



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 07:17 PM UTC

PDB ID : 7A7D / pdb_00007a7d
EMDB ID : EMD-11678
Title : Cadherin fit into cryo-ET map
Authors : Sikora, M.; Ermel, U.H.; Seybold, A.; Kunz, M.; Calloni, G.; Reitz, J.; Vabulas, R.M.; Hummer, G.; Frangakis, A.S.
Deposited on : 2020-08-28
Resolution : 26.00 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:

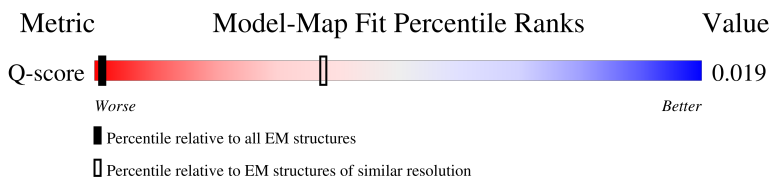
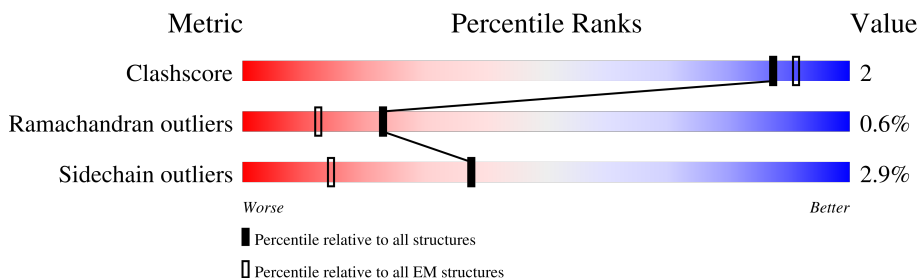
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 26.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8 (26.00 - 26.50)

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

Mol	Chain	Length	Quality of chain
1	A	554	42% 66% 32% .
1	B	554	70% 66% 32% .
1	C	554	77% 66% 32% .
1	D	554	66% 63% 34% .

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Mol	Chain	Length	Quality of chain
1	E	554	60% 61% 33% 5%
1	F	554	68% 63% 34%
1	G	554	64% 65% 33%
2	a	544	61% 61% 35%
2	b	544	80% 65% 32%
2	c	544	51% 60% 35% 5%
2	d	544	34% 65% 33%
2	e	544	60% 60% 36%
2	f	544	87% 61% 36%
2	g	544	55% 62% 36%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 119497 atoms, of which 59136 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 Desmoglein-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	B	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	C	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	D	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	E	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	F	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	G	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	HIS	GLN	conflict	UNP Q14126
B	2252	HIS	GLN	conflict	UNP Q14126
C	1120	HIS	GLN	conflict	UNP Q14126
D	1686	HIS	GLN	conflict	UNP Q14126
E	2252	HIS	GLN	conflict	UNP Q14126
F	1686	HIS	GLN	conflict	UNP Q14126
G	1120	HIS	GLN	conflict	UNP Q14126

- Molecule 2 is a protein called Desmocollin-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	a	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	b	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		

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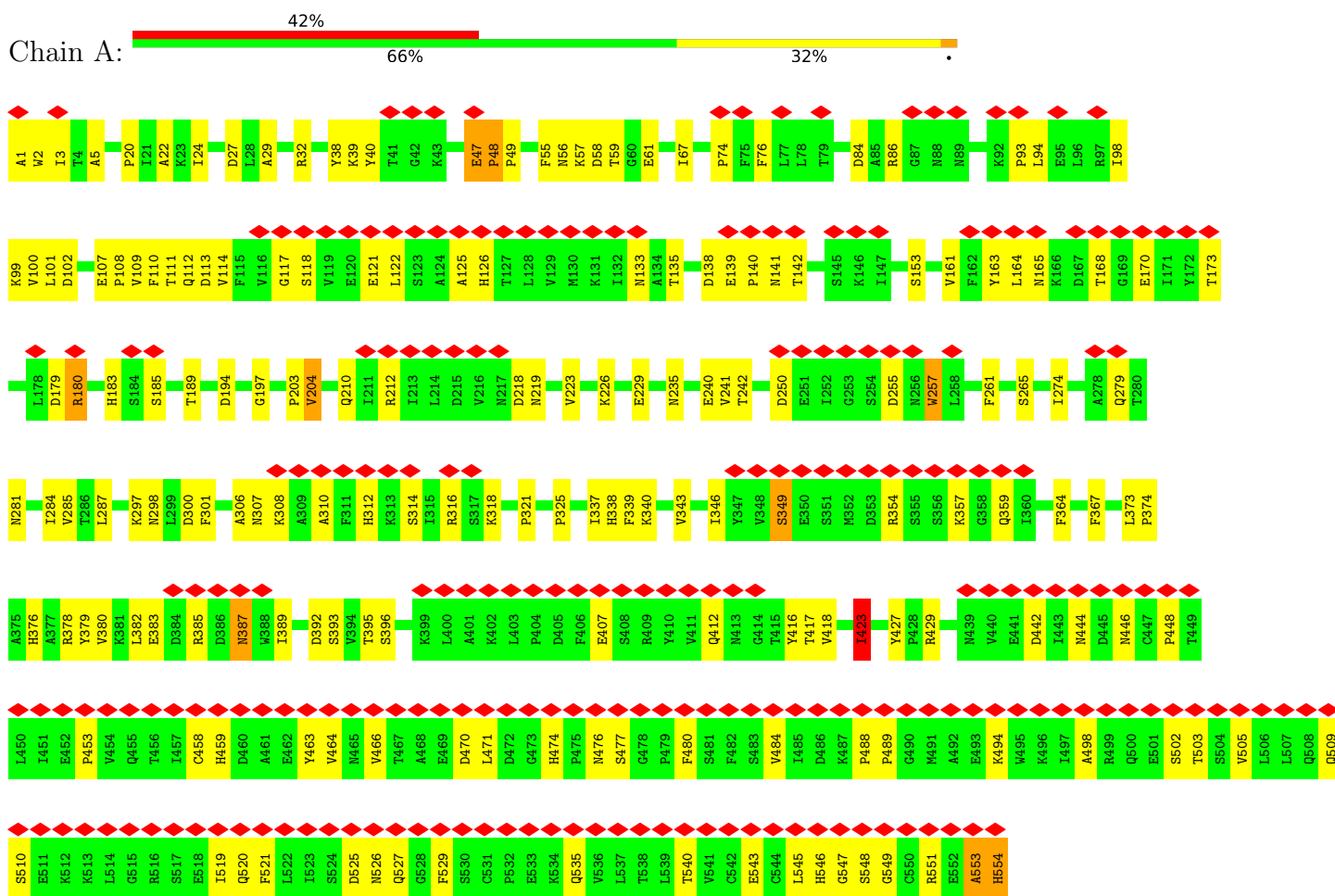
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Mol	Chain	Residues	Atoms						AltConf	Trace
2	c	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	d	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	e	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	f	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	g	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		

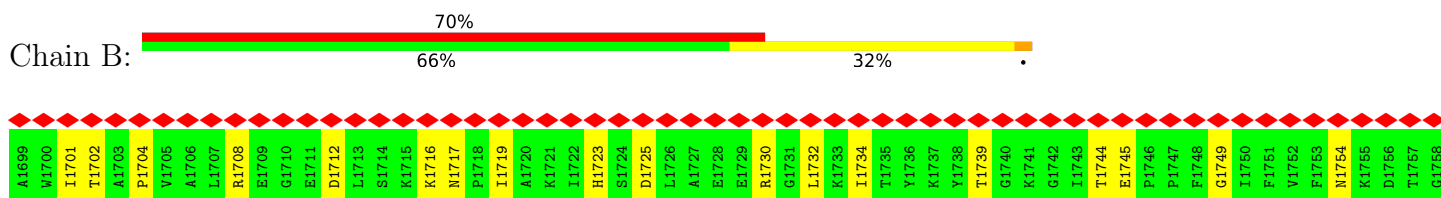
3 Residue-property plots

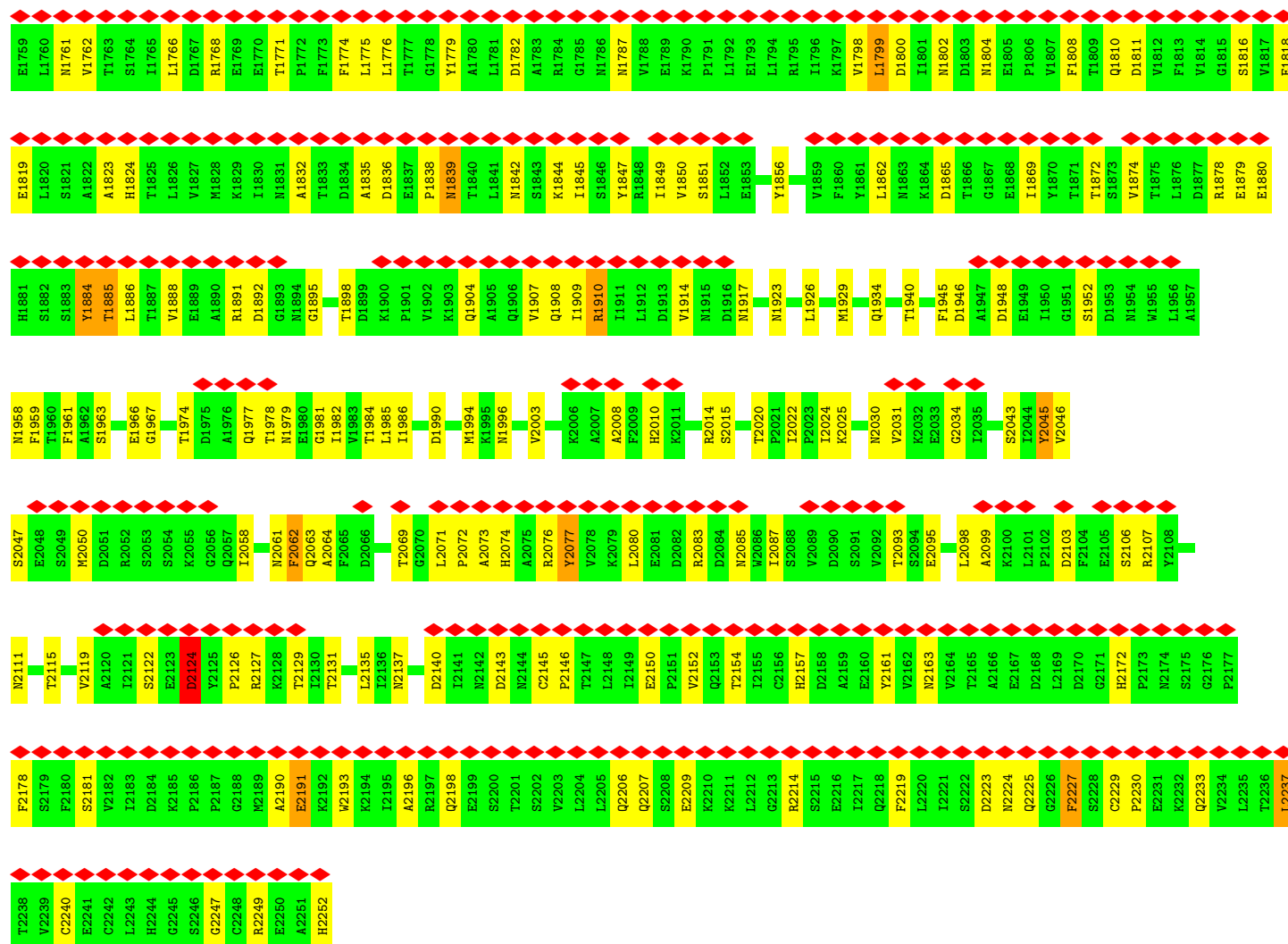
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Desmoglein-2

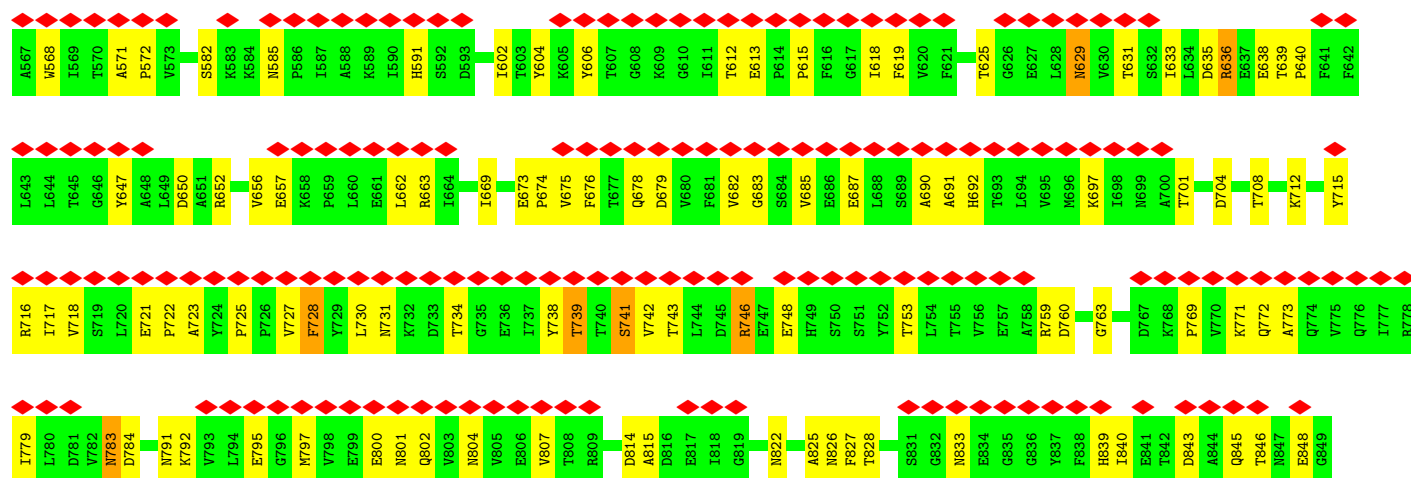
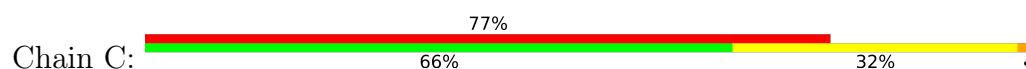


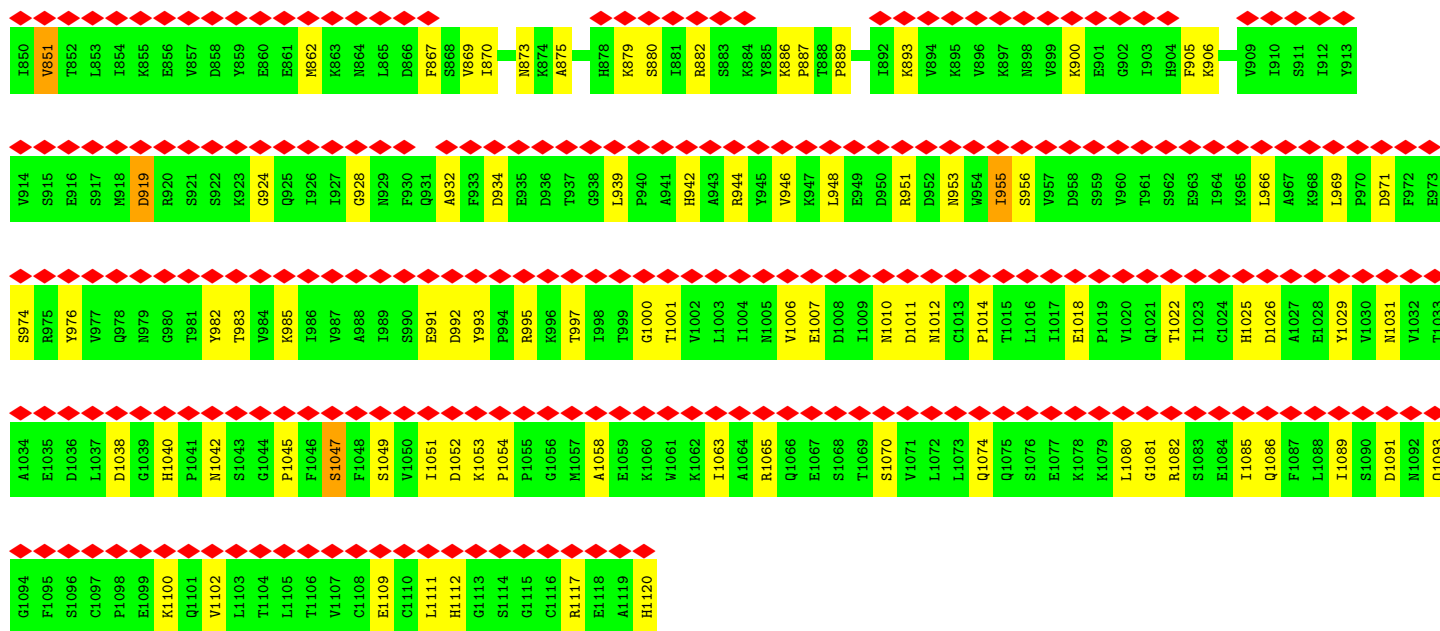
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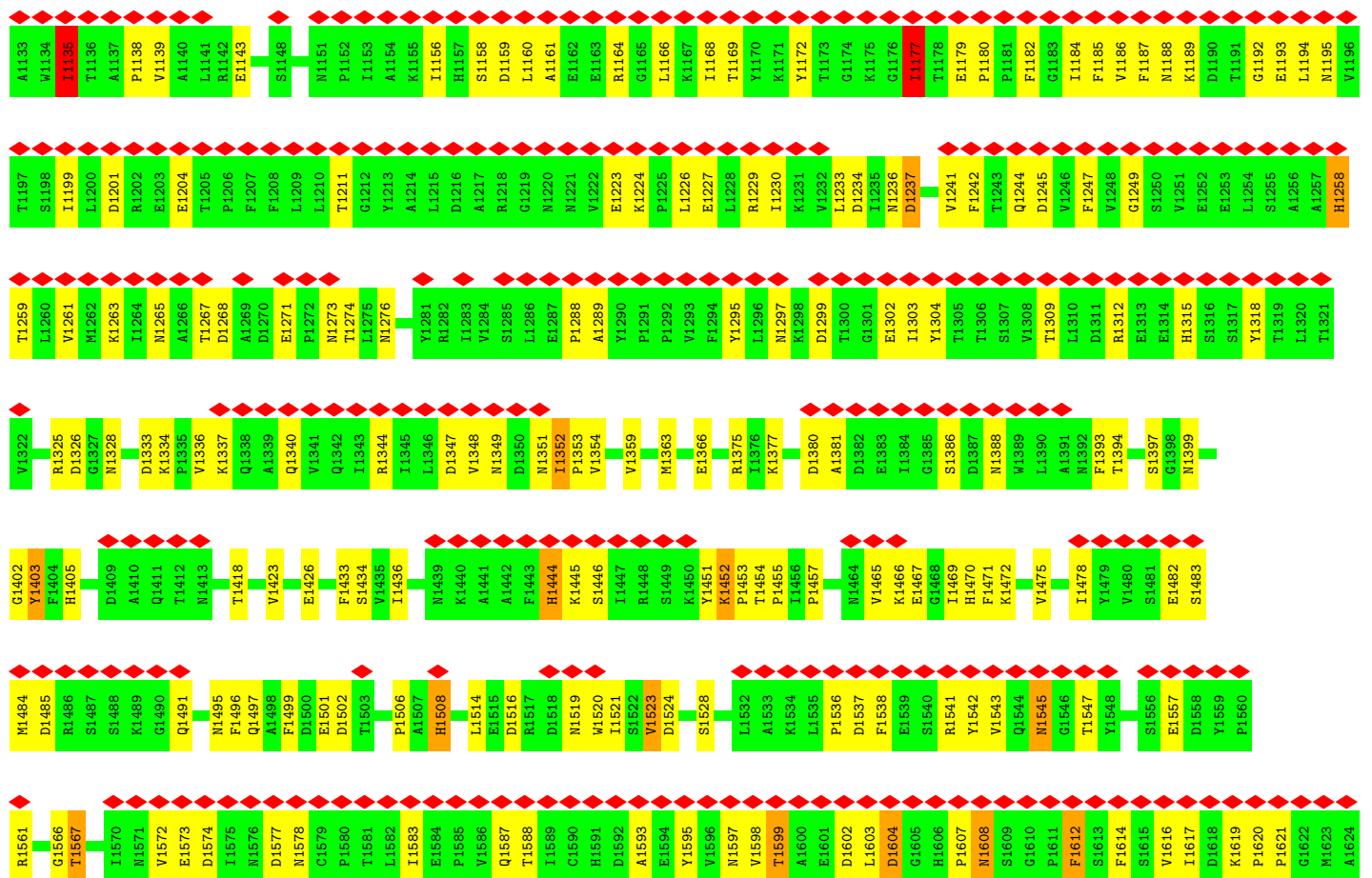


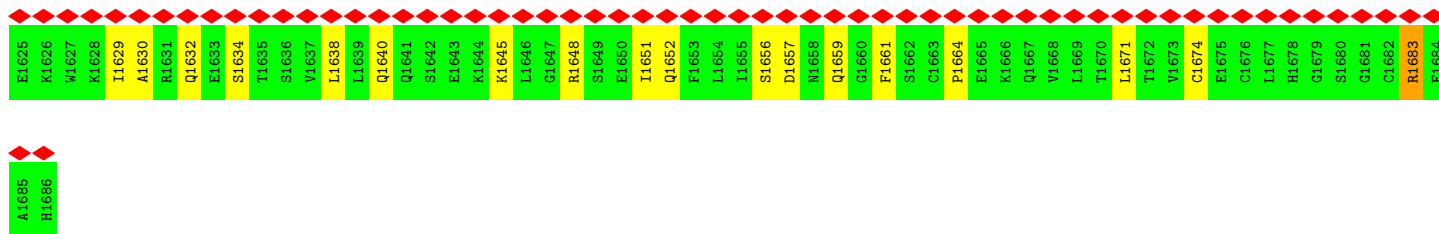
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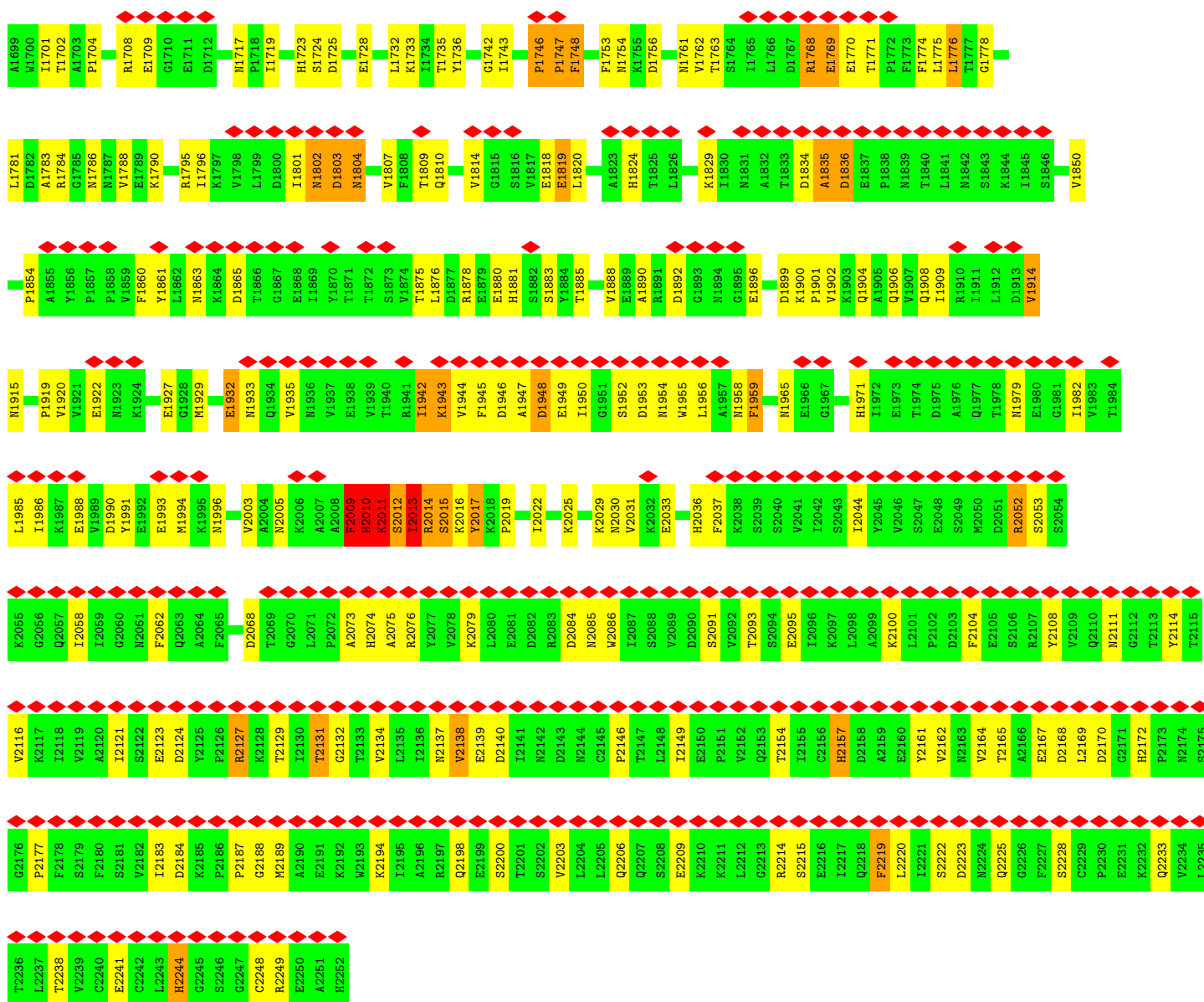


