	120.36	109.34
2	q	9	ARG	N-CA-C	-5.30	105.50	111.28
2	D	108	ARG	CA-C-N	-5.30	112.77	120.29
2	D	108	ARG	C-N-CA	-5.30	112.77	120.29
3	1	32	VAL	N-CA-C	5.30	115.53	108.11
3	1	516	MET	CA-C-N	5.30	124.96	119.56
3	1	516	MET	C-N-CA	5.30	124.96	119.56
7	Bm	186	ARG	CB-CA-C	-5.30	102.20	110.94
16	Aq	109	ARG	N-CA-C	5.30	117.44	109.23
7	Bm	165	PHE	N-CA-C	-5.30	101.02	109.07
1	Ca	200	ILE	N-CA-C	5.30	116.02	110.62
1	i	174	PHE	N-CA-C	5.29	118.06	108.69
5	Bt	38	VAL	CA-C-N	-5.29	113.19	121.87
5	Bt	38	VAL	C-N-CA	-5.29	113.19	121.87
2	s	265	ASP	O-C-N	-5.29	116.51	122.12
5	AO	291	ILE	N-CA-C	5.29	115.58	108.17
2	z	14	LEU	CA-C-N	5.29	127.37	120.28
2	z	14	LEU	C-N-CA	5.29	127.37	120.28
5	AU	141	GLN	CA-C-N	5.29	129.65	122.19
5	AU	141	GLN	C-N-CA	5.29	129.65	122.19
2	Ch	278	GLY	N-CA-C	5.29	118.86	111.19
7	J	158	TRP	N-CA-C	5.29	122.06	110.80
3	1	339	GLN	N-CA-C	5.29	117.05	111.28
5	AB	242	THR	N-CA-C	-5.29	107.48	114.04
7	AM	285	TYR	CA-C-N	-5.29	114.60	122.74
7	AM	285	TYR	C-N-CA	-5.29	114.60	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ca	414	LYS	N-CA-C	-5.29	105.60	111.36
2	s	14	LEU	CA-C-N	5.29	127.36	120.28
2	s	14	LEU	C-N-CA	5.29	127.36	120.28
5	v	762	LEU	N-CA-C	-5.29	106.33	112.89
2	y	86	ASN	N-CA-C	-5.29	105.19	111.69
5	AE	622	ILE	CA-C-O	-5.29	115.89	121.44
5	Bf	764	ARG	N-CA-C	-5.29	105.60	111.36
7	Bm	202	LEU	CA-C-O	-5.29	112.89	119.28
16	Z	172	ASP	N-CA-CB	5.28	119.48	110.50
3	1	144	SER	N-CA-C	-5.28	102.37	110.14
3	7	816	ASP	N-CA-C	-5.28	105.60	111.36
16	CB	35	TYR	CB-CA-C	-5.28	108.76	116.53
3	n	752	LYS	CA-C-N	5.28	129.05	120.60
3	n	752	LYS	C-N-CA	5.28	129.05	120.60
5	AO	249	PHE	N-CA-C	5.28	118.30	110.48
1	i	131	ASN	CA-C-N	5.28	125.20	119.76
1	i	131	ASN	C-N-CA	5.28	125.20	119.76
3	BY	660	ILE	CA-C-O	-5.28	114.95	120.76
16	CT	186	LEU	N-CA-C	-5.28	105.69	111.82
16	c	60	GLU	N-CA-C	5.28	118.29	110.48
16	Ai	132	GLN	CA-C-N	-5.28	113.87	121.42
16	Ai	132	GLN	C-N-CA	-5.28	113.87	121.42
3	BY	736	ASN	N-CA-C	-5.28	105.61	111.36
7	J	524	PRO	N-CA-C	-5.28	103.16	111.34
2	z	308	LEU	CA-C-N	5.28	131.20	121.70
2	z	308	LEU	C-N-CA	5.28	131.20	121.70
3	n	331	ILE	CB-CA-C	-5.28	105.22	111.97
5	9	618	THR	N-CA-C	-5.28	105.42	111.07
5	AU	289	PHE	N-CA-C	5.28	117.09	109.07
3	BY	331	ILE	CB-CA-C	-5.28	105.22	111.97
5	v	765	GLN	CA-C-O	-5.27	112.36	119.11
2	z	86	ASN	N-CA-C	-5.27	105.20	111.69
7	J	314	ASP	CB-CA-C	-5.27	104.80	111.86
1	CP	281	SER	N-CA-C	5.27	115.09	108.45
3	1	331	ILE	N-CA-CB	5.27	116.71	110.55
2	BR	48	GLY	N-CA-C	-5.27	106.27	113.27
5	Bt	209	SER	N-CA-C	-5.27	106.36	112.89
5	M	237	LEU	CA-C-N	5.26	125.26	119.89
5	M	237	LEU	C-N-CA	5.26	125.26	119.89
3	n	493	TYR	N-CA-C	-5.26	105.71	111.82
16	Ai	71	SER	N-CA-C	-5.26	105.54	111.28
16	CM	141	LYS	O-C-N	-5.26	115.59	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASP	CA-C-N	5.26	129.61	122.19
1	A	59	ASP	C-N-CA	5.26	129.61	122.19
3	1	294	GLU	N-CA-C	5.26	119.25	112.41
16	Z	68	THR	N-CA-C	5.26	117.32	110.53
2	y	308	LEU	CA-C-N	5.26	131.17	121.70
2	y	308	LEU	C-N-CA	5.26	131.17	121.70
16	Ai	118	HIS	N-CA-C	5.26	122.00	110.80
5	AO	242	THR	N-CA-C	-5.26	107.41	113.88
1	Ca	196	TRP	CB-CA-C	-5.26	101.44	110.22
3	E	32	VAL	N-CA-C	5.25	115.47	108.11
5	AE	756	TYR	CA-C-O	-5.25	113.41	119.56
5	Bt	349	LEU	N-CA-CB	5.25	119.21	111.43
1	i	90	GLN	N-CA-C	5.25	119.69	113.28
7	Bm	513	ASN	N-CA-C	5.25	118.49	111.24
3	1	493	TYR	N-CA-C	-5.25	105.73	111.82
3	1	125	THR	N-CA-C	-5.25	101.39	109.52
3	1	666	LEU	CA-C-N	-5.25	111.86	121.52
3	1	666	LEU	C-N-CA	-5.25	111.86	121.52
5	AU	59	VAL	O-C-N	-5.25	116.96	123.10
7	AM	126	ILE	CB-CA-C	-5.25	104.61	110.96
3	I	51	ASP	N-CA-C	5.24	117.63	110.55
5	v	474	LYS	N-CA-C	-5.24	106.57	113.12
5	L	474	LYS	N-CA-C	-5.24	106.95	113.55
7	O	46	HIS	CA-C-N	5.24	128.99	120.60
7	O	46	HIS	C-N-CA	5.24	128.99	120.60
1	A	131	ASN	CA-C-N	5.24	125.16	119.76
1	A	131	ASN	C-N-CA	5.24	125.16	119.76
5	AE	435	PRO	N-CA-C	-5.24	102.97	111.19
5	AU	290	ASP	CB-CA-C	-5.24	102.71	110.62
2	BK	20	GLU	N-CA-C	-5.24	106.39	112.89
5	Bt	322	GLN	N-CA-C	-5.24	105.47	111.07
3	I	128	ILE	N-CA-C	-5.24	101.98	108.89
2	BR	274	ARG	CA-C-N	5.24	131.13	121.70
2	BR	274	ARG	C-N-CA	5.24	131.13	121.70
7	J	76	PHE	CA-C-O	-5.24	113.02	120.51
7	O	51	THR	CB-CA-C	-5.24	100.55	109.03
5	9	611	PRO	CA-C-O	-5.24	117.35	121.38
3	E	740	GLN	CB-CA-C	-5.23	102.56	110.83
3	n	445	PRO	N-CA-C	5.23	118.55	111.22
1	BD	202	TYR	CA-C-N	-5.23	113.66	122.29
1	BD	202	TYR	C-N-CA	-5.23	113.66	122.29
16	CI	132	GLN	N-CA-C	-5.23	99.66	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BY	301	ILE	N-CA-C	5.23	115.84	108.36
7	Bm	169	PHE	N-CA-C	5.23	116.36	108.46
2	Cd	308	LEU	CA-C-N	5.23	131.11	121.70
2	Cd	308	LEU	C-N-CA	5.23	131.11	121.70
5	9	612	GLU	CA-C-N	-5.23	111.99	120.72
5	9	612	GLU	C-N-CA	-5.23	111.99	120.72
5	AE	584	LEU	CA-C-O	-5.23	113.65	119.40
2	BK	360	GLN	N-CA-C	5.23	121.94	110.80
3	n	735	LEU	N-CA-C	-5.22	105.67	111.36
3	7	211	LYS	N-CA-C	-5.22	105.19	112.45
7	AM	187	LEU	N-CA-C	5.22	118.46	110.20
3	I	837	MET	O-C-N	-5.22	117.21	123.27
5	AE	729	ILE	N-CA-C	-5.22	105.62	110.53
7	Bm	98	SER	CB-CA-C	5.22	118.90	109.61
1	C	417	LYS	N-CA-C	-5.22	107.58	114.31
5	M	207	ASP	N-CA-C	-5.22	97.20	107.69
3	1	114	SER	N-CA-C	-5.22	106.15	112.88
16	An	97	ILE	N-CA-C	-5.22	105.76	110.82
2	Cd	272	LYS	CA-C-N	5.22	129.43	120.72
2	Cd	272	LYS	C-N-CA	5.22	129.43	120.72
3	7	677	PRO	N-CA-C	-5.21	105.46	110.47
7	AM	180	VAL	N-CA-C	5.21	115.36	107.75
3	n	660	ILE	CA-C-O	-5.21	115.03	120.76
1	A	76	LYS	N-CA-C	5.21	116.89	108.34
5	AO	124	THR	N-CA-C	-5.21	106.83	114.39
7	4	541	GLN	O-C-N	-5.21	116.12	122.22
16	Z	29	LEU	CA-C-N	5.21	125.72	119.94
16	Z	29	LEU	C-N-CA	5.21	125.72	119.94
2	Ch	280	ILE	O-C-N	-5.21	116.06	122.57
7	AM	345	PHE	CA-C-O	-5.21	112.99	119.18
1	C	398	LEU	CA-C-N	5.20	126.55	120.98
1	C	398	LEU	C-N-CA	5.20	126.55	120.98
3	E	526	LEU	O-C-N	-5.20	116.76	122.38
7	4	88	HIS	CB-CA-C	-5.20	104.08	112.09
3	BY	833	ILE	CA-C-N	5.20	127.25	120.28
3	BY	833	ILE	C-N-CA	5.20	127.25	120.28
1	C	217	ILE	N-CA-C	-5.20	100.27	108.23
7	AG	328	TYR	N-CA-CB	-5.20	103.00	111.22
5	Bt	235	PHE	N-CA-C	5.20	116.43	108.42
2	CW	325	ILE	N-CA-CB	-5.20	107.38	111.64
2	Cd	310	LYS	N-CA-C	-5.20	106.33	113.30
7	AG	200	TRP	CA-C-N	5.20	129.33	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AG	200	TRP	C-N-CA	5.20	129.33	122.42
2	Ch	93	LEU	CA-C-O	-5.20	112.46	119.11
3	I	110	TYR	N-CA-CB	-5.20	102.09	110.71
7	J	76	PHE	CA-C-N	-5.20	109.12	121.80
7	J	76	PHE	C-N-CA	-5.20	109.12	121.80
7	AM	325	SER	CA-C-N	-5.20	113.79	122.62
7	AM	325	SER	C-N-CA	-5.20	113.79	122.62
1	A	69	ASN	N-CA-C	-5.19	106.90	113.18
5	G	506	PHE	N-CA-C	-5.19	107.08	113.41
5	L	588	PHE	N-CA-C	5.19	119.48	113.20
5	R	237	LEU	CA-C-N	5.19	125.18	119.89
5	R	237	LEU	C-N-CA	5.19	125.18	119.89
1	BD	60	ASN	N-CA-CB	-5.19	104.29	112.13
3	BY	538	ILE	CA-C-N	-5.19	113.32	120.28
3	BY	538	ILE	C-N-CA	-5.19	113.32	120.28
3	7	128	ILE	N-CA-C	-5.19	102.04	108.89
2	BR	313	THR	CA-C-O	-5.19	114.00	119.97
5	G	622	ILE	CA-C-O	-5.19	116.22	121.67
7	AM	239	HIS	N-CA-C	-5.19	102.63	109.84
5	Bf	583	PHE	N-CA-C	-5.19	107.02	113.55
3	E	147	ASN	N-CA-C	5.18	117.05	108.13
7	4	38	ALA	CA-C-N	-5.18	113.51	120.82
7	4	38	ALA	C-N-CA	-5.18	113.51	120.82
5	AO	181	ASN	N-CA-C	-5.18	100.64	108.67
16	A7	129	LEU	N-CA-C	5.18	117.01	111.36
3	BY	90	PHE	CA-C-N	5.18	129.79	123.10
3	BY	90	PHE	C-N-CA	5.18	129.79	123.10
1	Ca	388	TRP	N-CA-CB	5.18	117.57	110.57
1	i	164	TYR	N-CA-C	-5.18	100.72	108.96
5	v	577	VAL	CA-C-N	5.18	127.53	120.54
5	v	577	VAL	C-N-CA	5.18	127.53	120.54
5	AB	138	TRP	N-CA-C	5.18	116.94	109.07
3	E	599	VAL	CA-C-N	-5.18	114.39	122.05
3	E	599	VAL	C-N-CA	-5.18	114.39	122.05
3	I	670	LEU	CA-C-O	-5.18	112.89	119.31
5	AB	267	ILE	N-CA-C	5.18	115.36	108.11
3	BY	493	TYR	N-CA-C	-5.18	105.76	111.71
7	Bm	306	GLN	N-CA-C	-5.18	102.62	110.28
3	n	765	GLU	N-CA-C	5.17	119.65	113.23
2	CW	29	ILE	CA-C-N	-5.17	113.36	120.71
2	CW	29	ILE	C-N-CA	-5.17	113.36	120.71
3	E	97	TYR	N-CA-C	-5.17	104.56	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	756	TYR	CA-C-O	-5.17	113.51	119.56
7	4	76	PHE	CA-C-N	-5.17	109.19	121.80
7	4	76	PHE	C-N-CA	-5.17	109.19	121.80
3	E	331	ILE	CB-CA-C	-5.17	105.36	111.97
5	L	645	GLN	CA-C-N	5.17	127.67	120.65
5	L	645	GLN	C-N-CA	5.17	127.67	120.65
2	s	332	VAL	N-CA-C	-5.17	105.37	111.00
1	CP	414	LYS	N-CA-C	-5.17	105.73	111.36
3	BY	803	ALA	N-CA-C	-5.17	106.66	113.17
7	AM	521	ASN	CA-C-N	5.16	127.15	120.44
7	AM	521	ASN	C-N-CA	5.16	127.15	120.44
1	C	334	ALA	N-CA-C	-5.16	102.05	110.20
3	7	797	GLU	N-CA-C	-5.16	105.66	111.28
7	Bm	305	ARG	N-CA-C	5.16	116.92	109.07
5	AO	186	GLU	CA-C-N	-5.16	116.30	122.90
5	AO	186	GLU	C-N-CA	-5.16	116.30	122.90
2	s	136	GLU	CA-C-N	-5.16	111.76	120.58
2	s	136	GLU	C-N-CA	-5.16	111.76	120.58
5	R	208	SER	N-CA-C	5.16	118.69	110.70
5	AO	59	VAL	CA-C-O	-5.16	114.81	120.48
5	AO	235	PHE	N-CA-C	5.15	116.68	108.79
1	BD	90	GLN	N-CA-C	5.15	119.57	113.28
3	E	491	LYS	N-CA-C	-5.15	107.54	113.88
3	7	676	THR	CA-C-N	5.15	123.42	119.66
3	7	676	THR	C-N-CA	5.15	123.42	119.66
16	CI	40	GLN	CA-C-N	-5.15	115.04	122.36
16	CI	40	GLN	C-N-CA	-5.15	115.04	122.36
3	1	147	ASN	N-CA-C	5.15	116.99	108.13
7	4	332	GLY	CA-C-O	-5.15	118.87	122.22
5	AO	43	ASN	N-CA-C	5.15	121.77	110.80
2	BK	279	GLY	CA-C-N	5.15	131.24	121.97
2	BK	279	GLY	C-N-CA	5.15	131.24	121.97
2	z	265	ASP	O-C-N	-5.15	115.93	122.27
16	A7	146	GLN	CA-C-N	-5.15	112.98	120.29
16	A7	146	GLN	C-N-CA	-5.15	112.98	120.29
3	7	479	LEU	N-CA-C	5.15	119.64	112.90
5	R	270	SER	CA-C-O	-5.15	113.05	119.38
3	7	324	VAL	N-CA-CB	-5.14	104.98	111.41
16	Av	132	GLN	N-CA-C	-5.14	99.84	110.80
16	CB	142	ASN	N-CA-CB	5.14	119.25	110.50
1	Ca	287	GLN	CA-C-N	5.14	128.60	123.04
1	Ca	287	GLN	C-N-CA	5.14	128.60	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	805	LEU	N-CA-CB	-5.14	102.52	110.13
3	1	559	SER	O-C-N	-5.14	116.17	122.34
5	AE	504	ASP	N-CA-C	-5.14	106.16	112.90
1	BD	258	ILE	CB-CA-C	-5.14	107.46	113.22
5	R	291	ILE	N-CA-C	5.14	115.37	108.17
2	k	350	GLU	N-CA-C	5.14	118.01	107.37
5	L	486	MET	N-CA-C	-5.14	106.27	112.54
2	y	265	ASP	O-C-N	-5.14	115.95	122.27
3	1	538	ILE	CA-C-N	-5.14	113.39	120.28
3	1	538	ILE	C-N-CA	-5.14	113.39	120.28
5	Bf	521	GLU	N-CA-C	5.14	116.57	111.07
16	Z	98	LEU	CA-C-O	-5.14	112.39	119.12
7	4	513	ASN	N-CA-C	5.14	118.33	111.24
1	C	10	ALA	CA-C-N	5.14	127.16	120.28
1	C	10	ALA	C-N-CA	5.14	127.16	120.28
1	C	117	THR	CA-C-N	-5.14	115.95	122.37
1	C	117	THR	C-N-CA	-5.14	115.95	122.37
2	D	158	LYS	N-CA-C	-5.14	105.59	111.14
2	y	307	TYR	N-CA-C	5.14	119.26	112.89
3	7	625	LEU	CA-C-N	-5.14	112.38	120.60
3	7	625	LEU	C-N-CA	-5.14	112.38	120.60
5	Bf	468	PHE	N-CA-C	5.14	117.56	109.39
2	z	307	TYR	N-CA-C	5.14	119.26	112.89
5	AU	56	THR	CA-C-N	-5.13	115.95	122.37
5	AU	56	THR	C-N-CA	-5.13	115.95	122.37
2	Cd	235	GLU	CA-C-N	5.13	127.42	120.38
2	Cd	235	GLU	C-N-CA	5.13	127.42	120.38
5	G	503	SER	O-C-N	-5.13	116.95	123.01
3	7	153	ILE	CB-CA-C	-5.13	105.21	112.14
5	9	504	ASP	N-CA-C	-5.13	105.38	111.69
7	J	114	ARG	CA-C-N	-5.13	115.55	123.14
7	J	114	ARG	C-N-CA	-5.13	115.55	123.14
1	CP	117	THR	CA-C-N	-5.13	115.96	122.37
1	CP	117	THR	C-N-CA	-5.13	115.96	122.37
1	CP	222	TYR	CA-C-O	-5.13	113.32	121.94
3	1	211	LYS	N-CA-C	-5.13	105.32	112.45
7	4	324	GLN	CA-C-N	5.13	131.34	121.54
7	4	324	GLN	C-N-CA	5.13	131.34	121.54
5	Bt	252	GLY	CA-C-N	-5.13	114.39	122.08
5	Bt	252	GLY	C-N-CA	-5.13	114.39	122.08
1	CP	213	LEU	N-CA-C	5.13	117.67	110.23
2	s	25	GLN	CA-C-N	5.12	125.04	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	s	25	GLN	C-N-CA	5.12	125.04	119.76
7	AG	541	GLN	O-C-N	-5.12	115.44	122.46
7	AG	544	TYR	N-CA-C	-5.12	107.20	113.50
7	Bm	252	HIS	N-CA-CB	-5.12	102.40	110.49
3	I	173	CYS	N-CA-C	5.12	116.08	108.60
7	4	346	ASP	CA-C-N	5.12	130.92	121.70
7	4	346	ASP	C-N-CA	5.12	130.92	121.70
2	BK	93	LEU	CA-C-O	-5.12	112.56	119.11
2	BK	265	ASP	N-CA-C	-5.12	105.88	111.82
16	CB	38	LYS	N-CA-C	-5.12	105.82	111.71
1	Ca	425	ARG	CB-CA-C	-5.12	104.13	111.91
7	J	126	ILE	CB-CA-C	-5.12	104.77	110.96
16	CM	123	PHE	N-CA-C	-5.12	105.78	111.36
3	E	662	ILE	N-CA-C	-5.12	105.86	110.82
5	R	233	SER	N-CA-C	5.12	116.85	109.07
3	BY	32	VAL	N-CA-C	5.12	115.28	108.11
1	C	434	ILE	CB-CA-C	-5.12	105.65	112.46
5	9	602	ASP	N-CA-C	-5.12	105.78	112.23
3	n	133	VAL	N-CA-C	5.12	115.27	108.11
7	AM	506	GLN	CA-C-N	5.12	124.78	119.56
7	AM	506	GLN	C-N-CA	5.12	124.78	119.56
7	AM	534	GLU	CA-C-N	-5.12	113.43	120.28
7	AM	534	GLU	C-N-CA	-5.12	113.43	120.28
7	Bm	38	ALA	CA-C-N	-5.12	113.61	120.82
7	Bm	38	ALA	C-N-CA	-5.12	113.61	120.82
5	R	43	ASN	N-CA-C	5.11	121.69	110.80
2	k	158	LYS	N-CA-C	-5.11	105.78	111.36
5	9	489	ILE	CB-CA-C	-5.11	105.16	112.22
5	AU	63	ASN	CA-C-N	5.11	131.41	122.82
5	AU	63	ASN	C-N-CA	5.11	131.41	122.82
5	Bt	300	ILE	CA-C-N	-5.11	116.36	122.90
5	Bt	300	ILE	C-N-CA	-5.11	116.36	122.90
5	9	435	PRO	N-CA-C	-5.11	103.16	111.19
3	E	43	TRP	N-CA-C	5.11	116.25	108.12
3	E	670	LEU	CA-C-O	-5.11	112.97	119.31
5	L	581	TRP	N-CA-C	5.11	121.11	109.81
7	4	154	THR	N-CA-C	5.11	116.44	109.18
5	AB	329	ARG	N-CA-C	-5.11	107.17	113.41
7	Bm	146	LEU	CB-CA-C	-5.11	104.14	111.70
1	C	126	GLN	N-CA-C	5.11	117.41	108.52
3	7	775	TYR	N-CA-C	-5.11	105.71	111.28
1	A	208	HIS	N-CA-C	-5.11	103.60	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AG	76	PHE	N-CA-C	-5.11	102.02	109.63
7	AG	113	ILE	N-CA-C	-5.11	100.53	108.86
5	Bf	496	PHE	N-CA-C	-5.11	105.17	111.40
1	CP	388	TRP	N-CA-CB	5.11	117.46	110.57
7	O	81	ARG	CA-C-N	5.11	125.01	119.85
7	O	81	ARG	C-N-CA	5.11	125.01	119.85
5	R	309	LYS	N-CA-CB	5.11	119.18	110.50
7	4	56	ASP	CA-C-N	5.11	126.22	119.84
7	4	56	ASP	C-N-CA	5.11	126.22	119.84
5	Bt	194	GLU	CA-C-N	-5.11	115.41	122.30
5	Bt	194	GLU	C-N-CA	-5.11	115.41	122.30
5	G	625	PHE	CA-C-N	-5.10	112.13	121.52
5	G	625	PHE	C-N-CA	-5.10	112.13	121.52
5	R	337	TYR	CA-C-O	-5.10	113.11	119.18
16	c	129	LEU	N-CA-C	5.10	116.92	111.36
1	i	71	ASN	CA-C-N	-5.10	114.88	122.74
1	i	71	ASN	C-N-CA	-5.10	114.88	122.74
16	A7	132	GLN	N-CA-C	-5.10	99.93	110.80
5	Bt	1	MET	CA-C-N	5.10	130.88	121.70
5	Bt	1	MET	C-N-CA	5.10	130.88	121.70
2	Ch	22	HIS	N-CA-C	5.10	118.63	111.74
5	AB	332	GLU	N-CA-C	5.10	117.61	109.96
5	G	512	PRO	CA-C-N	-5.10	113.45	120.28
5	G	512	PRO	C-N-CA	-5.10	113.45	120.28
5	L	741	GLU	N-CA-C	-5.10	105.80	111.36
5	M	155	TYR	CA-C-N	5.10	128.11	120.87
5	M	155	TYR	C-N-CA	5.10	128.11	120.87
3	n	144	SER	N-CA-C	-5.10	102.64	110.14
3	n	326	ASP	CA-C-O	-5.10	114.95	120.81
5	AB	125	LYS	CA-C-N	-5.10	114.89	122.74
5	AB	125	LYS	C-N-CA	-5.10	114.89	122.74
1	BD	358	ILE	N-CA-C	5.10	115.25	108.11
16	CM	29	LEU	CA-C-N	5.10	125.60	119.94
16	CM	29	LEU	C-N-CA	5.10	125.60	119.94
2	z	82	ARG	N-CA-C	-5.10	105.81	112.23
7	J	534	GLU	N-CA-C	-5.10	107.61	113.88
2	f	32	ALA	O-C-N	-5.10	116.72	122.12
2	k	93	LEU	CA-C-N	-5.10	114.49	122.49
2	k	93	LEU	C-N-CA	-5.10	114.49	122.49
3	7	110	TYR	N-CA-CB	-5.10	102.25	110.71
3	7	143	VAL	N-CA-C	5.10	115.19	107.80
5	AU	21	ARG	CA-C-N	-5.10	116.01	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AU	21	ARG	C-N-CA	-5.10	116.01	122.43
1	Ca	282	THR	N-CA-C	-5.10	102.01	109.81
3	E	807	ALA	N-CA-C	-5.10	105.91	111.82
1	i	161	GLY	N-CA-C	-5.09	103.64	111.64
5	v	626	LYS	CA-C-N	-5.09	113.82	120.44
5	v	626	LYS	C-N-CA	-5.09	113.82	120.44
7	4	333	GLY	CA-C-N	5.09	129.23	120.72
7	4	333	GLY	C-N-CA	5.09	129.23	120.72
7	AM	252	HIS	N-CA-CB	-5.09	102.44	110.49
1	BD	237	PHE	CA-C-N	-5.09	116.87	123.19
1	BD	237	PHE	C-N-CA	-5.09	116.87	123.19
1	A	287	GLN	CA-C-N	5.09	128.54	123.04
1	A	287	GLN	C-N-CA	5.09	128.54	123.04
5	v	576	PHE	CB-CA-C	-5.09	99.11	109.65
5	AB	130	ILE	CB-CA-C	-5.09	104.18	111.31
16	CI	40	GLN	O-C-N	-5.09	116.73	122.03
1	CP	282	THR	N-CA-C	-5.09	102.02	109.81
2	Cd	86	ASN	CA-C-N	-5.09	112.02	120.68
2	Cd	86	ASN	C-N-CA	-5.09	112.02	120.68
5	Bf	464	LEU	CA-C-N	5.09	130.86	121.70
5	Bf	464	LEU	C-N-CA	5.09	130.86	121.70
2	CW	326	ALA	N-CA-C	5.09	116.83	111.28
3	I	544	GLN	N-CA-CB	5.08	117.35	110.59
7	J	239	HIS	N-CA-C	-5.08	103.18	109.64
3	n	278	ILE	CB-CA-C	-5.08	103.92	110.84
3	E	211	LYS	N-CA-C	-5.08	105.38	112.45
2	k	93	LEU	CA-C-O	-5.08	112.60	119.11
5	AB	44	HIS	N-CA-C	5.08	117.72	111.82
16	Ai	29	LEU	CA-C-N	5.08	125.58	119.94
16	Ai	29	LEU	C-N-CA	5.08	125.58	119.94
1	CP	343	ALA	N-CA-C	5.08	117.11	109.23
7	J	202	LEU	CA-C-N	-5.08	112.04	120.68
7	J	202	LEU	C-N-CA	-5.08	112.04	120.68
2	f	328	SER	N-CA-C	-5.08	103.82	110.53
2	y	82	ARG	N-CA-C	-5.08	105.83	112.23
16	Av	49	VAL	N-CA-C	-5.08	105.59	110.72
5	M	63	ASN	CA-C-N	5.08	130.49	122.36
5	M	63	ASN	C-N-CA	5.08	130.49	122.36
5	AU	181	ASN	N-CA-C	-5.08	99.05	107.99
1	CP	95	LEU	N-CA-C	-5.08	105.83	112.23
3	E	799	GLU	CA-C-N	-5.08	112.97	120.28
3	E	799	GLU	C-N-CA	-5.08	112.97	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	621	PHE	CA-C-N	5.08	130.73	123.27
5	L	621	PHE	C-N-CA	5.08	130.73	123.27
2	Ch	34	LEU	N-CA-C	-5.08	105.66	111.14
1	C	5	ASN	CA-C-N	-5.07	114.66	121.66
1	C	5	ASN	C-N-CA	-5.07	114.66	121.66
5	L	468	PHE	CA-C-N	5.07	127.59	120.28
5	L	468	PHE	C-N-CA	5.07	127.59	120.28
3	n	274	SER	CA-C-N	5.07	129.19	120.72
3	n	274	SER	C-N-CA	5.07	129.19	120.72
5	v	585	SER	N-CA-C	-5.07	107.14	113.38
5	AB	267	ILE	CA-C-N	5.07	129.55	121.99
5	AB	267	ILE	C-N-CA	5.07	129.55	121.99
16	A7	133	ASN	CA-C-N	5.07	127.97	120.82
16	A7	133	ASN	C-N-CA	5.07	127.97	120.82
1	BD	131	ASN	CA-C-N	5.07	125.00	119.78
1	BD	131	ASN	C-N-CA	5.07	125.00	119.78
1	i	288	HIS	CA-C-O	5.07	121.53	118.33
5	9	633	LYS	N-CA-C	-5.07	107.75	114.04
5	AE	611	PRO	CA-C-N	5.07	130.83	121.70
5	AE	611	PRO	C-N-CA	5.07	130.83	121.70
1	C	250	VAL	N-CA-C	5.07	115.21	108.11
3	n	529	THR	N-CA-C	-5.07	105.20	111.33
16	Ai	98	LEU	CA-C-O	-5.07	112.48	119.12
5	R	279	ARG	N-CA-C	5.07	117.08	109.23
2	f	87	LEU	N-CA-C	-5.07	105.84	112.23
2	q	93	LEU	CA-C-O	-5.07	112.46	119.05
5	AB	290	ASP	CA-C-N	-5.07	116.53	123.12
5	AB	290	ASP	C-N-CA	-5.07	116.53	123.12
3	BY	313	LEU	CA-C-N	-5.07	116.50	123.14
3	BY	313	LEU	C-N-CA	-5.07	116.50	123.14
1	CP	386	TYR	CA-C-N	-5.07	114.71	122.62
1	CP	386	TYR	C-N-CA	-5.07	114.71	122.62
3	E	481	LEU	N-CA-C	5.07	117.53	111.71
16	CI	178	SER	N-CA-C	-5.07	105.22	111.40
1	Ca	281	SER	N-CA-C	5.07	114.83	108.45
5	G	621	PHE	CA-C-N	5.06	130.68	122.68
5	G	621	PHE	C-N-CA	5.06	130.68	122.68
7	O	38	ALA	CA-C-N	-5.06	113.68	120.82
7	O	38	ALA	C-N-CA	-5.06	113.68	120.82
3	1	155	THR	N-CA-C	-5.06	108.13	114.56
16	An	136	GLU	N-CA-C	-5.06	105.84	111.36
16	CM	169	PRO	CA-C-N	-5.06	113.70	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	CM	169	PRO	C-N-CA	-5.06	113.70	122.10
2	Cd	291	TYR	CA-C-O	-5.06	112.19	120.80
7	J	267	HIS	CA-C-N	-5.06	115.97	123.05
7	J	267	HIS	C-N-CA	-5.06	115.97	123.05
5	v	650	VAL	N-CA-C	5.06	119.87	109.34
7	AM	125	SER	CA-C-N	5.06	128.70	122.37
7	AM	125	SER	C-N-CA	5.06	128.70	122.37
1	CP	26	ASN	N-CA-C	-5.06	102.30	110.14
3	n	602	ASP	N-CA-C	-5.06	106.79	113.17
3	1	598	VAL	N-CA-CB	-5.06	105.84	111.41
2	k	25	GLN	N-CA-C	5.06	117.84	108.94
2	s	29	ILE	O-C-N	-5.06	112.58	121.84
5	R	93	HIS	CA-C-N	-5.06	116.55	123.12
5	R	93	HIS	C-N-CA	-5.06	116.55	123.12
3	n	51	ASP	N-CA-C	5.06	117.38	110.55
5	AE	608	ASN	O-C-N	-5.06	115.23	122.41
2	Cd	321	SER	N-CA-C	5.06	119.32	112.04
5	v	583	PHE	CA-C-N	-5.05	114.68	121.71
5	v	583	PHE	C-N-CA	-5.05	114.68	121.71
7	AG	125	SER	CA-C-N	5.05	128.69	122.37
7	AG	125	SER	C-N-CA	5.05	128.69	122.37
7	AM	294	SER	CA-C-O	-5.05	113.31	119.32
16	Ai	139	LYS	CA-C-O	-5.05	113.34	119.61
5	Bf	504	ASP	N-CA-C	-5.05	106.28	112.90
7	Bm	166	MET	CB-CA-C	5.05	118.09	109.24
1	C	196	TRP	N-CA-CB	-5.05	102.03	110.37
5	AB	135	CYS	CA-C-N	-5.05	116.03	123.00
5	AB	135	CYS	C-N-CA	-5.05	116.03	123.00
1	A	388	TRP	N-CA-CB	5.05	117.39	110.57
5	Bf	567	GLN	N-CA-C	-5.05	105.77	111.28
16	CB	136	GLU	N-CA-C	-5.05	105.85	111.36
16	CM	40	GLN	N-CA-C	5.05	115.00	107.88
1	Ca	250	VAL	N-CA-C	5.05	115.18	108.11
1	Ca	334	ALA	N-CA-C	-5.05	102.22	110.20
1	A	10	ALA	CA-C-N	5.05	127.05	120.28
1	A	10	ALA	C-N-CA	5.05	127.05	120.28
5	9	581	TRP	N-CA-C	5.05	120.47	113.45
7	AG	38	ALA	CA-C-N	-5.05	113.70	120.82
7	AG	38	ALA	C-N-CA	-5.05	113.70	120.82
5	M	98	LEU	N-CA-C	-5.05	102.17	109.59
7	4	345	PHE	CA-C-O	-5.05	113.17	119.18
7	AG	205	GLN	CB-CA-C	-5.05	104.56	111.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AG	534	GLU	CA-C-N	-5.05	113.52	120.28
7	AG	534	GLU	C-N-CA	-5.05	113.52	120.28
5	AU	295	ASN	N-CA-C	-5.05	106.27	114.09
5	Bf	584	LEU	CA-C-N	-5.05	113.19	121.92
5	Bf	584	LEU	C-N-CA	-5.05	113.19	121.92
1	CP	270	TYR	N-CA-C	-5.05	101.08	109.46
7	Bm	324	GLN	CA-C-N	5.04	131.17	121.54
7	Bm	324	GLN	C-N-CA	5.04	131.17	121.54
5	G	756	TYR	CA-C-O	-5.04	113.66	119.56
5	AO	121	ASN	CA-C-N	5.04	124.70	119.56
5	AO	121	ASN	C-N-CA	5.04	124.70	119.56
16	Aq	89	ILE	CA-C-N	5.04	131.17	121.54
16	Aq	89	ILE	C-N-CA	5.04	131.17	121.54
3	BY	97	TYR	N-CA-C	-5.04	104.28	111.24
5	Bf	519	GLN	N-CA-C	5.04	119.52	113.17
1	C	213	LEU	N-CA-C	5.04	117.54	110.23
3	E	313	LEU	CA-C-N	-5.04	116.54	123.14
3	E	313	LEU	C-N-CA	-5.04	116.54	123.14
3	n	36	LYS	O-C-N	-5.04	116.78	122.12
5	R	4	ILE	N-CA-C	5.04	115.83	108.58
5	R	162	THR	CA-C-N	5.04	124.70	119.56
5	R	162	THR	C-N-CA	5.04	124.70	119.56
16	Ai	172	ASP	CA-C-N	5.04	131.03	121.97
16	Ai	172	ASP	C-N-CA	5.04	131.03	121.97
3	BY	36	LYS	O-C-N	-5.04	116.78	122.12
1	A	386	TYR	CA-C-N	-5.03	114.77	122.62
1	A	386	TYR	C-N-CA	-5.03	114.77	122.62
1	C	258	ILE	N-CA-C	-5.03	106.25	111.58
3	E	232	TYR	N-CA-C	5.03	117.45	109.50
5	AB	252	GLY	CA-C-N	-5.03	114.53	122.08
5	AB	252	GLY	C-N-CA	-5.03	114.53	122.08
5	AO	122	PRO	CA-C-N	-5.03	115.13	122.28
5	AO	122	PRO	C-N-CA	-5.03	115.13	122.28
2	z	249	THR	N-CA-C	-5.03	105.87	111.36
2	D	280	ILE	O-C-N	-5.03	116.28	122.57
5	R	282	LYS	CA-C-O	-5.03	114.65	120.49
2	D	113	GLN	N-CA-C	-5.03	105.88	111.36
5	G	581	TRP	N-CA-C	5.03	120.44	113.45
1	i	222	TYR	CA-C-O	-5.03	113.49	121.94
5	v	715	SER	N-CA-C	-5.03	105.80	111.28
16	A7	139	LYS	N-CA-C	-5.03	106.92	113.16
3	BY	551	GLU	N-CA-C	5.03	117.49	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Av	57	ARG	CA-C-N	-5.03	115.16	122.65
16	Av	57	ARG	C-N-CA	-5.03	115.16	122.65
7	Bm	332	GLY	CA-C-O	-5.03	118.76	122.23
3	I	255	ILE	N-CA-C	-5.03	103.09	109.58
2	k	31	SER	N-CA-C	5.03	121.51	110.80
1	BD	414	LYS	N-CA-C	-5.03	105.88	111.36
5	Bf	756	TYR	CA-C-O	-5.03	113.68	119.56
3	1	520	VAL	N-CA-C	-5.03	105.50	110.62
7	AG	113	ILE	CA-C-N	-5.03	115.78	122.72
7	AG	113	ILE	C-N-CA	-5.03	115.78	122.72
2	y	249	THR	N-CA-C	-5.02	105.88	111.36
5	AU	337	TYR	CA-C-O	-5.02	113.39	119.27
16	CB	98	LEU	CA-C-O	-5.02	112.54	119.12
3	n	312	TYR	N-CA-C	5.02	117.16	109.07
5	9	423	LYS	N-CA-C	-5.02	105.89	111.36
1	C	414	LYS	N-CA-C	-5.02	105.89	111.36
7	O	243	THR	N-CA-C	-5.02	103.31	110.59
16	Az	97	ILE	N-CA-C	-5.02	105.53	111.00
16	CM	56	GLU	N-CA-C	5.02	119.25	113.18
5	AB	316	PHE	N-CA-C	-5.02	105.89	111.36
2	BR	83	GLU	N-CA-C	-5.02	105.81	111.28
2	CW	34	LEU	N-CA-C	-5.02	105.52	111.69
5	M	251	HIS	N-CA-C	5.02	116.56	111.14
7	O	56	ASP	CA-C-N	5.02	126.11	119.84
7	O	56	ASP	C-N-CA	5.02	126.11	119.84
5	Bf	430	LYS	N-CA-C	5.02	120.05	113.88
5	M	13	TYR	N-CA-C	-5.01	105.26	112.13
3	1	526	LEU	O-C-N	-5.01	116.96	122.38
5	AE	741	GLU	N-CA-C	-5.01	105.89	111.36
5	AU	153	ALA	CA-C-N	-5.01	113.75	120.82
5	AU	153	ALA	C-N-CA	-5.01	113.75	120.82
3	1	309	ASP	N-CA-C	-5.01	99.61	108.23
3	7	326	ASP	CA-C-O	-5.01	115.05	120.81
5	AU	328	GLU	N-CA-C	-5.01	107.11	113.18
3	E	837	MET	CA-C-O	-5.01	115.65	121.26
3	1	235	ILE	N-CA-C	5.01	115.19	108.17
16	Aq	146	GLN	O-C-N	-5.01	116.44	122.15
16	Az	98	LEU	CA-C-O	-5.01	112.69	119.11
7	Bm	318	THR	N-CA-C	-5.01	107.55	113.97
7	J	202	LEU	O-C-N	-5.01	116.11	122.27
2	BK	21	LEU	N-CA-C	-5.01	106.42	112.88
3	n	784	GLN	CA-C-O	-5.01	113.35	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Bm	154	THR	CA-C-N	-5.01	114.81	122.87
7	Bm	154	THR	C-N-CA	-5.01	114.81	122.87
5	G	608	ASN	O-C-N	-5.00	115.30	122.41
7	AG	230	MET	N-CA-C	5.00	117.51	111.40
7	AM	324	GLN	CA-C-N	5.00	131.10	121.54
7	AM	324	GLN	C-N-CA	5.00	131.10	121.54
7	Bm	48	ASP	CA-C-O	-5.00	113.36	120.51
1	A	26	ASN	N-CA-C	-5.00	102.00	109.95
2	D	93	LEU	CA-C-O	-5.00	112.71	119.11
2	BK	357	ARG	CA-C-O	-5.00	114.50	120.55
5	Bt	279	ARG	N-CA-C	5.00	117.88	110.48