• Molecule 1: Desmoglein-2



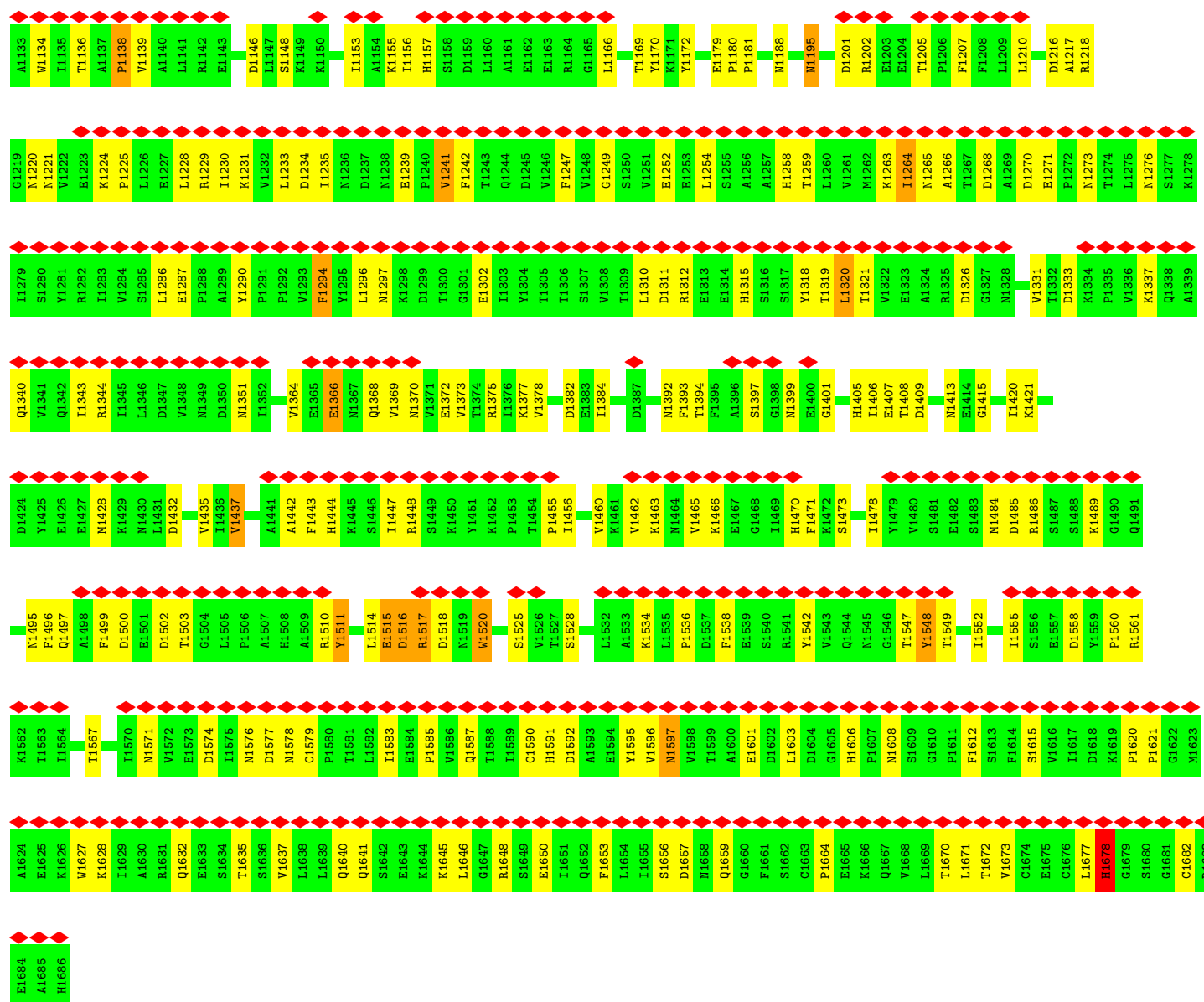


• Molecule 1: Desmoglein-2

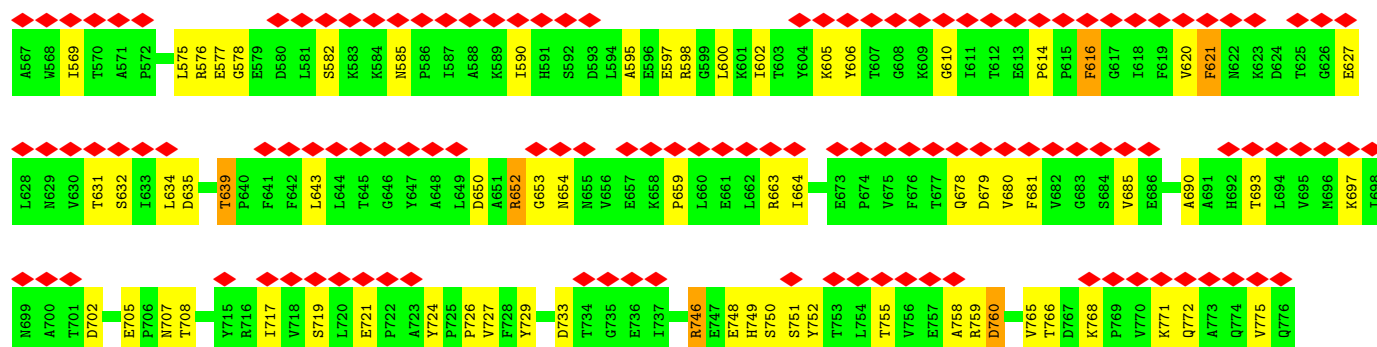


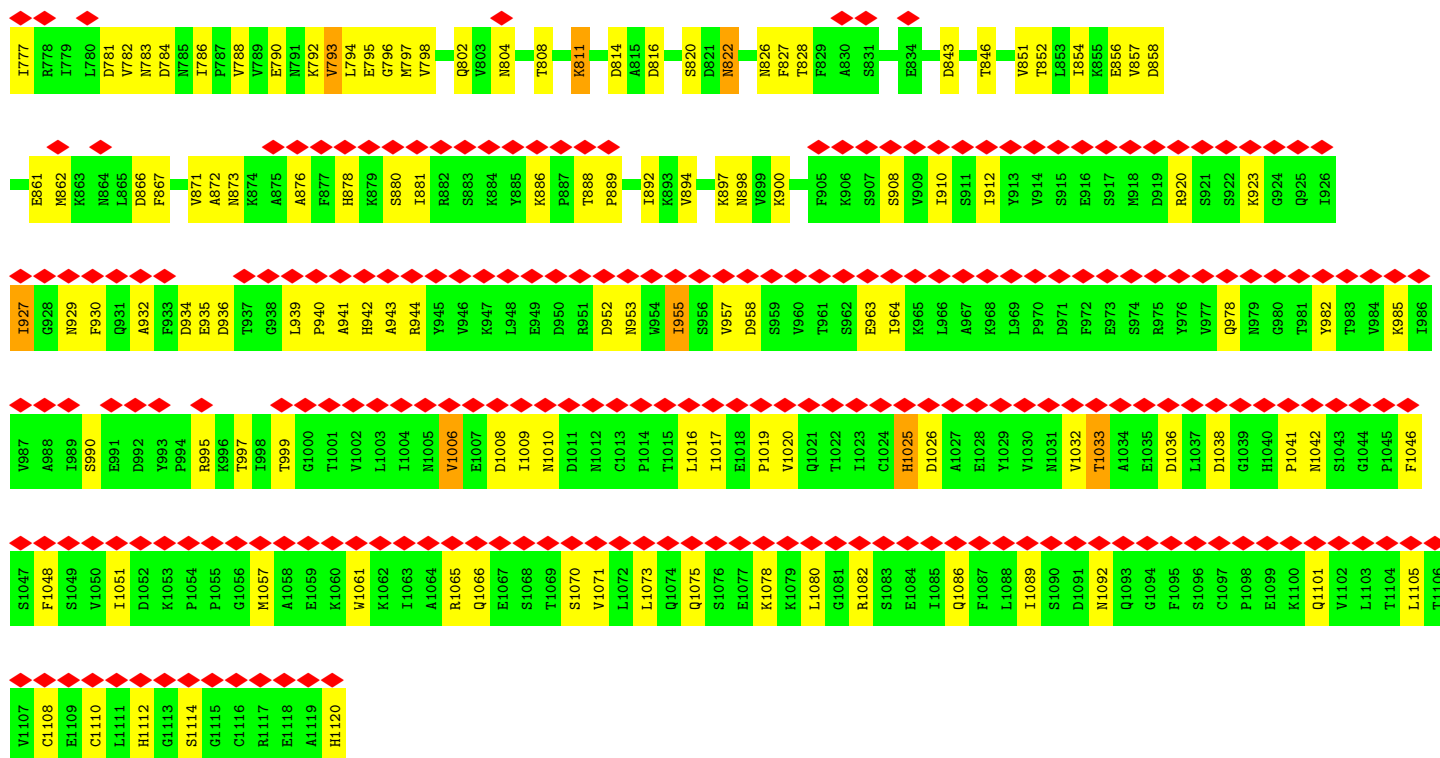
• Molecule 1: Desmoglein-2



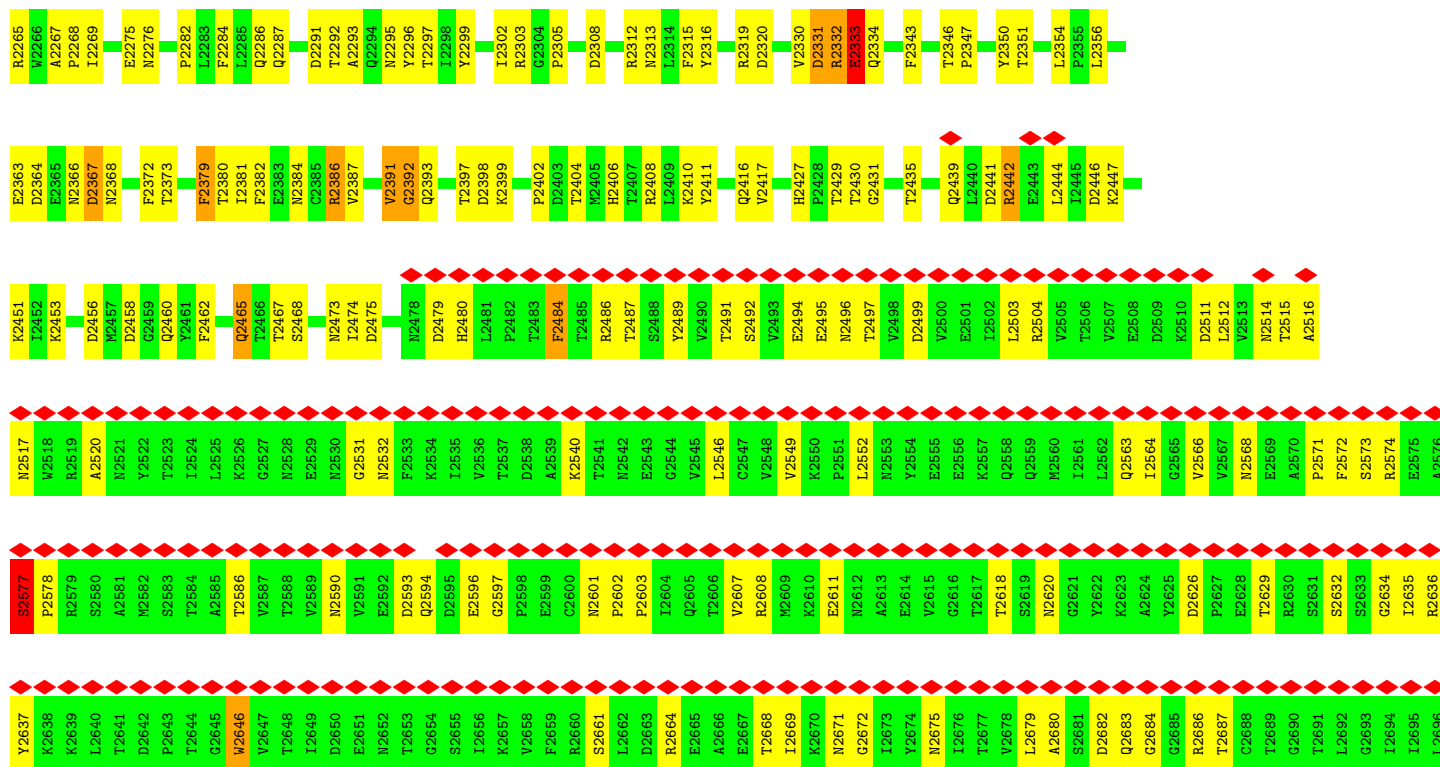


• Molecule 1: Desmoglein-2



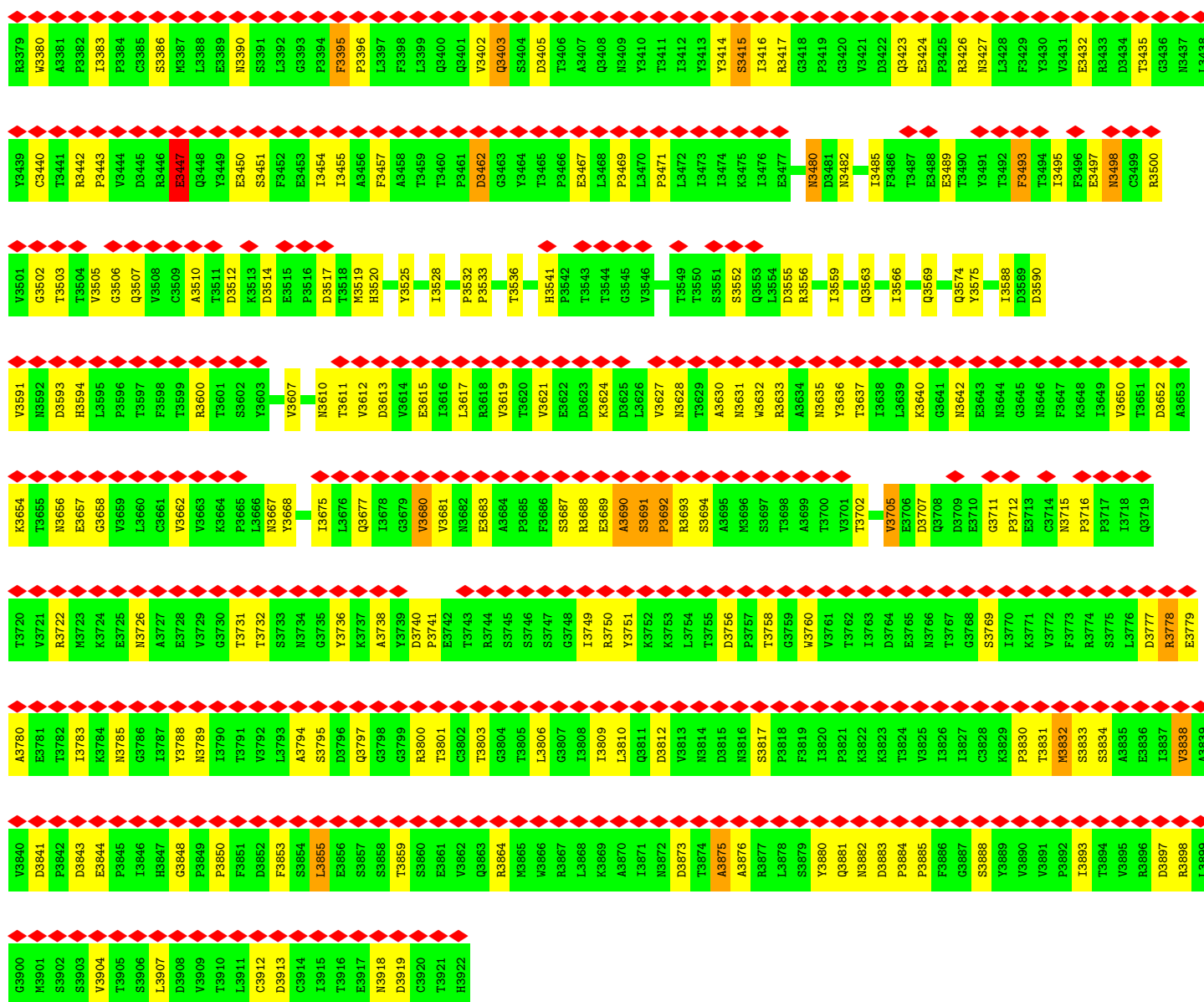
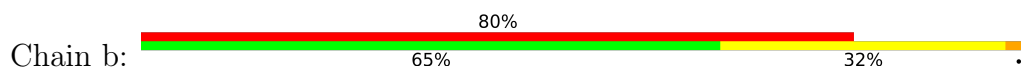


• Molecule 2: Desmocollin-2



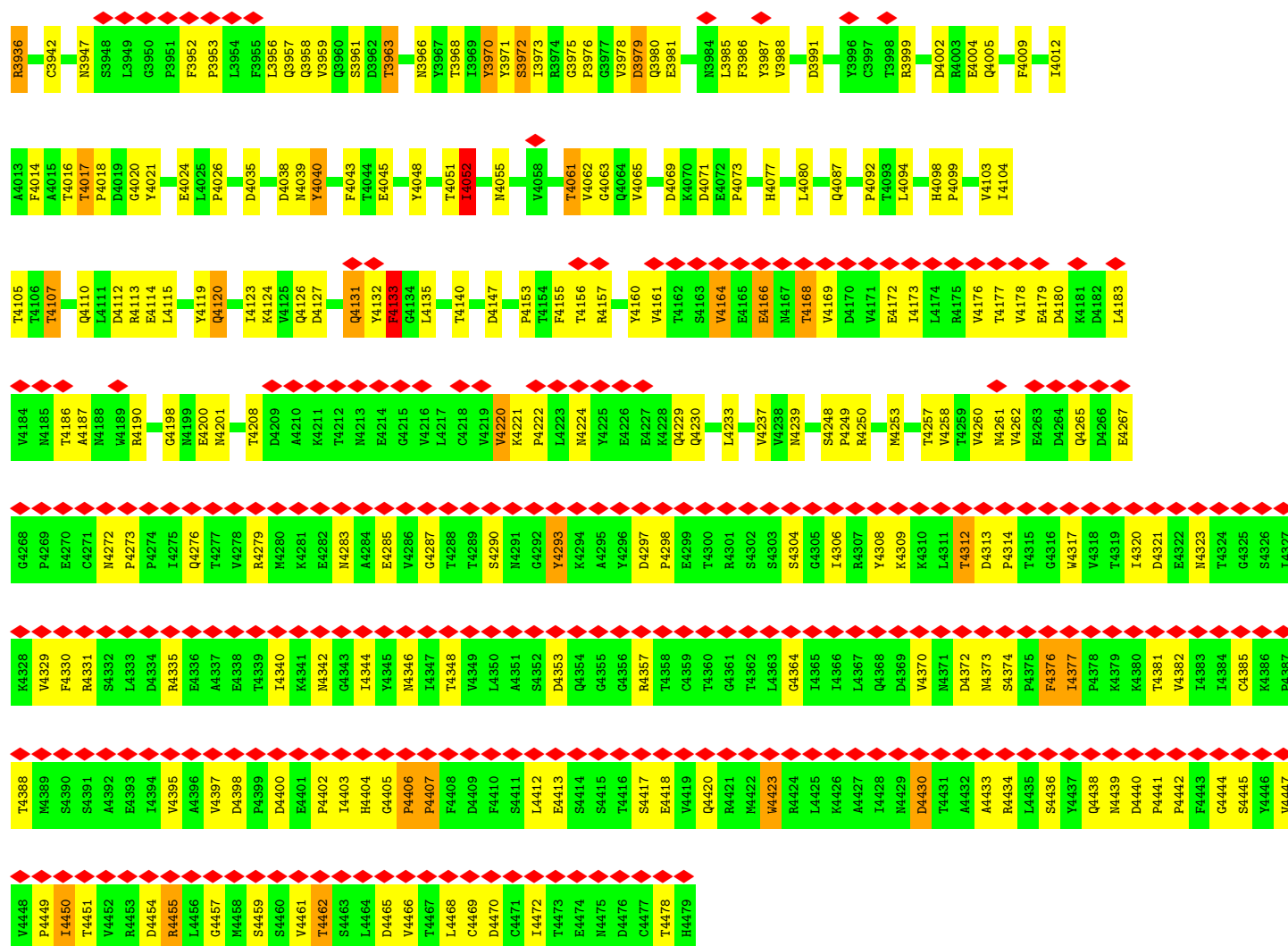


• Molecule 2: Desmocollin-2

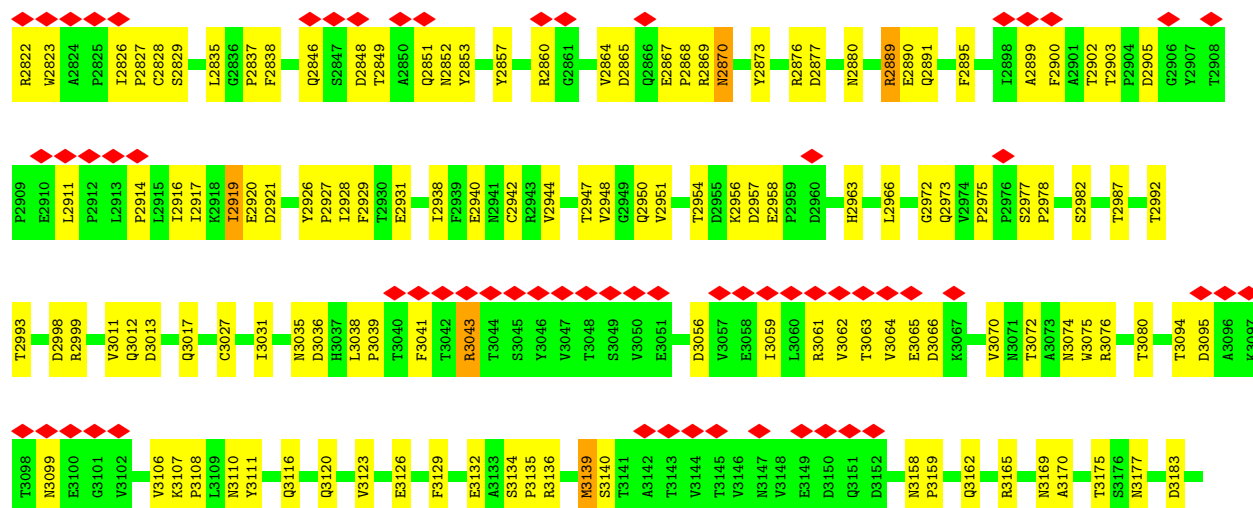


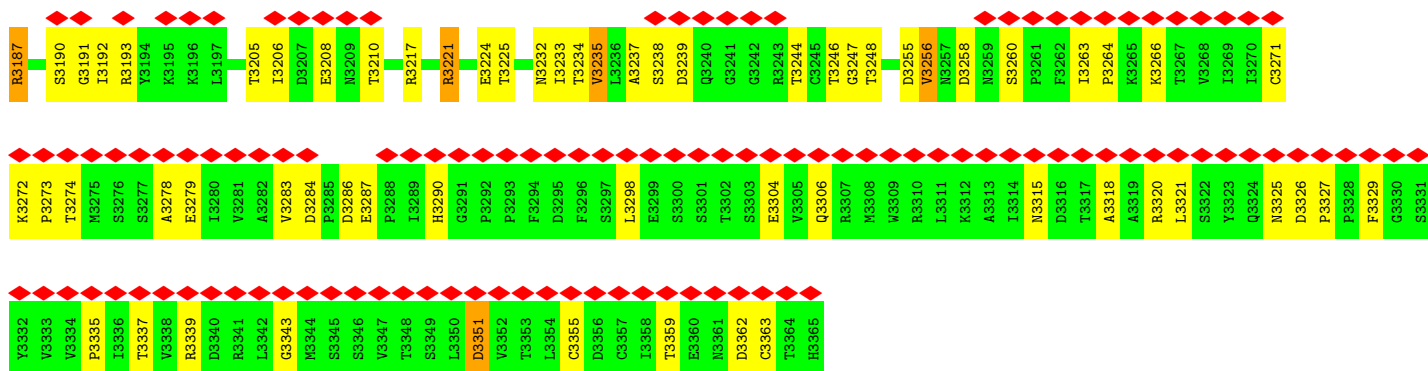
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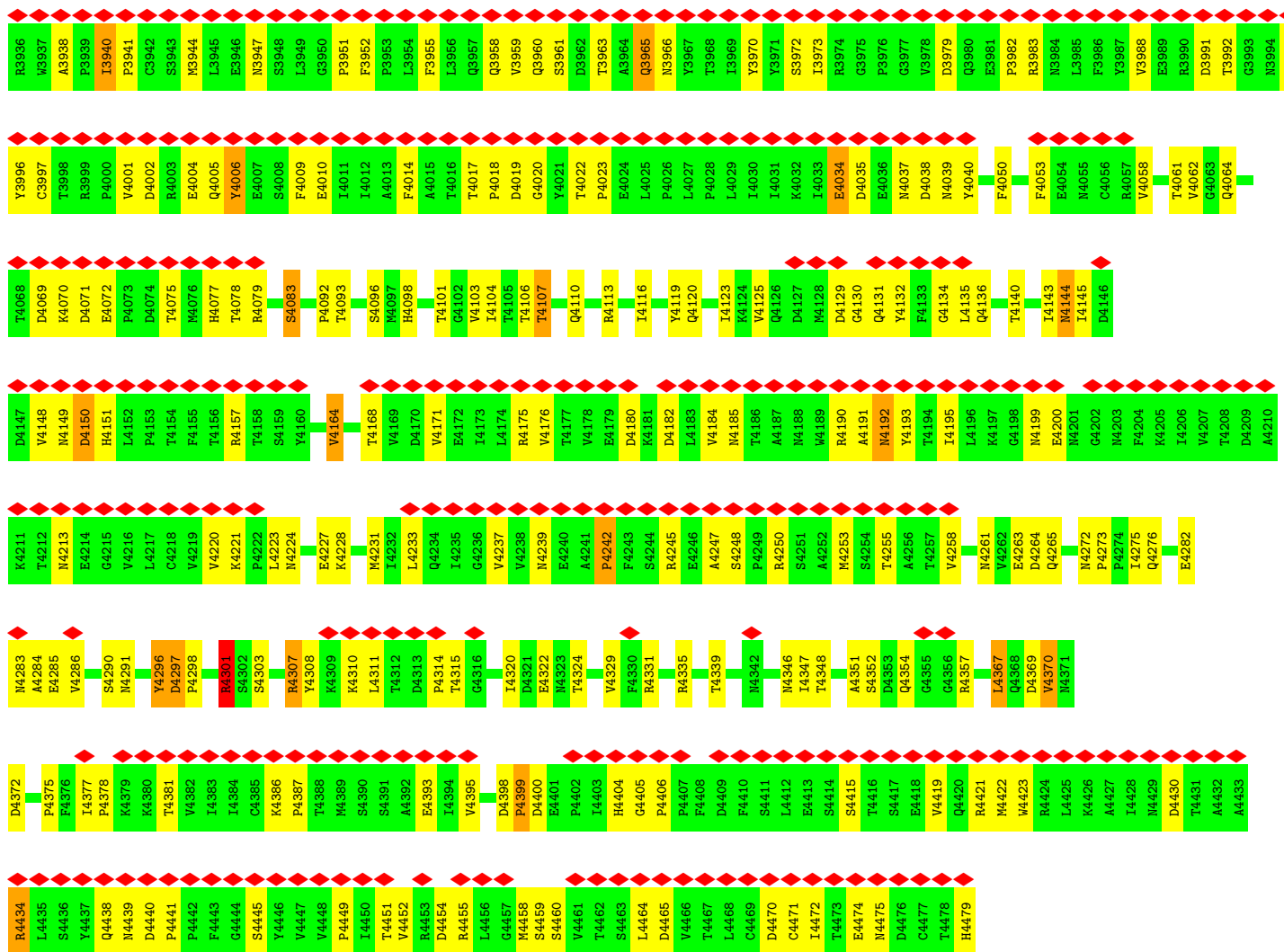


• Molecule 2: Desmocollin-2

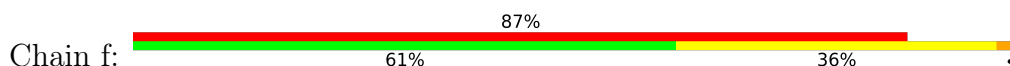


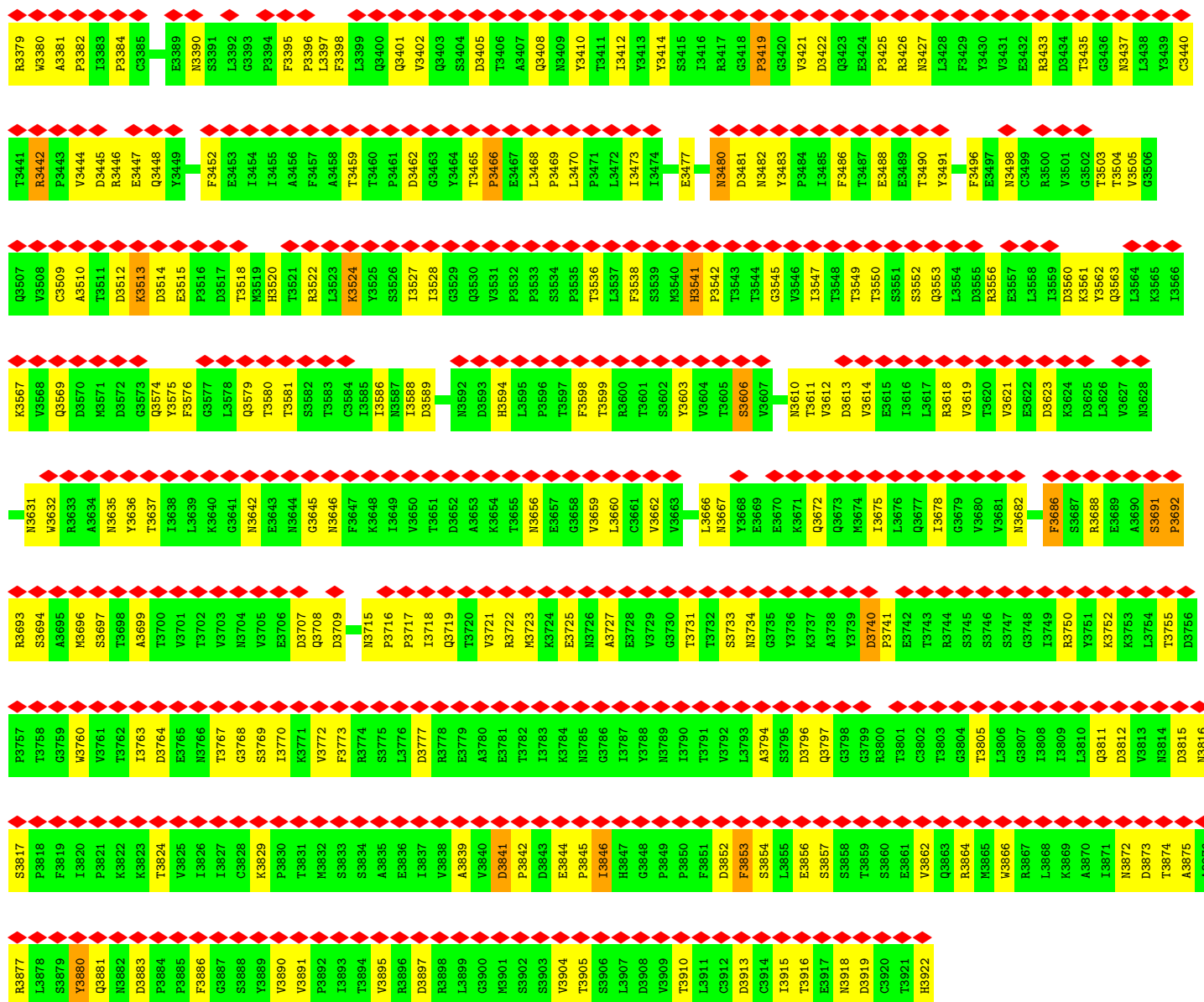


• Molecule 2: Desmocollin-2

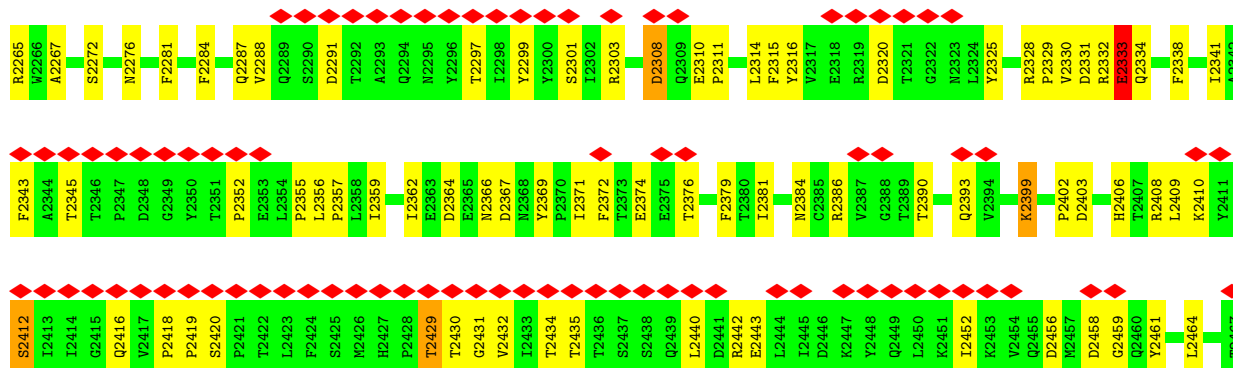


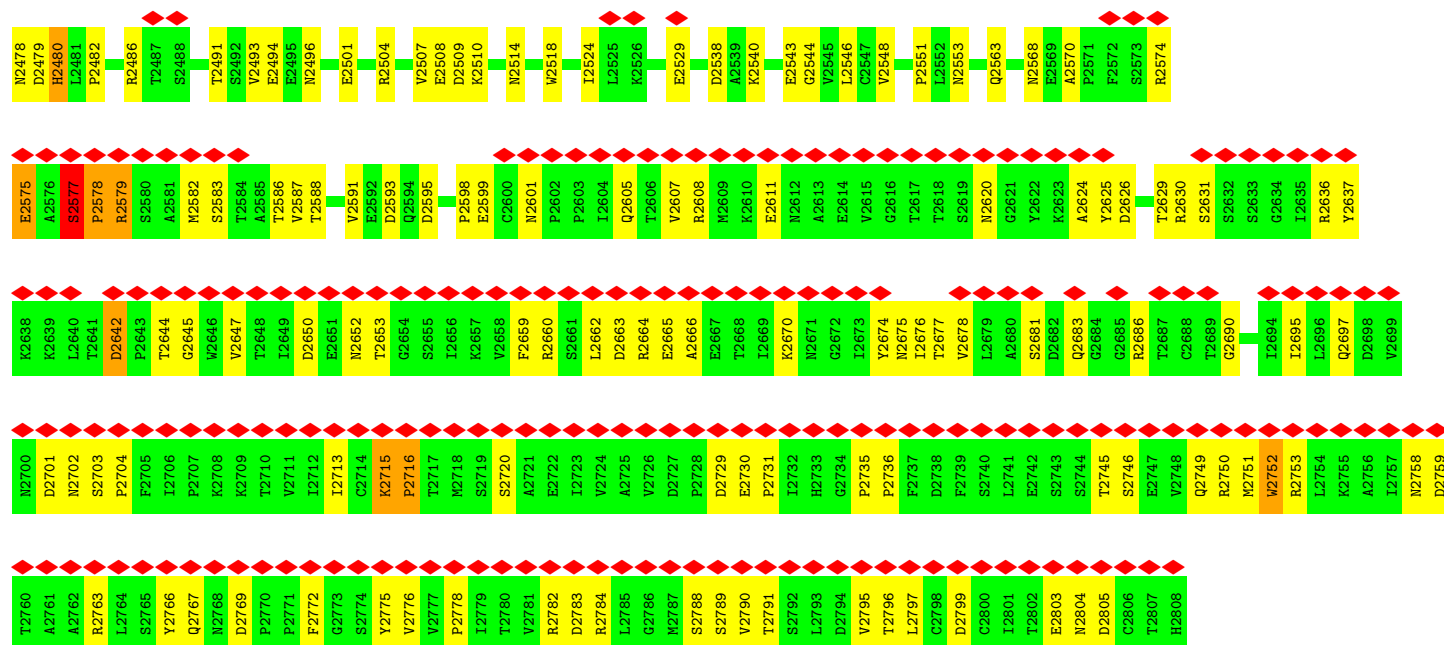
• Molecule 2: Desmocollin-2





• Molecule 2: Desmocollin-2





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	3656	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0133	Depositor
Map size (Å)	550.4, 550.4, 550.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.3, 4.3, 4.3	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	0.60	0/4438	2.38	226/6026 (3.8%)
1	B	0.59	0/4438	2.37	243/6026 (4.0%)
1	C	0.59	0/4438	2.37	247/6026 (4.1%)
1	D	0.60	0/4438	2.39	254/6026 (4.2%)
1	E	1.46	14/4438 (0.3%)	2.75	280/6026 (4.6%)
1	F	0.60	0/4438	2.36	247/6026 (4.1%)
1	G	0.60	0/4438	2.35	216/6026 (3.6%)
2	a	0.64	1/4355 (0.0%)	2.42	251/5943 (4.2%)
2	b	0.61	0/4355	2.35	235/5943 (4.0%)
2	c	0.61	0/4355	2.44	281/5943 (4.7%)
2	d	0.61	0/4355	2.38	236/5943 (4.0%)
2	e	0.61	0/4355	2.43	265/5943 (4.5%)
2	f	0.61	0/4355	2.36	243/5943 (4.1%)
2	g	0.63	2/4355 (0.0%)	2.40	245/5943 (4.1%)
All	All	0.71	17/61551 (0.0%)	2.41	3469/83783 (4.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	15
1	C	0	13
1	D	0	15
1	E	0	18
1	F	0	12
1	G	0	9
2	a	0	15
2	b	0	11
2	c	0	11
2	d	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	e	0	12
2	f	0	11
2	g	0	13
All	All	0	168