There are no chirality outliers.

All (579) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	0	46	UNK	Mainchain
3	1	326	ASP	Mainchain
3	1	36	LYS	Mainchain
3	1	445	PRO	Mainchain
3	1	471	ARG	Mainchain
3	1	526	LEU	Mainchain
3	1	609	TRP	Mainchain
3	1	631	VAL	Mainchain
3	1	666	LEU	Mainchain
3	1	733	LYS	Mainchain,Peptide
7	4	202	LEU	Mainchain
7	4	325	SER	Mainchain,Peptide
7	4	345	PHE	Mainchain
7	4	48	ASP	Mainchain,Peptide
7	4	522	PHE	Mainchain
7	4	533	THR	Mainchain
7	4	541	GLN	Mainchain
7	4	557	LEU	Mainchain,Peptide
7	4	76	PHE	Mainchain,Peptide
3	7	326	ASP	Mainchain
3	7	36	LYS	Mainchain
3	7	445	PRO	Mainchain
3	7	453	TRP	Mainchain
3	7	471	ARG	Mainchain
3	7	526	LEU	Mainchain
3	7	609	TRP	Mainchain

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Mol	Chain	Res	Type	Group
3	7	733	LYS	Mainchain
3	7	784	GLN	Mainchain,Peptide
3	7	792	GLN	Mainchain
3	7	803	ALA	Mainchain
3	7	808	GLU	Mainchain
3	7	837	MET	Mainchain,Peptide
3	7	847	LEU	Mainchain
3	7	863	ASP	Mainchain
3	7	880	LEU	Mainchain
5	9	483	TYR	Mainchain
5	9	492	CYS	Mainchain
5	9	503	SER	Mainchain
5	9	584	LEU	Mainchain,Peptide
5	9	597	TRP	Mainchain
5	9	608	ASN	Mainchain
5	9	649	SER	Mainchain,Peptide
1	A	155	ASP	Mainchain
1	A	222	TYR	Mainchain,Peptide
1	A	301	GLU	Mainchain
1	A	349	VAL	Mainchain,Peptide
1	A	94	LEU	Mainchain
16	A7	132	GLN	Mainchain,Peptide
16	A7	154	THR	Mainchain,Peptide
16	A7	40	GLN	Mainchain
5	AB	124	THR	Mainchain
5	AB	236	ALA	Mainchain
5	AB	253	ASN	Mainchain
5	AB	270	SER	Mainchain
5	AB	31	ASN	Mainchain,Peptide
5	AB	337	TYR	Mainchain
5	AB	59	VAL	Mainchain,Peptide
5	AE	475	TYR	Mainchain
5	AE	483	TYR	Mainchain
5	AE	492	CYS	Mainchain
5	AE	503	SER	Mainchain
5	AE	584	LEU	Mainchain
5	AE	597	TRP	Mainchain
5	AE	608	ASN	Mainchain
5	AE	649	SER	Mainchain,Peptide
5	AE	728	GLN	Mainchain
5	AE	756	TYR	Mainchain
5	AE	765	GLN	Mainchain

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Mol	Chain	Res	Type	Group
5	AE	782	LYS	Mainchain
5	AE	857	ARG	Mainchain
5	AE	876	GLN	Mainchain
5	AE	893	LYS	Mainchain
5	AE	919	THR	Mainchain
5	AE	927	MET	Mainchain
7	AG	202	LEU	Mainchain
7	AG	325	SER	Mainchain
7	AG	345	PHE	Mainchain
7	AG	48	ASP	Mainchain
7	AG	522	PHE	Mainchain
7	AG	533	THR	Mainchain
7	AG	541	GLN	Mainchain
7	AG	557	LEU	Mainchain
7	AG	76	PHE	Mainchain,Peptide
7	AM	294	SER	Mainchain
7	AM	304	GLY	Mainchain
7	AM	325	SER	Mainchain,Peptide
7	AM	345	PHE	Mainchain
7	AM	48	ASP	Mainchain,Peptide
7	AM	522	PHE	Mainchain
7	AM	533	THR	Mainchain
7	AM	541	GLN	Mainchain
7	AM	557	LEU	Mainchain
7	AM	76	PHE	Mainchain,Peptide
5	AO	191	SER	Mainchain,Peptide
5	AO	236	ALA	Mainchain
5	AO	253	ASN	Mainchain
5	AO	270	SER	Mainchain
5	AO	31	ASN	Mainchain,Peptide
5	AO	337	TYR	Mainchain
5	AO	59	VAL	Mainchain
15	AP	30	UNK	Mainchain
15	AP	44	UNK	Mainchain
13	AS	75	UNK	Mainchain
5	AU	124	THR	Mainchain
5	AU	236	ALA	Mainchain
5	AU	253	ASN	Mainchain
5	AU	283	ASN	Mainchain,Peptide
5	AU	31	ASN	Mainchain,Peptide
5	AU	337	TYR	Mainchain
5	AU	59	VAL	Mainchain

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Mol	Chain	Res	Type	Group
14	AZ	11	UNK	Mainchain
14	AZ	62	UNK	Mainchain
14	AZ	84	UNK	Mainchain
15	Aa	30	UNK	Mainchain
15	Aa	44	UNK	Mainchain
16	Ai	125	ALA	Mainchain
16	Ai	132	GLN	Mainchain
16	Ai	139	LYS	Mainchain
16	Ai	146	GLN	Mainchain
16	Ai	98	LEU	Mainchain
14	Am	11	UNK	Mainchain
14	Am	64	UNK	Mainchain
14	Am	84	UNK	Mainchain
16	An	125	ALA	Mainchain
16	An	132	GLN	Mainchain
16	An	139	LYS	Mainchain
16	An	35	TYR	Mainchain,Peptide
16	Aq	132	GLN	Mainchain,Peptide
16	Aq	146	GLN	Mainchain
16	Aq	154	THR	Mainchain,Peptide
16	Aq	40	GLN	Mainchain
14	As	11	UNK	Mainchain
14	As	62	UNK	Mainchain
14	As	84	UNK	Mainchain
16	Av	127	LYS	Mainchain
16	Av	132	GLN	Mainchain,Peptide
16	Av	154	THR	Mainchain,Peptide
16	Av	37	ILE	Mainchain
16	Az	132	GLN	Mainchain
16	Az	139	LYS	Mainchain
16	Az	98	LEU	Mainchain
11	B2	46	UNK	Mainchain
6	B4	105	UNK	Mainchain
6	B4	78	UNK	Mainchain,Peptide
15	B5	30	UNK	Mainchain
15	B5	44	UNK	Mainchain
1	BD	155	ASP	Mainchain
1	BD	222	TYR	Mainchain,Peptide
1	BD	301	GLU	Mainchain
1	BD	349	VAL	Mainchain,Peptide
1	BD	94	LEU	Mainchain
2	BK	12	LEU	Mainchain

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Mol	Chain	Res	Type	Group
2	BK	233	ILE	Mainchain,Peptide
2	BK	318	ILE	Mainchain
2	BK	331	ASN	Mainchain
2	BK	357	ARG	Mainchain,Peptide
2	BK	82	ARG	Mainchain
2	BK	93	LEU	Mainchain
4	BO	68	UNK	Mainchain
2	BR	117	GLN	Mainchain
2	BR	136	GLU	Mainchain
2	BR	239	GLN	Mainchain
2	BR	240	LEU	Mainchain
2	BR	265	ASP	Mainchain
2	BR	29	ILE	Mainchain,Peptide
2	BR	313	THR	Mainchain
2	BR	37	LYS	Mainchain
2	BR	53	LYS	Mainchain
6	BV	105	UNK	Mainchain
6	BV	78	UNK	Mainchain,Peptide
3	BY	326	ASP	Mainchain
3	BY	36	LYS	Mainchain
3	BY	445	PRO	Mainchain
3	BY	471	ARG	Mainchain
3	BY	526	LEU	Mainchain
3	BY	533	PHE	Mainchain
3	BY	556	PRO	Peptide
3	BY	609	TRP	Mainchain
3	BY	631	VAL	Mainchain
3	BY	670	LEU	Mainchain
3	BY	733	LYS	Mainchain
3	BY	755	ALA	Mainchain
3	BY	785	VAL	Mainchain
3	BY	792	GLN	Mainchain
3	BY	803	ALA	Mainchain
3	BY	837	MET	Mainchain
3	BY	847	LEU	Mainchain
3	BY	880	LEU	Mainchain
4	BZ	68	UNK	Mainchain
5	Bf	483	TYR	Mainchain
5	Bf	492	CYS	Mainchain
5	Bf	503	SER	Mainchain
5	Bf	584	LEU	Mainchain
5	Bf	597	TRP	Mainchain

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Mol	Chain	Res	Type	Group
5	Bf	608	ASN	Mainchain
5	Bf	649	SER	Mainchain
5	Bf	749	ILE	Mainchain
5	Bf	756	TYR	Mainchain
5	Bf	765	GLN	Mainchain
5	Bf	858	MET	Mainchain
6	Bg	105	UNK	Mainchain
6	Bg	78	UNK	Mainchain,Peptide
7	Bm	202	LEU	Mainchain
7	Bm	294	SER	Mainchain
7	Bm	325	SER	Mainchain,Peptide
7	Bm	345	PHE	Mainchain
7	Bm	48	ASP	Mainchain,Peptide
7	Bm	522	PHE	Mainchain
7	Bm	533	THR	Mainchain
7	Bm	541	GLN	Mainchain
7	Bm	557	LEU	Mainchain
7	Bm	76	PHE	Mainchain,Peptide
11	Bq	46	UNK	Mainchain
5	Bt	124	THR	Mainchain
5	Bt	236	ALA	Mainchain
5	Bt	253	ASN	Mainchain
5	Bt	270	SER	Mainchain
5	Bt	31	ASN	Mainchain,Peptide
5	Bt	337	TYR	Mainchain
5	Bt	59	VAL	Mainchain
4	Bw	68	UNK	Mainchain
1	C	222	TYR	Mainchain
1	C	301	GLU	Mainchain
1	C	349	VAL	Mainchain,Peptide
1	C	94	LEU	Mainchain
16	CB	125	ALA	Mainchain
16	CB	132	GLN	Mainchain
16	CB	139	LYS	Mainchain
16	CB	175	GLY	Mainchain
16	CB	98	LEU	Mainchain
14	CE	11	UNK	Mainchain
14	CE	62	UNK	Mainchain
14	CE	84	UNK	Mainchain
15	CF	30	UNK	Mainchain
15	CF	44	UNK	Mainchain
16	CI	132	GLN	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
16	CI	154	THR	Mainchain,Peptide
16	CI	40	GLN	Mainchain
16	CM	125	ALA	Mainchain
16	CM	132	GLN	Mainchain
16	CM	139	LYS	Mainchain
16	CM	98	LEU	Mainchain
11	CO	46	UNK	Mainchain
1	CP	155	ASP	Mainchain
1	CP	222	TYR	Mainchain,Peptide
1	CP	301	GLU	Mainchain
1	CP	349	VAL	Mainchain,Peptide
1	CP	94	LEU	Mainchain
16	CT	132	GLN	Mainchain,Peptide
16	CT	154	THR	Mainchain,Peptide
16	CT	40	GLN	Mainchain
2	CW	101	LYS	Mainchain
2	CW	12	LEU	Mainchain
2	CW	123	LEU	Mainchain
2	CW	233	ILE	Mainchain,Peptide
2	CW	318	ILE	Mainchain
2	CW	331	ASN	Mainchain
2	CW	357	ARG	Mainchain,Peptide
2	CW	82	ARG	Mainchain
2	CW	93	LEU	Mainchain
1	Ca	132	PRO	Mainchain
1	Ca	155	ASP	Mainchain
1	Ca	222	TYR	Mainchain,Peptide
1	Ca	301	GLU	Mainchain
1	Ca	349	VAL	Mainchain,Peptide
1	Ca	94	LEU	Mainchain
15	Cc	30	UNK	Mainchain
15	Cc	44	UNK	Mainchain
2	Cd	136	GLU	Mainchain
2	Cd	265	ASP	Mainchain
2	Cd	29	ILE	Mainchain
2	Cd	291	TYR	Mainchain
2	Cd	32	ALA	Mainchain
2	Cd	329	GLN	Mainchain,Peptide
2	Cd	347	LYS	Mainchain
2	Cd	354	GLU	Mainchain,Peptide
2	Cd	37	LYS	Mainchain
2	Cd	44	LYS	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
2	Cd	53	LYS	Mainchain
2	Cd	86	ASN	Mainchain
2	Ch	12	LEU	Mainchain
2	Ch	233	ILE	Mainchain,Peptide
2	Ch	237	GLN	Mainchain
2	Ch	318	ILE	Mainchain,Peptide
2	Ch	331	ASN	Mainchain
2	Ch	342	LEU	Mainchain
2	Ch	357	ARG	Mainchain
2	Ch	82	ARG	Mainchain
2	Ch	93	LEU	Mainchain
2	D	12	LEU	Mainchain
2	D	233	ILE	Mainchain,Peptide
2	D	318	ILE	Mainchain
2	D	331	ASN	Mainchain
2	D	357	ARG	Mainchain
2	D	82	ARG	Mainchain
2	D	93	LEU	Mainchain
3	E	326	ASP	Mainchain
3	E	36	LYS	Mainchain
3	E	445	PRO	Mainchain
3	E	471	ARG	Mainchain
3	E	526	LEU	Mainchain
3	E	609	TRP	Mainchain
3	E	631	VAL	Mainchain
3	E	662	ILE	Mainchain
3	E	670	LEU	Mainchain
3	E	733	LYS	Mainchain
3	E	784	GLN	Mainchain,Peptide
3	E	785	VAL	Mainchain
3	E	791	GLN	Mainchain
3	E	803	ALA	Mainchain
3	E	837	MET	Mainchain,Peptide
4	F	68	UNK	Mainchain
5	G	483	TYR	Mainchain
5	G	492	CYS	Mainchain
5	G	503	SER	Mainchain
5	G	584	LEU	Mainchain
5	G	597	TRP	Mainchain
5	G	608	ASN	Mainchain
5	G	625	PHE	Mainchain
5	G	649	SER	Mainchain