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2010	HIS	ND1-CE1	66.64	1.99	1.32
1	E	2010	HIS	CG-ND1	34.51	1.76	1.38
1	E	2011	LYS	C-N	27.15	1.70	1.33
1	E	2010	HIS	N-CA	21.43	1.73	1.46
1	E	2010	HIS	CG-CD2	-12.77	1.21	1.35
1	E	2012	SER	CB-OG	-11.30	1.19	1.42
2	a	2333	GLU	CD-OE1	-11.27	1.03	1.25
1	E	2010	HIS	CE1-NE2	10.36	1.43	1.32
1	E	2012	SER	C-N	9.49	1.46	1.33
1	E	2010	HIS	CA-C	9.27	1.65	1.52
1	E	2010	HIS	C-O	8.18	1.34	1.24
1	E	2012	SER	CA-C	-7.77	1.43	1.52
1	E	2010	HIS	CD2-NE2	7.65	1.46	1.37
1	E	2010	HIS	CA-CB	-7.58	1.40	1.53
2	g	2333	GLU	CD-OE2	-7.23	1.11	1.25
1	E	2012	SER	C-O	-6.33	1.16	1.24
2	g	2333	GLU	CD-OE1	-5.25	1.15	1.25

All (3469) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2010	HIS	CA-CB-CG	-48.66	65.14	113.80
1	E	2010	HIS	CE1-NE2-CD2	-48.20	60.80	109.00
1	E	2010	HIS	CG-ND1-CE1	-37.53	45.49	109.30
1	E	2012	SER	N-CA-CB	28.88	151.94	110.07
1	E	2010	HIS	ND1-CE1-NE2	-23.52	84.88	108.40
1	E	2012	SER	CA-C-O	22.58	143.96	120.70
1	E	2011	LYS	CA-CB-CG	17.43	148.96	114.10
1	E	2013	ILE	N-CA-CB	16.62	139.75	111.50
1	E	1819	GLU	CA-C-O	-16.29	103.95	121.87
2	e	4406	PRO	N-CA-CB	16.23	111.66	103.22
1	E	1899	ASP	CA-CB-CG	15.54	128.15	112.60
1	E	2010	HIS	CB-CG-ND1	-13.85	101.92	122.70
1	G	866	ASP	CA-CB-CG	13.79	126.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1819	GLU	CB-CG-CD	13.65	135.80	112.60
1	F	1632	GLN	OE1-CD-NE2	-13.55	109.05	122.60
1	E	2010	HIS	O-C-N	-13.49	104.64	122.59
2	d	3017	GLN	OE1-CD-NE2	-13.19	109.41	122.60
1	A	48	PRO	O-C-N	13.17	127.37	121.31
1	E	2011	LYS	CA-C-N	-13.10	102.63	120.44
1	E	2011	LYS	C-N-CA	-13.10	102.63	120.44
2	g	2783	ASP	CA-CB-CG	13.08	125.68	112.60
2	d	3246	THR	CA-C-N	12.88	132.66	121.58
2	d	3246	THR	C-N-CA	12.88	132.66	121.58
1	G	760	ASP	CA-CB-CG	12.62	125.22	112.60
1	E	2013	ILE	CA-C-O	-12.39	99.74	120.80
1	E	2012	SER	CA-C-N	12.37	143.96	121.70
1	E	2012	SER	C-N-CA	12.37	143.96	121.70
2	a	2486	ARG	NE-CZ-NH2	12.36	130.33	119.20
1	E	2010	HIS	CB-CA-C	12.33	134.95	110.42
1	E	2012	SER	CB-CA-C	-12.30	91.46	110.90
1	A	525	ASP	CA-CB-CG	12.29	124.89	112.60
1	C	731	ASN	OD1-CG-ND2	-12.16	110.44	122.60
1	D	1348	VAL	O-C-N	11.84	136.18	123.04
2	e	4110	GLN	OE1-CD-NE2	-11.55	111.05	122.60
1	G	784	ASP	CA-CB-CG	11.53	124.13	112.60
2	g	2381	ILE	CA-C-O	-11.36	107.94	120.67
1	G	726	PRO	N-CA-CB	11.33	109.27	102.92
1	E	2012	SER	CA-CB-OG	-11.32	88.45	111.10
1	E	1786	ASN	OD1-CG-ND2	-11.25	111.35	122.60
1	E	2010	HIS	CA-C-O	-11.22	104.46	120.51
2	e	4120	GLN	OE1-CD-NE2	-11.19	111.41	122.60
2	c	4346	ASN	CA-CB-CG	11.14	123.74	112.60
2	g	2329	PRO	N-CA-CB	11.03	113.67	103.19
2	d	2877	ASP	CA-CB-CG	11.02	123.62	112.60
1	B	2223	ASP	CA-CB-CG	10.98	123.58	112.60
2	d	2865	ASP	CA-CB-CG	10.91	123.51	112.60
1	F	1202	ARG	CD-NE-CZ	10.85	139.58	124.40
1	D	1604	ASP	CA-CB-CG	10.84	123.44	112.60
2	a	2564	ILE	CA-C-N	10.82	129.94	121.61
2	a	2564	ILE	C-N-CA	10.82	129.94	121.61
1	D	1444	HIS	N-CA-CB	10.73	125.60	110.26
1	B	2072	PRO	N-CA-CB	10.73	112.86	103.31
1	A	255	ASP	CA-CB-CG	10.70	123.30	112.60
1	G	936	ASP	CA-CB-CG	10.66	123.26	112.60
2	e	4064	GLN	OE1-CD-NE2	-10.60	112.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2124	ASP	CA-CB-CG	10.60	123.19	112.60
2	c	4133	PHE	CA-C-N	10.57	130.07	119.92
2	c	4133	PHE	C-N-CA	10.57	130.07	119.92
1	A	502	SER	N-CA-C	10.48	122.70	111.28
2	a	2320	ASP	CA-CB-CG	10.46	123.06	112.60
1	B	1725	ASP	CA-CB-CG	10.46	123.06	112.60
1	E	1914	VAL	N-CA-C	10.39	125.64	108.81
2	b	3726	ASN	OD1-CG-ND2	-10.36	112.24	122.60
2	g	2291	ASP	CA-CB-CG	10.36	122.96	112.60
1	A	261	PHE	CA-CB-CG	10.32	124.12	113.80
2	g	2735	PRO	N-CA-CB	10.28	108.94	103.19
1	E	2177	PRO	N-CA-CB	10.27	112.45	103.31
1	A	374	PRO	N-CA-CB	10.24	112.43	103.31
1	E	2013	ILE	CA-CB-CG1	10.23	127.80	110.40
2	b	3498	ASN	CA-CB-CG	10.21	122.81	112.60
2	e	4185	ASN	CA-CB-CG	10.19	122.79	112.60
2	e	4014	PHE	CA-CB-CG	10.09	123.89	113.80
1	E	2011	LYS	O-C-N	10.06	135.97	122.59
1	A	48	PRO	N-CA-C	10.03	120.10	110.47
1	F	1659	GLN	OE1-CD-NE2	-10.03	112.57	122.60
1	E	2010	HIS	CB-CG-CD2	9.99	144.19	131.20
1	A	480	PHE	CA-CB-CG	9.92	123.72	113.80
1	E	1820	LEU	CB-CA-C	9.81	129.94	110.42
1	D	1465	VAL	O-C-N	9.80	134.10	123.02
2	d	2860	ARG	NE-CZ-NH2	9.78	128.00	119.20
1	D	1349	ASN	OD1-CG-ND2	-9.74	112.86	122.60
1	F	1620	PRO	CA-C-N	9.73	130.12	119.90
1	F	1620	PRO	C-N-CA	9.73	130.12	119.90
2	b	3795	SER	CA-C-N	9.70	136.68	123.00
2	b	3795	SER	C-N-CA	9.70	136.68	123.00
2	e	4331	ARG	NE-CZ-NH2	9.69	127.92	119.20
2	a	2727	ASP	CA-CB-CG	9.68	122.28	112.60
2	a	2517	ASN	CA-CB-CG	9.67	122.27	112.60
1	A	110	PHE	N-CA-C	9.63	123.82	110.24
1	C	728	PHE	CA-CB-CG	9.63	123.43	113.80
1	E	1906	GLN	OE1-CD-NE2	-9.63	112.97	122.60
1	G	1026	ASP	CA-CB-CG	9.62	122.22	112.60
1	E	1803	ASP	CA-CB-CG	9.61	122.21	112.60
2	a	2737	PHE	CA-CB-CG	9.60	123.40	113.80
1	D	1211	THR	CA-C-N	9.59	132.06	122.66
1	D	1211	THR	C-N-CA	9.59	132.06	122.66
2	b	3883	ASP	CA-C-N	9.58	126.56	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	3883	ASP	C-N-CA	9.58	126.56	119.66
2	a	2366	ASN	CA-CB-CG	9.55	122.16	112.60
2	g	2686	ARG	NE-CZ-NH2	9.55	127.80	119.20
1	A	183	HIS	CB-CG-CD2	-9.52	118.82	131.20
1	G	795	GLU	CA-C-N	9.52	131.99	122.66
1	G	795	GLU	C-N-CA	9.52	131.99	122.66
1	E	2223	ASP	CA-CB-CG	9.50	122.10	112.60
2	g	2486	ARG	NE-CZ-NH2	9.49	127.74	119.20
2	f	3796	ASP	CA-CB-CG	9.48	122.08	112.60
1	C	679	ASP	CA-CB-CG	9.47	122.08	112.60
2	c	4449	PRO	CA-C-N	9.47	133.18	122.48
2	c	4449	PRO	C-N-CA	9.47	133.18	122.48
2	d	3264	PRO	N-CA-CB	9.42	113.14	103.25
1	C	801	ASN	CA-CB-CG	9.40	122.00	112.60
1	G	1038	ASP	CA-CB-CG	9.38	121.98	112.60
2	g	2543	GLU	CA-C-N	9.36	130.60	121.62
2	g	2543	GLU	C-N-CA	9.36	130.60	121.62
2	d	3351	ASP	CA-CB-CG	9.33	121.93	112.60
2	e	3960	GLN	OE1-CD-NE2	-9.33	113.27	122.60
2	f	3437	ASN	CA-CB-CG	9.31	121.91	112.60
1	B	2143	ASP	CA-CB-CG	9.30	121.90	112.60
2	f	3405	ASP	CA-CB-CG	9.29	121.89	112.60
2	f	3852	ASP	CA-CB-CG	9.29	121.89	112.60
2	d	2846	GLN	OE1-CD-NE2	-9.29	113.31	122.60
1	B	1712	ASP	CA-CB-CG	9.28	121.88	112.60
1	D	1333	ASP	CA-CB-CG	9.26	121.86	112.60
2	f	3815	ASP	CA-CB-CG	9.24	121.84	112.60
2	g	2416	GLN	OE1-CD-NE2	-9.24	113.36	122.60
1	A	139	GLU	O-C-N	-9.23	113.28	121.31
2	a	2486	ARG	NE-CZ-NH1	-9.23	112.27	121.50
2	d	2848	ASP	CA-CB-CG	9.22	121.82	112.60
2	g	2320	ASP	CA-CB-CG	9.21	121.81	112.60
2	d	2950	GLN	OE1-CD-NE2	-9.21	113.39	122.60
2	a	2590	ASN	OD1-CG-ND2	-9.20	113.40	122.60
2	a	2439	GLN	OE1-CD-NE2	-9.17	113.43	122.60
2	b	3480	ASN	CA-C-N	9.14	135.35	120.63
2	b	3480	ASN	C-N-CA	9.14	135.35	120.63
1	F	1485	ASP	CA-CB-CG	9.11	121.71	112.60
1	G	952	ASP	CA-CB-CG	9.10	121.70	112.60
2	a	2794	ASP	CA-CB-CG	9.08	121.68	112.60
1	A	219	ASN	OD1-CG-ND2	-9.07	113.53	122.60
1	G	873	ASN	OD1-CG-ND2	-9.06	113.54	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2061	ASN	OD1-CG-ND2	-9.04	113.56	122.60
2	e	4192	ASN	CA-CB-CG	9.04	121.64	112.60
2	a	2417	VAL	CA-C-O	-9.03	115.24	119.94
1	C	839	HIS	ND1-CE1-NE2	9.03	117.43	108.40
1	F	1621	PRO	N-CA-CB	9.02	111.30	103.36
2	b	3881	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	D	1347	ASP	CA-CB-CG	9.00	121.60	112.60
2	d	3056	ASP	CA-CB-CG	8.98	121.58	112.60
1	D	1593	ALA	CA-C-O	-8.97	111.11	121.16
2	a	2770	PRO	CB-CA-C	8.97	119.83	111.39
2	e	4406	PRO	CA-C-O	-8.96	113.65	120.73
1	C	1026	ASP	CA-CB-CG	8.96	121.56	112.60
2	e	4077	HIS	CA-C-N	8.95	135.95	121.99
2	e	4077	HIS	C-N-CA	8.95	135.95	121.99
2	g	2736	PRO	N-CA-CB	8.95	112.45	102.60
2	e	4339	THR	CA-C-O	-8.94	111.07	120.55
1	G	598	ARG	N-CA-C	8.93	124.01	113.20
2	a	2473	ASN	OD1-CG-ND2	-8.93	113.67	122.60
1	C	571	ALA	CA-C-N	8.91	128.76	120.21
1	C	571	ALA	C-N-CA	8.91	128.76	120.21
1	F	1455	PRO	N-CA-CB	8.91	111.62	103.34
2	a	2410	LYS	CA-C-N	8.90	135.91	122.65
2	a	2410	LYS	C-N-CA	8.90	135.91	122.65
2	c	4313	ASP	O-C-N	-8.89	115.16	121.65
1	D	1247	PHE	CA-CB-CG	8.87	122.67	113.80
1	A	359	GLN	OE1-CD-NE2	-8.84	113.76	122.60
1	E	2030	ASN	CA-CB-CG	-8.83	103.77	112.60
2	g	2328	ARG	CA-C-N	8.83	129.53	119.99
2	g	2328	ARG	C-N-CA	8.83	129.53	119.99
1	E	2068	ASP	CA-CB-CG	8.83	121.43	112.60
2	e	4079	ARG	NE-CZ-NH2	8.82	127.14	119.20
1	B	2224	ASN	OD1-CG-ND2	-8.82	113.78	122.60
1	F	1315	HIS	CB-CG-CD2	-8.80	119.76	131.20
2	b	3883	ASP	CB-CA-C	8.79	117.44	111.20
2	c	4127	ASP	CA-CB-CG	8.79	121.39	112.60
1	B	2178	PHE	CA-CB-CG	8.78	122.58	113.80
2	a	2742	GLU	O-C-N	8.77	131.22	122.09
1	B	1811	ASP	CA-CB-CG	8.77	121.37	112.60
2	e	4406	PRO	O-C-N	8.77	125.27	121.15
1	D	1237	ASP	CA-CB-CG	8.76	121.36	112.60
2	g	2538	ASP	CA-CB-CG	8.76	121.36	112.60
1	C	1091	ASP	CA-C-N	8.76	132.89	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1091	ASP	C-N-CA	8.76	132.89	120.28
2	d	2869	ARG	NE-CZ-NH2	8.76	127.08	119.20
2	e	4475	ASN	OD1-CG-ND2	-8.76	113.84	122.60
2	c	4357	ARG	CD-NE-CZ	8.75	136.65	124.40
2	d	2826	ILE	CA-C-N	8.73	128.67	119.85
2	d	2826	ILE	C-N-CA	8.73	128.67	119.85
2	c	4179	GLU	CB-CG-CD	-8.73	97.76	112.60
1	C	948	LEU	CA-C-N	8.71	134.73	122.36
1	C	948	LEU	C-N-CA	8.71	134.73	122.36
2	e	3991	ASP	CA-CB-CG	8.71	121.31	112.60
1	B	2140	ASP	CA-CB-CG	8.69	121.29	112.60
1	A	110	PHE	CA-CB-CG	8.68	122.48	113.80
2	e	4354	GLN	OE1-CD-NE2	-8.68	113.92	122.60
1	A	118	SER	CA-C-N	8.66	135.20	121.95
1	A	118	SER	C-N-CA	8.66	135.20	121.95
1	B	2107	ARG	NE-CZ-NH2	8.66	126.99	119.20
2	f	3505	VAL	CA-C-N	8.66	132.84	121.23
2	f	3505	VAL	C-N-CA	8.66	132.84	121.23
2	f	3637	THR	CA-C-O	-8.63	112.01	121.33
2	b	3803	THR	CA-C-N	8.63	133.51	121.26
2	b	3803	THR	C-N-CA	8.63	133.51	121.26
2	d	2860	ARG	NH1-CZ-NH2	-8.63	108.08	119.30
2	d	2963	HIS	CA-C-N	8.62	135.28	122.08
2	d	2963	HIS	C-N-CA	8.62	135.28	122.08
2	c	3947	ASN	CA-CB-CG	8.62	121.22	112.60
1	G	811	LYS	CB-CA-C	8.62	123.93	109.80
1	A	93	PRO	N-CA-CB	8.61	110.97	103.31
2	a	2770	PRO	O-C-N	-8.60	117.35	121.31
2	c	4002	ASP	CA-CB-CG	8.59	121.19	112.60
1	A	503	THR	OG1-CB-CG2	-8.58	92.13	109.30
1	A	459	HIS	ND1-CE1-NE2	8.55	116.95	108.40
2	a	2330	VAL	CA-CB-CG1	8.54	124.93	110.40
2	e	3951	PRO	N-CA-CB	8.54	111.99	102.60
2	g	2408	ARG	NE-CZ-NH2	8.54	126.88	119.20
1	F	1373	VAL	N-CA-C	8.53	119.29	112.12
1	D	1508	HIS	CB-CG-CD2	-8.53	120.11	131.20
2	c	4353	ASP	CA-CB-CG	8.51	121.11	112.60
2	a	2594	GLN	OE1-CD-NE2	-8.50	114.10	122.60
1	D	1192	GLY	CA-C-N	8.49	132.93	120.87
1	D	1192	GLY	C-N-CA	8.49	132.93	120.87
1	E	2011	LYS	CA-C-O	-8.49	108.37	120.51
2	a	2346	THR	CA-C-N	8.47	128.12	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	2346	THR	C-N-CA	8.47	128.12	119.56
2	e	4419	VAL	CB-CA-C	8.46	122.39	111.81
1	C	741	SER	CA-C-N	8.46	134.01	123.10
1	C	741	SER	C-N-CA	8.46	134.01	123.10
1	A	325	PRO	CA-C-N	8.44	134.71	123.06
1	A	325	PRO	C-N-CA	8.44	134.71	123.06
1	A	312	HIS	CB-CG-CD2	-8.44	120.23	131.20
2	g	2458	ASP	CA-CB-CG	8.43	121.03	112.60
1	A	47	GLU	CA-C-N	8.43	125.81	119.66
1	A	47	GLU	C-N-CA	8.43	125.81	119.66
1	E	1761	ASN	CA-C-N	8.43	133.64	123.19
1	E	1761	ASN	C-N-CA	8.43	133.64	123.19
1	G	1066	GLN	OE1-CD-NE2	-8.42	114.18	122.60
2	c	4314	PRO	CB-CA-C	8.42	121.13	110.27
1	E	1746	PRO	N-CA-C	8.42	119.59	110.58
2	d	3246	THR	CA-C-O	8.42	129.79	120.70
2	d	3110	ASN	OD1-CG-ND2	-8.42	114.18	122.60
2	f	3611	THR	CA-C-N	8.41	134.63	122.69
2	f	3611	THR	C-N-CA	8.41	134.63	122.69
1	G	804	ASN	OD1-CG-ND2	-8.40	114.20	122.60
2	b	3635	ASN	CA-CB-CG	8.39	120.99	112.60
1	E	2014	ARG	CA-C-N	8.39	137.56	121.54
1	E	2014	ARG	C-N-CA	8.39	137.56	121.54
2	b	3405	ASP	CA-CB-CG	8.39	120.99	112.60
1	B	1917	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	B	1934	GLN	OE1-CD-NE2	-8.38	114.22	122.60
1	G	852	THR	CA-CB-OG1	-8.37	97.05	109.60
2	c	4051	THR	CA-C-N	8.37	134.57	122.69
2	c	4051	THR	C-N-CA	8.37	134.57	122.69
2	g	2675	ASN	CA-CB-CG	8.36	120.96	112.60
1	E	1835	ALA	N-CA-C	8.35	123.03	113.01
1	D	1657	ASP	CA-CB-CG	8.34	120.94	112.60
1	D	1276	ASN	CA-CB-CG	8.33	120.93	112.60
2	b	3628	ASN	CA-CB-CG	-8.33	104.27	112.60
2	e	4019	ASP	CA-CB-CG	8.32	120.92	112.60
1	A	321	PRO	N-CA-CB	8.32	111.09	103.19
1	B	2030	ASN	CA-CB-CG	8.31	120.91	112.60
1	B	2252	HIS	CA-CB-CG	8.31	122.11	113.80
2	g	2419	PRO	N-CA-CB	8.31	111.22	103.41
1	E	1863	ASN	OD1-CG-ND2	-8.30	114.30	122.60
1	F	1571	ASN	CA-CB-CG	8.30	120.90	112.60
1	D	1375	ARG	CD-NE-CZ	8.29	136.00	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	727	VAL	N-CA-C	8.28	121.13	113.10
1	F	1606	HIS	CB-CG-CD2	-8.28	120.44	131.20
2	a	2661	SER	N-CA-C	8.27	122.16	110.50
2	c	4440	ASP	CA-CB-CG	8.27	120.87	112.60
2	g	2334	GLN	OE1-CD-NE2	-8.27	114.33	122.60
1	B	2076	ARG	NE-CZ-NH1	8.27	129.77	121.50
2	a	2295	ASN	CA-CB-CG	8.27	120.87	112.60
2	a	2634	GLY	CA-C-N	8.26	133.36	121.80
2	a	2634	GLY	C-N-CA	8.26	133.36	121.80
2	b	3600	ARG	NE-CZ-NH1	8.26	129.76	121.50
1	F	1470	HIS	ND1-CG-CD2	8.26	114.36	106.10
2	g	2769	ASP	CA-CB-CG	8.26	120.86	112.60
2	a	2675	ASN	CA-CB-CG	8.25	120.85	112.60
1	A	140	PRO	N-CA-CB	8.25	111.91	103.25
1	E	1824	HIS	CA-CB-CG	8.24	122.04	113.80
1	E	2187	PRO	N-CA-CB	8.24	111.00	103.34
1	E	2172	HIS	CA-CB-CG	8.23	122.03	113.80
1	A	141	ASN	CB-CA-C	8.23	124.58	111.66
1	C	629	ASN	CA-CB-CG	8.23	120.83	112.60
2	b	3403	GLN	OE1-CD-NE2	-8.22	114.38	122.60
2	e	4248	SER	O-C-N	-8.21	112.88	120.51
1	G	771	LYS	O-C-N	-8.19	113.51	122.85
2	e	3983	ARG	NH1-CZ-NH2	-8.18	108.66	119.30
2	g	2496	ASN	OD1-CG-ND2	-8.18	114.42	122.60
2	g	2745	THR	O-C-N	-8.18	113.18	122.75
1	D	1543	VAL	CA-C-N	8.18	134.26	121.26
1	D	1543	VAL	C-N-CA	8.18	134.26	121.26
1	G	920	ARG	NE-CZ-NH1	-8.18	113.33	121.50
1	E	1818	GLU	CA-CB-CG	-8.16	97.77	114.10
1	C	704	ASP	CA-C-N	8.16	131.74	120.65
1	C	704	ASP	C-N-CA	8.16	131.74	120.65
2	e	4395	VAL	CA-CB-CG1	8.15	124.26	110.40
1	C	779	ILE	CA-C-N	8.15	132.44	120.87
1	C	779	ILE	C-N-CA	8.15	132.44	120.87
2	d	3238	SER	CA-C-O	8.15	130.51	121.06
1	A	535	GLN	OE1-CD-NE2	-8.14	114.46	122.60
1	G	934	ASP	CA-CB-CG	8.14	120.74	112.60
1	E	2014	ARG	NE-CZ-NH1	8.14	129.64	121.50
1	G	749	HIS	CB-CG-CD2	-8.13	120.63	131.20
2	c	3979	ASP	CA-CB-CG	8.13	120.73	112.60
1	C	683	GLY	O-C-N	-8.13	116.01	123.57
2	d	2852	ASN	CA-CB-CG	8.13	120.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	2750	ARG	NE-CZ-NH2	8.12	126.51	119.20
1	D	1405	HIS	ND1-CE1-NE2	8.11	116.51	108.40
1	D	1608	ASN	O-C-N	-8.12	111.80	122.59
2	g	2686	ARG	NE-CZ-NH1	-8.11	113.39	121.50
1	B	2193	TRP	CE2-CD2-CE3	-8.11	110.69	118.80
2	g	2328	ARG	CD-NE-CZ	8.11	135.75	124.40
2	a	2618	THR	CA-C-O	-8.10	111.95	120.70
1	G	726	PRO	CB-CA-C	8.10	118.67	111.87
2	a	2552	LEU	O-C-N	-8.08	113.83	122.96
2	b	3541	HIS	CB-CG-CD2	-8.08	120.70	131.20
2	b	3677	GLN	OE1-CD-NE2	-8.07	114.53	122.60
1	E	2058	ILE	N-CA-CB	8.07	119.78	110.82
2	a	2727	ASP	CA-C-O	-8.07	112.12	119.86
1	E	1761	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	D	1648	ARG	NE-CZ-NH2	8.05	126.44	119.20
2	c	4272	ASN	CA-CB-CG	8.05	120.65	112.60
2	c	4455	ARG	CA-C-O	-8.04	111.01	120.10
1	D	1588	THR	CA-CB-CG2	8.03	124.15	110.50
2	e	4164	VAL	N-CA-C	8.03	118.33	108.53
2	f	3812	ASP	CA-CB-CG	8.03	120.63	112.60
1	E	1836	ASP	CA-CB-CG	8.02	120.62	112.60
2	d	3327	PRO	N-CA-CB	8.02	110.86	103.08
1	A	76	PHE	CA-CB-CG	8.01	121.81	113.80
2	g	2272	SER	N-CA-C	8.01	120.89	108.96
1	G	822	ASN	OD1-CG-ND2	-8.00	114.60	122.60
2	e	4010	GLU	CA-CB-CG	8.00	130.11	114.10
2	e	4069	ASP	CA-CB-CG	8.00	120.60	112.60
2	g	2702	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	F	1333	ASP	CA-CB-CG	7.99	120.58	112.60
2	b	3873	ASP	CA-CB-CG	7.98	120.58	112.60
1	D	1478	ILE	O-C-N	-7.98	114.56	123.10
1	E	1701	ILE	CA-CB-CG2	7.98	124.06	110.50
2	c	4470	ASP	CA-CB-CG	7.98	120.58	112.60
1	D	1344	ARG	CA-C-N	7.97	132.66	122.37
1	D	1344	ARG	C-N-CA	7.97	132.66	122.37
1	F	1597	ASN	CB-CA-C	7.97	122.88	109.48
1	E	2012	SER	N-CA-C	-7.97	102.53	111.14
2	g	2456	ASP	CA-CB-CG	7.97	120.57	112.60
2	e	4439	ASN	CB-CA-C	7.96	124.09	111.51
2	f	3606	SER	CA-C-O	-7.96	111.50	120.66
1	C	679	ASP	CA-C-N	7.96	134.09	123.11
1	C	679	ASP	C-N-CA	7.96	134.09	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	3740	ASP	N-CA-C	7.95	119.66	109.72
1	B	1958	ASN	OD1-CG-ND2	-7.95	114.65	122.60
2	d	2905	ASP	CA-CB-CG	7.93	120.53	112.60
2	c	4198	GLY	CA-C-N	7.92	134.97	123.17
2	c	4198	GLY	C-N-CA	7.92	134.97	123.17
1	D	1497	GLN	N-CA-C	7.91	120.79	110.43
2	b	3469	PRO	N-CA-CB	7.91	110.69	103.33
2	g	2729	ASP	CA-CB-CG	7.91	120.51	112.60
2	c	4276	GLN	OE1-CD-NE2	-7.90	114.70	122.60
1	D	1189	LYS	CA-C-N	7.90	131.51	120.29
1	D	1189	LYS	C-N-CA	7.90	131.51	120.29
1	C	690	ALA	N-CA-C	7.90	120.77	110.43
2	e	4472	ILE	N-CA-C	-7.89	105.03	111.81
2	b	3569	GLN	OE1-CD-NE2	-7.88	114.72	122.60
2	c	4126	GLN	OE1-CD-NE2	-7.88	114.72	122.60
2	g	2432	VAL	CB-CA-C	7.88	120.30	111.08
1	F	1218	ARG	NE-CZ-NH1	7.86	129.35	121.50
2	g	2716	PRO	N-CA-CB	7.85	112.09	103.30
2	g	2508	GLU	CA-C-O	-7.85	111.91	120.30
1	C	839	HIS	CB-CG-CD2	-7.83	121.02	131.20
2	d	3255	ASP	CA-C-N	7.82	135.12	122.69
2	d	3255	ASP	C-N-CA	7.82	135.12	122.69
2	c	4094	LEU	O-C-N	-7.82	114.14	122.19
1	A	3	ILE	O-C-N	-7.81	114.77	122.97
2	b	3693	ARG	CB-CA-C	7.81	119.23	109.16
1	C	771	LYS	CA-C-N	7.80	134.84	122.21
1	C	771	LYS	C-N-CA	7.80	134.84	122.21
2	c	4005	GLN	OE1-CD-NE2	-7.80	114.80	122.60
2	c	4092	PRO	N-CA-CB	7.79	111.17	102.60
2	b	3897	ASP	CA-C-N	7.79	131.75	120.38
2	b	3897	ASP	C-N-CA	7.79	131.75	120.38
2	c	4420	GLN	OE1-CD-NE2	-7.78	114.82	122.60
2	a	2680	ALA	CA-C-N	7.77	133.94	122.99
2	a	2680	ALA	C-N-CA	7.77	133.94	122.99
2	f	3734	ASN	CA-CB-CG	7.76	120.36	112.60
2	f	3446	ARG	CD-NE-CZ	7.76	135.27	124.40
1	G	858	ASP	CA-CB-CG	7.76	120.36	112.60
2	e	4253	MET	CA-C-O	-7.76	112.19	120.80
1	F	1415	GLY	CA-C-O	-7.76	114.35	121.18
2	d	3362	ASP	CA-CB-CG	7.76	120.36	112.60
2	g	2804	ASN	OD1-CG-ND2	-7.76	114.84	122.60
1	B	1984	THR	CA-CB-CG2	7.75	123.67	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	953	ASN	OD1-CG-ND2	-7.74	114.86	122.60
2	c	4335	ARG	CD-NE-CZ	7.74	135.24	124.40
1	D	1502	ASP	CA-CB-CG	7.74	120.34	112.60
2	e	4335	ARG	CD-NE-CZ	7.72	135.21	124.40
1	E	2009	PHE	O-C-N	-7.72	114.42	123.22
2	b	3380	TRP	CA-C-N	7.72	131.12	120.39
2	b	3380	TRP	C-N-CA	7.72	131.12	120.39
1	F	1448	ARG	NE-CZ-NH2	7.71	126.14	119.20
2	c	3991	ASP	CA-CB-CG	7.71	120.31	112.60
1	D	1263	LYS	CA-C-N	7.71	134.35	122.25
1	D	1263	LYS	C-N-CA	7.71	134.35	122.25
2	g	2704	PRO	N-CA-CB	7.70	110.05	103.35
1	C	585	ASN	CA-C-O	-7.70	112.38	120.23
2	d	2972	GLY	CA-C-N	7.68	134.88	122.81
2	d	2972	GLY	C-N-CA	7.68	134.88	122.81
2	f	3631	ASN	OD1-CG-ND2	-7.68	114.92	122.60
2	a	2397	THR	CA-CB-CG2	7.68	123.56	110.50
1	B	1977	GLN	OE1-CD-NE2	-7.68	114.92	122.60
1	G	782	VAL	O-C-N	7.67	131.08	123.03
1	D	1164	ARG	NE-CZ-NH2	-7.67	112.30	119.20
1	B	1734	ILE	O-C-N	-7.66	114.91	123.18
2	a	2532	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	E	1996	ASN	OD1-CG-ND2	-7.65	114.95	122.60
2	c	4312	THR	CA-CB-OG1	7.65	121.08	109.60
1	B	2146	PRO	N-CD-CG	7.65	114.67	103.20
1	B	2031	VAL	CA-CB-CG2	7.65	123.40	110.40
2	e	4378	PRO	N-CA-CB	7.65	112.01	103.44
1	C	882	ARG	NE-CZ-NH2	7.65	126.08	119.20
2	b	3884	PRO	O-C-N	-7.64	117.56	121.15
2	f	3919	ASP	CA-C-O	-7.64	112.53	121.16
1	B	1804	ASN	CA-CB-CG	7.64	120.24	112.60
2	e	4151	HIS	CB-CG-CD2	-7.64	121.27	131.20
1	C	919	ASP	CA-CB-CG	7.63	120.23	112.60
2	e	4185	ASN	OD1-CG-ND2	-7.63	114.97	122.60
2	f	3632	TRP	CE2-CD2-CE3	-7.63	111.17	118.80
2	f	3524	LYS	O-C-N	-7.62	113.94	123.17
1	G	978	GLN	OE1-CD-NE2	-7.62	114.98	122.60
1	E	1988	GLU	CA-C-N	7.62	131.09	122.48
1	E	1988	GLU	C-N-CA	7.62	131.09	122.48
2	a	2593	ASP	CA-CB-CG	7.61	120.21	112.60
2	c	4331	ARG	CD-NE-CZ	7.59	135.03	124.40
2	e	4479	HIS	CB-CG-CD2	-7.59	121.34	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1786	ASN	CA-C-N	7.58	131.57	120.95
1	E	1786	ASN	C-N-CA	7.58	131.57	120.95
1	G	733	ASP	CA-CB-CG	7.58	120.18	112.60
2	d	3359	THR	CA-C-N	7.58	136.02	121.54
2	d	3359	THR	C-N-CA	7.58	136.02	121.54
1	E	2014	ARG	CA-C-O	-7.58	109.68	120.51
2	b	3778	ARG	NH1-CZ-NH2	-7.58	109.45	119.30
1	B	1865	ASP	CA-CB-CG	7.57	120.17	112.60
1	E	1896	GLU	CA-C-N	7.57	132.53	121.18
1	E	1896	GLU	C-N-CA	7.57	132.53	121.18
2	d	3170	ALA	N-CA-CB	-7.57	97.70	110.49
2	d	3287	GLU	CA-C-N	7.56	127.59	119.28
2	d	3287	GLU	C-N-CA	7.56	127.59	119.28
1	D	1201	ASP	CA-CB-CG	7.55	120.15	112.60
2	d	3136	ARG	NH1-CZ-NH2	-7.55	109.48	119.30
1	G	678	GLN	O-C-N	-7.55	114.51	123.27
1	C	969	LEU	CA-C-N	7.54	129.27	119.84
1	C	969	LEU	C-N-CA	7.54	129.27	119.84
2	b	3600	ARG	NE-CZ-NH2	-7.54	112.41	119.20
1	A	527	GLN	OE1-CD-NE2	-7.54	115.06	122.60
1	G	679	ASP	CA-CB-CG	7.54	120.14	112.60
2	a	2540	LYS	CA-C-N	7.54	134.06	122.23
2	a	2540	LYS	C-N-CA	7.54	134.06	122.23
2	a	2777	VAL	CA-C-N	7.54	129.50	120.23
2	a	2777	VAL	C-N-CA	7.54	129.50	120.23
2	f	3883	ASP	CA-C-N	7.54	125.16	119.66
2	f	3883	ASP	C-N-CA	7.54	125.16	119.66
1	E	2013	ILE	O-C-N	7.53	135.05	123.00
2	b	3532	PRO	CA-C-N	7.53	127.91	119.32
2	b	3532	PRO	C-N-CA	7.53	127.91	119.32
2	b	3467	GLU	CA-C-O	-7.53	112.30	121.11
2	d	3107	LYS	CA-C-N	7.53	127.97	119.92
2	d	3107	LYS	C-N-CA	7.53	127.97	119.92
1	C	827	PHE	CA-CB-CG	7.52	121.32	113.80
2	b	3789	ASN	OD1-CG-ND2	-7.52	115.08	122.60
2	e	4157	ARG	NE-CZ-NH1	7.51	129.01	121.50
2	g	2343	PHE	CA-C-O	7.51	129.40	120.99
1	D	1195	ASN	OD1-CG-ND2	-7.51	115.09	122.60
2	c	4039	ASN	CA-CB-CG	7.51	120.11	112.60
2	d	3320	ARG	CD-NE-CZ	7.51	134.91	124.40
1	D	1236	ASN	OD1-CG-ND2	-7.50	115.10	122.60
2	a	2774	SER	CA-C-O	-7.50	112.03	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	4018	PRO	N-CA-CB	7.50	111.49	103.39
1	F	1369	VAL	CA-CB-CG1	7.50	123.15	110.40
2	e	4171	VAL	CA-CB-CG2	7.50	123.14	110.40
1	F	1659	GLN	CG-CD-NE2	7.49	127.64	116.40
1	C	725	PRO	N-CD-CG	7.49	112.79	103.80
2	a	2700	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	C	1025	HIS	ND1-CG-CD2	7.48	113.58	106.10
2	c	3999	ARG	CA-C-O	-7.48	113.70	120.13
1	A	279	GLN	OE1-CD-NE2	-7.47	115.12	122.60
1	D	1340	GLN	OE1-CD-NE2	-7.47	115.12	122.60
2	g	2586	THR	CA-C-N	7.47	132.93	123.14
2	g	2586	THR	C-N-CA	7.47	132.93	123.14
1	G	944	ARG	NE-CZ-NH2	7.47	125.92	119.20
2	c	4126	GLN	CG-CD-NE2	7.47	127.60	116.40
2	c	3987	TYR	N-CA-CB	-7.46	99.77	111.56
1	A	48	PRO	N-CA-CB	7.46	107.37	103.19
1	E	1770	GLU	CA-C-N	7.45	128.84	122.28
1	E	1770	GLU	C-N-CA	7.45	128.84	122.28
2	d	3013	ASP	CA-CB-CG	7.45	120.05	112.60
1	B	1966	GLU	CA-C-N	7.44	128.18	120.00
1	B	1966	GLU	C-N-CA	7.44	128.18	120.00
2	c	4430	ASP	CA-CB-CG	7.44	120.04	112.60
2	g	2390	THR	CA-C-N	7.43	130.97	120.42
2	g	2390	THR	C-N-CA	7.43	130.97	120.42
1	A	194	ASP	O-C-N	7.43	132.16	123.17
2	b	3624	LYS	N-CA-C	7.42	121.98	113.15
2	f	3797	GLN	OE1-CD-NE2	-7.42	115.18	122.60
2	d	2851	GLN	OE1-CD-NE2	-7.42	115.19	122.60
2	g	2598	PRO	CA-C-N	7.42	133.22	122.77
2	g	2598	PRO	C-N-CA	7.42	133.22	122.77
1	D	1380	ASP	CA-CB-CG	7.41	120.01	112.60
2	b	3512	ASP	CA-CB-CG	7.41	120.01	112.60
2	b	3611	THR	CA-CB-OG1	7.41	120.72	109.60
2	c	4395	VAL	CA-C-O	-7.41	114.61	121.72
1	B	2198	GLN	OE1-CD-NE2	-7.41	115.19	122.60
1	C	971	ASP	CA-CB-CG	7.41	120.00	112.60
1	F	1276	ASN	N-CA-C	7.41	121.89	113.01
2	g	2605	GLN	OE1-CD-NE2	-7.40	115.20	122.60
1	G	582	SER	N-CA-CB	7.40	120.97	109.94
1	G	1092	ASN	CA-CB-CG	-7.40	105.20	112.60
2	f	3688	ARG	CD-NE-CZ	7.40	134.75	124.40
1	B	1816	SER	N-CA-C	7.39	120.46	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	4470	ASP	O-C-N	-7.39	114.69	123.27
2	f	3444	VAL	CA-C-N	7.39	132.28	122.30
2	f	3444	VAL	C-N-CA	7.39	132.28	122.30
1	G	772	GLN	OE1-CD-NE2	-7.38	115.22	122.60
2	c	4404	HIS	CB-CG-CD2	-7.38	121.61	131.20
1	B	1946	ASP	CA-CB-CG	7.38	119.98	112.60
2	b	3875	ALA	N-CA-C	7.38	120.38	109.24
1	A	378	ARG	CA-C-O	-7.37	112.83	121.16
1	D	1204	GLU	CA-C-N	7.37	133.40	123.46
1	D	1204	GLU	C-N-CA	7.37	133.40	123.46
2	f	3763	ILE	CA-CB-CG2	7.37	123.02	110.50
2	g	2480	HIS	CB-CG-CD2	-7.36	121.63	131.20
1	A	20	PRO	N-CA-CB	7.36	110.70	102.60
2	c	4364	GLY	O-C-N	-7.36	117.90	123.35
2	c	4342	ASN	OD1-CG-ND2	-7.36	115.24	122.60
2	f	3672	GLN	N-CA-C	7.36	122.35	113.23
2	a	2441	ASP	O-C-N	-7.35	114.44	123.33
2	f	3612	VAL	CA-C-N	7.34	132.55	122.19
2	f	3612	VAL	C-N-CA	7.34	132.55	122.19
2	f	3381	ALA	CA-C-N	7.34	127.27	119.85
2	f	3381	ALA	C-N-CA	7.34	127.27	119.85
2	f	3514	ASP	CA-C-N	7.34	130.59	120.39
2	f	3514	ASP	C-N-CA	7.34	130.59	120.39
2	f	3621	VAL	CA-C-N	7.34	133.13	123.00
2	f	3621	VAL	C-N-CA	7.34	133.13	123.00
2	e	4180	ASP	O-C-N	-7.34	114.76	123.27
2	e	4237	VAL	N-CA-C	7.33	118.03	108.35
2	e	4150	ASP	CA-CB-CG	7.33	119.93	112.60
2	f	3482	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	E	1935	VAL	N-CA-CB	-7.32	102.27	112.52
2	a	2293	ALA	N-CA-C	-7.32	103.30	111.28
1	G	826	ASN	OD1-CG-ND2	-7.32	115.28	122.60
2	c	4120	GLN	O-C-N	-7.32	114.65	123.29
1	G	816	ASP	CA-CB-CG	7.31	119.91	112.60
1	F	1263	LYS	CA-C-O	7.31	129.42	121.16
1	C	944	ARG	NE-CZ-NH1	7.30	128.80	121.50
1	F	1534	LYS	O-C-N	-7.30	114.93	123.25
1	C	692	HIS	ND1-CG-CD2	7.30	113.40	106.10
1	C	791	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	G	1086	GLN	OE1-CD-NE2	-7.30	115.30	122.60
1	A	470	ASP	CA-C-O	-7.29	112.82	120.70
2	e	4190	ARG	N-CA-C	7.29	121.07	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	4454	ASP	CA-CB-CG	7.29	119.89	112.60
2	b	3760	TRP	CG-CD2-CE3	7.28	141.18	133.90
2	b	3812	ASP	CA-CB-CG	7.28	119.88	112.60
1	D	1159	ASP	CA-C-N	7.27	131.00	120.38
1	D	1159	ASP	C-N-CA	7.27	131.00	120.38
1	D	1543	VAL	CA-CB-CG2	7.27	122.76	110.40
2	a	2268	PRO	CA-C-N	7.27	129.66	123.33
2	a	2268	PRO	C-N-CA	7.27	129.66	123.33
1	C	676	PHE	CA-CB-CG	7.27	121.07	113.80
2	c	4087	GLN	OE1-CD-NE2	-7.27	115.33	122.60
1	B	1800	ASP	CA-CB-CG	7.27	119.87	112.60
1	B	1824	HIS	CB-CG-CD2	-7.26	121.76	131.20
1	D	1634	SER	N-CA-C	7.26	120.06	111.71
1	F	1239	GLU	CA-C-N	7.26	128.91	119.84
1	F	1239	GLU	C-N-CA	7.26	128.91	119.84
1	A	140	PRO	CA-C-N	7.25	132.74	122.08
1	A	140	PRO	C-N-CA	7.25	132.74	122.08
1	A	387	ASN	CA-CB-CG	7.25	119.85	112.60
1	C	942	HIS	CB-CG-CD2	-7.25	121.78	131.20
1	F	1548	TYR	O-C-N	-7.24	114.03	123.16
1	G	898	ASN	OD1-CG-ND2	-7.24	115.36	122.60
2	e	4098	HIS	CB-CG-CD2	-7.24	121.79	131.20
2	f	3422	ASP	CA-CB-CG	7.24	119.84	112.60
2	e	3983	ARG	NE-CZ-NH2	7.23	125.71	119.20
1	F	1608	ASN	OD1-CG-ND2	-7.23	115.37	122.60
2	d	3099	ASN	OD1-CG-ND2	-7.23	115.37	122.60
2	e	4242	PRO	N-CA-CB	7.23	110.84	103.25
2	f	3481	ASP	N-CA-C	7.23	121.54	112.87
1	C	571	ALA	CB-CA-C	7.22	119.94	109.11
2	d	3123	VAL	CA-C-N	7.21	130.18	122.11
2	d	3123	VAL	C-N-CA	7.21	130.18	122.11
2	e	4322	GLU	N-CA-C	7.21	120.18	111.82
1	B	1774	PHE	CA-C-O	-7.20	113.55	121.33
1	F	1641	GLN	CA-C-O	7.20	129.18	121.55
2	g	2393	GLN	OE1-CD-NE2	-7.20	115.40	122.60
2	d	2867	GLU	CB-CG-CD	-7.20	100.37	112.60
2	d	3278	ALA	N-CA-CB	-7.20	99.03	111.55
2	f	3841	ASP	CA-CB-CG	7.20	119.80	112.60
1	B	2140	ASP	CA-C-N	7.19	134.75	122.67
1	B	2140	ASP	C-N-CA	7.19	134.75	122.67
1	D	1478	ILE	CA-C-N	7.19	133.07	122.86
1	D	1478	ILE	C-N-CA	7.19	133.07	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	LEU	N-CA-C	7.19	116.41	108.14
1	E	1892	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	2010	HIS	N-CA-C	7.19	120.13	110.35
2	e	3947	ASN	CA-CB-CG	7.19	119.79	112.60
1	A	56	ASN	CA-C-O	-7.18	112.07	120.62
2	c	4439	ASN	OD1-CG-ND2	-7.18	115.42	122.60
2	g	2644	THR	CA-CB-OG1	7.18	120.38	109.60
1	C	748	GLU	N-CA-CB	-7.18	99.44	110.42
1	D	1446	SER	CA-C-N	7.18	132.28	121.65
1	D	1446	SER	C-N-CA	7.18	132.28	121.65
2	g	2579	ARG	NE-CZ-NH2	7.17	125.66	119.20
2	c	4168	THR	CA-CB-CG2	7.17	122.69	110.50
1	G	768	LYS	N-CA-C	7.17	116.38	108.14
1	B	2076	ARG	CD-NE-CZ	7.16	134.43	124.40
2	e	3979	ASP	CA-CB-CG	7.16	119.76	112.60
2	a	2384	ASN	OD1-CG-ND2	-7.16	115.44	122.60
2	g	2504	ARG	CD-NE-CZ	7.16	134.42	124.40
2	b	3402	VAL	N-CA-CB	7.16	120.78	112.40
2	e	4022	THR	CA-C-N	7.16	126.65	118.85
2	e	4022	THR	C-N-CA	7.16	126.65	118.85
1	D	1185	PHE	CA-CB-CG	7.15	120.95	113.80
1	B	1754	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	F	1340	GLN	CA-C-N	7.15	132.32	123.10
1	F	1340	GLN	C-N-CA	7.15	132.32	123.10
1	C	591	HIS	CB-CG-CD2	-7.15	121.91	131.20
1	D	1299	ASP	CA-CB-CG	7.14	119.75	112.60
1	E	2025	LYS	O-C-N	-7.14	114.83	123.19
2	f	3402	VAL	CA-C-O	-7.14	112.46	120.74
1	F	1326	ASP	CA-CB-CG	7.14	119.74	112.60
2	e	3997	CYS	CB-CA-C	7.14	123.01	109.37
2	c	4020	GLY	N-CA-C	7.14	124.85	115.36
2	d	3139	MET	CB-CA-C	7.13	121.50	109.80
2	f	3872	ASN	OD1-CG-ND2	-7.13	115.47	122.60
2	g	2338	PHE	CA-CB-CG	7.13	120.93	113.80
1	C	974	SER	N-CA-C	7.13	119.77	110.43
2	g	2653	THR	CA-CB-CG2	7.13	122.62	110.50
1	D	1242	PHE	CA-CB-CG	7.13	120.93	113.80
2	e	4175	ARG	NH1-CZ-NH2	-7.13	110.04	119.30
2	f	3547	ILE	O-C-N	-7.12	115.38	122.93
1	F	1297	ASN	CB-CA-C	7.12	121.49	110.67
2	c	4176	VAL	N-CA-C	7.12	118.73	108.48
1	A	470	ASP	CA-CB-CG	7.11	119.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	2749	GLN	OE1-CD-NE2	-7.11	115.49	122.60
2	g	2372	PHE	CA-C-O	-7.11	113.21	120.96
1	G	822	ASN	CA-CB-CG	7.11	119.71	112.60
1	G	941	ALA	N-CA-C	7.10	120.14	110.55
1	F	1558	ASP	CA-CB-CG	7.10	119.70	112.60
2	g	2364	ASP	N-CA-C	7.09	120.49	109.07
2	a	2406	HIS	CA-C-N	7.09	133.53	122.26
2	a	2406	HIS	C-N-CA	7.09	133.53	122.26
2	b	3517	ASP	CA-CB-CG	7.09	119.69	112.60
1	F	1515	GLU	N-CA-C	7.09	121.26	112.47
1	G	707	ASN	OD1-CG-ND2	-7.09	115.51	122.60
2	a	2291	ASP	CA-CB-CG	7.08	119.68	112.60
1	G	995	ARG	NE-CZ-NH1	7.08	128.58	121.50
2	c	4423	TRP	CG-CD2-CE3	-7.08	126.82	133.90
2	d	3258	ASP	CB-CA-C	7.07	122.81	110.64
2	g	2588	THR	O-C-N	-7.07	114.23	123.21
1	C	833	ASN	OD1-CG-ND2	-7.07	115.53	122.60
2	f	3709	ASP	CA-C-N	7.07	134.68	122.81
2	f	3709	ASP	C-N-CA	7.07	134.68	122.81
1	B	1730	ARG	CD-NE-CZ	7.06	134.29	124.40
1	F	1406	ILE	CB-CA-C	7.06	120.64	110.33
1	F	1671	LEU	O-C-N	-7.06	114.96	123.29
2	e	4227	GLU	CA-C-N	7.06	134.34	121.85
2	e	4227	GLU	C-N-CA	7.06	134.34	121.85
1	E	2079	LYS	CA-C-O	-7.06	112.95	121.28
2	b	3848	GLY	CA-C-O	-7.06	111.43	121.52
2	b	3740	ASP	CA-C-N	7.05	126.75	119.56
2	b	3740	ASP	C-N-CA	7.05	126.75	119.56
2	f	3473	ILE	CB-CA-C	7.05	120.21	111.25
2	e	4077	HIS	CA-CB-CG	7.05	120.85	113.80
1	C	934	ASP	CA-C-N	7.05	130.43	120.28
1	C	934	ASP	C-N-CA	7.05	130.43	120.28
1	A	484	VAL	CA-C-N	7.05	132.37	123.14
1	A	484	VAL	C-N-CA	7.05	132.37	123.14
1	E	2203	VAL	CA-C-N	7.04	132.92	122.99
1	E	2203	VAL	C-N-CA	7.04	132.92	122.99
1	F	1678	HIS	CB-CG-CD2	-7.04	122.05	131.20
2	d	3066	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	126	HIS	CB-CG-CD2	-7.03	122.07	131.20
1	F	1224	LYS	CB-CA-C	7.02	120.25	109.50
2	f	3522	ARG	NE-CZ-NH2	7.02	125.52	119.20
1	B	2157	HIS	CB-CG-CD2	-7.02	122.08	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2157	HIS	CA-CB-CG	7.02	120.82	113.80
2	e	4245	ARG	NE-CZ-NH2	-7.02	112.89	119.20
2	a	2572	PHE	CA-CB-CG	7.01	120.81	113.80
1	F	1516	ASP	CA-CB-CG	7.01	119.61	112.60
1	F	1657	ASP	CA-CB-CG	7.01	119.61	112.60
1	G	854	ILE	N-CA-C	7.01	119.63	112.90
2	d	3095	ASP	CA-CB-CG	7.01	119.61	112.60
1	G	878	HIS	CB-CG-CD2	-7.00	122.10	131.20
2	d	3074	ASN	CA-CB-CG	7.00	119.60	112.60
1	G	820	SER	N-CA-C	7.00	119.56	110.53
2	f	3666	LEU	CA-C-N	7.00	132.58	122.44
2	f	3666	LEU	C-N-CA	7.00	132.58	122.44
1	E	1725	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	141	ASN	N-CA-CB	-6.99	101.53	112.08
2	c	4400	ASP	CA-CB-CG	6.99	119.59	112.60
1	F	1382	ASP	CA-C-N	6.99	130.67	120.82
1	F	1382	ASP	C-N-CA	6.99	130.67	120.82
2	b	3510	ALA	CA-C-O	-6.99	113.51	121.40
2	g	2767	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	F	1392	ASN	CA-CB-CG	-6.98	105.62	112.60
1	B	1847	TYR	N-CA-C	6.97	120.39	110.14
1	G	999	THR	CA-CB-OG1	6.97	120.05	109.60
2	b	3443	PRO	N-CA-CB	6.96	109.91	103.15
1	B	2247	GLY	CA-C-N	6.96	131.26	120.75
1	B	2247	GLY	C-N-CA	6.96	131.26	120.75
2	f	3520	HIS	CB-CG-CD2	-6.96	122.15	131.20
1	E	1818	GLU	O-C-N	-6.96	114.90	123.04
2	f	3864	ARG	NE-CZ-NH1	6.96	128.46	121.50
2	a	2635	ILE	CB-CA-C	6.95	119.22	111.08
1	D	1561	ARG	CD-NE-CZ	6.95	134.12	124.40
2	a	2697	GLN	OE1-CD-NE2	-6.94	115.66	122.60
2	e	4297	ASP	CA-CB-CG	6.94	119.54	112.60
2	g	2538	ASP	CA-C-O	-6.94	112.83	120.81
2	f	3718	ILE	CA-CB-CG1	6.94	122.19	110.40
1	D	1353	PRO	N-CA-CB	6.93	109.77	103.33
1	D	1164	ARG	NE-CZ-NH1	6.92	128.42	121.50
2	b	3594	HIS	CG-CD2-NE2	-6.92	100.28	107.20
1	C	1070	SER	N-CA-C	6.91	119.68	108.76
2	g	2403	ASP	N-CA-C	6.91	121.09	112.24
2	d	3177	ASN	OD1-CG-ND2	-6.91	115.69	122.60
2	a	2768	ASN	CA-CB-CG	6.91	119.51	112.60
1	E	2091	SER	N-CA-C	6.90	119.65	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ASN	OD1-CG-ND2	-6.90	115.70	122.60
2	a	2753	ARG	O-C-N	-6.90	114.86	123.27
1	A	2	TRP	CG-CD2-CE3	6.89	140.79	133.90
1	E	1748	PHE	CA-CB-CG	-6.89	106.91	113.80
1	G	826	ASN	CA-CB-CG	6.89	119.49	112.60
1	B	1802	ASN	CA-CB-CG	6.88	119.48	112.60
2	a	2456	ASP	CA-CB-CG	6.88	119.48	112.60
2	d	2919	ILE	CA-CB-CG1	6.87	122.08	110.40
1	A	392	ASP	CA-CB-CG	6.87	119.47	112.60
1	D	1612	PHE	CA-C-O	-6.87	113.17	121.89
2	a	2451	LYS	CA-C-O	6.87	128.46	120.49
1	A	141	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	C	1085	ILE	O-C-N	-6.87	115.77	123.18
1	B	1708	ARG	NE-CZ-NH1	6.86	128.36	121.50
1	B	2047	SER	O-C-N	-6.86	115.03	122.85
2	b	3630	ALA	N-CA-CB	-6.86	99.01	110.39
2	c	4406	PRO	O-C-N	6.86	124.37	121.15
2	f	3382	PRO	N-CA-CB	6.85	109.70	103.33
1	F	1368	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	C	802	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	G	765	VAL	N-CA-C	6.85	119.94	109.12
1	E	1914	VAL	CB-CA-C	-6.84	98.46	110.71
2	d	2902	THR	CA-CB-CG2	6.84	122.12	110.50
1	C	1074	GLN	N-CA-C	6.83	120.06	109.07
1	G	985	LYS	CA-C-O	-6.83	113.22	120.80
2	f	3768	GLY	CA-C-N	6.83	130.85	120.82
2	f	3768	GLY	C-N-CA	6.83	130.85	120.82
2	f	3875	ALA	N-CA-C	6.83	120.10	109.52
1	A	285	VAL	CA-CB-CG1	6.82	122.00	110.40
1	C	743	THR	CA-CB-CG2	6.82	122.10	110.50
1	B	1940	THR	N-CA-C	6.82	118.56	108.60
2	d	2920	GLU	CA-C-N	6.82	132.81	122.65
2	d	2920	GLU	C-N-CA	6.82	132.81	122.65
2	f	3750	ARG	CD-NE-CZ	6.82	133.95	124.40
2	c	4045	GLU	CA-C-N	6.82	130.67	120.31
2	c	4045	GLU	C-N-CA	6.82	130.67	120.31
1	G	1006	VAL	CA-CB-CG2	6.81	121.98	110.40
2	b	3442	ARG	CA-C-N	6.81	127.36	120.14
2	b	3442	ARG	C-N-CA	6.81	127.36	120.14
1	D	1651	ILE	O-C-N	-6.81	115.83	123.18
1	E	2015	SER	O-C-N	-6.81	113.53	122.59
2	c	4373	ASN	OD1-CG-ND2	-6.81	115.79	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	4186	THR	CA-CB-OG1	6.80	119.79	109.60
2	e	4079	ARG	NH1-CZ-NH2	-6.80	110.47	119.30
2	b	3656	ASN	OD1-CG-ND2	-6.79	115.81	122.60
2	c	4382	VAL	CA-CB-CG2	6.79	121.94	110.40
2	f	3904	VAL	O-C-N	-6.79	116.21	123.14
2	c	3966	ASN	O-C-N	6.79	130.38	122.17
1	E	2086	TRP	CE2-CD2-CE3	-6.79	112.01	118.80
2	c	4418	GLU	CA-C-N	6.79	129.24	122.66
2	c	4418	GLU	C-N-CA	6.79	129.24	122.66
1	E	1771	THR	CA-C-N	6.78	126.38	119.19
1	E	1771	THR	C-N-CA	6.78	126.38	119.19
1	E	1756	ASP	CA-CB-CG	6.78	119.38	112.60
1	C	613	GLU	CA-C-N	6.78	127.36	120.38
1	C	613	GLU	C-N-CA	6.78	127.36	120.38
1	D	1166	LEU	N-CA-C	6.78	120.31	110.28
1	F	1517	ARG	N-CA-C	6.78	119.50	111.71
2	d	3284	ASP	CA-C-O	-6.78	112.78	119.69
2	d	3339	ARG	NE-CZ-NH2	6.77	125.29	119.20
2	b	3913	ASP	CA-CB-CG	6.76	119.36	112.60
2	f	3589	ASP	CA-CB-CG	6.76	119.36	112.60
2	f	3635	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	A	446	ASN	OD1-CG-ND2	-6.76	115.84	122.60
2	c	4071	ASP	CA-CB-CG	6.76	119.36	112.60
1	D	1309	THR	CA-C-O	-6.76	113.59	121.16
1	C	955	ILE	N-CA-C	6.76	116.78	108.53
2	e	4347	ILE	CA-C-N	6.76	132.04	122.72
2	e	4347	ILE	C-N-CA	6.76	132.04	122.72
2	f	3708	GLN	OE1-CD-NE2	-6.76	115.84	122.60
2	g	2435	THR	O-C-N	-6.75	115.33	122.96
2	c	3976	PRO	N-CA-CB	6.75	110.33	103.25
2	f	3844	GLU	CA-C-N	6.75	127.30	119.47