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Mol	Chain	Res	Type	Group
5	G	733	GLU	Mainchain
5	G	749	ILE	Mainchain
5	G	756	TYR	Mainchain
5	G	765	GLN	Mainchain
6	H	105	UNK	Mainchain
6	H	78	UNK	Mainchain,Peptide
3	I	326	ASP	Mainchain
3	I	36	LYS	Mainchain
3	I	445	PRO	Mainchain
3	I	471	ARG	Mainchain
3	I	526	LEU	Mainchain
3	I	609	TRP	Mainchain
3	I	631	VAL	Mainchain
3	I	662	ILE	Mainchain
3	I	670	LEU	Mainchain
3	I	784	GLN	Mainchain,Peptide
3	I	785	VAL	Mainchain
3	I	826	ARG	Mainchain
3	I	833	ILE	Mainchain
3	I	837	MET	Mainchain,Peptide
3	I	847	LEU	Mainchain
3	I	921	LYS	Mainchain
7	J	202	LEU	Mainchain
7	J	294	SER	Mainchain
7	J	325	SER	Mainchain
7	J	345	PHE	Mainchain
7	J	48	ASP	Mainchain
7	J	522	PHE	Mainchain
7	J	533	THR	Mainchain
7	J	541	GLN	Mainchain
7	J	76	PHE	Mainchain,Peptide
5	L	483	TYR	Mainchain
5	L	492	CYS	Mainchain
5	L	503	SER	Mainchain
5	L	584	LEU	Mainchain
5	L	597	TRP	Mainchain
5	L	608	ASN	Mainchain
5	L	649	SER	Mainchain,Peptide
5	L	749	ILE	Mainchain
5	L	756	TYR	Mainchain
5	L	765	GLN	Mainchain
5	L	858	MET	Mainchain

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Mol	Chain	Res	Type	Group
5	L	875	ILE	Mainchain
5	L	893	LYS	Mainchain
5	L	908	GLU	Mainchain
5	L	919	THR	Mainchain
5	L	927	MET	Mainchain
5	M	236	ALA	Mainchain
5	M	253	ASN	Mainchain
5	M	270	SER	Mainchain
5	M	31	ASN	Mainchain,Peptide
5	M	320	MET	Mainchain
5	M	337	TYR	Mainchain
5	M	341	LYS	Peptide
5	M	59	VAL	Mainchain
7	O	202	LEU	Mainchain
7	O	294	SER	Mainchain
7	O	325	SER	Mainchain,Peptide
7	O	345	PHE	Mainchain
7	O	48	ASP	Mainchain
7	O	522	PHE	Mainchain
7	O	533	THR	Mainchain
7	O	541	GLN	Mainchain
7	O	557	LEU	Mainchain
7	O	76	PHE	Mainchain,Peptide
5	R	124	THR	Mainchain
5	R	236	ALA	Mainchain
5	R	253	ASN	Mainchain
5	R	270	SER	Mainchain
5	R	282	LYS	Mainchain,Peptide
5	R	283	ASN	Mainchain
5	R	31	ASN	Mainchain,Peptide
5	R	337	TYR	Mainchain
5	R	59	VAL	Mainchain
14	V	11	UNK	Mainchain
14	V	64	UNK	Mainchain
14	V	84	UNK	Mainchain
15	W	30	UNK	Mainchain
15	W	44	UNK	Mainchain
16	Z	125	ALA	Mainchain
16	Z	132	GLN	Mainchain
16	Z	139	LYS	Mainchain
16	Z	147	LYS	Mainchain
16	Z	98	LEU	Mainchain

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Mol	Chain	Res	Type	Group
14	a	11	UNK	Mainchain
14	a	64	UNK	Mainchain
14	a	84	UNK	Mainchain
16	c	132	GLN	Mainchain,Peptide
16	c	154	THR	Mainchain,Peptide
16	c	40	GLN	Mainchain
4	d	68	UNK	Mainchain
2	f	136	GLU	Mainchain
2	f	265	ASP	Mainchain
2	f	29	ILE	Mainchain
2	f	32	ALA	Mainchain
2	f	347	LYS	Mainchain
2	f	354	GLU	Mainchain,Peptide
2	f	37	LYS	Mainchain
2	f	44	LYS	Mainchain
2	f	53	LYS	Mainchain
2	f	86	ASN	Mainchain
1	i	155	ASP	Mainchain
1	i	222	TYR	Mainchain
1	i	301	GLU	Mainchain
1	i	349	VAL	Mainchain,Peptide
1	i	94	LEU	Mainchain
2	k	12	LEU	Mainchain
2	k	233	ILE	Mainchain,Peptide
2	k	318	ILE	Mainchain
2	k	331	ASN	Mainchain
2	k	350	GLU	Mainchain,Peptide
2	k	355	TYR	Mainchain
2	k	357	ARG	Mainchain
2	k	82	ARG	Mainchain
2	k	93	LEU	Mainchain
6	l	105	UNK	Mainchain
6	l	78	UNK	Mainchain,Peptide
3	n	326	ASP	Mainchain
3	n	36	LYS	Mainchain
3	n	445	PRO	Mainchain
3	n	471	ARG	Mainchain
3	n	526	LEU	Mainchain
3	n	609	TRP	Mainchain
3	n	631	VAL	Mainchain
3	n	662	ILE	Mainchain
3	n	670	LEU	Mainchain

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Mol	Chain	Res	Type	Group
3	n	733	LYS	Mainchain
3	n	784	GLN	Mainchain,Peptide
4	o	68	UNK	Mainchain
2	q	12	LEU	Mainchain
2	q	233	ILE	Mainchain,Peptide
2	q	318	ILE	Mainchain
2	q	357	ARG	Mainchain
2	q	82	ARG	Mainchain
2	q	93	LEU	Mainchain
2	s	136	GLU	Mainchain
2	s	239	GLN	Mainchain
2	s	265	ASP	Mainchain
2	s	29	ILE	Mainchain,Peptide
2	s	314	GLU	Mainchain
2	s	32	ALA	Mainchain
2	s	354	GLU	Mainchain,Peptide
2	s	37	LYS	Mainchain
5	v	483	TYR	Mainchain
5	v	492	CYS	Mainchain
5	v	503	SER	Mainchain
5	v	584	LEU	Mainchain
5	v	597	TRP	Mainchain
5	v	608	ASN	Mainchain
5	v	649	SER	Mainchain
5	v	749	ILE	Mainchain
5	v	756	TYR	Mainchain
5	v	765	GLN	Mainchain
6	w	105	UNK	Mainchain
6	w	78	UNK	Mainchain,Peptide
2	y	239	GLN	Mainchain
2	y	265	ASP	Mainchain
2	y	32	ALA	Mainchain
2	y	329	GLN	Mainchain
2	y	347	LYS	Mainchain
2	y	354	GLU	Mainchain
2	y	37	LYS	Mainchain
2	y	44	LYS	Mainchain,Peptide
2	y	53	LYS	Mainchain
2	y	86	ASN	Mainchain
2	z	239	GLN	Mainchain
2	z	265	ASP	Mainchain
2	z	32	ALA	Mainchain