2	f	3844	GLU	C-N-CA	6.75	127.30	119.47
2	b	3732	THR	CA-CB-OG1	6.74	119.72	109.60
1	E	1723	HIS	CB-CG-CD2	-6.74	122.44	131.20
2	e	4151	HIS	CA-CB-CG	-6.74	107.06	113.80
1	F	1401	GLY	O-C-N	-6.74	115.07	122.68
1	D	1234	ASP	CA-CB-CG	6.74	119.34	112.60
2	f	3794	ALA	O-C-N	-6.73	114.39	123.15
2	f	3486	PHE	CA-CB-CG	6.73	120.53	113.80
2	e	4083	SER	CA-CB-OG	6.73	124.56	111.10
1	B	2046	VAL	N-CA-C	6.72	118.86	108.44
1	D	1135	ILE	N-CA-C	6.72	118.25	109.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	3574	GLN	OE1-CD-NE2	-6.72	115.88	122.60
2	c	4459	SER	N-CA-C	6.72	120.36	109.40
1	A	117	GLY	O-C-N	-6.72	116.33	123.45
1	D	1326	ASP	CA-CB-CG	6.72	119.32	112.60
1	C	840	ILE	CA-C-O	6.71	128.09	120.90
2	f	3549	THR	O-C-N	-6.71	115.20	122.85
2	g	2478	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	C	692	HIS	ND1-CE1-NE2	6.71	115.11	108.40
2	a	2465	GLN	OE1-CD-NE2	-6.71	115.89	122.60
2	a	2749	GLN	OE1-CD-NE2	-6.71	115.89	122.60
2	f	3811	GLN	O-C-N	-6.71	115.69	123.27
2	b	3482	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	C	636	ARG	N-CA-CB	-6.70	99.27	110.39
2	c	4230	GLN	OE1-CD-NE2	-6.70	115.90	122.60
2	f	3637	THR	O-C-N	6.70	130.89	123.25
1	E	2076	ARG	NE-CZ-NH2	6.70	125.23	119.20
1	F	1312	ARG	CD-NE-CZ	6.70	133.78	124.40
1	E	1985	LEU	N-CA-CB	-6.69	99.57	110.21
1	D	1521	ILE	O-C-N	-6.69	115.84	123.00
2	c	4224	ASN	CA-C-N	6.69	129.24	120.28
2	c	4224	ASN	C-N-CA	6.69	129.24	120.28
2	d	2870	ASN	CB-CA-C	6.69	123.73	110.42
2	f	3470	LEU	CA-C-N	6.68	126.92	119.90
2	f	3470	LEU	C-N-CA	6.68	126.92	119.90
1	A	38	TYR	CA-C-O	-6.68	113.49	120.70
2	g	2715	LYS	CA-C-N	6.68	127.22	119.47
2	g	2715	LYS	C-N-CA	6.68	127.22	119.47
1	C	991	GLU	CA-C-N	6.68	134.29	121.54
1	C	991	GLU	C-N-CA	6.68	134.29	121.54
1	E	2017	TYR	N-CA-CB	-6.67	101.23	110.38
2	f	3515	GLU	CB-CA-C	6.67	120.06	109.52
1	G	693	THR	N-CA-CB	6.67	120.29	109.95
1	C	612	THR	CA-CB-OG1	6.67	119.60	109.60
2	a	2363	GLU	CA-C-N	6.67	130.34	120.87
2	a	2363	GLU	C-N-CA	6.67	130.34	120.87
2	e	4471	CYS	N-CA-C	6.67	120.49	108.69
2	f	3693	ARG	N-CA-C	6.67	121.01	112.34
1	B	1891	ARG	CD-NE-CZ	6.67	133.73	124.40
2	b	3652	ASP	CA-CB-CG	6.67	119.27	112.60
2	d	3158	ASN	CA-CB-CG	6.67	119.27	112.60
1	G	920	ARG	NH1-CZ-NH2	6.66	127.96	119.30
1	E	2169	LEU	CD1-CG-CD2	-6.66	96.15	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	2791	THR	O-C-N	-6.66	113.73	122.59
2	c	4434	ARG	CD-NE-CZ	6.65	133.71	124.40
2	c	4115	LEU	CB-CA-C	6.65	118.12	109.28
1	C	701	THR	CA-C-O	-6.64	113.34	121.11
2	a	2404	THR	CA-CB-OG1	6.64	119.57	109.60
2	c	4113	ARG	NH1-CZ-NH2	-6.64	110.66	119.30
2	f	3435	THR	CB-CA-C	-6.64	100.44	109.28
2	e	4193	TYR	CA-C-O	-6.63	113.62	121.11
1	D	1325	ARG	NE-CZ-NH2	6.62	125.16	119.20
2	f	3646	ASN	N-CA-C	6.62	121.10	112.89
1	F	1210	LEU	CA-C-N	6.62	132.32	122.99
1	F	1210	LEU	C-N-CA	6.62	132.32	122.99
1	F	1413	ASN	OD1-CG-ND2	-6.62	115.98	122.60
2	d	3094	THR	O-C-N	-6.62	115.79	123.27
2	f	3561	LYS	N-CA-C	6.62	119.48	109.23
1	C	678	GLN	CA-C-N	6.61	129.68	120.29
1	C	678	GLN	C-N-CA	6.61	129.68	120.29
1	E	1994	MET	CA-C-N	6.61	130.88	121.42
1	E	1994	MET	C-N-CA	6.61	130.88	121.42
1	E	1746	PRO	N-CA-CB	6.61	106.66	103.22
2	d	3271	CYS	CA-C-N	6.61	127.93	120.06
2	d	3271	CYS	C-N-CA	6.61	127.93	120.06
2	e	4441	PRO	N-CA-C	6.61	118.76	110.70
1	D	1528	SER	N-CA-C	6.61	120.92	112.86
1	G	1089	ILE	O-C-N	-6.61	116.20	123.20
2	a	2736	PRO	N-CA-CB	6.61	109.87	102.60
1	G	828	THR	CA-CB-CG2	6.60	121.73	110.50
2	a	2479	ASP	CA-CB-CG	6.60	119.20	112.60
1	E	1795	ARG	CD-NE-CZ	6.60	133.64	124.40
1	A	549	GLY	CA-C-N	6.59	130.12	120.82
1	A	549	GLY	C-N-CA	6.59	130.12	120.82
1	E	2012	SER	O-C-N	6.59	129.21	122.09
2	a	2380	THR	CA-CB-CG2	6.59	121.70	110.50
2	e	4009	PHE	O-C-N	-6.59	115.56	123.27
2	g	2412	SER	CA-C-N	6.59	129.33	120.50
2	g	2412	SER	C-N-CA	6.59	129.33	120.50
1	D	1514	LEU	CA-C-N	6.59	134.12	121.54
1	D	1514	LEU	C-N-CA	6.59	134.12	121.54
1	A	138	ASP	CA-CB-CG	6.58	119.18	112.60
1	D	1159	ASP	CA-CB-CG	6.58	119.18	112.60
1	C	1045	PRO	CA-C-N	6.58	130.91	121.50
1	C	1045	PRO	C-N-CA	6.58	130.91	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	582	SER	N-CA-C	6.58	119.29	111.33
1	D	1405	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	B	1963	SER	CA-CB-OG	6.57	124.23	111.10
1	C	942	HIS	CA-CB-CG	6.57	120.37	113.80
2	c	4157	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	E	1950	ILE	CB-CG1-CD1	6.56	127.58	113.80
1	B	1892	ASP	O-C-N	-6.56	115.56	123.10
1	C	953	ASN	N-CA-C	6.56	120.22	111.30
1	E	1965	ASN	CA-C-N	6.56	129.07	120.28
1	E	1965	ASN	C-N-CA	6.56	129.07	120.28
2	a	2682	ASP	CA-CB-CG	6.56	119.16	112.60
2	f	3740	ASP	CA-CB-CG	6.56	119.16	112.60
1	C	867	PHE	CA-CB-CG	6.56	120.36	113.80
1	B	2106	SER	CA-C-O	-6.55	113.99	121.07
1	E	2154	THR	CA-CB-CG2	6.55	121.64	110.50
2	d	3286	ASP	CA-CB-CG	6.55	119.15	112.60
2	g	2288	VAL	CB-CA-C	6.55	119.19	111.59
1	B	1766	LEU	CA-C-O	6.55	129.47	121.94
2	a	2460	GLN	O-C-N	-6.55	115.09	122.75
2	f	3545	GLY	O-C-N	-6.55	115.99	122.41
2	b	3454	ILE	CA-C-N	6.55	131.90	123.13
2	b	3454	ILE	C-N-CA	6.55	131.90	123.13
2	e	4050	PHE	CA-CB-CG	-6.54	107.26	113.80
1	B	2126	PRO	N-CA-CB	6.54	109.80	102.60
2	e	4231	MET	CA-C-O	-6.54	114.23	121.23
1	A	189	THR	CA-C-O	-6.54	113.14	120.66
1	C	928	GLY	N-CA-C	6.54	118.74	110.96
2	c	4331	ARG	NE-CZ-NH1	-6.54	114.96	121.50
2	c	4423	TRP	CB-CG-CD2	6.54	135.96	126.80
2	e	4455	ARG	CD-NE-CZ	-6.54	115.25	124.40
1	G	828	THR	O-C-N	-6.54	115.76	123.41
1	C	619	PHE	N-CA-C	6.53	119.35	109.23
2	a	2514	ASN	OD1-CG-ND2	-6.53	116.07	122.60
2	b	3789	ASN	N-CA-C	6.53	119.88	109.24
2	f	3682	ASN	OD1-CG-ND2	-6.53	116.07	122.60
2	g	2410	LYS	CA-C-N	6.53	132.01	123.00
2	g	2410	LYS	C-N-CA	6.53	132.01	123.00
1	C	712	LYS	N-CA-C	6.53	119.69	109.96
1	D	1288	PRO	N-CA-CB	6.53	109.78	102.60
2	d	2903	THR	CA-C-N	6.53	127.04	119.47
2	d	2903	THR	C-N-CA	6.53	127.04	119.47
2	a	2596	GLU	O-C-N	6.52	130.65	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1704	PRO	O-C-N	-6.52	115.19	123.14
2	f	3922	HIS	CB-CG-CD2	-6.52	122.73	131.20
1	B	1774	PHE	N-CA-C	6.52	118.98	109.07
2	e	4017	THR	CA-C-N	6.51	126.45	119.28
2	e	4017	THR	C-N-CA	6.51	126.45	119.28
1	A	466	VAL	CA-CB-CG2	6.51	121.47	110.40
2	e	4144	ASN	OD1-CG-ND2	-6.51	116.09	122.60
2	d	3318	ALA	N-CA-C	6.51	119.07	109.24
2	e	3988	VAL	O-C-N	-6.51	116.15	123.18
1	D	1337	LYS	CB-CA-C	6.50	122.04	111.05
2	e	4071	ASP	CA-C-N	6.50	129.39	120.67
2	e	4071	ASP	C-N-CA	6.50	129.39	120.67
2	a	2444	LEU	CB-CA-C	6.50	121.11	110.83
2	c	4120	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	G	843	ASP	N-CA-C	6.50	118.88	108.41
2	c	4317	TRP	NE1-CE2-CD2	-6.50	98.95	107.40
1	F	1252	GLU	O-C-N	6.50	130.30	122.96
1	D	1386	SER	CA-C-O	-6.49	114.67	121.55
1	B	2150	GLU	CA-C-N	6.49	126.12	119.56
1	B	2150	GLU	C-N-CA	6.49	126.12	119.56
1	G	1073	LEU	CA-C-N	6.49	132.75	122.62
1	G	1073	LEU	C-N-CA	6.49	132.75	122.62
2	c	4038	ASP	N-CA-C	6.49	122.33	113.37
2	a	2520	ALA	N-CA-C	6.49	119.27	109.41
1	E	1754	ASN	OD1-CG-ND2	-6.49	116.11	122.60
2	e	4157	ARG	CA-C-N	6.49	131.71	120.68
2	e	4157	ARG	C-N-CA	6.49	131.71	120.68
1	B	1967	GLY	CA-C-O	-6.49	113.78	120.66
2	f	3716	PRO	N-CA-CB	6.49	109.73	102.60
1	D	1336	VAL	N-CA-C	6.48	117.64	108.17
2	f	3660	LEU	N-CA-C	6.48	119.69	109.96
2	b	3627	VAL	N-CA-C	6.48	118.12	109.37
2	f	3520	HIS	CA-CB-CG	6.48	120.28	113.80
1	D	1574	ASP	CA-CB-CG	6.48	119.08	112.60
2	b	3624	LYS	N-CA-CB	-6.48	100.48	110.46
2	b	3758	THR	N-CA-CB	6.48	120.61	111.15
2	e	4035	ASP	CA-C-N	6.48	132.72	122.62
2	e	4035	ASP	C-N-CA	6.48	132.72	122.62
2	g	2697	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	D	1602	ASP	CA-CB-CG	6.48	119.08	112.60
1	F	1343	ILE	CB-CA-C	6.48	120.19	111.19
1	B	2020	THR	CA-CB-CG2	6.47	121.51	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1454	THR	CA-C-N	6.47	126.65	120.31
1	D	1454	THR	C-N-CA	6.47	126.65	120.31
2	a	2265	ARG	NH1-CZ-NH2	-6.47	110.89	119.30
2	b	3617	LEU	CD1-CG-CD2	-6.47	96.57	110.80
2	a	2427	HIS	CB-CG-CD2	-6.47	122.79	131.20
2	f	3563	GLN	OE1-CD-NE2	-6.47	116.13	122.60
2	a	2706	ILE	O-C-N	6.46	125.44	121.37
1	E	2010	HIS	ND1-CG-CD2	6.46	112.56	106.10
2	f	3678	ILE	CA-C-N	6.46	127.25	121.82
2	f	3678	ILE	C-N-CA	6.46	127.25	121.82
1	G	1061	TRP	CG-CD2-CE3	6.46	140.36	133.90
2	e	3938	ALA	CA-C-N	6.46	126.41	120.21
2	e	3938	ALA	C-N-CA	6.46	126.41	120.21
1	E	1735	THR	CA-CB-OG1	6.45	119.28	109.60
2	c	3988	VAL	O-C-N	-6.45	115.89	123.05
2	f	3642	ASN	CB-CA-C	6.45	122.44	111.35
2	b	3631	ASN	N-CA-C	6.45	119.12	111.71
2	a	2611	GLU	N-CA-C	6.44	119.12	111.71
2	c	4229	GLN	OE1-CD-NE2	-6.44	116.16	122.60
1	A	61	GLU	CA-C-O	-6.44	114.11	121.19
2	c	4372	ASP	CB-CA-C	6.44	121.26	110.44
1	A	29	ALA	N-CA-C	6.44	119.12	111.33
1	G	585	ASN	CA-CB-CG	6.44	119.04	112.60
2	a	2496	ASN	CA-CB-CG	6.44	119.04	112.60
2	d	3326	ASP	CB-CA-C	6.44	116.60	111.00
2	g	2704	PRO	CA-C-O	6.44	129.03	121.56
2	g	2763	ARG	NE-CZ-NH1	6.44	127.94	121.50
2	d	2837	PRO	N-CD-CG	6.44	111.52	103.80
1	E	2127	ARG	CA-CB-CG	6.43	126.96	114.10
1	G	717	ILE	CA-C-N	6.43	129.11	121.84
1	G	717	ILE	C-N-CA	6.43	129.11	121.84
1	A	444	ASN	CA-C-N	6.43	130.07	120.17
1	A	444	ASN	C-N-CA	6.43	130.07	120.17
2	g	2287	GLN	CA-C-O	6.43	127.24	120.36
1	G	1101	GLN	OE1-CD-NE2	-6.43	116.17	122.60
2	c	4262	VAL	O-C-N	-6.43	115.62	122.95
1	B	1717	ASN	OD1-CG-ND2	-6.42	116.17	122.60
1	B	1723	HIS	N-CA-C	6.42	118.53	107.93
1	C	1100	LYS	N-CA-C	6.42	119.34	110.35
1	A	168	THR	CA-CB-CG2	6.42	121.42	110.50
1	B	2193	TRP	CD2-CE3-CZ3	6.42	126.94	118.60
1	C	791	ASN	CA-CB-CG	6.42	119.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ASP	N-CA-C	6.42	120.97	113.20
1	E	1743	ILE	CA-C-O	-6.42	112.76	120.78
2	e	4250	ARG	CB-CA-C	6.42	117.44	109.16
2	g	2406	HIS	CA-CB-CG	6.42	120.22	113.80
1	D	1180	PRO	N-CA-CB	6.42	109.30	103.08
2	d	2902	THR	CA-CB-OG1	-6.41	99.98	109.60
1	D	1354	VAL	O-C-N	-6.41	116.14	123.00
1	C	934	ASP	CA-CB-CG	6.41	119.01	112.60
1	D	1652	GLN	OE1-CD-NE2	-6.41	116.19	122.60
2	c	4220	VAL	CA-C-O	-6.41	114.51	120.34
2	f	3717	PRO	N-CA-CB	6.41	109.98	103.25
1	A	418	VAL	CA-CB-CG1	6.41	121.29	110.40
1	C	1109	GLU	O-C-N	6.40	130.52	123.22
2	f	3877	ARG	NE-CZ-NH1	6.40	127.90	121.50
2	c	4438	GLN	OE1-CD-NE2	-6.40	116.20	122.60
2	g	2593	ASP	CA-CB-CG	6.40	119.00	112.60
1	E	2074	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	F	1241	VAL	CA-C-O	-6.40	113.58	120.36
2	g	2468	SER	O-C-N	-6.40	115.44	122.92
2	g	2652	ASN	CA-CB-CG	-6.39	106.20	112.60
1	F	1153	ILE	CA-CB-CG2	-6.39	99.63	110.50
1	F	1230	ILE	O-C-N	-6.39	115.71	123.00
2	b	3705	VAL	N-CA-CB	6.39	117.50	110.53
1	A	346	ILE	CA-C-O	-6.39	113.51	120.67
1	F	1375	ARG	CA-C-O	6.39	127.48	120.71
1	F	1470	HIS	CG-CD2-NE2	-6.39	100.81	107.20
2	c	4441	PRO	N-CA-CB	6.39	109.28	103.08
1	G	690	ALA	N-CA-C	6.38	118.79	110.43
2	d	3283	VAL	CA-CB-CG2	6.38	121.25	110.40
2	e	4136	GLN	CG-CD-NE2	6.38	125.97	116.40
1	C	760	ASP	CA-CB-CG	6.37	118.97	112.60
2	d	3191	GLY	CA-C-N	6.37	130.46	121.66
2	d	3191	GLY	C-N-CA	6.37	130.46	121.66
1	B	2071	LEU	O-C-N	6.37	128.57	121.43
1	C	822	ASN	CA-CB-CG	6.37	118.97	112.60
1	B	1986	ILE	CB-CA-C	6.37	118.87	111.55
1	B	1749	GLY	CA-C-N	6.37	129.18	120.46
1	B	1749	GLY	C-N-CA	6.37	129.18	120.46
2	a	2686	ARG	CD-NE-CZ	6.37	133.31	124.40
2	b	3594	HIS	CB-CG-CD2	-6.37	122.93	131.20
2	f	3513	LYS	N-CA-C	6.36	119.97	112.72
1	B	2229	CYS	CA-C-N	6.36	126.05	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2229	CYS	C-N-CA	6.36	126.05	119.56
2	c	3958	GLN	OE1-CD-NE2	-6.36	116.24	122.60
2	f	3845	PRO	N-CA-CB	6.36	110.42	103.30
1	B	2137	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	G	827	PHE	CA-CB-CG	6.36	120.16	113.80
2	b	3882	ASN	OD1-CG-ND2	-6.36	116.24	122.60
2	c	4221	LYS	CA-C-N	6.36	126.81	120.52
2	c	4221	LYS	C-N-CA	6.36	126.81	120.52
2	d	3107	LYS	O-C-N	-6.36	115.73	121.39
1	A	307	ASN	CB-CG-ND2	6.35	125.93	116.40
1	G	1041	PRO	N-CD-CG	6.35	111.42	103.80
1	G	1112	HIS	CB-CG-CD2	-6.35	122.94	131.20
1	E	2223	ASP	CA-C-N	6.35	129.11	120.54
1	E	2223	ASP	C-N-CA	6.35	129.11	120.54
1	D	1426	GLU	N-CA-C	6.35	120.74	113.19
1	F	1134	TRP	CA-C-N	6.35	129.61	120.98
1	F	1134	TRP	C-N-CA	6.35	129.61	120.98
1	G	577	GLU	CA-C-O	-6.35	114.64	121.56
2	c	3972	SER	CA-C-O	-6.35	114.40	121.51
2	c	4257	THR	N-CA-C	-6.35	99.47	109.50
2	d	3208	GLU	N-CA-C	6.35	122.13	113.37
2	f	3613	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	153	SER	CA-C-O	-6.34	113.91	120.89
2	b	3658	GLY	CA-C-N	6.34	131.87	123.11
2	b	3658	GLY	C-N-CA	6.34	131.87	123.11
1	E	2033	GLU	N-CA-C	6.34	117.80	108.86
2	e	4430	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	2252	HIS	ND1-CE1-NE2	6.34	114.74	108.40
2	d	3192	ILE	N-CA-C	6.34	117.26	108.89
2	g	2276	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	F	1421	LYS	O-C-N	-6.34	114.26	122.94
2	a	2393	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	A	526	ASN	OD1-CG-ND2	-6.34	116.26	122.60
2	g	2587	VAL	CA-CB-CG1	6.34	121.17	110.40
1	C	640	PRO	O-C-N	6.33	131.35	122.55
2	d	2998	ASP	CA-CB-CG	6.33	118.93	112.60
2	e	4465	ASP	CA-C-O	-6.33	113.96	120.54
2	f	3569	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	D	1444	HIS	CB-CG-CD2	-6.33	122.97	131.20
2	a	2303	ARG	NH1-CZ-NH2	-6.33	111.08	119.30
1	F	1640	GLN	OE1-CD-NE2	-6.32	116.28	122.60
2	c	4304	SER	N-CA-C	6.32	118.46	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	3477	GLU	CA-C-N	6.32	131.45	122.72
2	f	3477	GLU	C-N-CA	6.32	131.45	122.72
2	e	4023	PRO	N-CA-CB	6.32	110.52	103.44
1	D	1577	ASP	CA-CB-CG	6.32	118.92	112.60
1	B	2249	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	F	1576	ASN	CA-C-N	6.32	131.26	120.72
1	F	1576	ASN	C-N-CA	6.32	131.26	120.72
2	e	4116	ILE	CA-CB-CG1	6.32	121.14	110.40
1	C	953	ASN	N-CA-CB	-6.31	102.59	111.62
2	a	2715	LYS	CA-C-O	-6.31	111.86	117.98
1	D	1470	HIS	ND1-CG-CD2	6.31	112.41	106.10
2	b	3760	TRP	CE2-CD2-CE3	-6.31	112.49	118.80
1	G	935	GLU	N-CA-C	6.31	120.18	112.23
2	d	3183	ASP	CA-C-O	-6.31	113.79	119.59
2	f	3866	TRP	CA-CB-CG	6.31	125.59	113.60
1	C	625	THR	CA-CB-CG2	6.31	121.22	110.50
1	E	2129	THR	CA-CB-OG1	6.31	119.06	109.60
2	d	2914	PRO	N-CA-CB	6.31	109.21	103.34
2	d	3066	ASP	OD1-CG-OD2	-6.31	107.76	122.90
2	f	3562	TYR	N-CA-C	6.31	119.41	110.14
2	f	3610	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	G	955	ILE	N-CA-C	6.31	119.14	108.86
2	d	3263	ILE	CA-C-N	6.31	127.72	119.84
2	d	3263	ILE	C-N-CA	6.31	127.72	119.84
2	a	2549	VAL	CA-C-O	6.30	124.38	119.46
2	a	2574	ARG	NE-CZ-NH1	6.30	127.80	121.50
2	d	3126	GLU	O-C-N	6.30	129.39	122.20
2	g	2374	GLU	CA-C-N	6.30	129.24	120.29
2	g	2374	GLU	C-N-CA	6.30	129.24	120.29
1	G	569	ILE	CB-CA-C	6.30	119.77	111.33
1	B	1885	THR	O-C-N	-6.30	115.22	123.16
1	C	932	ALA	CA-C-N	6.30	133.39	122.81
1	C	932	ALA	C-N-CA	6.30	133.39	122.81
2	b	3432	GLU	CA-C-O	-6.30	114.18	120.98
1	F	1377	LYS	CB-CA-C	6.29	121.09	109.70
2	e	4037	ASN	N-CA-C	6.29	120.68	113.19
1	B	2058	ILE	CA-CB-CG2	6.29	121.19	110.50
2	a	2760	THR	O-C-N	-6.29	114.63	122.24
2	c	4344	ILE	CA-CB-CG2	6.29	121.19	110.50
1	B	2098	LEU	CA-C-N	6.29	131.80	121.99
1	B	2098	LEU	C-N-CA	6.29	131.80	121.99
2	a	2549	VAL	N-CA-C	6.29	119.23	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1926	LEU	N-CA-C	6.28	118.73	109.24
2	f	3512	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	540	THR	CA-C-N	6.28	131.73	123.06
1	A	540	THR	C-N-CA	6.28	131.73	123.06
2	d	2868	PRO	N-CA-CB	6.28	109.51	102.60
1	A	464	VAL	CA-CB-CG2	6.28	121.07	110.40
1	B	2129	THR	CA-C-N	6.28	131.75	122.71
1	B	2129	THR	C-N-CA	6.28	131.75	122.71
1	C	974	SER	O-C-N	-6.28	115.40	122.75
1	C	1031	ASN	OD1-CG-ND2	6.28	128.88	122.60
2	g	2664	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	A	94	LEU	CB-CA-C	6.28	120.10	109.75
1	E	1948	ASP	O-C-N	-6.28	115.64	122.79
1	C	1049	SER	N-CA-CB	-6.27	101.84	111.56
2	f	3599	THR	N-CA-CB	6.27	119.88	110.22
2	g	2575	GLU	N-CA-CB	-6.27	102.77	112.30
1	B	1761	ASN	O-C-N	-6.27	114.35	122.94
2	d	3244	THR	OG1-CB-CG2	-6.27	96.76	109.30
1	B	1799	LEU	CA-C-N	6.27	132.34	122.94
1	B	1799	LEU	C-N-CA	6.27	132.34	122.94
2	a	2675	ASN	CA-C-N	6.27	132.65	122.69
2	a	2675	ASN	C-N-CA	6.27	132.65	122.69
2	e	4062	VAL	CB-CA-C	6.27	121.57	111.29
1	B	2214	ARG	CA-C-N	6.26	132.62	122.29
1	B	2214	ARG	C-N-CA	6.26	132.62	122.29
2	b	3471	PRO	N-CA-CB	6.26	109.83	103.25
1	G	1008	ASP	CA-CB-CG	6.26	118.86	112.60
2	d	3056	ASP	CA-C-N	6.26	131.70	123.06
2	d	3056	ASP	C-N-CA	6.26	131.70	123.06
2	d	3232	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	C	1102	VAL	CA-CB-CG2	6.26	121.04	110.40
2	e	4058	VAL	N-CA-C	-6.26	101.50	109.58
1	E	2184	ASP	CA-CB-CG	6.26	118.86	112.60
1	G	768	LYS	CA-C-O	-6.26	115.27	120.71
2	a	2430	THR	CA-CB-CG2	6.25	121.13	110.50
1	D	1187	PHE	CA-CB-CG	6.25	120.05	113.80
2	c	4253	MET	CA-C-O	6.25	127.45	120.70
1	C	807	VAL	O-C-N	-6.25	115.59	121.97
2	a	2491	THR	CA-CB-CG2	6.25	121.13	110.50
2	b	3424	GLU	N-CA-C	6.25	117.58	109.64
1	E	2209	GLU	CA-C-N	6.25	131.55	122.36
1	E	2209	GLU	C-N-CA	6.25	131.55	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	4200	GLU	CA-C-N	6.25	132.02	122.08
2	c	4200	GLU	C-N-CA	6.25	132.02	122.08
1	F	1590	CYS	CA-C-N	6.25	133.47	121.54
1	F	1590	CYS	C-N-CA	6.25	133.47	121.54
1	A	240	GLU	CB-CG-CD	-6.25	101.98	112.60
1	B	1952	SER	CA-C-N	6.25	129.27	120.28
1	B	1952	SER	C-N-CA	6.25	129.27	120.28
2	c	4077	HIS	CA-C-N	6.25	131.73	121.99
2	c	4077	HIS	C-N-CA	6.25	131.73	121.99
1	C	652	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	C	669	ILE	CA-C-O	-6.24	115.05	121.67
2	c	4018	PRO	N-CA-CB	6.24	109.50	103.51
1	E	1971	HIS	CB-CG-CD2	-6.24	123.08	131.20
2	c	3972	SER	O-C-N	6.24	130.82	122.96
2	c	3956	LEU	O-C-N	-6.24	114.29	122.59
2	e	4098	HIS	CA-C-N	6.24	126.43	119.32
2	e	4098	HIS	C-N-CA	6.24	126.43	119.32
2	f	3750	ARG	NE-CZ-NH2	6.24	124.81	119.20
2	g	2697	GLN	CG-CD-NE2	6.24	125.76	116.40
1	A	387	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	D	1536	PRO	CA-C-O	-6.24	114.10	122.08
2	a	2366	ASN	CA-C-N	6.24	133.45	121.54
2	a	2366	ASN	C-N-CA	6.24	133.45	121.54
1	D	1226	LEU	CB-CA-C	6.24	120.51	109.72
1	G	1009	ILE	CA-C-O	-6.24	113.48	121.40
2	f	3491	TYR	O-C-N	-6.24	115.57	123.24
2	a	2515	THR	N-CA-CB	6.23	120.45	110.85
1	C	631	THR	CA-CB-CG2	6.23	121.09	110.50
1	A	463	TYR	CB-CG-CD2	-6.23	111.45	120.80
1	F	1635	THR	O-C-N	-6.23	115.49	122.34
2	c	4124	LYS	N-CA-CB	-6.23	101.11	111.20
1	C	846	THR	CA-C-N	6.23	131.43	122.40
1	C	846	THR	C-N-CA	6.23	131.43	122.40
1	E	1820	LEU	N-CA-CB	-6.22	99.97	110.49
2	d	2827	PRO	N-CA-CB	6.22	109.12	103.33
1	D	1434	SER	CA-C-N	6.22	132.51	122.68
1	D	1434	SER	C-N-CA	6.22	132.51	122.68
2	g	2788	SER	CA-C-N	6.22	132.89	121.94
2	g	2788	SER	C-N-CA	6.22	132.89	121.94
2	f	3696	MET	N-CA-C	6.22	119.67	109.72
1	E	1904	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	F	1520	TRP	N-CA-C	6.22	118.85	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	3758	THR	CB-CA-C	-6.21	101.15	109.16
2	f	3465	THR	CA-C-N	6.21	128.02	120.94
2	f	3465	THR	C-N-CA	6.21	128.02	120.94
1	D	1621	PRO	N-CA-CB	6.21	109.23	103.39
1	A	417	THR	OG1-CB-CG2	6.21	121.72	109.30
1	C	1052	ASP	CA-CB-CG	6.21	118.81	112.60
1	D	1599	THR	N-CA-C	6.21	119.31	109.50
1	G	786	ILE	N-CA-CB	6.21	116.38	109.99
1	E	1863	ASN	CA-CB-CG	-6.20	106.40	112.60
2	c	3963	THR	CA-C-N	6.20	130.62	120.63
2	c	3963	THR	C-N-CA	6.20	130.62	120.63
2	f	3579	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	D	1393	PHE	CA-CB-CG	6.20	120.00	113.80
2	e	4075	THR	CA-C-N	6.20	129.21	120.28
2	e	4075	THR	C-N-CA	6.20	129.21	120.28
2	e	4136	GLN	OE1-CD-NE2	-6.20	116.40	122.60
2	g	2758	ASN	CA-CB-CG	-6.20	106.40	112.60
2	e	4378	PRO	CA-N-CD	-6.20	103.32	112.00
1	C	1074	GLN	OE1-CD-NE2	-6.20	116.40	122.60
2	a	2367	ASP	CA-CB-CG	6.20	118.80	112.60
2	e	4283	ASN	N-CA-C	6.20	120.10	112.54
1	C	1080	LEU	CA-C-N	6.20	130.14	121.22
1	C	1080	LEU	C-N-CA	6.20	130.14	121.22
2	b	3726	ASN	CB-CG-ND2	6.20	125.69	116.40
1	C	1025	HIS	CB-CG-CD2	-6.19	123.15	131.20
1	G	920	ARG	CD-NE-CZ	6.19	133.07	124.40
2	b	3693	ARG	CD-NE-CZ	6.19	133.07	124.40
1	B	2045	TYR	CA-C-N	6.19	130.62	122.51
1	B	2045	TYR	C-N-CA	6.19	130.62	122.51
1	C	889	PRO	CA-C-N	6.19	133.59	122.13
1	C	889	PRO	C-N-CA	6.19	133.59	122.13
1	E	1742	GLY	CA-C-O	-6.19	114.17	119.56
2	a	2313	ASN	OD1-CG-ND2	-6.19	116.41	122.60
2	b	3500	ARG	NE-CZ-NH2	-6.19	113.63	119.20
2	c	4417	SER	N-CA-C	6.19	118.82	111.33
2	e	4405	GLY	CA-C-N	6.19	124.12	119.66
2	e	4405	GLY	C-N-CA	6.19	124.12	119.66
1	G	1010	ASN	CA-CB-CG	6.19	118.79	112.60
2	f	3856	GLU	O-C-N	-6.19	114.14	122.43
1	B	2163	ASN	N-CA-CB	-6.19	100.86	110.57
1	E	2031	VAL	O-C-N	-6.18	116.54	123.03
2	d	2870	ASN	OD1-CG-ND2	-6.18	116.42	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	2957	ASP	CA-C-O	-6.18	115.07	121.87
2	f	3682	ASN	CA-C-N	6.18	128.56	120.28
2	f	3682	ASN	C-N-CA	6.18	128.56	120.28
1	F	1408	THR	N-CA-C	6.18	118.81	109.41
2	a	2777	VAL	O-C-N	-6.18	114.05	121.10
1	A	316	ARG	NE-CZ-NH1	6.18	127.68	121.50
2	a	2343	PHE	CA-CB-CG	6.18	119.98	113.80
2	c	4164	VAL	O-C-N	-6.18	117.59	122.97
2	d	3321	LEU	CB-CA-C	6.18	119.86	109.48
1	B	2223	ASP	CA-C-O	-6.18	114.66	121.89
1	B	2076	ARG	NH1-CZ-NH2	-6.17	111.27	119.30
1	E	1946	ASP	CA-CB-CG	6.17	118.78	112.60
2	d	3193	ARG	CD-NE-CZ	6.17	133.04	124.40
2	g	2529	GLU	CA-C-O	6.17	126.97	119.38
1	A	194	ASP	CA-CB-CG	6.17	118.77	112.60
2	a	2480	HIS	ND1-CE1-NE2	6.17	114.57	108.40
1	E	1814	VAL	CA-C-N	6.17	130.57	120.51
1	E	1814	VAL	C-N-CA	6.17	130.57	120.51
1	G	1089	ILE	CA-C-O	6.17	126.81	120.39
2	f	3553	GLN	OE1-CD-NE2	-6.17	116.43	122.60
2	d	2977	SER	N-CA-C	6.17	118.17	108.55
1	A	494	LYS	CA-C-N	6.17	132.27	122.59
1	A	494	LYS	C-N-CA	6.17	132.27	122.59
2	e	4393	GLU	CA-C-N	6.17	130.70	122.93
2	e	4393	GLU	C-N-CA	6.17	130.70	122.93
1	C	773	ALA	N-CA-C	6.17	118.79	109.23
2	d	2895	PHE	CA-C-O	-6.17	114.08	120.99
2	d	3036	ASP	CA-CB-CG	6.17	118.77	112.60
1	D	1567	THR	N-CA-CB	-6.17	99.84	111.00
1	D	1661	PHE	CA-C-N	6.17	133.47	121.63
1	D	1661	PHE	C-N-CA	6.17	133.47	121.63
1	F	1447	ILE	N-CA-C	6.17	117.11	111.81
2	f	3496	PHE	CA-C-O	-6.17	114.53	121.81
2	a	2733	HIS	CA-CB-CG	6.16	119.96	113.80
2	d	3159	PRO	N-CA-CB	6.16	109.38	102.60
1	D	1491	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	D	1671	LEU	CA-C-N	6.16	131.22	122.72
1	D	1671	LEU	C-N-CA	6.16	131.22	122.72
1	A	250	ASP	CA-C-N	6.16	129.57	120.95
1	A	250	ASP	C-N-CA	6.16	129.57	120.95
2	b	3493	PHE	CA-C-N	6.16	132.48	122.81
2	b	3493	PHE	C-N-CA	6.16	132.48	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	4449	PRO	N-CA-CB	6.16	108.22	103.30
2	b	3612	VAL	O-C-N	-6.16	115.19	122.58
1	F	1201	ASP	O-C-N	-6.15	116.11	123.31
1	D	1495	ASN	CB-CA-C	6.15	121.53	109.35
2	c	3999	ARG	N-CA-C	6.15	113.67	108.13
2	e	4119	TYR	CA-C-N	6.15	131.49	123.00
2	e	4119	TYR	C-N-CA	6.15	131.49	123.00
1	C	1093	GLN	OE1-CD-NE2	-6.15	116.45	122.60
2	c	4403	ILE	CA-C-N	6.15	131.84	122.37
2	c	4403	ILE	C-N-CA	6.15	131.84	122.37
2	d	3062	VAL	CB-CA-C	6.15	119.90	110.55
2	c	3959	VAL	O-C-N	-6.15	116.21	123.03
2	e	3952	PHE	CA-C-O	-6.15	114.31	120.64
1	E	2116	VAL	CA-C-O	-6.15	115.30	121.45
1	A	376	HIS	N-CA-C	6.14	120.28	109.96
1	B	1981	GLY	CA-C-O	-6.14	116.05	121.58
1	A	459	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	A	545	LEU	CB-CA-C	6.14	117.44	109.28
1	E	2140	ASP	CA-C-N	6.14	132.53	122.64
1	E	2140	ASP	C-N-CA	6.14	132.53	122.64
1	G	798	VAL	CA-CB-CG2	6.14	120.84	110.40
2	c	4309	LYS	N-CA-C	6.14	118.49	108.55
2	a	2446	ASP	CA-CB-CG	6.14	118.74	112.60
1	D	1455	PRO	N-CA-CB	6.13	110.16	103.23
2	b	3711	GLY	CA-C-N	6.13	127.09	119.98
2	b	3711	GLY	C-N-CA	6.13	127.09	119.98
2	f	3760	TRP	N-CA-C	6.13	118.76	111.71
2	g	2769	ASP	CB-CA-C	6.13	115.55	111.20
1	F	1608	ASN	N-CA-C	6.13	120.48	113.19
1	A	498	ALA	CB-CA-C	6.13	118.84	109.34
1	G	900	LYS	N-CA-C	6.13	118.77	108.23
2	d	2876	ARG	N-CA-C	6.13	120.31	112.34
2	f	3380	TRP	CD2-CE3-CZ3	6.13	126.57	118.60
2	f	3688	ARG	N-CA-C	6.12	119.87	111.54
2	g	2630	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	B	2008	ALA	CA-C-N	6.12	131.77	122.65
1	B	2008	ALA	C-N-CA	6.12	131.77	122.65
1	G	1033	THR	O-C-N	-6.12	116.11	123.03
1	B	2069	THR	CA-C-O	-6.12	111.49	118.47
2	b	3640	LYS	CA-C-O	-6.12	113.96	121.06
2	d	3140	SER	O-C-N	-6.12	116.03	123.19
1	E	1943	LYS	CA-C-N	6.12	131.44	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1943	LYS	C-N-CA	6.12	131.44	122.94
1	G	729	TYR	CA-C-O	-6.12	114.09	120.70
1	C	1081	GLY	N-CA-C	6.11	119.92	110.88
1	F	1567	THR	OG1-CB-CG2	-6.11	97.08	109.30
2	a	2480	HIS	CE1-NE2-CD2	-6.11	102.89	109.00
2	c	4157	ARG	NH1-CZ-NH2	-6.11	111.36	119.30
2	g	2630	ARG	NH1-CZ-NH2	-6.11	111.36	119.30
1	F	1310	LEU	CA-C-N	6.11	132.15	122.74
1	F	1310	LEU	C-N-CA	6.11	132.15	122.74
1	F	1344	ARG	NE-CZ-NH1	6.11	127.61	121.50
1	C	650	ASP	CA-CB-CG	6.11	118.70	112.60
2	c	4404	HIS	CB-CG-ND1	6.10	131.86	122.70
1	E	2206	GLN	OE1-CD-NE2	-6.10	116.50	122.60
2	a	2494	GLU	N-CA-C	6.10	118.58	110.53
2	d	3337	THR	CA-C-O	-6.10	113.78	120.43
2	a	2800	CYS	N-CA-C	6.10	118.98	109.52
2	d	3076	ARG	NH1-CZ-NH2	-6.10	111.37	119.30
2	e	4140	THR	CA-CB-CG2	6.10	120.86	110.50
2	f	3662	VAL	CA-C-O	-6.10	113.77	120.84
1	B	2064	ALA	CA-C-O	6.09	127.17	120.71
2	g	2331	ASP	CA-C-N	6.09	129.05	120.28
2	g	2331	ASP	C-N-CA	6.09	129.05	120.28
2	g	2333	GLU	CB-CG-CD	-6.09	102.24	112.60
1	E	1958	ASN	CA-C-O	-6.09	113.99	121.06
2	a	2738	ASP	CA-CB-CG	6.09	118.69	112.60
2	d	3247	GLY	O-C-N	-6.09	117.88	123.42
2	d	3339	ARG	CD-NE-CZ	6.09	132.93	124.40
2	c	4450	ILE	CA-C-O	6.09	127.56	121.72
1	C	769	PRO	N-CA-CB	6.09	108.99	103.33
1	D	1541	ARG	CB-CA-C	6.09	121.34	110.81
2	e	4378	PRO	O-C-N	-6.09	114.62	122.23
2	f	3709	ASP	O-C-N	-6.08	116.13	123.13
1	B	1744	THR	CA-CB-OG1	6.08	118.72	109.60
2	d	2860	ARG	CA-C-N	6.08	131.42	121.87
2	d	2860	ARG	C-N-CA	6.08	131.42	121.87
2	f	3805	THR	CA-CB-CG2	6.08	120.84	110.50
1	B	2034	GLY	CA-C-N	6.08	128.65	120.50
1	B	2034	GLY	C-N-CA	6.08	128.65	120.50
2	b	3607	VAL	CA-C-N	6.08	130.49	120.94
2	b	3607	VAL	C-N-CA	6.08	130.49	120.94
1	B	1818	GLU	O-C-N	-6.08	116.11	123.10
1	E	2198	GLN	CA-CB-CG	-6.08	101.94	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	3435	THR	CA-CB-OG1	6.08	118.72	109.60
2	c	4239	ASN	CA-CB-CG	6.08	118.68	112.60
2	c	4039	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	F	1155	LYS	N-CA-CB	-6.08	100.62	110.71
2	a	2484	PHE	N-CA-CB	-6.08	101.04	109.97
2	a	2571	PRO	N-CA-CB	6.07	108.70	103.36
1	F	1378	VAL	N-CA-C	6.07	117.33	108.53
2	c	4335	ARG	NE-CZ-NH1	-6.07	115.43	121.50
2	c	4377	ILE	CA-CB-CG2	6.07	120.81	110.50
2	f	3426	ARG	NE-CZ-NH2	6.07	124.66	119.20
1	A	170	GLU	CB-CA-C	6.06	119.88	109.51
1	G	635	ASP	N-CA-CB	-6.06	100.31	110.80
2	e	4140	THR	CA-C-N	6.06	132.63	122.87
2	e	4140	THR	C-N-CA	6.06	132.63	122.87
2	e	4228	LYS	CA-C-N	6.06	132.94	122.09
2	e	4228	LYS	C-N-CA	6.06	132.94	122.09
1	G	857	VAL	CA-CB-CG2	6.06	120.70	110.40
2	d	2870	ASN	N-CA-CB	-6.06	100.25	110.49
1	B	2237	LEU	CA-C-O	6.06	127.73	120.28
1	E	2157	HIS	N-CA-C	6.06	120.28	113.01
1	G	927	ILE	CA-C-N	6.06	130.81	121.42
1	G	927	ILE	C-N-CA	6.06	130.81	121.42
2	d	2938	ILE	O-C-N	-6.06	116.67	123.03
2	f	3796	ASP	O-C-N	-6.06	114.64	122.94
1	B	1804	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	D	1179	GLU	OE1-CD-OE2	-6.06	108.36	122.90
1	F	1315	HIS	ND1-CE1-NE2	6.06	114.46	108.40
1	G	997	THR	OG1-CB-CG2	-6.06	97.19	109.30
2	b	3810	LEU	O-C-N	-6.06	116.17	123.13
2	f	3541	HIS	CA-C-N	6.06	125.77	119.05
2	f	3541	HIS	C-N-CA	6.06	125.77	119.05
1	C	606	TYR	O-C-N	-6.05	116.33	123.41
2	a	2366	ASN	OD1-CG-ND2	-6.05	116.55	122.60
2	d	3190	SER	N-CA-C	6.05	117.70	110.19
2	f	3469	PRO	N-CA-CB	6.05	108.97	103.34
2	b	3688	ARG	N-CA-C	6.05	119.98	112.47
2	b	3594	HIS	ND1-CG-CD2	6.05	112.15	106.10
2	f	3610	ASN	CA-CB-CG	6.05	118.65	112.60
2	g	2636	ARG	NH1-CZ-NH2	-6.05	111.43	119.30
1	B	2062	PHE	CA-C-N	6.05	129.30	120.71
1	B	2062	PHE	C-N-CA	6.05	129.30	120.71
1	D	1184	ILE	N-CA-C	-6.05	105.23	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1040	HIS	CB-CG-CD2	-6.05	123.34	131.20
1	F	1216	ASP	CA-CB-CG	6.05	118.65	112.60
2	e	4148	VAL	CA-CB-CG2	6.04	120.67	110.40
2	g	2366	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	B	1836	ASP	CA-CB-CG	6.04	118.64	112.60
1	D	1607	PRO	N-CD-CG	6.04	111.05	103.80
1	E	2085	ASN	CA-C-N	6.04	128.87	120.29
1	E	2085	ASN	C-N-CA	6.04	128.87	120.29
2	b	3447	GLU	CB-CG-CD	6.04	122.87	112.60
2	g	2746	SER	N-CA-C	6.04	119.48	111.75
1	E	1818	GLU	N-CA-CB	6.04	119.31	109.95
2	a	2762	ALA	N-CA-CB	-6.04	101.84	111.62
1	G	621	PHE	CA-CB-CG	6.04	119.84	113.80
2	c	4222	PRO	N-CA-C	6.04	120.12	111.13
2	f	3722	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	E	1929	MET	CA-C-N	6.04	131.55	122.98
1	E	1929	MET	C-N-CA	6.04	131.55	122.98
2	a	2778	PRO	CA-C-N	6.04	130.89	123.10
2	a	2778	PRO	C-N-CA	6.04	130.89	123.10
2	g	2434	THR	CA-C-N	6.04	131.41	121.39
2	g	2434	THR	C-N-CA	6.04	131.41	121.39
1	D	1497	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	B	2152	VAL	N-CA-C	6.03	116.97	108.17
1	A	554	HIS	CA-CB-CG	6.03	119.83	113.80
2	d	3041	PHE	CA-CB-CG	6.03	119.83	113.80
2	g	2366	ASN	CA-C-N	6.03	133.06	121.54
2	g	2366	ASN	C-N-CA	6.03	133.06	121.54
2	g	2659	PHE	CA-C-O	6.03	126.22	119.41
2	b	3875	ALA	O-C-N	-6.03	115.88	123.17
1	D	1520	TRP	CA-CB-CG	6.03	125.05	113.60
1	G	932	ALA	CB-CA-C	6.03	119.47	109.53
2	b	3612	VAL	CA-C-N	6.03	130.69	122.07
2	b	3612	VAL	C-N-CA	6.03	130.69	122.07
2	b	3797	GLN	OE1-CD-NE2	-6.03	116.58	122.60
2	e	4220	VAL	CA-CB-CG1	6.03	120.64	110.40
2	d	3111	TYR	N-CA-C	-6.02	104.83	111.82
2	g	2381	ILE	N-CA-C	6.02	117.44	108.46
1	C	656	VAL	CA-C-N	6.02	132.45	122.33
1	C	656	VAL	C-N-CA	6.02	132.45	122.33
1	D	1333	ASP	CA-C-N	6.02	129.04	120.49
1	D	1333	ASP	C-N-CA	6.02	129.04	120.49
2	g	2791	THR	OG1-CB-CG2	-6.02	97.25	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	3225	THR	CA-C-N	6.02	131.31	122.94
2	d	3225	THR	C-N-CA	6.02	131.31	122.94
1	A	58	ASP	CA-CB-CG	6.02	118.62	112.60
1	F	1538	PHE	N-CA-C	-6.02	105.02	112.90
2	d	3263	ILE	N-CA-CB	6.02	119.64	111.21
2	g	2329	PRO	CA-N-CD	-6.02	103.58	112.00
1	C	674	PRO	N-CA-C	6.02	120.67	111.34
1	F	1597	ASN	CA-CB-CG	6.02	118.62	112.60
2	a	2333	GLU	OE1-CD-OE2	-6.02	108.46	122.90
1	E	1900	LYS	CA-C-N	6.01	127.36	119.84
1	E	1900	LYS	C-N-CA	6.01	127.36	119.84
2	c	4285	GLU	CB-CA-C	6.01	120.36	109.83
2	f	3862	VAL	CG1-CB-CG2	-6.01	97.57	110.80
1	E	1786	ASN	CB-CG-ND2	6.01	125.42	116.40
2	e	4320	ILE	CB-CA-C	6.01	117.72	111.23
1	A	197	GLY	CA-C-N	6.01	129.24	120.71
1	A	197	GLY	C-N-CA	6.01	129.24	120.71
2	c	4320	ILE	CA-CB-CG2	6.01	120.72	110.50
2	d	3059	ILE	O-C-N	-6.01	115.06	122.57
1	A	407	GLU	O-C-N	6.01	129.55	122.34
1	F	1273	ASN	CA-CB-CG	6.01	118.61	112.60
1	G	858	ASP	CA-C-N	6.01	129.44	120.31
1	G	858	ASP	C-N-CA	6.01	129.44	120.31
2	f	3772	VAL	CB-CA-C	6.01	118.23	110.96
1	G	1036	ASP	CA-CB-CG	6.00	118.61	112.60
2	e	4037	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	D	1156	ILE	CA-C-N	6.00	132.79	121.69
1	D	1156	ILE	C-N-CA	6.00	132.79	121.69
1	G	889	PRO	CA-C-N	6.00	129.26	123.02
1	G	889	PRO	C-N-CA	6.00	129.26	123.02
1	B	1888	VAL	N-CA-C	6.00	118.85	108.95
2	a	2683	GLN	OE1-CD-NE2	-6.00	116.60	122.60
2	f	3642	ASN	CA-C-O	-6.00	114.96	121.20
1	E	2075	ALA	N-CA-C	6.00	117.65	108.42
2	a	2573	SER	CA-C-N	6.00	130.87	122.36
2	a	2573	SER	C-N-CA	6.00	130.87	122.36
2	a	2741	LEU	CA-C-N	6.00	128.63	120.54
2	a	2741	LEU	C-N-CA	6.00	128.63	120.54
2	c	4331	ARG	NE-CZ-NH2	6.00	124.60	119.20
2	c	4445	SER	CA-C-N	6.00	131.23	122.77
2	c	4445	SER	C-N-CA	6.00	131.23	122.77
2	e	4276	GLN	OE1-CD-NE2	-6.00	116.61	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	730	LEU	CA-C-O	-5.99	113.85	120.38
1	F	1270	ASP	O-C-N	-5.99	115.28	122.65
2	b	3502	GLY	CA-C-O	-5.99	112.37	119.02
2	e	4248	SER	CA-C-O	5.99	124.07	118.44
1	G	1020	VAL	N-CA-C	5.99	117.32	108.45
2	e	4020	GLY	CA-C-O	-5.99	113.27	119.20
2	f	3632	TRP	CD2-CE2-CZ2	5.99	128.39	122.40
2	g	2418	PRO	CA-C-N	5.99	126.10	119.87
2	g	2418	PRO	C-N-CA	5.99	126.10	119.87
1	C	640	PRO	CA-C-O	-5.99	110.40	118.78
1	D	1418	THR	CA-C-N	5.99	130.91	121.99
1	D	1418	THR	C-N-CA	5.99	130.91	121.99
1	G	886	LYS	O-C-N	-5.99	117.88	121.71
2	c	4043	PHE	CA-C-O	-5.99	114.58	121.47
1	G	600	LEU	CA-C-O	-5.99	114.22	121.05
2	g	2683	GLN	OE1-CD-NE2	-5.99	116.61	122.60
2	f	3667	ASN	N-CA-C	5.99	118.16	107.80
2	c	4073	PRO	N-CA-CB	5.98	108.56	103.35
2	g	2582	MET	N-CA-CB	-5.98	101.28	111.69
2	g	2701	ASP	CA-CB-CG	5.98	118.58	112.60
1	C	662	LEU	N-CA-CB	-5.98	100.43	111.13
2	d	3187	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	E	1875	THR	CA-C-O	-5.98	114.13	121.78
2	b	3687	SER	O-C-N	-5.98	115.81	122.86
2	d	3017	GLN	CG-CD-NE2	5.98	125.37	116.40
2	e	4103	VAL	CA-C-N	5.98	130.46	122.93
2	e	4103	VAL	C-N-CA	5.98	130.46	122.93
1	A	301	PHE	N-CA-C	5.98	117.86	108.96
1	C	663	ARG	O-C-N	-5.97	115.62	123.21
1	C	1018	GLU	CA-C-N	5.97	126.92	120.83
1	C	1018	GLU	C-N-CA	5.97	126.92	120.83
2	e	4071	ASP	O-C-N	-5.97	115.36	122.65
1	D	1227	GLU	CB-CA-C	5.97	119.38	109.53
1	E	2184	ASP	O-C-N	5.97	129.25	122.20
2	b	3683	GLU	O-C-N	5.97	128.48	122.03
2	b	3702	THR	CA-C-N	5.97	131.04	123.10
2	b	3702	THR	C-N-CA	5.97	131.04	123.10
2	g	2341	ILE	CA-CB-CG1	5.97	120.55	110.40
2	f	3922	HIS	ND1-CG-CD2	5.97	112.07	106.10
2	b	3780	ALA	N-CA-C	5.97	118.46	108.73
2	b	3841	ASP	CA-CB-CG	5.97	118.57	112.60
2	e	4440	ASP	CA-CB-CG	5.97	118.57	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1961	PHE	CA-CB-CG	5.96	119.77	113.80
2	e	4221	LYS	O-C-N	-5.96	117.68	121.85
2	e	4421	ARG	CD-NE-CZ	5.96	132.75	124.40
1	F	1471	PHE	O-C-N	-5.96	116.28	123.13
2	b	3555	ASP	CA-CB-CG	5.96	118.56	112.60
2	d	3175	THR	OG1-CB-CG2	-5.96	97.38	109.30
1	G	627	GLU	N-CA-C	5.96	119.62	110.20
2	d	3120	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	287	LEU	N-CA-CB	-5.96	100.72	109.95
2	a	2391	VAL	N-CA-C	-5.96	107.08	111.90
2	a	2773	GLY	O-C-N	-5.96	118.06	123.96
2	b	3749	ILE	O-C-N	-5.96	116.79	122.98
2	a	2319	ARG	O-C-N	-5.95	115.66	122.09
2	c	4098	HIS	CA-C-O	-5.95	115.42	119.29
1	C	826	ASN	CA-CB-CG	5.95	118.55	112.60
1	G	653	GLY	CA-C-N	5.95	130.35	121.72
1	G	653	GLY	C-N-CA	5.95	130.35	121.72
2	e	4377	ILE	CA-C-N	5.95	125.34	118.85
2	e	4377	ILE	C-N-CA	5.95	125.34	118.85
1	E	1880	GLU	CA-C-O	-5.95	114.55	120.80
1	F	1503	THR	CA-CB-OG1	5.95	118.53	109.60
2	c	4444	GLY	N-CA-C	5.95	118.65	110.56
1	C	887	PRO	CB-CA-C	5.95	119.12	111.21
2	c	4177	THR	CB-CA-C	5.95	119.47	109.48
1	C	843	ASP	CA-C-O	5.94	126.72	120.54
1	A	241	VAL	N-CA-CB	5.94	121.03	111.23
2	b	3417	ARG	NE-CZ-NH1	5.94	127.44	121.50
1	E	2146	PRO	O-C-N	5.94	126.95	122.73
2	a	2331	ASP	O-C-N	-5.94	116.38	123.27
2	g	2767	GLN	CA-C-N	5.94	130.60	122.34
2	g	2767	GLN	C-N-CA	5.94	130.60	122.34
2	e	4346	ASN	O-C-N	-5.94	116.15	123.33
1	B	1878	ARG	NH1-CZ-NH2	5.94	127.02	119.30
1	D	1519	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	B	1979	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	B	2214	ARG	NH1-CZ-NH2	-5.93	111.59	119.30
1	C	804	ASN	CA-CB-CG	5.93	118.53	112.60
2	a	2492	SER	CA-C-O	-5.93	113.48	120.60
1	F	1270	ASP	CA-C-N	5.93	129.67	120.60
1	F	1270	ASP	C-N-CA	5.93	129.67	120.60
2	b	3832	MET	CA-C-O	5.93	127.11	120.70
2	a	2603	PRO	O-C-N	5.93	129.35	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	3637	THR	O-C-N	-5.93	115.49	122.96
1	D	1211	THR	CA-CB-CG2	-5.93	100.42	110.50
1	E	1919	PRO	N-CD-CG	5.92	112.08	103.20
1	G	990	SER	N-CA-C	5.92	119.29	110.52
2	b	3712	PRO	N-CA-CB	5.92	108.44	103.17
1	C	1058	ALA	CA-C-O	5.92	126.88	119.12
1	D	1621	PRO	CB-CA-C	-5.92	103.48	111.12
2	d	3106	VAL	N-CA-C	5.92	117.86	111.58