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Mol	Chain	Res	Type	Group
2	z	329	GLN	Mainchain
2	z	347	LYS	Mainchain
2	z	354	GLU	Mainchain
2	z	37	LYS	Mainchain
2	z	44	LYS	Mainchain,Peptide
2	z	53	LYS	Mainchain
2	z	86	ASN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2129	0	926	2	0
1	BD	2129	0	926	2	0
1	C	2129	0	926	7	0
1	CP	2129	0	926	4	0
1	Ca	2129	0	926	5	0
1	i	2129	0	926	1	0
2	BK	1415	0	597	4	0
2	BR	1288	0	542	5	0
2	CW	1415	0	596	6	0
2	Cd	1288	0	542	10	0
2	Ch	1415	0	597	8	0
2	D	1415	0	597	4	0
2	f	1288	0	542	9	0
2	k	1415	0	597	9	0
2	q	1415	0	597	4	0
2	s	1288	0	542	10	0
2	y	1288	0	542	5	0
2	z	1288	0	542	5	0
3	1	3082	0	1317	8	0
3	7	4040	0	1741	15	0
3	BY	3841	0	1655	18	0
3	E	3597	0	1547	14	0
3	I	4040	0	1741	10	0
3	n	3302	0	1411	12	0
4	BO	755	0	158	7	0
4	BZ	755	0	158	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Bw	755	0	158	5	0
4	F	755	0	157	5	0
4	d	755	0	159	6	0
4	o	755	0	157	3	0
5	9	1510	0	629	6	0
5	AB	1752	0	772	1	0
5	AE	2584	0	1093	11	0
5	AO	1752	0	772	3	0
5	AU	1752	0	772	7	0
5	Bf	2334	0	990	8	0
5	Bt	1752	0	772	5	0
5	G	2064	0	867	9	0
5	L	2584	0	1093	10	0
5	M	1752	0	772	6	0
5	R	1752	0	772	4	0
5	v	1790	0	744	5	0
6	B4	820	0	167	0	0
6	BV	820	0	167	0	0
6	Bg	820	0	167	0	0
6	H	820	0	167	0	0
6	l	820	0	167	0	0
6	w	820	0	166	0	0
7	4	1806	0	792	15	0
7	AG	1806	0	792	17	0
7	AM	1806	0	792	17	0
7	Bm	1806	0	792	17	0
7	J	1806	0	792	10	0
7	O	1806	0	792	10	0
8	5	835	0	169	0	0
8	Bc	835	0	169	0	0
8	Bn	835	0	169	0	0
8	CA	835	0	169	0	0
8	K	835	0	169	0	0
8	t	835	0	169	0	0
9	2	805	0	165	2	0
9	AC	805	0	165	1	0
9	Bj	805	0	165	0	0
9	Bu	805	0	165	0	0
9	CH	805	0	165	0	0
9	N	805	0	165	0	0
10	AJ	160	0	34	0	0
10	AW	160	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Ac	160	0	35	0	0
10	B1	160	0	34	0	0
10	P	160	0	34	0	0
10	U	160	0	34	0	0
11	O	525	0	107	0	0
11	AK	525	0	107	1	0
11	B2	525	0	107	0	0
11	Bq	525	0	107	0	0
11	CO	525	0	107	0	0
11	Q	525	0	107	1	0
12	AR	165	0	35	0	0
12	Ae	165	0	35	0	0
12	Ak	165	0	35	0	0
12	B8	165	0	35	0	0
12	S	165	0	35	0	0
12	X	165	0	35	0	0
13	AH	635	0	129	1	0
13	AS	635	0	130	0	0
13	B9	635	0	129	1	0
13	Bx	635	0	129	1	0
13	CV	635	0	129	1	0
13	T	635	0	129	1	0
14	AZ	765	0	158	3	0
14	Am	765	0	157	7	0
14	As	765	0	158	3	0
14	CE	765	0	157	4	0
14	V	765	0	157	2	0
14	a	765	0	158	3	0
15	AP	510	0	105	3	0
15	Aa	510	0	104	0	0
15	B5	510	0	104	2	0
15	CF	510	0	104	2	0
15	Cc	510	0	104	1	0
15	W	510	0	104	1	0
16	A7	783	0	350	3	0
16	Ai	748	0	330	1	0
16	An	748	0	330	2	0
16	Aq	783	0	350	4	0
16	Av	783	0	350	3	0
16	Az	748	0	330	1	0
16	CB	748	0	330	1	0
16	CI	783	0	350	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CM	748	0	330	3	0
16	CT	783	0	350	4	0
16	Z	748	0	330	2	0
16	c	783	0	350	4	0
All	All	130144	0	48035	442	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 (442) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cd:330:ALA:H	2:Cd:332:VAL:H	1.41	0.69
1:BD:234:THR:O	1:BD:235:PRO:C	2.43	0.62
1:CP:234:THR:O	1:CP:235:PRO:C	2.43	0.62
1:A:234:THR:O	1:A:235:PRO:C	2.43	0.61
14:CE:72:UNK:O	14:CE:73:UNK:C	2.48	0.61
14:AZ:72:UNK:O	14:AZ:73:UNK:C	2.49	0.60
2:q:152:TYR:O	2:q:153:LEU:C	2.41	0.60
2:BK:152:TYR:O	2:BK:153:LEU:C	2.44	0.60
2:Ch:152:TYR:O	2:Ch:153:LEU:C	2.44	0.60
14:a:72:UNK:O	14:a:73:UNK:C	2.50	0.59
3:E:799:GLU:O	3:E:803:ALA:N	2.36	0.59
14:V:72:UNK:O	14:V:73:UNK:C	2.48	0.59
14:Am:72:UNK:O	14:Am:73:UNK:C	2.49	0.59
14:a:5:UNK:HA	14:a:6:UNK:C	2.33	0.58
3:I:682:GLN:O	3:I:683:ALA:C	2.44	0.58
2:k:152:TYR:O	2:k:153:LEU:C	2.46	0.58
14:As:72:UNK:O	14:As:73:UNK:C	2.49	0.58
14:CE:5:UNK:HA	14:CE:6:UNK:C	2.34	0.58
7:AG:142:ASP:O	7:AG:144:GLY:N	2.38	0.56
3:BY:555:ASN:C	3:BY:556:PRO:O	2.42	0.56
5:Bt:230:LEU:N	5:Bt:351:PHE:O	2.39	0.56
7:AG:146:LEU:N	7:AG:157:LEU:O	2.39	0.56
7:Bm:231:ASP:O	7:Bm:232:THR:C	2.48	0.56
14:As:5:UNK:HA	14:As:6:UNK:C	2.36	0.56
1:Ca:234:THR:O	1:Ca:235:PRO:C	2.48	0.56
5:AU:230:LEU:N	5:AU:351:PHE:O	2.40	0.55
5:Bt:317:ILE:O	5:Bt:321:ASN:N	2.39	0.55
7:AM:553:TYR:O	7:AM:557:LEU:N	2.40	0.55
3:BY:799:GLU:O	3:BY:803:ALA:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:230:LEU:N	5:R:351:PHE:O	2.40	0.55
2:s:44:LYS:O	2:s:45:THR:C	2.48	0.55
5:M:230:LEU:N	5:M:351:PHE:O	2.39	0.55
5:AO:230:LEU:N	5:AO:351:PHE:O	2.40	0.55
3:n:754:ASP:O	3:n:755:ALA:C	2.50	0.54
2:y:84:ASN:O	2:y:88:GLN:N	2.38	0.54
2:z:84:ASN:O	2:z:88:GLN:N	2.38	0.54
5:AU:153:ALA:O	5:AU:154:SER:C	2.46	0.54
3:E:746:GLU:O	3:E:747:LYS:CB	2.56	0.54
3:1:287:MET:O	3:1:288:GLU:C	2.50	0.54
5:AB:230:LEU:N	5:AB:351:PHE:O	2.41	0.54
7:AM:544:TYR:O	7:AM:545:SER:C	2.51	0.54
3:1:682:GLN:O	3:1:683:ALA:C	2.50	0.54
5:v:626:LYS:O	5:v:627:HIS:C	2.49	0.53
2:BR:90:GLU:O	2:BR:92:ILE:N	2.42	0.53
5:M:320:MET:O	5:M:323:GLN:N	2.41	0.53
3:7:682:GLN:O	3:7:683:ALA:C	2.51	0.53
5:Bt:323:GLN:O	5:Bt:327:LEU:N	2.42	0.53
5:L:597:TRP:O	5:L:600:LEU:N	2.41	0.52
7:J:544:TYR:O	7:J:545:SER:C	2.52	0.52
1:C:38:GLU:O	1:C:39:LEU:C	2.52	0.52
2:D:152:TYR:O	2:D:153:LEU:C	2.51	0.52
1:C:37:GLN:O	1:C:38:GLU:C	2.47	0.52
7:O:201:ASP:O	7:O:205:GLN:N	2.43	0.52
3:BY:682:GLN:O	3:BY:684:VAL:N	2.43	0.51
3:I:287:MET:O	3:I:288:GLU:C	2.54	0.51
7:Bm:178:SER:CB	7:Bm:236:VAL:H	2.22	0.51
3:7:287:MET:O	3:7:288:GLU:C	2.53	0.51
5:AE:466:PRO:O	5:AE:705:GLU:N	2.44	0.51
16:CI:53:ALA:O	16:CI:54:PRO:C	2.53	0.51
5:L:706:THR:O	5:L:707:GLU:C	2.53	0.51
16:Aq:93:ILE:C	16:Aq:94:PRO:O	2.48	0.50
2:Ch:296:ASP:C	2:Ch:297:LYS:O	2.46	0.50
1:C:234:THR:O	1:C:235:PRO:C	2.54	0.50
2:f:83:GLU:O	2:f:87:LEU:N	2.44	0.50
5:9:597:TRP:O	5:9:600:LEU:N	2.45	0.50
5:v:556:GLU:C	5:v:557:ILE:O	2.51	0.50
7:AM:553:TYR:O	7:AM:554:MET:C	2.53	0.50
7:AG:163:LYS:O	7:AG:164:LYS:C	2.55	0.50
2:BR:41:ASP:O	2:BR:45:THR:N	2.45	0.50
3:BY:559:SER:HA	3:BY:562:LYS:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:682:GLN:O	3:E:683:ALA:C	2.54	0.50
7:O:38:ALA:O	7:O:39:LEU:C	2.54	0.50
3:E:287:MET:O	3:E:288:GLU:C	2.55	0.49
5:L:575:LYS:C	5:L:576:PHE:O	2.51	0.49
3:7:792:GLN:O	3:7:795:LYS:N	2.44	0.49
7:J:524:PRO:O	7:J:525:LYS:CB	2.61	0.49
5:M:323:GLN:O	5:M:327:LEU:N	2.46	0.49
7:O:524:PRO:O	7:O:525:LYS:CB	2.61	0.49
5:L:927:MET:O	5:L:930:ILE:N	2.46	0.49
2:y:328:SER:C	2:y:330:ALA:H	2.19	0.49
5:AU:285:GLY:HA3	7:Bm:143:GLY:HA3	1.94	0.49
7:J:138:SER:O	7:J:147:LEU:N	2.44	0.49
7:AG:231:ASP:O	7:AG:232:THR:C	2.55	0.49
7:AM:524:PRO:O	7:AM:525:LYS:CB	2.61	0.49
2:z:328:SER:C	2:z:330:ALA:H	2.19	0.49
5:v:706:THR:O	5:v:707:GLU:C	2.55	0.49
5:AU:282:LYS:HA	7:Bm:140:SER:O	2.13	0.49
2:y:304:GLN:O	2:y:308:LEU:N	2.41	0.48
7:Bm:159:ARG:H	7:Bm:166:MET:CB	2.26	0.48
2:Cd:28:GLN:C	2:Cd:30:GLU:H	2.21	0.48
3:7:799:GLU:O	3:7:803:ALA:N	2.47	0.48
5:AE:927:MET:O	5:AE:930:ILE:N	2.46	0.48
7:AG:144:GLY:O	7:AG:160:LEU:N	2.44	0.48
7:AG:524:PRO:O	7:AG:525:LYS:CB	2.62	0.48
4:BO:15:UNK:O	4:BO:19:UNK:N	2.46	0.48
15:B5:44:UNK:O	15:B5:45:UNK:C	2.61	0.48
2:z:304:GLN:O	2:z:308:LEU:N	2.41	0.48
7:J:144:GLY:O	7:J:160:LEU:N	2.44	0.48
2:y:328:SER:C	2:y:330:ALA:N	2.71	0.48
2:z:328:SER:C	2:z:330:ALA:N	2.71	0.48
3:n:682:GLN:O	3:n:684:VAL:N	2.47	0.48
7:4:159:ARG:H	7:4:166:MET:CB	2.27	0.48
14:Am:-16:UNK:O	14:Am:-12:UNK:N	2.46	0.48
7:Bm:524:PRO:O	7:Bm:525:LYS:CB	2.62	0.48
16:CT:42:TYR:O	16:CT:43:LYS:C	2.55	0.48
7:4:524:PRO:O	7:4:525:LYS:CB	2.62	0.48
15:AP:44:UNK:O	15:AP:45:UNK:C	2.61	0.48
5:AE:575:LYS:C	5:AE:576:PHE:O	2.53	0.48
7:AM:517:THR:O	7:AM:518:TYR:C	2.56	0.47
2:BK:108:ARG:O	2:BK:112:LEU:N	2.42	0.47
5:Bf:575:LYS:C	5:Bf:576:PHE:O	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Bm:163:LYS:O	7:Bm:164:LYS:C	2.57	0.47
3:BY:792:GLN:O	3:BY:795:LYS:N	2.47	0.47
5:Bf:483:TYR:O	5:Bf:486:MET:N	2.46	0.47
2:f:136:GLU:O	2:f:139:ALA:N	2.47	0.47
16:CM:173:ILE:CB	16:CM:174:GLU:HA	2.44	0.47
3:E:799:GLU:O	3:E:800:SER:C	2.54	0.47
5:G:575:LYS:C	5:G:576:PHE:O	2.51	0.47
5:9:626:LYS:O	5:9:627:HIS:C	2.56	0.47
5:L:803:ASP:O	5:L:804:LEU:C	2.55	0.47
5:R:53:GLY:O	5:R:54:ASN:C	2.58	0.47
3:n:631:VAL:O	3:n:634:PHE:N	2.48	0.47
3:BY:631:VAL:O	3:BY:634:PHE:N	2.46	0.47
3:n:765:GLU:C	3:n:767:ILE:H	2.23	0.47
4:Bw:15:UNK:O	4:Bw:19:UNK:N	2.47	0.47
16:c:53:ALA:O	16:c:54:PRO:C	2.57	0.47
3:1:429:LEU:O	3:1:430:ASP:CB	2.63	0.47
7:O:544:TYR:O	7:O:545:SER:C	2.55	0.47
11:Q:55:UNK:O	11:Q:59:UNK:N	2.48	0.47
7:4:201:ASP:O	7:4:205:GLN:N	2.48	0.47
2:Ch:342:LEU:O	2:Ch:345:LEU:N	2.48	0.47
3:E:92:GLU:O	3:E:93:LYS:C	2.58	0.46
4:F:15:UNK:O	4:F:19:UNK:N	2.48	0.46
3:n:287:MET:O	3:n:288:GLU:C	2.58	0.46
14:a:11:UNK:O	14:a:14:UNK:N	2.48	0.46
3:7:595:SER:O	3:7:599:VAL:HA	2.15	0.46
7:AG:142:ASP:C	7:AG:144:GLY:H	2.23	0.46
7:AM:280:ILE:O	7:AM:281:HIS:C	2.56	0.46
14:Am:-28:UNK:O	14:Am:-24:UNK:N	2.48	0.46
15:Cc:44:UNK:O	15:Cc:45:UNK:C	2.62	0.46
4:d:15:UNK:O	4:d:19:UNK:N	2.48	0.46
7:4:108:GLY:C	7:4:110:ASP:H	2.22	0.46
7:AM:342:LYS:O	7:AM:343:THR:C	2.57	0.46
16:CT:73:LEU:O	16:CT:74:VAL:C	2.54	0.46
5:M:317:ILE:O	5:M:321:ASN:N	2.49	0.46
2:k:331:ASN:O	2:k:332:VAL:C	2.59	0.46
2:q:246:GLN:HA	2:q:248:HIS:N	2.30	0.46
7:O:163:LYS:O	7:O:164:LYS:C	2.58	0.46
4:d:33:UNK:CB	4:d:34:UNK:HA	2.46	0.46
2:k:270:ARG:O	2:k:271:LEU:C	2.58	0.46
2:CW:152:TYR:O	2:CW:153:LEU:C	2.57	0.46
7:J:38:ALA:O	7:J:39:LEU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:285:GLY:O	5:R:303:GLY:N	2.48	0.46
15:W:44:UNK:O	15:W:45:UNK:C	2.63	0.46
5:9:424:LEU:O	5:9:425:ARG:C	2.57	0.46
16:CI:42:TYR:O	16:CI:43:LYS:C	2.56	0.46
2:Cd:327:LEU:O	2:Cd:329:GLN:N	2.49	0.46
2:s:291:TYR:O	2:s:292:MET:C	2.58	0.46
7:4:87:GLY:O	7:4:88:HIS:C	2.59	0.46
2:BR:117:GLN:O	2:BR:120:LYS:N	2.48	0.46
2:Cd:240:LEU:O	2:Cd:241:ARG:C	2.57	0.46
5:L:893:LYS:O	5:L:896:LYS:N	2.48	0.46
4:o:16:UNK:O	4:o:17:UNK:C	2.63	0.46
2:s:41:ASP:O	2:s:45:THR:N	2.47	0.46
2:s:44:LYS:O	2:s:47:GLU:N	2.49	0.46
5:9:523:LEU:O	5:9:524:ALA:C	2.55	0.46
7:AG:559:ASN:O	7:AG:560:ARG:C	2.57	0.46
16:CI:178:SER:C	16:CI:179:TYR:O	2.53	0.46
16:CT:93:ILE:C	16:CT:94:PRO:O	2.46	0.46
7:AM:231:ASP:O	7:AM:232:THR:C	2.59	0.46
16:Av:53:ALA:O	16:Av:54:PRO:C	2.55	0.46
4:d:32:UNK:O	4:d:33:UNK:C	2.64	0.45
7:4:534:GLU:C	7:4:535:ALA:O	2.47	0.45
7:AG:517:THR:O	7:AG:518:TYR:C	2.58	0.45
3:BY:558:VAL:O	3:BY:562:LYS:N	2.49	0.45
16:c:42:TYR:O	16:c:43:LYS:C	2.57	0.45
5:v:575:LYS:C	5:v:576:PHE:O	2.54	0.45
7:Bm:280:ILE:O	7:Bm:281:HIS:C	2.54	0.45
3:n:96:GLY:O	3:n:97:TYR:C	2.59	0.45
16:An:30:GLY:O	16:An:31:LYS:C	2.57	0.45
16:Aq:42:TYR:O	16:Aq:43:LYS:C	2.56	0.45
16:A7:42:TYR:O	16:A7:43:LYS:C	2.58	0.45
3:BY:745:LEU:C	3:BY:746:GLU:O	2.53	0.45
5:AU:285:GLY:O	5:AU:303:GLY:N	2.48	0.45
4:F:16:UNK:O	4:F:20:UNK:N	2.50	0.45
5:G:598:LEU:O	5:G:599:GLN:C	2.56	0.45
4:o:-2:UNK:O	4:o:-1:UNK:C	2.64	0.45
7:4:342:LYS:O	7:4:343:THR:C	2.58	0.45
5:M:266:ALA:O	5:M:275:ALA:N	2.49	0.45
2:s:136:GLU:O	2:s:139:ALA:N	2.49	0.45
3:1:92:GLU:O	3:1:93:LYS:C	2.59	0.45
7:4:144:GLY:O	7:4:160:LEU:N	2.49	0.45
1:BD:375:ASN:O	1:BD:376:LEU:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:11:UNK:O	14:V:14:UNK:N	2.49	0.45
2:f:78:GLN:O	2:f:82:ARG:N	2.47	0.45
2:s:32:ALA:O	2:s:34:LEU:N	2.50	0.45
5:G:610:THR:C	5:G:612:GLU:HA	2.42	0.45
5:Bf:858:MET:O	5:Bf:861:ASP:N	2.48	0.45
2:Ch:108:ARG:O	2:Ch:109:LEU:C	2.56	0.45
7:AG:342:LYS:O	7:AG:343:THR:C	2.59	0.45
5:Bf:881:GLU:O	5:Bf:882:ASP:C	2.57	0.45
3:n:732:LEU:C	3:n:734:GLU:H	2.24	0.45
7:4:517:THR:O	7:4:518:TYR:C	2.59	0.45
3:7:795:LYS:O	3:7:799:GLU:N	2.50	0.45
16:Aq:146:GLN:O	16:Aq:147:LYS:C	2.56	0.45
3:BY:287:MET:O	3:BY:288:GLU:C	2.58	0.45
1:CP:374:ASN:O	1:CP:375:ASN:C	2.60	0.45
7:O:69:SER:HA	7:O:88:HIS:O	2.17	0.44
2:f:265:ASP:O	2:f:268:ILE:N	2.50	0.44
7:Bm:245:LEU:N	7:Bm:257:THR:O	2.49	0.44
3:BY:555:ASN:O	3:BY:556:PRO:C	2.58	0.44
3:I:826:ARG:O	3:I:829:ASP:N	2.50	0.44
16:c:95:ASP:O	16:c:96:ARG:C	2.61	0.44
2:k:111:GLN:O	2:k:115:GLU:N	2.51	0.44
3:7:828:ASN:O	3:7:832:PHE:N	2.44	0.44
7:J:243:THR:O	7:J:244:CYS:C	2.60	0.44
2:s:312:ASN:O	2:s:313:THR:C	2.59	0.44
9:2:25:UNK:O	9:2:29:UNK:N	2.51	0.44
5:AU:320:MET:C	5:AU:321:ASN:O	2.56	0.44
7:Bm:320:VAL:O	7:Bm:321:GLN:C	2.57	0.44
2:Cd:286:VAL:O	2:Cd:287:GLN:C	2.60	0.44
7:Bm:342:LYS:O	7:Bm:343:THR:C	2.58	0.44
7:AM:45:GLY:O	7:AM:46:HIS:C	2.57	0.44