1	A	1	ALA	CA-C-N	5.92	129.88	121.42
1	A	1	ALA	C-N-CA	5.92	129.88	121.42
2	a	2532	ASN	CA-C-O	-5.92	113.41	120.10
2	a	2771	PRO	N-CD-CG	5.92	112.08	103.20
2	e	4190	ARG	NE-CZ-NH2	5.92	124.53	119.20
2	f	3659	VAL	CA-CB-CG2	5.92	120.46	110.40
1	B	2083	ARG	NH1-CZ-NH2	-5.92	111.61	119.30
1	D	1664	PRO	CA-C-N	5.92	129.23	120.95
1	D	1664	PRO	C-N-CA	5.92	129.23	120.95
1	F	1321	THR	CA-CB-OG1	5.92	118.48	109.60
2	c	4169	VAL	CA-CB-CG1	5.92	120.46	110.40
1	D	1557	GLU	CA-C-N	5.92	132.84	121.54
1	D	1557	GLU	C-N-CA	5.92	132.84	121.54
2	c	4348	THR	CA-CB-CG2	5.92	120.56	110.50
2	d	2940	GLU	CA-C-N	5.92	130.78	122.08
2	d	2940	GLU	C-N-CA	5.92	130.78	122.08
1	B	1745	GLU	CA-C-N	5.91	126.47	120.38
1	B	1745	GLU	C-N-CA	5.91	126.47	120.38
1	D	1567	THR	CB-CA-C	5.91	121.06	109.35
2	d	3315	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	F	1370	ASN	CA-C-N	5.91	131.36	122.91
1	F	1370	ASN	C-N-CA	5.91	131.36	122.91
1	B	1768	ARG	CD-NE-CZ	5.91	132.67	124.40
1	F	1612	PHE	CA-CB-CG	5.91	119.71	113.80
2	g	2607	VAL	O-C-N	-5.91	115.18	122.57
1	E	1747	PRO	N-CA-CB	5.91	109.10	102.60
1	E	1809	THR	N-CA-CB	5.91	119.66	110.44
1	F	1188	ASN	CB-CA-C	5.91	120.64	110.77
2	e	4005	GLN	OE1-CD-NE2	-5.91	116.69	122.60
2	g	2332	ARG	NE-CZ-NH1	5.91	127.41	121.50
2	a	2568	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	B	1787	ASN	CA-CB-CG	-5.90	106.70	112.60
1	G	758	ALA	N-CA-C	5.90	118.14	108.52
1	B	2025	LYS	CA-C-O	-5.90	114.46	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1117	ARG	NH1-CZ-NH2	-5.90	111.63	119.30
2	f	3862	VAL	CA-CB-CG1	5.90	120.42	110.40
1	F	1399	ASN	CA-CB-CG	5.90	118.50	112.60
2	a	2351	THR	CA-C-N	5.90	125.44	119.19
2	a	2351	THR	C-N-CA	5.90	125.44	119.19
1	F	1547	THR	CA-CB-CG2	5.89	120.52	110.50
1	A	203	PRO	N-CA-CB	5.89	108.48	103.35
1	D	1619	LYS	CA-C-O	-5.89	115.08	120.50
1	F	1264	ILE	CA-C-O	-5.89	115.48	121.67
1	F	1603	LEU	CA-C-O	-5.89	114.17	120.42
1	G	781	ASP	N-CA-C	5.89	118.55	110.24
2	a	2772	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	212	ARG	CD-NE-CZ	5.89	132.65	124.40
2	a	2781	VAL	CB-CA-C	5.89	119.59	110.28
1	B	2111	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	D	1349	ASN	CA-CB-CG	-5.89	106.71	112.60
1	A	510	SER	O-C-N	-5.88	114.48	122.19
1	D	1271	GLU	CA-C-N	5.88	127.20	119.84
1	D	1271	GLU	C-N-CA	5.88	127.20	119.84
2	c	4110	GLN	CA-C-N	5.88	130.97	122.44
2	c	4110	GLN	C-N-CA	5.88	130.97	122.44
2	f	3918	ASN	CA-C-N	5.88	132.34	122.87
2	f	3918	ASN	C-N-CA	5.88	132.34	122.87
2	g	2626	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	2207	GLN	N-CA-C	5.88	118.98	109.40
1	D	1139	VAL	O-C-N	-5.88	115.90	122.66
2	e	4125	VAL	CB-CA-C	5.88	120.19	111.31
1	A	39	LYS	O-C-N	-5.88	116.69	123.33
2	a	2474	ILE	N-CA-C	-5.88	101.22	109.21
2	c	4080	LEU	CD1-CG-CD2	-5.88	97.87	110.80
2	e	3965	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	A	453	PRO	CA-C-N	5.87	130.69	123.17
1	A	453	PRO	C-N-CA	5.87	130.69	123.17
1	D	1273	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	E	1728	GLU	CA-C-N	5.87	132.60	122.09
1	E	1728	GLU	C-N-CA	5.87	132.60	122.09
1	G	997	THR	CA-C-N	5.87	131.27	122.58
1	G	997	THR	C-N-CA	5.87	131.27	122.58
2	g	2553	ASN	CA-CB-CG	5.87	118.47	112.60
1	C	893	LYS	N-CA-CB	-5.87	101.20	110.06
1	F	1510	ARG	O-C-N	-5.87	115.71	122.93
2	e	4018	PRO	CA-N-CD	-5.87	103.78	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	3905	THR	CA-CB-CG2	5.87	120.48	110.50
1	F	1615	SER	CA-C-N	5.87	131.16	122.71
1	F	1615	SER	C-N-CA	5.87	131.16	122.71
2	c	4140	THR	N-CA-C	5.87	119.11	109.72
1	A	489	PRO	CA-C-O	-5.87	114.57	122.08
1	G	748	GLU	CA-C-O	5.87	126.83	120.55
1	A	27	ASP	N-CA-C	5.86	119.62	112.23
1	F	1170	TYR	O-C-N	-5.86	116.41	123.03
2	b	3844	GLU	CA-C-O	-5.86	114.07	120.87
1	D	1265	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	B	2252	HIS	CB-CG-CD2	-5.86	123.58	131.20
2	b	3503	THR	CA-CB-CG2	5.86	120.46	110.50
1	F	1447	ILE	O-C-N	5.86	131.42	122.16
1	C	1111	LEU	CA-C-N	5.86	130.57	121.26
1	C	1111	LEU	C-N-CA	5.86	130.57	121.26
1	F	1606	HIS	ND1-CG-CD2	5.86	111.96	106.10
2	a	2276	ASN	N-CA-CB	-5.86	103.24	111.62
2	a	2768	ASN	N-CA-C	5.86	119.65	111.74
1	E	1948	ASP	CA-CB-CG	5.86	118.46	112.60
1	G	751	SER	CA-C-O	5.86	126.68	120.36
2	c	4153	PRO	CA-C-N	5.86	131.62	123.07
2	c	4153	PRO	C-N-CA	5.86	131.62	123.07
1	C	721	GLU	O-C-N	-5.85	114.59	121.32
1	F	1549	THR	OG1-CB-CG2	-5.85	97.59	109.30
1	D	1180	PRO	CB-CA-C	-5.85	103.78	110.92
1	D	1593	ALA	O-C-N	5.85	130.03	122.89
1	F	1312	ARG	CB-CG-CD	5.85	124.75	111.30
1	D	1381	ALA	CB-CA-C	5.85	121.42	109.55
2	c	4113	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	B	2080	LEU	CA-C-O	5.84	127.38	120.66
2	a	2384	ASN	CB-CG-ND2	5.84	125.17	116.40
2	e	4378	PRO	N-CD-CG	5.84	111.97	103.20
2	c	4077	HIS	CA-CB-CG	-5.84	107.96	113.80
2	d	2975	PRO	N-CA-CB	5.84	109.03	102.60
1	C	995	ARG	NE-CZ-NH1	-5.84	115.66	121.50
2	c	4157	ARG	CA-C-O	-5.84	114.45	120.99
2	d	2944	VAL	CA-CB-CG2	5.84	120.33	110.40
1	D	1519	ASN	O-C-N	-5.84	115.96	122.91
1	F	1265	ASN	CA-CB-CG	5.84	118.44	112.60
2	d	3260	SER	CA-C-N	5.84	125.81	120.03
2	d	3260	SER	C-N-CA	5.84	125.81	120.03
2	e	4182	ASP	CB-CA-C	5.84	122.04	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1368	GLN	CG-CD-NE2	5.84	125.16	116.40
1	A	3	ILE	CB-CA-C	5.83	119.18	111.19
1	F	1470	HIS	CA-CB-CG	-5.83	107.97	113.80
2	g	2452	ILE	O-C-N	-5.83	116.90	123.03
2	c	4173	ILE	CB-CA-C	5.83	116.92	110.62
2	e	4010	GLU	N-CA-C	5.83	118.41	108.90
2	d	3306	GLN	OE1-CD-NE2	-5.83	116.77	122.60
2	f	3719	GLN	OE1-CD-NE2	-5.83	116.77	122.60
2	g	2805	ASP	CA-CB-CG	5.83	118.43	112.60
2	d	2919	ILE	O-C-N	5.83	129.60	122.95
2	c	4407	PRO	N-CA-CB	5.83	109.01	102.60
2	c	4061	THR	CA-CB-CG2	5.83	120.40	110.50
2	c	4335	ARG	NE-CZ-NH2	5.83	124.44	119.20
2	b	3416	ILE	CB-CA-C	5.82	119.79	110.82
2	g	2514	ASN	OD1-CG-ND2	-5.82	116.78	122.60
2	f	3538	PHE	N-CA-CB	-5.82	102.32	111.05
1	C	682	VAL	CA-C-O	-5.82	114.15	120.67
1	F	1428	MET	N-CA-C	5.82	118.30	111.02
2	f	3380	TRP	CE2-CD2-CE3	-5.82	112.98	118.80
1	E	1932	GLU	CA-C-N	5.82	130.43	122.34
1	E	1932	GLU	C-N-CA	5.82	130.43	122.34
2	e	4131	GLN	OE1-CD-NE2	-5.81	116.79	122.60
2	e	4195	ILE	N-CA-CB	5.81	119.20	111.64
1	D	1267	THR	CA-C-N	5.81	133.45	123.05
1	D	1267	THR	C-N-CA	5.81	133.45	123.05
2	c	3947	ASN	N-CA-CB	-5.81	103.18	111.84
2	d	2835	LEU	N-CA-CB	-5.81	101.89	110.49
1	A	382	LEU	CA-C-N	5.81	133.56	123.91
1	A	382	LEU	C-N-CA	5.81	133.56	123.91
1	D	1193	GLU	CA-CB-CG	-5.81	102.48	114.10
2	c	4283	ASN	CA-C-N	5.81	129.09	120.90
2	c	4283	ASN	C-N-CA	5.81	129.09	120.90
1	E	2073	ALA	O-C-N	-5.81	116.53	123.27
2	b	3566	ILE	N-CA-C	5.81	116.65	108.17
2	c	4304	SER	CA-C-N	5.81	132.04	120.77
2	c	4304	SER	C-N-CA	5.81	132.04	120.77
2	d	2987	THR	CA-CB-CG2	5.81	120.37	110.50
2	g	2544	GLY	CA-C-O	-5.81	116.06	120.76
1	F	1311	ASP	CA-CB-CG	5.80	118.41	112.60
2	e	4130	GLY	N-CA-C	5.80	123.66	115.30
2	f	3480	ASN	CA-C-N	5.80	131.79	120.99
2	f	3480	ASN	C-N-CA	5.80	131.79	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	650	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	442	ASP	CA-C-N	5.80	131.07	123.06
1	A	442	ASP	C-N-CA	5.80	131.07	123.06
1	B	1948	ASP	N-CA-C	5.80	117.55	110.41
1	G	908	SER	N-CA-C	5.80	120.08	112.89
2	a	2602	PRO	CA-C-N	5.80	125.49	119.05
2	a	2602	PRO	C-N-CA	5.80	125.49	119.05
1	D	1467	GLU	CA-C-N	5.80	129.58	120.65
1	D	1467	GLU	C-N-CA	5.80	129.58	120.65
2	a	2708	LYS	CB-CA-C	5.80	120.97	111.23
1	F	1442	ALA	N-CA-CB	-5.80	102.37	110.25
1	F	1664	PRO	CA-C-N	5.80	129.06	120.95
1	F	1664	PRO	C-N-CA	5.80	129.06	120.95
1	G	892	ILE	CB-CA-C	5.80	119.00	110.77
1	F	1216	ASP	CA-C-N	5.79	132.61	121.54
1	F	1216	ASP	C-N-CA	5.79	132.61	121.54
1	F	1271	GLU	CA-C-N	5.79	125.77	120.03
1	F	1271	GLU	C-N-CA	5.79	125.77	120.03
1	G	952	ASP	CA-C-O	5.79	125.53	119.51
2	d	3031	ILE	CA-C-N	5.79	131.00	123.00
2	d	3031	ILE	C-N-CA	5.79	131.00	123.00
1	F	1525	SER	CA-C-N	5.79	130.64	121.09
1	F	1525	SER	C-N-CA	5.79	130.64	121.09
1	E	1865	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	108	PRO	O-C-N	-5.79	115.84	123.13
2	a	2398	ASP	O-C-N	-5.79	116.56	123.27
2	b	3414	TYR	CA-C-N	5.79	131.65	122.62
2	b	3414	TYR	C-N-CA	5.79	131.65	122.62
2	e	4367	LEU	CB-CA-C	5.79	119.56	110.19
2	g	2730	GLU	CA-C-N	5.79	125.40	119.56
2	g	2730	GLU	C-N-CA	5.79	125.40	119.56
1	A	57	LYS	N-CA-CB	-5.78	100.27	110.39
1	C	1063	ILE	CA-CB-CG2	-5.78	100.67	110.50
1	G	861	GLU	CA-C-N	5.78	131.18	122.68
1	G	861	GLU	C-N-CA	5.78	131.18	122.68
2	a	2636	ARG	NE-CZ-NH2	5.78	124.41	119.20
2	b	3590	ASP	CA-C-N	5.78	132.38	122.67
2	b	3590	ASP	C-N-CA	5.78	132.38	122.67
2	c	3961	SER	CA-C-N	5.78	132.59	121.54
2	c	3961	SER	C-N-CA	5.78	132.59	121.54
2	c	4273	PRO	CA-C-N	5.78	125.32	119.19
2	c	4273	PRO	C-N-CA	5.78	125.32	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	4323	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	B	1994	MET	CB-CA-C	5.78	120.62	111.95
1	C	862	MET	CA-C-O	5.78	127.68	121.55
1	E	1982	ILE	CA-C-O	-5.78	114.35	120.48
2	c	4285	GLU	CB-CG-CD	-5.78	102.77	112.60
1	F	1233	LEU	N-CA-C	5.78	118.64	110.50
2	g	2494	GLU	CB-CG-CD	-5.78	102.78	112.60
1	C	618	ILE	CA-C-O	-5.78	113.56	120.78
2	c	4114	GLU	CA-C-N	5.78	132.66	121.63
2	c	4114	GLU	C-N-CA	5.78	132.66	121.63
1	D	1336	VAL	CA-CB-CG2	5.77	120.22	110.40
2	g	2563	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	F	1331	VAL	CA-C-O	-5.77	113.93	120.74
2	a	2611	GLU	N-CA-CB	-5.77	101.33	110.22
1	F	1518	ASP	CA-C-N	5.77	130.60	122.46
1	F	1518	ASP	C-N-CA	5.77	130.60	122.46
1	F	1595	TYR	CA-C-O	-5.77	114.59	121.11
2	b	3760	TRP	CD2-CE3-CZ3	5.77	126.10	118.60
1	C	708	THR	CA-CB-OG1	5.77	118.25	109.60
1	G	602	ILE	CA-C-O	-5.77	115.17	121.28
2	f	3891	VAL	O-C-N	-5.77	114.53	121.10
1	A	349	SER	CA-C-O	-5.76	115.05	121.51
1	D	1259	THR	CA-C-N	5.76	129.54	121.24
1	D	1259	THR	C-N-CA	5.76	129.54	121.24
1	D	1297	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	D	1423	VAL	N-CA-C	5.76	117.30	108.71
2	b	3707	ASP	O-C-N	-5.76	116.01	122.93
2	c	4402	PRO	N-CD-CG	5.76	111.85	103.20
2	f	3488	GLU	CB-CG-CD	-5.76	102.80	112.60
2	g	2642	ASP	CA-C-N	5.76	125.46	119.64
2	g	2642	ASP	C-N-CA	5.76	125.46	119.64
1	D	1249	GLY	O-C-N	-5.76	117.18	123.29
1	D	1366	GLU	CA-C-N	5.76	132.54	121.54
1	D	1366	GLU	C-N-CA	5.76	132.54	121.54
2	e	4132	TYR	N-CA-C	5.76	118.34	111.71
1	B	1708	ARG	NE-CZ-NH2	-5.76	114.02	119.20
2	g	2281	PHE	CB-CA-C	5.76	116.68	108.68
2	g	2645	GLY	CA-C-N	5.76	128.79	120.38
2	g	2645	GLY	C-N-CA	5.76	128.79	120.38
1	E	1829	LYS	CA-C-N	5.76	131.32	122.68
1	E	1829	LYS	C-N-CA	5.76	131.32	122.68
2	b	3795	SER	N-CA-C	5.76	118.15	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	4106	THR	N-CA-CB	5.76	118.75	110.06
1	G	783	ASN	OD1-CG-ND2	-5.75	116.84	122.60
1	G	858	ASP	O-C-N	-5.75	116.45	123.30
1	B	2146	PRO	CA-N-CD	-5.75	103.95	112.00
2	f	3397	LEU	CA-C-O	-5.75	114.20	120.36
2	g	2430	THR	N-CA-CB	-5.75	103.39	110.98
2	c	4208	THR	OG1-CB-CG2	-5.75	97.80	109.30
2	d	2849	THR	N-CA-C	5.75	119.99	113.15
2	d	3256	VAL	CB-CA-C	5.75	119.89	110.69
1	D	1351	ASN	OD1-CG-ND2	-5.75	116.85	122.60
2	e	4009	PHE	CB-CA-C	5.75	119.34	110.14
1	A	3	ILE	CA-C-N	5.75	132.46	122.81
1	A	3	ILE	C-N-CA	5.75	132.46	122.81
2	a	2763	ARG	CD-NE-CZ	5.75	132.45	124.40
2	d	3318	ALA	N-CA-CB	-5.75	101.69	111.69
1	B	2022	ILE	CA-C-O	-5.74	114.11	119.62
1	F	1637	VAL	CA-C-N	5.74	130.41	122.77
1	F	1637	VAL	C-N-CA	5.74	130.41	122.77
2	e	4370	VAL	CA-CB-CG1	5.74	120.16	110.40
2	g	2553	ASN	CA-C-N	5.74	128.44	120.29
2	g	2553	ASN	C-N-CA	5.74	128.44	120.29
1	A	86	ARG	CD-NE-CZ	5.74	132.44	124.40
2	b	3690	ALA	N-CA-CB	-5.74	101.67	110.16
2	d	3158	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	125	ALA	CA-C-N	5.74	130.28	122.07
1	A	125	ALA	C-N-CA	5.74	130.28	122.07
1	A	284	ILE	O-C-N	-5.74	117.06	123.26
1	F	1517	ARG	NE-CZ-NH1	5.74	127.24	121.50
2	d	2891	GLN	CA-C-O	-5.74	111.78	119.47
2	f	3688	ARG	CB-CA-C	5.74	120.18	111.80
2	f	3440	CYS	CA-C-O	-5.74	114.48	121.36
2	b	3657	GLU	CB-CG-CD	-5.74	102.85	112.60
2	e	3963	THR	CA-C-O	5.74	126.06	119.35
2	e	4175	ARG	O-C-N	-5.74	116.27	123.27
2	a	2499	ASP	CA-C-N	5.73	131.81	122.69
2	a	2499	ASP	C-N-CA	5.73	131.81	122.69
1	G	1110	CYS	CA-C-O	-5.73	114.88	121.47
2	b	3650	VAL	CA-CB-CG1	5.73	120.14	110.40
1	B	1923	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	F	1218	ARG	NE-CZ-NH2	-5.72	114.05	119.20
2	e	3966	ASN	OD1-CG-ND2	-5.72	116.88	122.60
2	f	3777	ASP	N-CA-C	5.72	117.76	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1186	VAL	O-C-N	-5.72	116.72	122.67
1	E	1850	VAL	N-CA-C	5.72	116.50	110.72
1	G	997	THR	CA-CB-OG1	5.72	118.18	109.60
2	f	3390	ASN	CA-CB-CG	5.72	118.32	112.60
2	g	2551	PRO	CA-C-N	5.72	131.43	123.07
2	g	2551	PRO	C-N-CA	5.72	131.43	123.07
2	b	3423	GLN	O-C-N	-5.72	116.56	123.03
1	C	800	GLU	N-CA-C	5.72	118.56	110.50
1	D	1405	HIS	CE1-NE2-CD2	-5.72	103.28	109.00
1	E	2052	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	E	2206	GLN	CG-CD-NE2	5.72	124.98	116.40
2	e	4002	ASP	N-CA-C	5.72	118.72	109.40
1	B	1771	THR	CA-C-N	5.72	125.25	119.19
1	B	1771	THR	C-N-CA	5.72	125.25	119.19
2	d	3129	PHE	CA-C-O	-5.72	114.75	121.44
1	E	1860	PHE	CA-CB-CG	5.71	119.52	113.80
1	F	1366	GLU	N-CA-C	5.71	118.56	110.50
1	F	1548	TYR	CA-C-O	5.71	127.62	121.16
2	a	2458	ASP	CA-CB-CG	5.71	118.31	112.60
2	b	3848	GLY	O-C-N	5.71	127.48	121.77
2	g	2778	PRO	O-C-N	-5.71	116.97	123.03
1	E	2139	GLU	N-CA-C	5.71	119.13	109.76
1	G	680	VAL	CA-C-N	5.71	130.54	122.09
1	G	680	VAL	C-N-CA	5.71	130.54	122.09
2	d	2900	PHE	O-C-N	-5.71	115.76	122.96
1	F	1409	ASP	CA-CB-CG	5.71	118.31	112.60
2	a	2607	VAL	CB-CA-C	-5.71	101.56	110.52
1	G	881	ILE	N-CA-C	5.71	118.64	113.10
2	c	4099	PRO	N-CA-CB	5.71	109.57	103.52
1	D	1188	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	G	597	GLU	N-CA-C	-5.71	105.14	111.36
1	G	746	ARG	NE-CZ-NH1	5.71	127.21	121.50
2	e	4458	MET	O-C-N	-5.71	116.28	123.01
2	f	3382	PRO	CA-N-CD	-5.71	104.01	112.00
2	g	2328	ARG	N-CA-CB	-5.71	105.41	111.29
1	B	2229	CYS	CA-C-O	-5.71	114.09	120.25
1	G	708	THR	N-CA-C	5.71	117.86	109.24
1	E	1947	ALA	CB-CA-C	5.70	119.62	110.09
1	E	2013	ILE	N-CA-C	-5.70	95.03	111.00
1	F	1408	THR	O-C-N	-5.70	115.13	122.94
2	a	2295	ASN	CA-C-O	-5.70	113.04	120.00
2	d	2829	SER	CA-C-O	-5.70	114.54	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	2386	ARG	N-CA-C	5.70	118.50	110.23
1	B	1990	ASP	CA-C-N	5.70	128.49	120.28
1	B	1990	ASP	C-N-CA	5.70	128.49	120.28
1	C	1065	ARG	NH1-CZ-NH2	-5.70	111.89	119.30
1	G	1108	CYS	O-C-N	-5.70	116.89	123.33
2	c	3966	ASN	CA-C-O	-5.70	114.45	120.55
1	D	1547	THR	N-CA-C	5.70	118.24	109.07
2	b	3593	ASP	CA-C-N	5.70	131.52	122.74
2	b	3593	ASP	C-N-CA	5.70	131.52	122.74
2	f	3466	PRO	CA-N-CD	-5.70	104.02	112.00
2	f	3873	ASP	CA-CB-CG	5.70	118.30	112.60
2	f	3576	PHE	CA-CB-CG	-5.70	108.10	113.80
1	E	1949	GLU	N-CA-C	5.70	118.59	110.10
2	a	2626	ASP	CA-CB-CG	5.70	118.30	112.60
2	f	3623	ASP	O-C-N	-5.70	117.81	123.62
2	g	2409	LEU	CA-C-N	5.70	131.90	122.33
2	g	2409	LEU	C-N-CA	5.70	131.90	122.33
1	F	1672	THR	CA-CB-CG2	5.69	120.18	110.50
2	a	2780	THR	CA-CB-CG2	5.69	120.18	110.50
2	b	3615	GLU	CB-CA-C	5.69	119.00	109.89
1	C	839	HIS	CE1-NE2-CD2	-5.69	103.31	109.00
1	D	1465	VAL	CA-C-O	-5.69	116.00	121.63
1	E	1952	SER	N-CA-C	5.69	118.23	110.55
1	B	2225	GLN	OE1-CD-NE2	-5.69	116.91	122.60
2	f	3560	ASP	CB-CA-C	5.69	118.62	109.07
1	C	633	ILE	N-CA-CB	5.68	117.55	110.05
1	D	1234	ASP	CA-C-O	-5.68	114.49	120.80
1	E	1945	PHE	CA-CB-CG	5.68	119.48	113.80
2	a	2778	PRO	CA-C-O	5.68	127.57	120.92
2	b	3574	GLN	CA-C-N	5.68	128.16	120.38
2	b	3574	GLN	C-N-CA	5.68	128.16	120.38
2	b	3680	VAL	CA-C-N	5.68	130.99	122.58
2	b	3680	VAL	C-N-CA	5.68	130.99	122.58
2	g	2431	GLY	O-C-N	-5.68	115.41	122.34
2	f	3522	ARG	CD-NE-CZ	5.68	132.35	124.40
2	g	2753	ARG	N-CA-CB	-5.68	100.96	111.53
1	D	1597	ASN	OD1-CG-ND2	-5.68	116.92	122.60
2	b	3520	HIS	CA-C-N	5.68	131.11	122.08
2	b	3520	HIS	C-N-CA	5.68	131.11	122.08
1	D	1241	VAL	N-CA-C	5.68	118.32	108.95
2	a	2728	PRO	N-CA-CB	5.68	109.03	102.33
1	C	1086	GLN	CA-C-O	5.68	127.98	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1908	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	F	1294	PHE	CA-CB-CG	5.68	119.48	113.80
1	G	826	ASN	CB-CG-ND2	5.68	124.91	116.40
2	e	3961	SER	O-C-N	-5.68	116.31	123.01
1	F	1263	LYS	O-C-N	-5.67	116.01	123.16
2	d	3224	GLU	CB-CG-CD	-5.67	102.95	112.60
2	b	3552	SER	O-C-N	-5.67	113.29	122.42
2	c	4413	GLU	CA-C-O	-5.67	112.40	119.38
1	A	520	GLN	CA-C-O	-5.67	114.22	120.69
2	g	2390	THR	CB-CA-C	5.67	120.24	110.77
1	B	1904	GLN	N-CA-CB	-5.67	101.69	111.55
2	e	4285	GLU	N-CA-CB	-5.67	102.61	110.38
2	e	4400	ASP	CA-CB-CG	5.67	118.27	112.60
2	d	2852	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	C	870	ILE	CA-C-O	5.67	127.29	121.28
1	F	1579	CYS	CB-CA-C	5.67	117.83	109.22
2	a	2788	SER	CA-C-N	5.67	131.44	122.94
2	a	2788	SER	C-N-CA	5.67	131.44	122.94
2	e	4459	SER	N-CA-CB	-5.67	101.83	111.69
1	A	458	CYS	CA-C-N	5.66	128.14	120.38
1	A	458	CYS	C-N-CA	5.66	128.14	120.38
1	F	1514	LEU	CA-C-N	5.66	131.44	122.61
1	F	1514	LEU	C-N-CA	5.66	131.44	122.61
1	G	939	LEU	CB-CA-C	-5.66	102.61	110.37
2	c	4052	ILE	N-CA-C	5.66	118.30	108.90
2	f	3433	ARG	CD-NE-CZ	5.66	132.33	124.40
2	f	3618	ARG	NH1-CZ-NH2	-5.66	111.94	119.30
2	g	2611	GLU	N-CA-C	-5.66	106.21	113.01
2	d	3061	ARG	NE-CZ-NH1	-5.66	115.84	121.50
2	d	3239	ASP	CA-CB-CG	5.66	118.26	112.60
2	g	2371	ILE	CA-CB-CG1	5.66	120.03	110.40
2	b	3838	VAL	CG1-CB-CG2	-5.66	98.35	110.80
1	A	546	HIS	N-CA-CB	-5.66	102.99	111.25
1	C	886	LYS	CA-C-N	5.66	125.42	119.76
1	C	886	LYS	C-N-CA	5.66	125.42	119.76
2	b	3402	VAL	CA-CB-CG2	5.66	120.02	110.40
2	f	3623	ASP	CA-CB-CG	5.66	118.26	112.60
2	g	2429	THR	N-CA-CB	5.66	118.82	110.33
1	B	1798	VAL	CA-C-O	5.66	127.17	120.72
1	C	663	ARG	CA-C-O	5.66	126.71	120.71