7:AM:320:VAL:O	7:AM:321:GLN:C	2.59	0.44
16:CM:172:ASP:O	16:CM:173:ILE:C	2.60	0.44
3:E:795:LYS:O	3:E:799:GLU:N	2.51	0.44
5:G:794:GLN:O	5:G:795:GLU:C	2.58	0.44
2:f:308:LEU:N	2:f:309:ASN:HA	2.32	0.44
14:AZ:5:UNK:HA	14:AZ:6:UNK:C	2.47	0.44
4:BO:33:UNK:CB	4:BO:34:UNK:HA	2.47	0.44
5:G:575:LYS:O	5:G:576:PHE:C	2.61	0.44
2:s:108:ARG:O	2:s:109:LEU:C	2.59	0.44
5:v:597:TRP:O	5:v:600:LEU:N	2.51	0.44
7:4:243:THR:O	7:4:244:CYS:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BY:92:GLU:O	3:BY:93:LYS:C	2.60	0.44
4:BZ:15:UNK:O	4:BZ:19:UNK:N	2.50	0.44
4:Bw:20:UNK:O	4:Bw:21:UNK:C	2.65	0.44
15:CF:44:UNK:O	15:CF:45:UNK:C	2.64	0.44
4:F:32:UNK:O	4:F:33:UNK:C	2.65	0.44
4:Bw:34:UNK:O	4:Bw:35:UNK:C	2.61	0.44
13:B9:-7:UNK:O	13:B9:-6:UNK:C	2.66	0.44
16:Av:42:TYR:O	16:Av:43:LYS:C	2.59	0.43
4:Bw:33:UNK:CB	4:Bw:34:UNK:HA	2.48	0.43
1:C:362:ASN:O	1:C:363:PRO:C	2.61	0.43
3:E:732:LEU:C	3:E:734:GLU:H	2.25	0.43
5:L:858:MET:O	5:L:861:ASP:N	2.51	0.43
16:Z:119:ARG:O	16:Z:120:CYS:C	2.59	0.43
7:4:69:SER:HA	7:4:88:HIS:O	2.18	0.43
7:O:320:VAL:O	7:O:321:GLN:C	2.60	0.43
16:Z:62:GLU:O	16:Z:63:LYS:C	2.61	0.43
7:AG:45:GLY:O	7:AG:46:HIS:C	2.60	0.43
16:CT:53:ALA:O	16:CT:54:PRO:C	2.60	0.43
3:I:884:TYR:O	3:I:885:LYS:C	2.61	0.43
3:1:152:ASN:O	3:1:156:TYR:N	2.51	0.43
14:CE:11:UNK:O	14:CE:14:UNK:N	2.51	0.43
13:CV:-7:UNK:O	13:CV:-6:UNK:C	2.65	0.43
5:L:431:HIS:O	5:L:432:LYS:C	2.62	0.43
5:R:308:PHE:HA	5:R:309:LYS:CB	2.49	0.43
5:AE:523:LEU:O	5:AE:524:ALA:C	2.58	0.43
5:AE:773:LYS:O	5:AE:774:GLN:C	2.60	0.43
13:AH:-7:UNK:O	13:AH:-6:UNK:C	2.66	0.43
4:BO:32:UNK:O	4:BO:33:UNK:C	2.67	0.43
1:CP:432:PRO:O	1:CP:434:ILE:N	2.52	0.43
2:CW:12:LEU:O	2:CW:15:ARG:N	2.51	0.43
2:k:351:ILE:O	2:k:352:LEU:C	2.59	0.43
3:1:631:VAL:O	3:1:634:PHE:N	2.47	0.43
5:AE:728:GLN:O	5:AE:731:SER:N	2.52	0.43
15:AP:50:UNK:O	15:AP:54:UNK:N	2.52	0.43
15:CF:50:UNK:O	15:CF:54:UNK:N	2.52	0.43
3:n:756:LEU:O	3:n:757:MET:C	2.61	0.43
4:F:33:UNK:CB	4:F:34:UNK:HA	2.49	0.43
16:c:116:PHE:O	16:c:117:GLU:C	2.59	0.43
2:k:310:LYS:O	2:k:311:GLU:C	2.61	0.43
3:n:307:ASN:O	3:n:308:ILE:C	2.60	0.43
5:AE:610:THR:C	5:AE:612:GLU:HA	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:55:UNK:O	11:AK:59:UNK:N	2.52	0.43
7:AM:534:GLU:O	7:AM:535:ALA:C	2.60	0.43
2:BK:111:GLN:O	2:BK:115:GLU:N	2.51	0.43
4:F:21:UNK:O	4:F:25:UNK:N	2.52	0.43
7:O:231:ASP:O	7:O:232:THR:C	2.61	0.43
13:T:-7:UNK:O	13:T:-6:UNK:C	2.67	0.43
5:9:566:HIS:O	5:9:567:GLN:C	2.55	0.43
5:AE:626:LYS:O	5:AE:627:HIS:C	2.60	0.43
7:AG:544:TYR:O	7:AG:545:SER:C	2.57	0.43
7:AG:553:TYR:O	7:AG:557:LEU:N	2.52	0.43
7:Bm:517:THR:O	7:Bm:518:TYR:C	2.59	0.43
16:CM:119:ARG:O	16:CM:120:CYS:C	2.60	0.43
2:Ch:297:LYS:O	2:Ch:299:LYS:N	2.51	0.43
5:G:786:LEU:O	5:G:787:THR:C	2.60	0.42
9:2:123:UNK:O	9:2:124:UNK:C	2.66	0.42
3:7:738:LEU:O	3:7:742:LEU:N	2.52	0.42
7:AM:163:LYS:O	7:AM:164:LYS:C	2.62	0.42
7:4:293:ASP:O	7:4:316:ASP:HA	2.19	0.42
14:Am:3:UNK:O	14:Am:4:UNK:C	2.67	0.42
4:BZ:16:UNK:O	4:BZ:17:UNK:C	2.63	0.42
5:L:442:ILE:O	5:L:443:TYR:C	2.62	0.42
7:O:534:GLU:O	7:O:535:ALA:C	2.55	0.42
4:d:16:UNK:O	4:d:17:UNK:C	2.67	0.42
7:AG:201:ASP:O	7:AG:205:GLN:N	2.52	0.42
4:BO:16:UNK:O	4:BO:17:UNK:C	2.67	0.42
2:BR:35:VAL:O	2:BR:36:ASP:C	2.61	0.42
5:Bf:531:PHE:O	5:Bf:532:ALA:C	2.60	0.42
5:G:803:ASP:O	5:G:804:LEU:C	2.59	0.42
16:Av:94:PRO:O	16:Av:95:ASP:CB	2.67	0.42
3:BY:125:THR:O	3:BY:126:PHE:CB	2.67	0.42
16:CI:44:HIS:O	16:CI:45:ALA:C	2.60	0.42
1:i:432:PRO:O	1:i:434:ILE:N	2.52	0.42
3:BY:126:PHE:O	3:BY:127:LYS:C	2.62	0.42
2:CW:247:VAL:O	2:CW:248:HIS:C	2.62	0.42
1:C:201:ASN:O	1:C:202:TYR:C	2.60	0.42
2:s:289:TYR:O	2:s:290:ASN:CB	2.68	0.42
5:AE:786:LEU:O	5:AE:787:THR:C	2.60	0.42
14:AZ:11:UNK:O	14:AZ:14:UNK:N	2.53	0.42
7:Bm:553:TYR:O	7:Bm:557:LEU:N	2.52	0.42
4:Bw:32:UNK:O	4:Bw:33:UNK:C	2.68	0.42
2:CW:331:ASN:O	2:CW:332:VAL:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:608:ASP:C	3:E:610:LEU:H	2.27	0.42
2:f:35:VAL:O	2:f:36:ASP:C	2.62	0.42
3:7:533:PHE:O	3:7:534:CYS:C	2.61	0.42
3:7:593:TRP:O	3:7:597:GLN:N	2.53	0.42
5:Bf:626:LYS:O	5:Bf:627:HIS:C	2.62	0.42
7:Bm:293:ASP:O	7:Bm:316:ASP:HA	2.20	0.42
3:E:631:VAL:O	3:E:633:TYR:N	2.53	0.42
5:L:626:LYS:O	5:L:627:HIS:C	2.60	0.42
5:M:85:LEU:O	5:M:96:GLN:HA	2.20	0.42
16:A7:169:PRO:O	16:A7:170:HIS:C	2.62	0.42
4:BO:25:UNK:O	4:BO:26:UNK:C	2.67	0.42
3:I:631:VAL:O	3:I:633:TYR:N	2.52	0.42
7:AM:138:SER:O	7:AM:147:LEU:N	2.53	0.42
4:BZ:33:UNK:CB	4:BZ:34:UNK:HA	2.49	0.42
1:C:154:ARG:O	1:C:155:ASP:C	2.62	0.42
4:BO:20:UNK:O	4:BO:21:UNK:C	2.68	0.42
2:BR:287:GLN:O	2:BR:291:TYR:N	2.53	0.42
7:J:554:MET:C	7:J:557:LEU:O	2.63	0.41
2:k:5:LEU:O	2:k:6:PHE:C	2.62	0.41
5:AU:9:HIS:CB	5:AU:279:ARG:H	2.33	0.41
16:Ai:119:ARG:O	16:Ai:120:CYS:C	2.60	0.41
3:BY:307:ASN:O	3:BY:308:ILE:C	2.60	0.41
13:Bx:-7:UNK:O	13:Bx:-6:UNK:C	2.68	0.41
15:B5:44:UNK:O	15:B5:46:UNK:N	2.53	0.41
2:Ch:331:ASN:O	2:Ch:332:VAL:C	2.63	0.41
3:I:96:GLY:O	3:I:97:TYR:C	2.64	0.41
2:f:41:ASP:O	2:f:45:THR:N	2.48	0.41
3:1:732:LEU:C	3:1:734:GLU:H	2.28	0.41
3:7:278:ILE:O	3:7:292:CYS:HA	2.20	0.41
7:AG:143:GLY:O	7:AG:144:GLY:C	2.62	0.41
3:BY:662:ILE:O	3:BY:663:GLN:C	2.61	0.41
4:BZ:32:UNK:O	4:BZ:33:UNK:C	2.68	0.41
7:Bm:553:TYR:O	7:Bm:554:MET:C	2.62	0.41
2:CW:321:SER:O	2:CW:322:LYS:C	2.63	0.41
2:q:246:GLN:HA	2:q:247:VAL:C	2.45	0.41
7:AM:69:SER:HA	7:AM:88:HIS:O	2.20	0.41
14:Am:-20:UNK:O	14:Am:-16:UNK:N	2.53	0.41
16:An:119:ARG:O	16:An:120:CYS:C	2.62	0.41
14:As:11:UNK:O	14:As:14:UNK:N	2.54	0.41
5:Bf:597:TRP:O	5:Bf:599:GLN:N	2.53	0.41
14:CE:5:UNK:CA	14:CE:6:UNK:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CI:73:LEU:O	16:CI:74:VAL:C	2.61	0.41
1:Ca:201:ASN:O	1:Ca:202:TYR:C	2.63	0.41
2:Cd:35:VAL:O	2:Cd:36:ASP:C	2.60	0.41
5:G:427:PHE:O	5:G:431:HIS:N	2.52	0.41
7:J:69:SER:HA	7:J:88:HIS:O	2.19	0.41
2:y:286:VAL:O	2:y:287:GLN:C	2.63	0.41
5:Bf:794:GLN:O	5:Bf:795:GLU:C	2.62	0.41
3:E:785:VAL:O	3:E:787:GLU:N	2.54	0.41
5:G:597:TRP:O	5:G:599:GLN:N	2.53	0.41
2:f:136:GLU:O	2:f:137:ASN:C	2.64	0.41
3:n:429:LEU:O	3:n:430:ASP:CB	2.67	0.41
2:s:71:ASN:O	2:s:75:ALA:N	2.46	0.41
7:4:331:THR:CB	7:4:339:MET:H	2.33	0.41
5:AE:706:THR:O	5:AE:707:GLU:C	2.63	0.41
4:BO:-1:UNK:O	4:BO:0:UNK:C	2.68	0.41
4:BZ:25:UNK:O	4:BZ:26:UNK:C	2.68	0.41
16:CB:30:GLY:O	16:CB:31:LYS:C	2.62	0.41
2:z:286:VAL:O	2:z:287:GLN:C	2.63	0.41
3:E:168:ARG:O	3:E:169:TYR:C	2.64	0.41
14:Am:77:UNK:O	14:Am:78:UNK:C	2.69	0.41
5:Bt:283:ASN:O	5:Bt:284:LYS:CB	2.68	0.41
3:1:96:GLY:O	3:1:97:TYR:C	2.61	0.41
7:4:546:ARG:O	7:4:547:LEU:C	2.62	0.41
3:7:625:LEU:O	3:7:626:LEU:C	2.62	0.41
3:7:732:LEU:C	3:7:734:GLU:H	2.28	0.41
5:AE:876:GLN:O	5:AE:879:ARG:N	2.54	0.41
15:AP:44:UNK:O	15:AP:46:UNK:N	2.54	0.41
4:BZ:-2:UNK:O	4:BZ:-1:UNK:C	2.69	0.41
2:Cd:289:TYR:O	2:Cd:290:ASN:CB	2.68	0.41
2:D:114:THR:O	2:D:115:GLU:C	2.63	0.41
2:D:321:SER:O	2:D:322:LYS:C	2.62	0.41
7:O:553:TYR:O	7:O:554:MET:C	2.61	0.41
4:d:25:UNK:O	4:d:26:UNK:C	2.68	0.41
7:AM:243:THR:O	7:AM:244:CYS:C	2.64	0.41
5:AO:7:SER:O	5:AO:9:HIS:N	2.54	0.41
5:AO:323:GLN:O	5:AO:327:LEU:N	2.54	0.41
16:A7:44:HIS:O	16:A7:45:ALA:C	2.63	0.41
2:Ch:321:SER:O	2:Ch:322:LYS:C	2.64	0.41
1:C:364:VAL:O	1:C:366:GLY:N	2.53	0.41
3:E:96:GLY:O	3:E:97:TYR:C	2.61	0.41
7:J:556:ASN:N	7:J:557:LEU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:290:ASN:O	2:q:291:TYR:C	2.63	0.41
9:AC:117:UNK:HA	9:AC:118:UNK:CB	2.51	0.41
7:AG:534:GLU:O	7:AG:535:ALA:C	2.59	0.41
3:BY:96:GLY:O	3:BY:97:TYR:C	2.61	0.41
1:Ca:432:PRO:O	1:Ca:434:ILE:N	2.53	0.41
3:I:92:GLU:O	3:I:93:LYS:C	2.65	0.41
2:k:10:LYS:O	2:k:11:TYR:C	2.64	0.41
3:n:528:GLY:O	3:n:529:THR:C	2.62	0.41
3:7:152:ASN:O	3:7:156:TYR:N	2.53	0.41
1:Ca:243:TYR:HA	1:Ca:320:GLY:HA2	2.03	0.41
1:Ca:374:ASN:O	1:Ca:375:ASN:C	2.64	0.41
2:Cd:328:SER:O	2:Cd:330:ALA:N	2.54	0.41
3:E:152:ASN:O	3:E:156:TYR:N	2.53	0.40
7:AM:536:ILE:O	7:AM:537:ALA:C	2.61	0.40
2:Cd:330:ALA:H	2:Cd:332:VAL:N	2.12	0.40
3:I:152:ASN:O	3:I:156:TYR:N	2.54	0.40
3:I:560:TYR:H	3:I:683:ALA:CB	2.35	0.40
4:d:34:UNK:O	4:d:35:UNK:C	2.65	0.40
3:n:732:LEU:C	3:n:734:GLU:N	2.79	0.40
16:Az:62:GLU:O	16:Az:63:LYS:C	2.62	0.40
7:Bm:69:SER:HA	7:Bm:88:HIS:O	2.21	0.40
2:CW:91:ILE:O	2:CW:95:SER:N	2.55	0.40
3:I:307:ASN:O	3:I:308:ILE:C	2.61	0.40
2:f:289:TYR:O	2:f:290:ASN:CB	2.70	0.40
7:4:45:GLY:O	7:4:46:HIS:C	2.64	0.40
5:9:617:ILE:O	5:9:618:THR:C	2.64	0.40
3:BY:799:GLU:O	3:BY:800:SER:C	2.62	0.40
7:Bm:138:SER:O	7:Bm:147:LEU:N	2.54	0.40
2:Ch:290:ASN:O	2:Ch:291:TYR:C	2.62	0.40
1:A:362:ASN:O	1:A:363:PRO:C	2.65	0.40
2:D:247:VAL:O	2:D:248:HIS:C	2.64	0.40
4:o:32:UNK:O	4:o:33:UNK:C	2.69	0.40
3:7:307:ASN:O	3:7:308:ILE:C	2.61	0.40
2:BK:30:GLU:O	2:BK:31:SER:CB	2.69	0.40
3:BY:631:VAL:O	3:BY:632:ALA:C	2.65	0.40
1:CP:70:SER:O	1:CP:71:ASN:C	2.64	0.40
7:J:342:LYS:O	7:J:343:THR:C	2.59	0.40
2:k:35:VAL:O	2:k:36:ASP:C	2.64	0.40
7:AG:553:TYR:O	7:AG:554:MET:C	2.58	0.40
7:AM:553:TYR:O	7:AM:556:ASN:N	2.52	0.40
14:Am:91:UNK:O	14:Am:92:UNK:C	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Aq:176:ILE:O	16:Aq:177:ARG:C	2.63	0.40
5:Bt:266:ALA:O	5:Bt:275:ALA:N	2.53	0.40
2:Cd:86:ASN:O	2:Cd:89:SER:N	2.52	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	425/452 (94%)	373 (88%)	41 (10%)	11 (3%)	4	27
1	BD	425/452 (94%)	374 (88%)	37 (9%)	14 (3%)	3	24
1	C	425/452 (94%)	369 (87%)	44 (10%)	12 (3%)	4	26
1	CP	425/452 (94%)	369 (87%)	43 (10%)	13 (3%)	3	25
1	Ca	425/452 (94%)	375 (88%)	40 (9%)	10 (2%)	4	29
1	i	425/452 (94%)	371 (87%)	45 (11%)	9 (2%)	5	31
2	BK	278/380 (73%)	269 (97%)	5 (2%)	4 (1%)	9	37
2	BR	252/380 (66%)	244 (97%)	7 (3%)	1 (0%)	30	62
2	CW	278/380 (73%)	262 (94%)	12 (4%)	4 (1%)	9	37
2	Cd	252/380 (66%)	243 (96%)	3 (1%)	6 (2%)	4	29
2	Ch	278/380 (73%)	263 (95%)	12 (4%)	3 (1%)	11	41
2	D	278/380 (73%)	266 (96%)	8 (3%)	4 (1%)	9	37
2	f	252/380 (66%)	244 (97%)	6 (2%)	2 (1%)	16	48
2	k	278/380 (73%)	262 (94%)	12 (4%)	4 (1%)	9	37
2	q	278/380 (73%)	266 (96%)	8 (3%)	4 (1%)	9	37
2	s	252/380 (66%)	244 (97%)	6 (2%)	2 (1%)	16	48
2	y	252/380 (66%)	244 (97%)	6 (2%)	2 (1%)	16	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	z	252/380 (66%)	244 (97%)	6 (2%)	2 (1%)	16	48
3	1	615/937 (66%)	577 (94%)	23 (4%)	15 (2%)	4	29
3	7	805/937 (86%)	761 (94%)	28 (4%)	16 (2%)	6	32
3	BY	767/937 (82%)	724 (94%)	27 (4%)	16 (2%)	5	31
3	E	718/937 (77%)	677 (94%)	25 (4%)	16 (2%)	5	30
3	I	805/937 (86%)	765 (95%)	26 (3%)	14 (2%)	7	34
3	n	659/937 (70%)	620 (94%)	25 (4%)	14 (2%)	5	31
5	9	299/1202 (25%)	272 (91%)	23 (8%)	4 (1%)	9	38
5	AB	352/1202 (29%)	332 (94%)	17 (5%)	3 (1%)	14	45
5	AE	514/1202 (43%)	479 (93%)	27 (5%)	8 (2%)	7	35
5	AO	352/1202 (29%)	335 (95%)	13 (4%)	4 (1%)	11	41
5	AU	352/1202 (29%)	334 (95%)	15 (4%)	3 (1%)	14	45
5	Bf	464/1202 (39%)	432 (93%)	27 (6%)	5 (1%)	11	41
5	Bt	352/1202 (29%)	330 (94%)	20 (6%)	2 (1%)	21	54
5	G	410/1202 (34%)	382 (93%)	26 (6%)	2 (0%)	24	57
5	L	514/1202 (43%)	484 (94%)	25 (5%)	5 (1%)	12	43
5	M	352/1202 (29%)	326 (93%)	23 (6%)	3 (1%)	14	45
5	R	352/1202 (29%)	329 (94%)	19 (5%)	4 (1%)	11	41
5	v	355/1202 (30%)	327 (92%)	22 (6%)	6 (2%)	7	34
7	4	359/634 (57%)	315 (88%)	38 (11%)	6 (2%)	7	34
7	AG	359/634 (57%)	316 (88%)	35 (10%)	8 (2%)	5	30
7	AM	359/634 (57%)	319 (89%)	36 (10%)	4 (1%)	11	41
7	Bm	359/634 (57%)	317 (88%)	37 (10%)	5 (1%)	9	37
7	J	359/634 (57%)	317 (88%)	34 (10%)	8 (2%)	5	30
7	O	359/634 (57%)	317 (88%)	36 (10%)	6 (2%)	7	34
16	A7	154/230 (67%)	143 (93%)	9 (6%)	2 (1%)	9	38
16	Ai	147/230 (64%)	133 (90%)	10 (7%)	4 (3%)	4	27
16	An	147/230 (64%)	133 (90%)	9 (6%)	5 (3%)	3	23
16	Aq	154/230 (67%)	141 (92%)	12 (8%)	1 (1%)	21	54
16	Av	154/230 (67%)	143 (93%)	7 (4%)	4 (3%)	4	27
16	Az	147/230 (64%)	129 (88%)	13 (9%)	5 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	CB	147/230 (64%)	130 (88%)	13 (9%)	4 (3%)	4	27
16	CI	154/230 (67%)	144 (94%)	9 (6%)	1 (1%)	21	54
16	CM	147/230 (64%)	127 (86%)	15 (10%)	5 (3%)	3	23
16	CT	154/230 (67%)	142 (92%)	11 (7%)	1 (1%)	21	54
16	Z	147/230 (64%)	133 (90%)	10 (7%)	4 (3%)	4	27
16	c	154/230 (67%)	143 (93%)	9 (6%)	2 (1%)	9	38
All	All	18727/33882 (55%)	17310 (92%)	1095 (6%)	322 (2%)	9	34

All (322) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	101	PRO
1	C	68	SER
1	C	101	PRO
2	D	234	LYS
3	E	72	ASP
3	E	295	LEU
3	E	430	ASP
3	E	704	PRO
3	I	72	ASP
3	I	295	LEU
3	I	430	ASP
3	I	704	PRO
3	I	838	GLU
7	J	325	SER
5	M	110	HIS
7	O	325	SER
5	R	110	HIS
16	Z	141	LYS
16	c	40	GLN
1	i	68	SER
2	k	234	LYS
3	n	72	ASP
3	n	295	LEU
3	n	430	ASP
3	n	755	ALA
2	s	45	THR
3	1	72	ASP
3	1	253	ASN

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Mol	Chain	Res	Type
3	1	430	ASP
7	4	167	CYS
7	4	325	SER
3	7	72	ASP
3	7	430	ASP
5	AE	583	PHE
5	AE	598	LEU
7	AG	143	GLY
7	AG	259	ILE
7	AG	325	SER
7	AM	325	SER
5	AO	8	THR
5	AO	110	HIS
5	AU	110	HIS
16	An	141	LYS
16	Aq	40	GLN
16	Av	27	THR
16	Az	141	LYS
16	A7	40	GLN
16	A7	95	ASP
1	BD	68	SER
1	BD	101	PRO
1	BD	259	THR
2	BK	234	LYS
3	BY	72	ASP
3	BY	253	ASN
3	BY	295	LEU
3	BY	430	ASP
3	BY	557	PRO
5	Bf	598	LEU
7	Bm	325	SER
5	Bt	110	HIS
16	CB	141	LYS
16	CM	141	LYS
16	CM	172	ASP
1	CP	68	SER
1	CP	101	PRO
1	CP	364	VAL
16	CT	40	GLN
2	CW	234	LYS
1	Ca	68	SER
1	Ca	101	PRO

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Mol	Chain	Res	Type
1	Ca	316	SER
2	Cd	328	SER
2	Cd	355	TYR
1	A	236	ASN
1	C	265	ALA
2	D	247	VAL
3	E	480	ASN
3	E	560	TYR
3	E	747	LYS
3	E	804	ILE
5	G	454	ASP
5	G	465	TYR
3	I	480	ASN
3	I	560	TYR
3	I	747	LYS
7	J	232	THR
7	J	512	ASN
5	L	454	ASP
5	L	465	TYR
5	L	650	VAL
7	O	244	CYS
5	R	54	ASN
16	Z	142	ASN
16	Z	172	ASP
1	i	101	PRO
1	i	316	SER
3	n	480	ASN
3	n	704	PRO
2	q	247	VAL
2	s	290	ASN
5	v	454	ASP
5	v	588	PHE
5	v	650	VAL
5	v	707	GLU
3	1	480	ASN
3	1	704	PRO
3	7	295	LEU
3	7	480	ASN
3	7	560	TYR
3	7	709	ASP
5	9	454	ASP
5	9	465	TYR

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Mol	Chain	Res	Type
5	AB	80	ILE
5	AB	110	HIS
5	AE	454	ASP
5	AE	650	VAL
5	AE	901	TYR
7	AG	232	THR
7	AG	244	CYS
7	AM	512	ASN
16	Ai	141	LYS
16	Ai	142	ASN
16	Ai	172	ASP
16	An	142	ASN
16	An	172	ASP
16	Az	142	ASN
16	Az	172	ASP
1	BD	236	ASN
1	BD	432	PRO
2	BR	290	ASN
3	BY	116	LYS
3	BY	480	ASN
3	BY	704	PRO
5	Bf	454	ASP
7	Bm	117	GLN
16	CB	142	ASN
16	CB	172	ASP
16	CM	142	ASN
16	CM	173	ILE
1	CP	236	ASN
1	CP	258	ILE
1	CP	265	ALA
2	Cd	29	ILE
2	Cd	45	THR
2	Cd	329	GLN
2	Ch	234	LYS
1	A	171	VAL
1	A	316	SER
1	C	171	VAL
7	J	171	GLY
5	R	309	LYS
2	f	45	THR
2	k	247	VAL
3	n	116	LYS

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Mol	Chain	Res	Type
2	q	280	ILE
5	v	465	TYR
2	y	290	ASN
3	1	116	LYS
3	1	560	TYR
3	1	709	ASP
7	4	512	ASN
3	7	116	LYS
3	7	286	ASN
3	7	704	PRO
5	AE	465	TYR
5	AE	642	ILE
7	AG	158	TRP
7	AM	158	TRP
7	AM	232	THR
5	AO	167	SER
5	AO	192	GLU
1	BD	156	ILE
1	BD	316	SER
2	BK	247	VAL
3	BY	126	PHE
3	BY	683	ALA
3	BY	804	ILE
5	Bf	465	TYR
7	Bm	232	THR
7	Bm	249	SER
5	Bt	282	LYS
1	CP	156	ILE
2	CW	247	VAL
2	CW	280	ILE
1	Ca	171	VAL
2	Cd	290	ASN
2	Ch	247	VAL
2	z	290	ASN
1	A	124	LYS
1	A	336	LYS
1	C	39	LEU
1	C	373	SER
2	D	280	ILE
3	E	116	LYS
3	E	286	ASN
3	E	709	ASP

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Mol	Chain	Res	Type
3	E	838	GLU
3	I	39	LYS
3	I	116	LYS
3	I	123	TRP
3	I	709	ASP
3	I	804	ILE
7	J	158	TRP
7	J	160	LEU
5	M	5	HIS
7	O	153	LYS
7	O	158	TRP
2	f	290	ASN
1	i	124	LYS
1	i	373	SER
2	k	280	ILE
2	k	351	ILE
3	n	39	LYS
2	q	246	GLN
2	y	45	THR
3	1	39	LYS
3	1	123	TRP
3	1	286	ASN
7	4	232	THR
7	4	249	SER
3	7	39	LYS
3	7	123	TRP
3	7	784	GLN
3	7	804	ILE
7	AG	249	SER
5	AU	309	LYS
16	Ai	69	THR
16	An	69	THR
16	Az	41	ASP
16	Az	69	THR
3	BY	39	LYS
3	BY	599	VAL
3	BY	604	LEU
3	BY	838	GLU
16	CB	69	THR
16	CM	69	THR
1	CP	124	LYS
1	Ca	124	LYS

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Mol	Chain	Res	Type
1	Ca	156	ILE
2	Ch	280	ILE
2	z	45	THR
1	C	124	LYS
1	C	291	ASP
1	C	362	ASN
1	C	432	PRO
3	E	39	LYS
3	E	126	PHE
3	I	126	PHE
7	J	249	SER
5	L	587	PHE
7	O	117	GLN
16	Z	69	THR
16	c	133	ASN
3	n	126	PHE
3	n	604	LEU
3	n	683	ALA
2	q	31	SER
5	v	649	SER
3	1	126	PHE
3	1	604	LEU
3	1	683	ALA
3	7	126	PHE
3	7	747	LYS
5	AE	649	SER
5	AU	153	ALA
16	Av	95	ASP
16	Av	133	ASN
1	BD	59	ASP
1	BD	124	LYS
1	BD	265	ALA
1	BD	356	TYR
3	BY	709	ASP
16	CI	133	ASN
1	Ca	131	ASN
1	Ca	236	ASN
1	A	235	PRO
1	A	407	VAL
1	A	432	PRO
1	C	407	VAL
2	D	324	TYR

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Mol	Chain	Res	Type
3	E	604	LEU
5	L	649	SER
1	i	59	ASP
3	n	560	TYR
3	n	599	VAL
7	4	117	GLN
5	9	587	PHE
1	BD	235	PRO
1	BD	291	ASP
2	BK	31	SER
5	Bf	587	PHE
7	Bm	158	TRP
1	CP	235	PRO
1	CP	291	ASP
1	CP	336	LYS
1	Ca	407	VAL
1	Ca	432	PRO
7	O	49	ILE
1	i	407	VAL
1	BD	407	VAL
1	CP	407	VAL
1	C	156	ILE
1	i	432	PRO
3	1	295	LEU
3	7	599	VAL
16	Av	128	ILE
1	CP	432	PRO
5	M	343	GLY
5	9	650	VAL
2	BK	280	ILE
3	E	599	VAL
5	R	341	LYS
1	i	156	ILE
3	n	558	VAL
5	AB	78	VAL
7	AG	49	ILE
16	An	37	ILE
5	Bf	650	VAL
2	CW	318	ILE
1	A	156	ILE
7	J	49	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

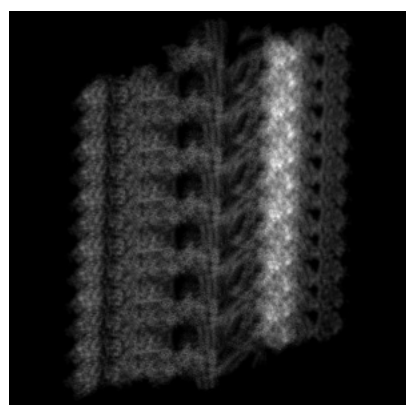
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53471. These allow visual inspection of the internal detail of the map and identification of artifacts.

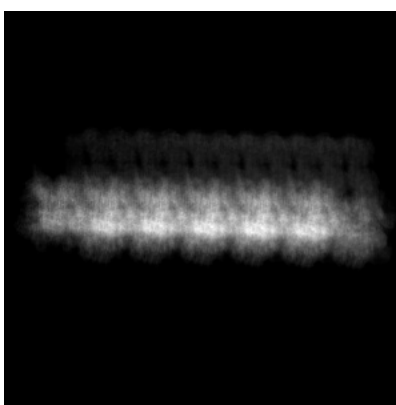
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

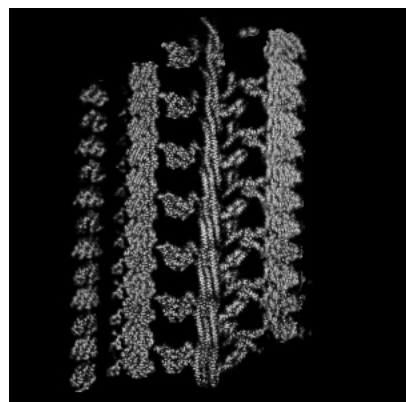


Z

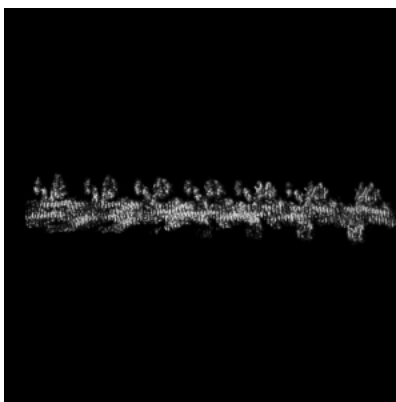
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240

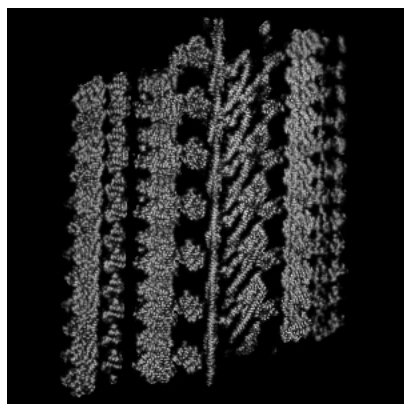


Z Index: 240

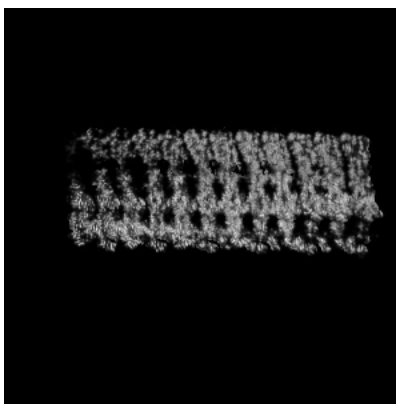
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

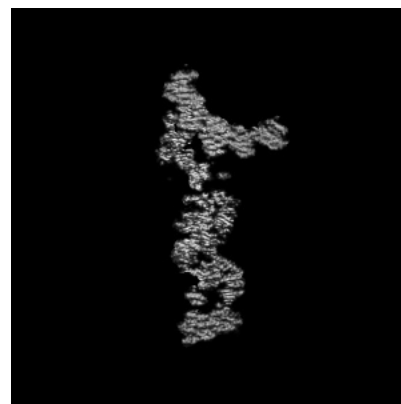
6.3.1 Primary map



X Index: 218



Y Index: 335

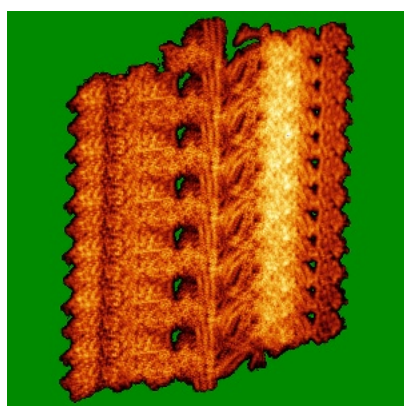


Z Index: 311

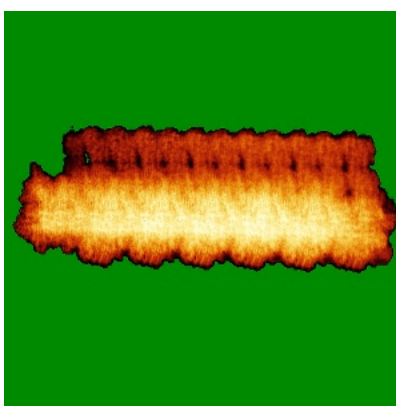
The images above show the largest variance slices of the map in three orthogonal directions.

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

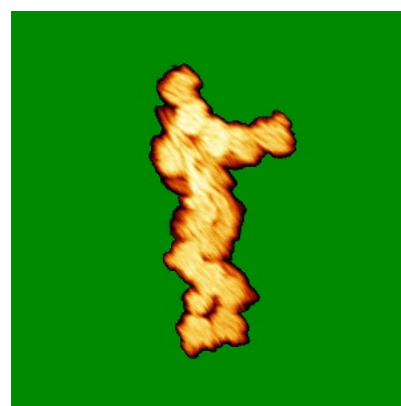
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

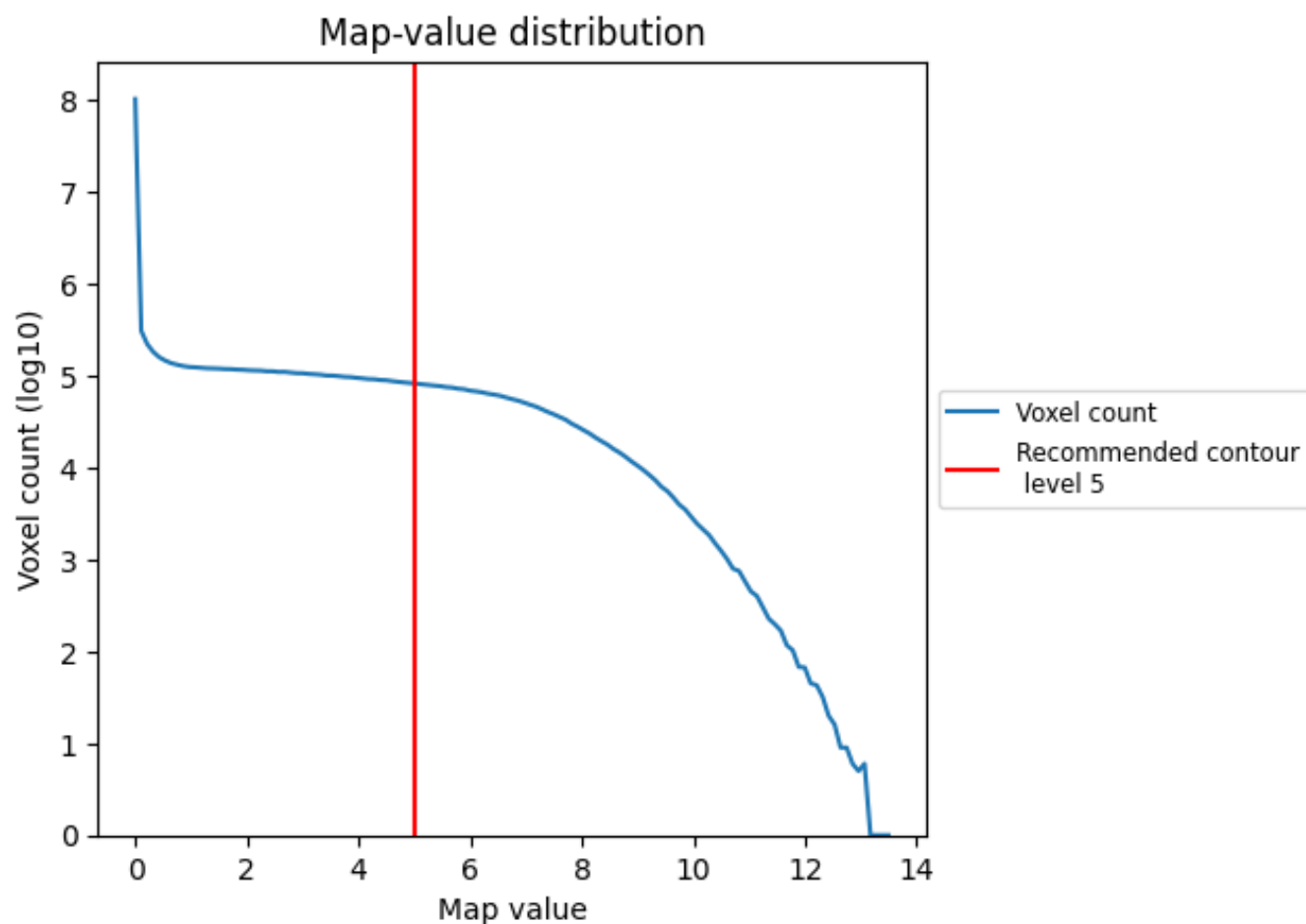
6.6 Mask visualisation

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

7 Map analysis [i](#)

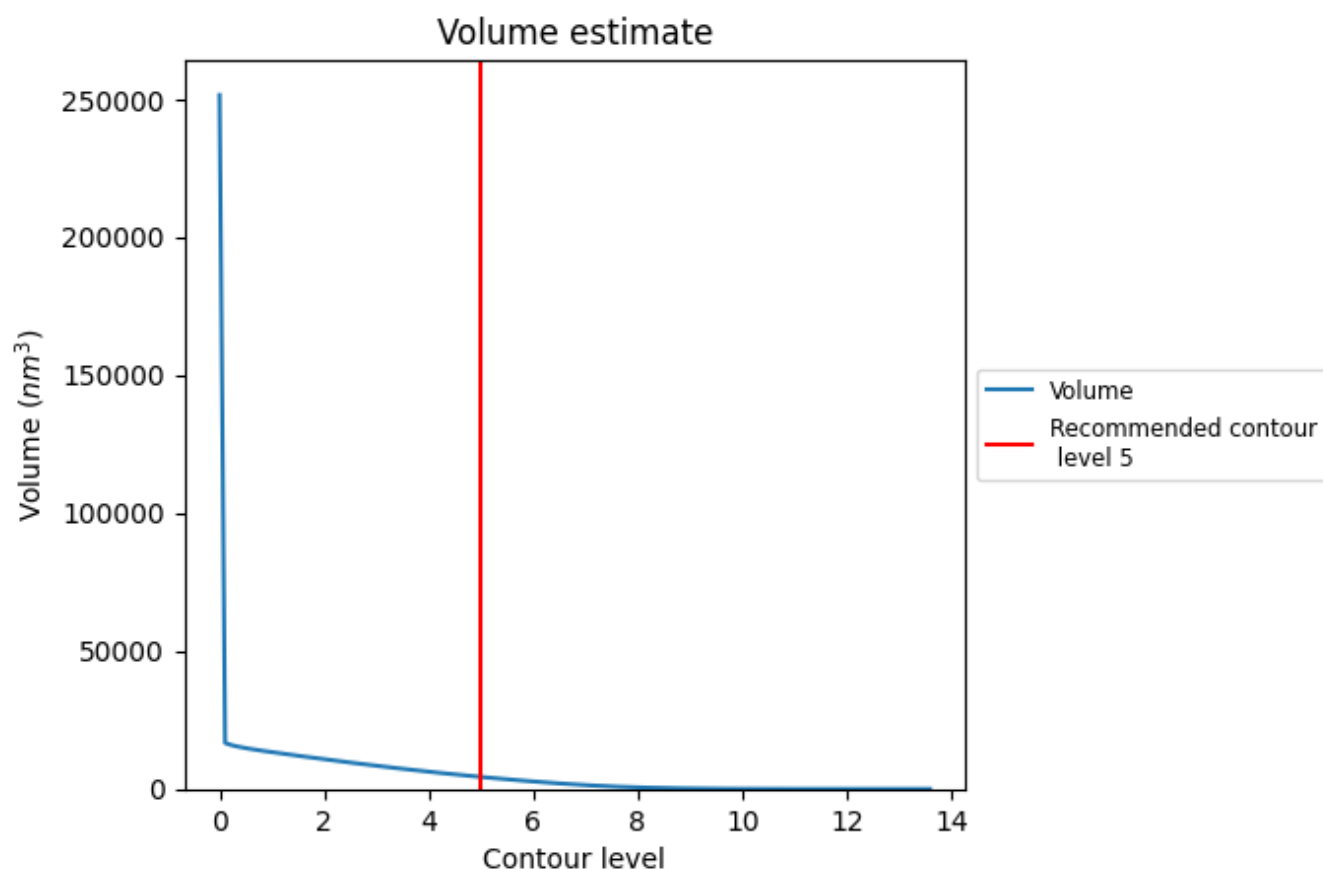
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

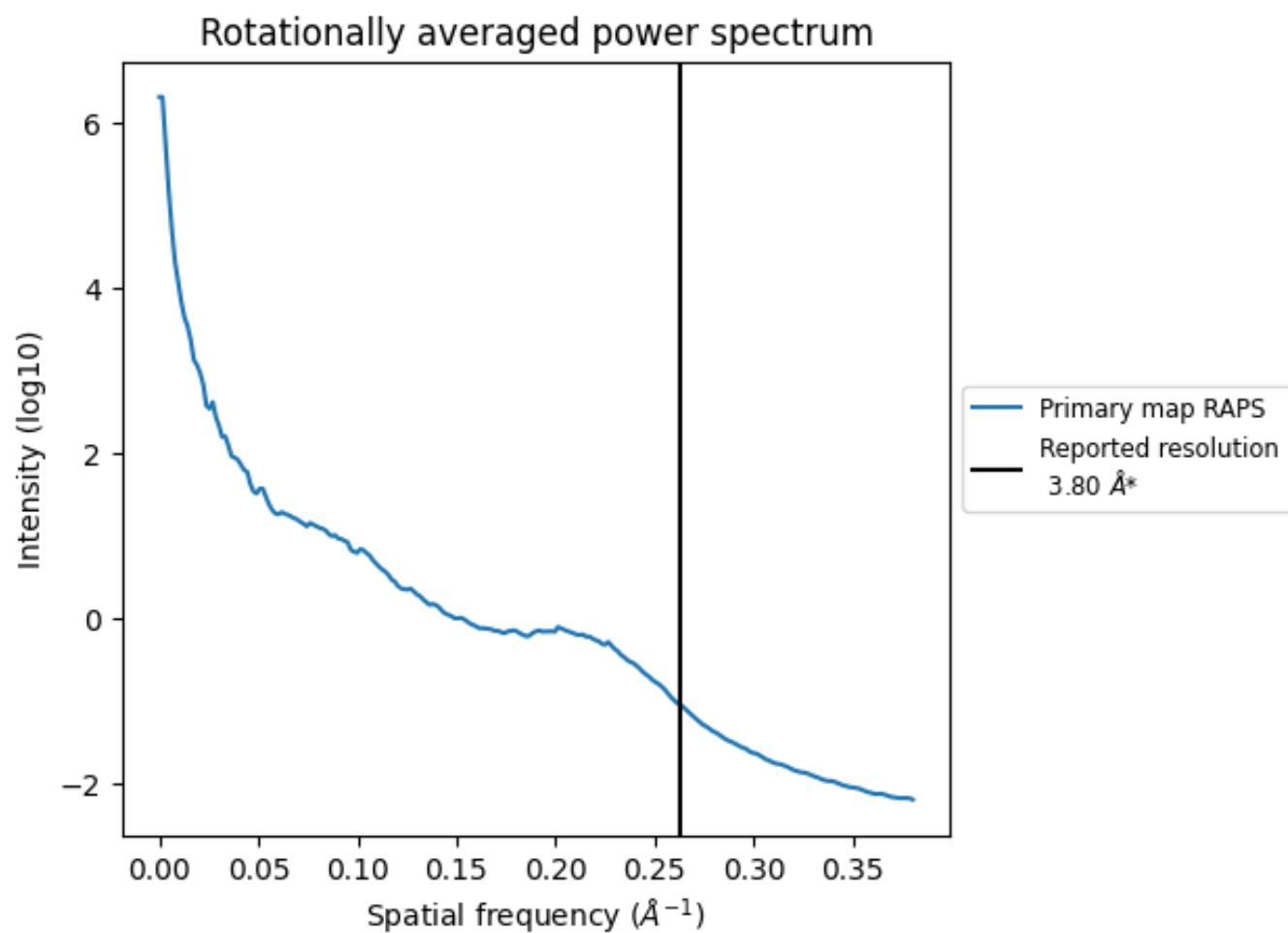
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4355 nm^3 ; this corresponds to an approximate mass of 3934 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 0.263 Å⁻¹

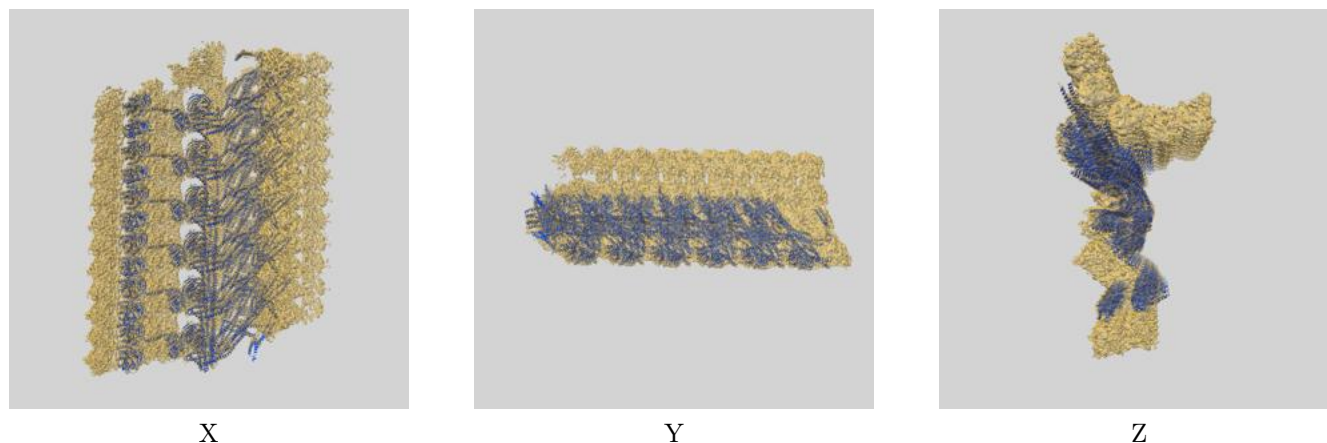
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

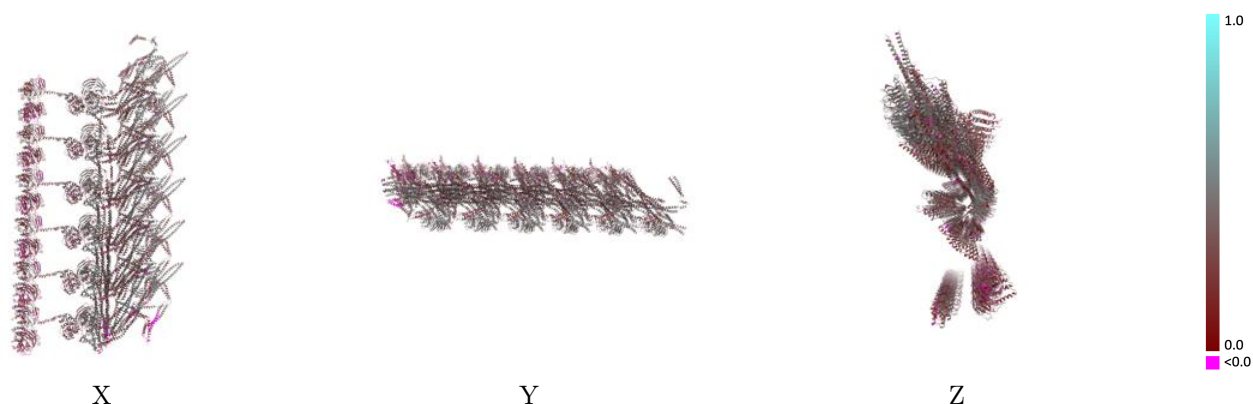
This section contains information regarding the fit between EMDB map EMD-53471 and PDB model 9QZF. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



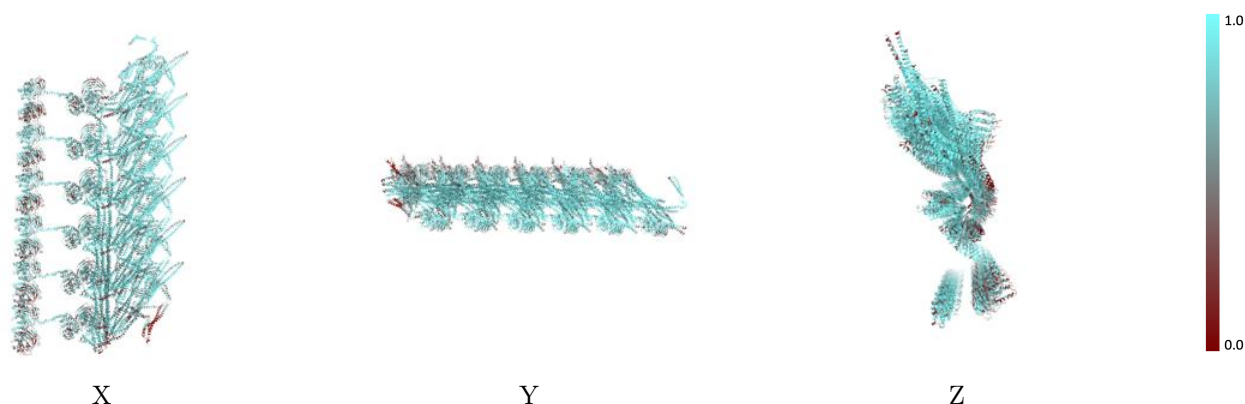
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



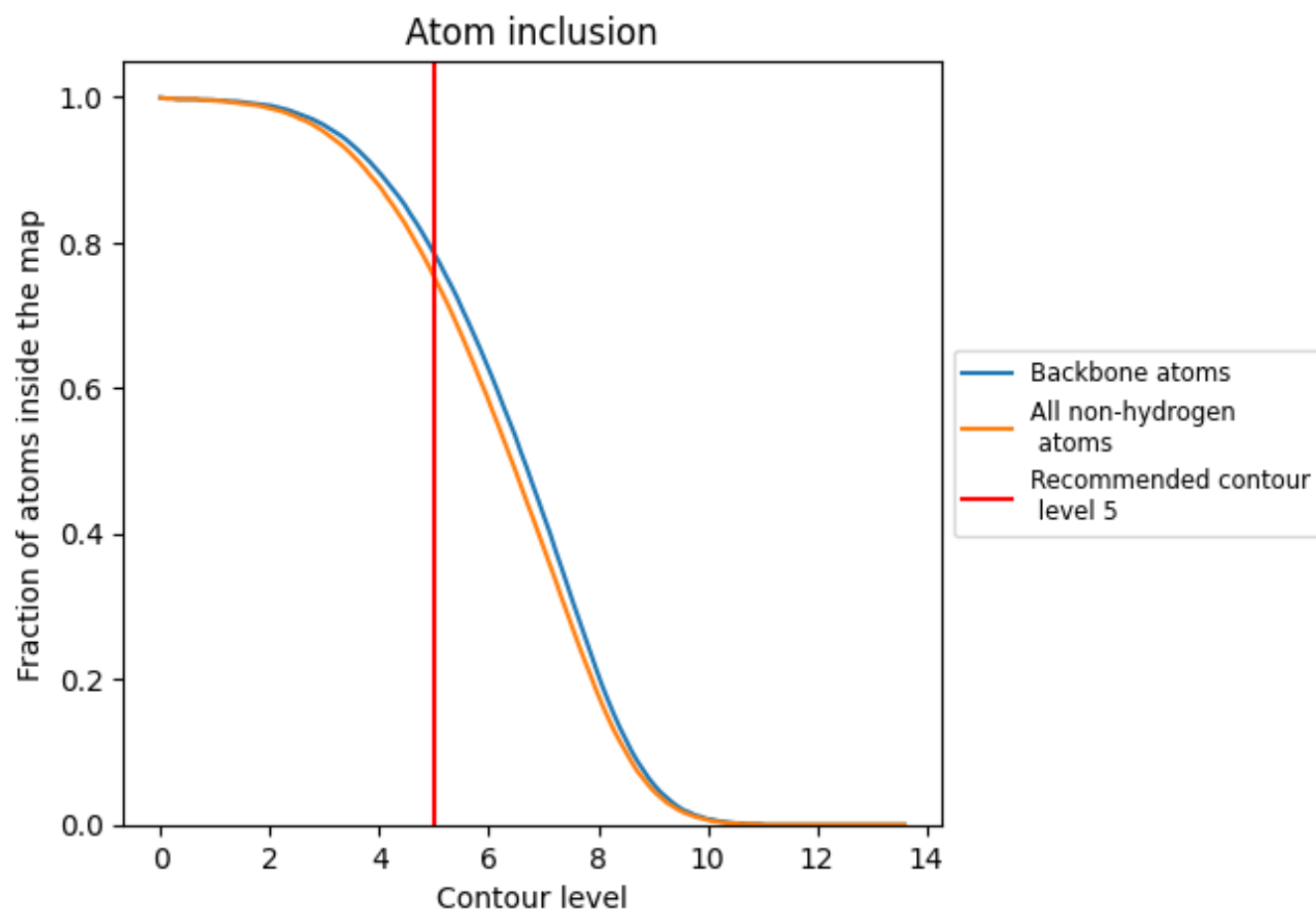
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 75% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.3370
0	 0.8930	 0.3640
1	 0.5950	 0.3520
2	 0.9020	 0.3790
4	 0.6570	 0.2890
5	 0.7290	 0.4000
7	 0.7440	 0.3410
9	 0.7150	 0.3350
A	 0.7590	 0.3960
A7	 0.7940	 0.3400
AB	 0.4420	 0.2140
AC	 0.8560	 0.4000
AE	 0.8500	 0.3580
AG	 0.6470	 0.2890
AH	 0.8900	 0.3500
AJ	 0.7690	 0.4220
AK	 0.8020	 0.3780
AM	 0.7320	 0.2870
AO	 0.4300	 0.2210
AP	 0.8800	 0.3710
AR	 0.8490	 0.3760
AS	 0.6830	 0.3720
AU	 0.5010	 0.2150
AW	 0.7810	 0.4480
AZ	 0.8180	 0.3400
Aa	 0.7060	 0.3870
Ac	 0.8440	 0.4140
Ae	 0.7880	 0.3640
Ai	 0.7740	 0.3300
Ak	 0.7880	 0.3420
Am	 0.5520	 0.2930
An	 0.7430	 0.3270
Aq	 0.7230	 0.3400
As	 0.8990	 0.3380
Av	 0.6900	 0.3360



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Chain	Atom inclusion	Q-score
Az	 0.7940	 0.3240
B1	 0.8500	 0.4240
B2	 0.9330	 0.3680
B4	 0.8520	 0.3670
B5	 0.9250	 0.3690
B8	 0.8730	 0.3710
B9	 0.9180	 0.3590
BD	 0.8410	 0.3990
BK	 0.8620	 0.3480
BO	 0.9420	 0.3710
BR	 0.8200	 0.3130
BV	 0.8540	 0.3530
BY	 0.7140	 0.3540
BZ	 0.9010	 0.3710
Bc	 0.8380	 0.3660
Bf	 0.8210	 0.3570
Bg	 0.8460	 0.3710
Bj	 0.9580	 0.3760
Bm	 0.6990	 0.2870
Bn	 0.8480	 0.3750
Bq	 0.9390	 0.3630
Bt	 0.4650	 0.1940
Bu	 0.9490	 0.3970
Bw	 0.9430	 0.3710
Bx	 0.9290	 0.3460
C	 0.7660	 0.4030
CA	 0.8520	 0.3760
CB	 0.8010	 0.3260
CE	 0.8850	 0.3430
CF	 0.9120	 0.3650
CH	 0.9430	 0.3910
CI	 0.7480	 0.3350
CM	 0.8050	 0.3230
CO	 0.9330	 0.3750
CP	 0.8500	 0.3950
CT	 0.8050	 0.3370
CV	 0.9200	 0.3590
CW	 0.8710	 0.3560
Ca	 0.7740	 0.3950
Cc	 0.9250	 0.3730
Cd	 0.8200	 0.3150
Ch	 0.8010	 0.3510

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Chain	Atom inclusion	Q-score
D	 0.8070	 0.3360
E	 0.7170	 0.3540
F	 0.8720	 0.3760
G	 0.8170	 0.3510
H	 0.7910	 0.3620
I	 0.6590	 0.3400
J	 0.7180	 0.2830
K	 0.7750	 0.3750
L	 0.8080	 0.3430
M	 0.5110	 0.2000
N	 0.9200	 0.3900
O	 0.6220	 0.2700
P	 0.8250	 0.4210
Q	 0.8910	 0.3580
R	 0.4080	 0.2080
S	 0.8610	 0.3590
T	 0.8740	 0.3600
U	 0.7810	 0.4140
V	 0.8690	 0.3470
W	 0.8760	 0.3700
X	 0.7390	 0.3470
Z	 0.8210	 0.3170
a	 0.8520	 0.3460
c	 0.7330	 0.3350
d	 0.8910	 0.3640
f	 0.7520	 0.3050
i	 0.8760	 0.3990
k	 0.7040	 0.3330
l	 0.7910	 0.3620
n	 0.5920	 0.3350
o	 0.4950	 0.2430
q	 0.8820	 0.3490
s	 0.6480	 0.2900
t	 0.7750	 0.3690
v	 0.7590	 0.3600
w	 0.7290	 0.3830
y	 0.8370	 0.3210
z	 0.7550	 0.3040