1	E	2131	THR	CA-CB-OG1	5.66	118.09	109.60
2	g	2772	PHE	CA-CB-CG	5.66	119.46	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2085	ASN	CA-CB-CG	-5.66	106.94	112.60
2	a	2747	GLU	CB-CA-C	-5.66	101.24	110.85
1	F	1138	PRO	CA-C-O	-5.65	115.00	121.56
1	C	1063	ILE	O-C-N	-5.65	116.50	122.95
2	g	2629	THR	CA-C-N	5.65	130.15	122.07
2	g	2629	THR	C-N-CA	5.65	130.15	122.07
1	E	1819	GLU	O-C-N	5.65	129.36	122.75
2	f	3817	SER	CA-C-N	5.65	125.56	119.85
2	f	3817	SER	C-N-CA	5.65	125.56	119.85
1	B	1838	PRO	CA-C-N	5.65	131.42	122.61
1	B	1838	PRO	C-N-CA	5.65	131.42	122.61
1	B	1909	ILE	CB-CA-C	5.65	118.87	111.53
1	D	1359	VAL	CA-C-N	5.65	131.12	122.93
1	D	1359	VAL	C-N-CA	5.65	131.12	122.93
1	E	1824	HIS	N-CA-C	5.65	119.19	111.39
1	C	985	LYS	CA-C-N	5.64	130.85	123.06
1	C	985	LYS	C-N-CA	5.64	130.85	123.06
1	F	1320	LEU	CA-C-O	-5.64	114.73	121.11
2	f	3504	THR	N-CA-C	-5.64	101.55	109.96
1	E	1701	ILE	CB-CA-C	5.64	120.54	111.29
1	E	1790	LYS	CA-C-N	5.64	125.61	120.03
1	E	1790	LYS	C-N-CA	5.64	125.61	120.03
2	a	2495	GLU	N-CA-C	5.64	117.35	110.41
2	e	4459	SER	N-CA-C	5.64	117.76	109.24
2	c	4061	THR	CA-C-N	5.64	128.40	122.14
2	c	4061	THR	C-N-CA	5.64	128.40	122.14
1	B	2237	LEU	CA-C-N	5.64	130.95	123.00
1	B	2237	LEU	C-N-CA	5.64	130.95	123.00
1	D	1506	PRO	N-CA-CB	5.64	108.26	103.35
1	E	2244	HIS	CB-CA-C	5.64	121.64	110.42
1	F	1229	ARG	CD-NE-CZ	5.64	132.29	124.40
1	G	929	ASN	CA-CB-CG	5.64	118.24	112.60
2	e	4422	MET	CB-CA-C	5.64	119.03	109.55
2	a	2484	PHE	O-C-N	5.64	129.76	122.89
1	C	784	ASP	CA-C-N	5.63	129.91	122.30
1	C	784	ASP	C-N-CA	5.63	129.91	122.30
1	D	1469	ILE	O-C-N	-5.63	116.47	122.61
1	G	766	THR	CA-C-N	5.63	131.84	122.66
1	G	766	THR	C-N-CA	5.63	131.84	122.66
2	b	3423	GLN	CA-CB-CG	-5.63	102.83	114.10
1	D	1377	LYS	N-CA-CB	-5.63	101.25	110.43
1	A	223	VAL	N-CA-CB	-5.63	103.30	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1347	ASP	N-CA-C	5.63	119.42	109.96
1	D	1629	ILE	CA-C-N	5.63	132.17	122.09
1	D	1629	ILE	C-N-CA	5.63	132.17	122.09
2	f	3509	CYS	N-CA-CB	-5.63	102.25	111.66
2	g	2784	ARG	NE-CZ-NH1	5.63	127.13	121.50
1	D	1328	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	F	1384	ILE	CA-CB-CG2	5.63	120.07	110.50
2	b	3740	ASP	CA-CB-CG	5.63	118.23	112.60
1	E	1804	ASN	N-CA-C	5.63	117.40	108.79
2	b	3907	LEU	CA-C-N	5.63	131.10	123.11
2	b	3907	LEU	C-N-CA	5.63	131.10	123.11
2	d	3116	GLN	N-CA-CB	-5.63	101.13	111.37
2	f	3752	LYS	N-CA-C	5.62	117.62	109.07
1	A	393	SER	N-CA-C	5.62	119.62	112.87
1	F	1500	ASP	CA-CB-CG	5.62	118.22	112.60
2	b	3918	ASN	CA-CB-CG	5.62	118.22	112.60
2	f	3755	THR	CA-CB-OG1	5.62	118.03	109.60
1	E	1733	LYS	N-CA-C	5.62	118.66	110.17
2	a	2808	HIS	CA-CB-CG	-5.62	108.18	113.80
1	B	2209	GLU	CA-C-N	5.62	130.72	122.63
1	B	2209	GLU	C-N-CA	5.62	130.72	122.63
2	b	3552	SER	CA-C-N	5.62	132.27	121.54
2	b	3552	SER	C-N-CA	5.62	132.27	121.54
2	a	2387	VAL	N-CA-CB	5.62	117.66	110.13
2	e	4315	THR	O-C-N	-5.62	115.44	122.35
2	b	3454	ILE	CB-CA-C	5.62	119.24	111.49
2	e	3983	ARG	O-C-N	-5.62	116.38	123.01
2	e	4164	VAL	CA-C-O	-5.62	115.54	121.44
2	e	4301	ARG	N-CA-C	5.62	119.43	112.24
1	A	173	THR	N-CA-C	5.61	118.79	110.48
1	A	459	HIS	CE1-NE2-CD2	-5.61	103.39	109.00
1	B	1762	VAL	CA-CB-CG1	5.61	119.94	110.40
1	D	1501	GLU	CA-C-O	5.61	126.37	120.42
2	a	2330	VAL	O-C-N	-5.61	116.96	122.97
2	c	4376	PHE	CA-CB-CG	5.61	119.41	113.80
2	c	4461	VAL	O-C-N	-5.61	116.09	122.72
2	g	2595	ASP	CA-C-N	5.61	132.24	122.81
2	g	2595	ASP	C-N-CA	5.61	132.24	122.81
2	g	2599	GLU	O-C-N	-5.61	116.70	123.27
1	B	2157	HIS	ND1-CE1-NE2	5.61	114.01	108.40
2	e	4331	ARG	NE-CZ-NH1	-5.61	115.89	121.50
2	e	4329	VAL	CA-C-N	5.61	132.13	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	4329	VAL	C-N-CA	5.61	132.13	122.09
1	F	1646	LEU	CA-C-O	-5.61	115.60	121.99
2	b	3722	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	c	4297	ASP	CA-CB-CG	5.61	118.21	112.60
1	C	1038	ASP	N-CA-C	5.61	117.97	110.35
2	a	2286	GLN	OE1-CD-NE2	-5.61	117.00	122.60
2	c	4166	GLU	N-CA-C	5.61	122.74	110.80
1	A	476	ASN	OD1-CG-ND2	-5.60	117.00	122.60
2	c	4445	SER	CB-CA-C	5.60	118.89	109.48
2	a	2597	GLY	CA-C-N	5.60	125.78	119.90
2	a	2597	GLY	C-N-CA	5.60	125.78	119.90
2	c	4454	ASP	CA-CB-CG	5.60	118.20	112.60
2	f	3586	ILE	CB-CA-C	5.60	118.72	110.77
2	g	2267	ALA	CA-C-N	5.60	126.39	120.11
2	g	2267	ALA	C-N-CA	5.60	126.39	120.11
2	g	2303	ARG	CD-NE-CZ	5.60	132.24	124.40
1	A	121	GLU	CB-CA-C	5.60	119.64	109.62
1	F	1632	GLN	CG-CD-NE2	5.60	124.80	116.40
2	e	4001	VAL	CA-CB-CG2	5.60	119.92	110.40
1	B	1835	ALA	CA-C-O	-5.60	113.08	119.41
1	E	2228	SER	CA-C-O	-5.60	115.07	121.40
2	c	4186	THR	O-C-N	-5.60	116.20	122.75
1	C	882	ARG	CA-C-N	5.60	130.51	122.40
1	C	882	ARG	C-N-CA	5.60	130.51	122.40
2	c	4147	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	939	LEU	CA-C-O	-5.59	114.20	119.91
2	a	2601	ASN	CA-CB-CG	-5.59	107.01	112.60
2	f	3767	THR	CA-C-O	-5.59	112.17	118.55
2	g	2650	ASP	CA-CB-CG	5.59	118.19	112.60
2	e	4078	THR	CA-CB-CG2	5.59	120.00	110.50
1	A	543	GLU	O-C-N	-5.59	115.16	122.59
1	G	602	ILE	CA-CB-CG2	5.59	120.00	110.50
2	e	4129	ASP	N-CA-CB	-5.59	103.63	111.62
1	F	1462	VAL	CA-CB-CG2	5.59	119.90	110.40
1	A	49	PRO	N-CA-CB	5.59	108.75	102.60
1	B	1929	MET	CA-C-N	5.59	130.85	122.58
1	B	1929	MET	C-N-CA	5.59	130.85	122.58
1	C	663	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	E	2194	LYS	CA-C-O	-5.59	115.09	121.40
1	F	1252	GLU	CB-CA-C	5.59	119.74	109.46
2	f	3581	THR	CA-CB-CG2	5.59	120.00	110.50
2	f	3750	ARG	NH1-CZ-NH2	-5.59	112.04	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	657	GLU	O-C-N	-5.58	116.55	123.36
2	e	4290	SER	CA-C-N	5.58	129.03	120.82
2	e	4290	SER	C-N-CA	5.58	129.03	120.82
1	C	572	PRO	N-CD-CG	5.58	111.58	103.20
2	f	3877	ARG	O-C-N	-5.58	116.96	123.27
1	B	1874	VAL	CA-CB-CG1	5.58	119.89	110.40
2	b	3440	CYS	CB-CA-C	5.58	120.32	109.33
2	d	3095	ASP	CA-C-O	5.58	127.01	120.98
2	g	2376	THR	CA-C-N	5.58	129.48	121.50
2	g	2376	THR	C-N-CA	5.58	129.48	121.50
2	b	3883	ASP	N-CA-CB	-5.58	105.47	111.66
1	B	2043	SER	CA-C-N	5.58	130.61	122.69
1	B	2043	SER	C-N-CA	5.58	130.61	122.69
1	G	639	THR	CB-CA-C	-5.58	101.37	109.45
1	C	697	LYS	CG-CD-CE	5.57	124.12	111.30
1	E	1732	LEU	CA-C-O	-5.57	115.10	121.40
1	F	1511	TYR	CA-CB-CG	5.57	123.93	113.90
1	D	1143	GLU	CA-C-N	5.57	130.59	122.46
1	D	1143	GLU	C-N-CA	5.57	130.59	122.46
2	e	3992	THR	CA-C-O	5.57	125.03	118.90
2	b	3843	ASP	CA-CB-CG	5.57	118.17	112.60
2	g	2631	SER	N-CA-CB	-5.57	102.42	111.22
1	A	84	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	1001	THR	CA-CB-CG2	5.57	119.96	110.50
1	F	1548	TYR	CA-C-N	5.57	130.63	122.39
1	F	1548	TYR	C-N-CA	5.57	130.63	122.39
2	a	2384	ASN	O-C-N	-5.57	115.18	122.59
1	C	880	SER	CA-C-N	5.57	131.99	121.97
1	C	880	SER	C-N-CA	5.57	131.99	121.97
1	A	185	SER	CA-C-O	-5.56	115.22	121.40
1	E	1881	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	B	1851	SER	CA-C-N	5.56	131.37	121.75
1	B	1851	SER	C-N-CA	5.56	131.37	121.75
2	d	3329	PHE	CA-CB-CG	5.56	119.36	113.80
2	g	2393	GLN	N-CA-C	5.56	118.52	109.06
2	g	2459	GLY	O-C-N	-5.56	116.96	122.41
2	f	3598	PHE	CA-CB-CG	-5.56	108.24	113.80
1	B	1959	PHE	CA-CB-CG	5.56	119.36	113.80
1	C	615	PRO	N-CA-CB	5.56	108.72	102.60
1	D	1403	TYR	O-C-N	5.56	130.47	122.13
1	E	1834	ASP	CA-C-N	5.56	132.19	121.18
1	E	1834	ASP	C-N-CA	5.56	132.19	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	4439	ASN	N-CA-CB	-5.56	103.85	112.30
1	F	1148	SER	O-C-N	-5.56	115.20	122.59
1	A	109	VAL	CA-C-O	5.55	125.75	120.31
1	A	540	THR	O-C-N	-5.55	115.96	122.96
1	E	2170	ASP	CA-CB-CG	5.55	118.15	112.60
1	G	1114	SER	N-CA-CB	-5.55	102.59	110.81
1	C	862	MET	O-C-N	-5.55	115.98	122.81
1	G	878	HIS	O-C-N	-5.55	115.98	122.81
2	d	2838	PHE	CA-C-O	-5.55	114.91	120.63
2	d	3169	ASN	CA-CB-CG	5.55	118.15	112.60
2	e	4263	GLU	CA-CB-CG	5.55	125.20	114.10
2	e	4354	GLN	CG-CD-OE1	5.55	131.90	120.80
1	B	2240	CYS	CA-C-N	5.55	129.44	121.50
1	B	2240	CYS	C-N-CA	5.55	129.44	121.50
1	C	1054	PRO	CA-C-N	5.55	125.31	119.76
1	C	1054	PRO	C-N-CA	5.55	125.31	119.76
1	D	1470	HIS	CG-CD2-NE2	-5.55	101.65	107.20
1	G	797	MET	CA-C-O	-5.55	114.83	120.71
2	d	3027	CYS	CB-CA-C	5.55	119.02	110.14
1	D	1524	ASP	CA-CB-CG	5.55	118.15	112.60
1	D	1399	ASN	CA-C-N	5.54	127.71	120.28
1	D	1399	ASN	C-N-CA	5.54	127.71	120.28
2	b	3779	GLU	CB-CG-CD	5.54	122.02	112.60
2	f	3442	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	A	98	ILE	CB-CA-C	5.54	117.32	110.73
1	C	1010	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	D	1516	ASP	CB-CA-C	5.54	121.45	110.42
1	E	1802	ASN	OD1-CG-ND2	-5.54	117.06	122.60
2	d	2926	TYR	CA-CB-CG	5.54	123.87	113.90
2	e	3963	THR	O-C-N	-5.54	115.42	122.34
1	B	1908	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	D	1169	THR	CA-CB-CG2	5.54	119.91	110.50
1	A	22	ALA	N-CA-CB	-5.54	102.81	111.56
1	E	2165	THR	CA-CB-CG2	5.54	119.91	110.50
2	f	3422	ASP	N-CA-C	-5.54	106.58	113.55
1	C	746	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	b	3662	VAL	CA-C-N	5.53	129.41	121.55
2	b	3662	VAL	C-N-CA	5.53	129.41	121.55
2	b	3888	SER	CA-CB-OG	-5.53	100.03	111.10
1	A	2	TRP	CD2-CE3-CZ3	5.53	125.79	118.60
1	C	1042	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	D	1302	GLU	CA-C-N	5.53	129.90	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1302	GLU	C-N-CA	5.53	129.90	122.93
1	B	2103	ASP	O-C-N	-5.53	116.80	123.27
1	E	2219	PHE	CA-CB-CG	5.53	119.33	113.80
1	F	1555	ILE	N-CA-C	5.53	115.95	107.77
2	b	3668	TYR	CA-C-O	5.53	126.32	119.79
2	e	4224	ASN	N-CA-C	5.53	117.23	107.61
2	e	4245	ARG	CA-C-N	5.53	130.21	122.36
2	e	4245	ARG	C-N-CA	5.53	130.21	122.36
2	e	4297	ASP	O-C-N	5.53	126.32	121.18
2	e	4406	PRO	CB-CA-C	-5.53	105.97	111.17
2	f	3692	PRO	N-CA-CB	5.53	109.41	103.33
1	E	1982	ILE	CA-CB-CG1	5.53	119.80	110.40
1	F	1297	ASN	OD1-CG-ND2	-5.53	117.07	122.60
2	a	2275	GLU	N-CA-C	5.53	118.29	110.50
2	g	2703	SER	N-CA-C	5.53	117.64	110.40
1	C	879	LYS	O-C-N	-5.53	116.26	122.12
1	C	924	GLY	CA-C-O	-5.53	113.18	119.04
1	D	1261	VAL	CA-CB-CG2	5.53	119.79	110.40
1	E	1708	ARG	CD-NE-CZ	5.53	132.13	124.40
1	E	2031	VAL	CA-CB-CG1	5.53	119.79	110.40
1	E	2167	GLU	CA-C-N	5.53	131.52	122.07
1	E	2167	GLU	C-N-CA	5.53	131.52	122.07
1	F	1228	LEU	CB-CA-C	5.53	119.48	109.37
1	G	681	PHE	CB-CA-C	5.53	118.65	109.53
2	d	3043	ARG	N-CA-C	5.53	118.20	108.75
2	g	2315	PHE	CA-CB-CG	5.53	119.33	113.80
2	g	2384	ASN	N-CA-CB	-5.53	103.61	111.84
2	e	4372	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	825	ALA	CB-CA-C	5.52	118.64	109.53
1	D	1645	LYS	CA-C-N	5.52	129.32	121.42
1	D	1645	LYS	C-N-CA	5.52	129.32	121.42
1	C	814	ASP	CA-CB-CG	5.52	118.12	112.60
2	c	3986	PHE	O-C-N	-5.52	116.75	123.10
1	B	2122	SER	N-CA-C	5.52	117.65	110.53
2	c	4123	ILE	CB-CA-C	5.52	119.83	110.95
2	f	3733	SER	O-C-N	-5.52	117.47	123.26
1	D	1394	THR	CA-C-N	5.51	129.31	121.42
1	D	1394	THR	C-N-CA	5.51	129.31	121.42
1	F	1448	ARG	N-CA-C	5.51	118.47	110.42
2	a	2267	ALA	N-CA-C	5.51	118.00	110.01
2	c	3975	GLY	O-C-N	-5.51	116.25	121.77
2	c	3999	ARG	CA-C-N	5.51	125.42	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	3999	ARG	C-N-CA	5.51	125.42	119.85
1	B	1723	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	B	2157	HIS	CA-C-N	5.51	131.03	122.49
1	B	2157	HIS	C-N-CA	5.51	131.03	122.49
1	B	2107	ARG	NH1-CZ-NH2	-5.51	112.14	119.30
1	D	1567	THR	CA-C-N	5.51	130.51	123.13
1	D	1567	THR	C-N-CA	5.51	130.51	123.13
2	b	3471	PRO	CA-C-N	5.51	130.00	122.84
2	b	3471	PRO	C-N-CA	5.51	130.00	122.84
2	c	4026	PRO	N-CD-CG	5.51	111.46	103.20
1	A	354	ARG	CA-C-N	5.51	130.56	121.86
1	A	354	ARG	C-N-CA	5.51	130.56	121.86
1	D	1258	HIS	CB-CA-C	5.51	120.46	111.26
1	D	1397	SER	CA-C-N	5.51	130.93	121.07
1	D	1397	SER	C-N-CA	5.51	130.93	121.07
1	D	1566	GLY	CA-C-N	5.50	131.65	122.73
1	D	1566	GLY	C-N-CA	5.50	131.65	122.73
2	g	2379	PHE	O-C-N	-5.50	116.89	123.27
1	F	1448	ARG	CD-NE-CZ	5.50	132.10	124.40
2	d	2954	THR	CA-CB-CG2	5.50	119.86	110.50
1	A	48	PRO	CA-C-O	-5.50	116.94	120.90
1	B	2233	GLN	CA-C-O	-5.50	114.39	120.33
2	a	2671	ASN	OD1-CG-ND2	-5.50	117.10	122.60
2	b	3610	ASN	OD1-CG-ND2	-5.50	117.10	122.60
2	f	3588	ILE	CB-CA-C	5.50	117.73	110.91
1	E	2084	ASP	CA-CB-CG	5.50	118.10	112.60
2	e	3944	MET	O-C-N	-5.50	117.11	122.99
2	g	2501	GLU	CA-C-N	5.50	128.31	121.71
2	g	2501	GLU	C-N-CA	5.50	128.31	121.71
1	A	505	VAL	CA-CB-CG2	5.50	119.75	110.40
2	c	3978	VAL	CB-CA-C	5.50	120.30	111.29
2	e	4213	ASN	OD1-CG-ND2	-5.50	117.11	122.60
2	e	4415	SER	O-C-N	-5.50	116.78	123.10
1	D	1483	SER	CA-C-O	5.49	126.42	120.32
1	G	597	GLU	O-C-N	-5.49	115.89	122.15
2	a	2772	PHE	O-C-N	-5.49	116.27	122.97
1	B	2083	ARG	CA-C-N	5.49	130.56	121.99
1	B	2083	ARG	C-N-CA	5.49	130.56	121.99
1	C	571	ALA	O-C-N	-5.49	114.67	121.64
1	C	731	ASN	CA-C-N	5.49	128.09	120.29
1	C	731	ASN	C-N-CA	5.49	128.09	120.29
1	G	1046	PHE	O-C-N	5.49	129.24	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	PHE	CA-C-O	5.49	127.53	121.11
1	A	521	PHE	CA-CB-CG	5.49	119.29	113.80
2	c	4388	THR	N-CA-C	5.49	121.75	114.12
2	f	3794	ALA	CA-C-O	5.49	127.86	121.44
1	C	875	ALA	CA-C-O	-5.49	114.61	120.92
1	A	179	ASP	CA-CB-CG	5.49	118.08	112.60
1	B	2172	HIS	CB-CG-CD2	-5.49	124.07	131.20
1	E	1776	LEU	CA-C-N	5.49	130.50	122.77
1	E	1776	LEU	C-N-CA	5.49	130.50	122.77
1	F	1326	ASP	N-CA-C	5.49	117.31	109.14
2	c	4063	GLY	N-CA-C	5.49	118.50	110.38
1	A	111	THR	CA-C-N	5.48	131.59	121.94
1	A	111	THR	C-N-CA	5.48	131.59	121.94
2	e	4399	PRO	N-CA-CB	5.48	108.67	103.19
2	e	4464	LEU	CA-C-N	5.48	129.97	122.84
2	e	4464	LEU	C-N-CA	5.48	129.97	122.84
2	f	3913	ASP	CA-CB-CG	5.48	118.08	112.60
1	E	1888	VAL	CA-C-O	-5.48	115.91	121.67
1	F	1139	VAL	CA-C-N	5.48	130.50	122.77
1	F	1139	VAL	C-N-CA	5.48	130.50	122.77
1	G	793	VAL	O-C-N	-5.48	116.97	123.00
2	a	2269	ILE	CA-C-O	-5.48	116.11	119.51
2	b	3912	CYS	N-CA-CB	-5.48	102.74	111.62
1	D	1388	ASN	CA-CB-CG	5.48	118.08	112.60
1	E	2017	TYR	N-CA-C	5.48	117.15	110.41
1	G	749	HIS	CB-CG-ND1	5.48	130.92	122.70
2	c	4077	HIS	CB-CG-CD2	-5.48	124.08	131.20
2	d	2966	LEU	CA-C-N	5.48	130.52	121.86
2	d	2966	LEU	C-N-CA	5.48	130.52	121.86
1	F	1221	ASN	CA-CB-CG	5.48	118.08	112.60
1	G	1016	LEU	CA-C-N	5.48	127.97	120.46
1	G	1016	LEU	C-N-CA	5.48	127.97	120.46
2	e	4284	ALA	N-CA-C	5.48	117.04	109.15
2	g	2716	PRO	CA-N-CD	-5.48	104.33	112.00
1	C	845	GLN	CG-CD-NE2	5.48	124.61	116.40
1	D	1471	PHE	O-C-N	-5.47	116.81	123.16
2	b	3800	ARG	N-CA-C	5.47	118.15	109.50
2	d	2978	PRO	CA-C-N	5.47	128.62	120.95
2	d	2978	PRO	C-N-CA	5.47	128.62	120.95
2	f	3686	PHE	N-CA-C	5.47	118.56	110.46
2	g	2384	ASN	N-CA-C	5.47	118.98	111.54
1	A	338	HIS	ND1-CG-CD2	5.47	111.57	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	2647	VAL	N-CA-C	5.47	117.21	108.89
1	F	1601	GLU	CA-C-N	5.47	130.49	122.39
1	F	1601	GLU	C-N-CA	5.47	130.49	122.39
2	a	2384	ASN	CB-CA-C	5.47	121.31	110.42
2	a	2392	GLY	CA-C-O	-5.47	116.13	121.05
2	c	4442	PRO	CB-CA-C	5.47	118.39	111.39
2	e	4470	ASP	N-CA-CB	-5.47	101.98	110.29
1	C	869	VAL	CA-C-N	5.47	130.67	122.58
1	C	869	VAL	C-N-CA	5.47	130.67	122.58
1	E	1933	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	226	LYS	N-CA-CB	-5.46	102.06	110.20
1	F	1571	ASN	OD1-CG-ND2	-5.46	117.14	122.60
2	g	2265	ARG	NE-CZ-NH1	5.46	126.96	121.50
2	g	2546	LEU	CD1-CG-CD2	-5.46	98.78	110.80
1	A	547	GLY	CA-C-N	5.46	129.84	120.72
1	A	547	GLY	C-N-CA	5.46	129.84	120.72
1	B	2074	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	C	635	ASP	CA-CB-CG	5.46	118.06	112.60
1	F	1234	ASP	CA-CB-CG	5.46	118.06	112.60
1	F	1592	ASP	CA-CB-CG	5.46	118.06	112.60
2	d	3012	GLN	CB-CG-CD	5.46	121.88	112.60
1	A	284	ILE	CA-C-O	5.46	126.12	120.39
2	c	4469	CYS	CA-C-N	5.46	131.30	122.29
2	c	4469	CYS	C-N-CA	5.46	131.30	122.29
1	B	1845	ILE	CA-C-O	-5.46	115.97	121.59
2	a	2379	PHE	CA-CB-CG	5.46	119.26	113.80
2	d	2911	LEU	CA-C-O	-5.46	115.69	120.60
2	d	3335	PRO	CB-CA-C	5.46	116.46	111.87
1	C	833	ASN	CA-CB-CG	5.46	118.06	112.60
1	G	814	ASP	CA-C-N	5.46	132.21	122.06
1	G	814	ASP	C-N-CA	5.46	132.21	122.06
2	d	3237	ALA	CA-C-N	5.46	131.29	122.29
2	d	3237	ALA	C-N-CA	5.46	131.29	122.29
1	G	876	ALA	N-CA-C	5.46	117.88	110.35
1	C	612	THR	OG1-CB-CG2	-5.45	98.39	109.30
2	c	4465	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	548	SER	CA-C-N	5.45	125.87	120.31
1	A	548	SER	C-N-CA	5.45	125.87	120.31
1	D	1359	VAL	CA-C-O	-5.45	114.58	120.36
1	E	2189	MET	CA-C-N	5.45	128.13	120.28
1	E	2189	MET	C-N-CA	5.45	128.13	120.28
1	F	1258	HIS	CA-C-N	5.45	130.24	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1258	HIS	C-N-CA	5.45	130.24	122.72
1	B	1879	GLU	N-CA-CB	5.45	120.01	110.42
1	C	839	HIS	ND1-CG-CD2	5.45	111.55	106.10
1	G	846	THR	CA-C-O	5.45	125.24	118.43
2	b	3683	GLU	CA-C-O	-5.45	115.29	120.90
2	b	3690	ALA	N-CA-C	5.45	117.30	111.36
2	g	2720	SER	N-CA-CB	-5.45	103.28	111.56
1	C	691	ALA	CA-C-N	5.45	130.14	122.46
1	C	691	ALA	C-N-CA	5.45	130.14	122.46
1	C	1040	HIS	ND1-CG-CD2	5.45	111.55	106.10
2	e	3972	SER	CA-C-O	-5.45	115.61	121.38
1	F	1648	ARG	NH1-CZ-NH2	-5.44	112.22	119.30
1	A	509	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	C	725	PRO	CA-N-CD	-5.44	103.88	111.50
1	E	2022	ILE	CA-CB-CG1	5.44	119.65	110.40
1	G	746	ARG	NH1-CZ-NH2	-5.44	112.22	119.30
2	a	2727	ASP	O-C-N	5.44	126.60	121.38
1	A	114	VAL	O-C-N	5.44	127.87	122.97
1	G	1051	ILE	CB-CA-C	5.44	118.65	110.98
2	a	2431	GLY	CA-C-N	5.44	129.17	121.66
2	a	2431	GLY	C-N-CA	5.44	129.17	121.66
2	f	3672	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	A	480	PHE	O-C-N	-5.44	116.59	122.79
1	E	1986	ILE	O-C-N	5.44	127.42	122.14
1	E	1956	LEU	O-C-N	-5.44	116.18	122.87
2	f	3881	GLN	N-CA-C	5.44	117.53	108.99
2	g	2591	VAL	O-C-N	5.44	128.89	123.18
2	g	2653	THR	N-CA-C	5.44	120.79	113.72
1	F	1478	ILE	CA-C-N	5.44	130.44	122.77
1	F	1478	ILE	C-N-CA	5.44	130.44	122.77
2	e	4120	GLN	CG-CD-NE2	5.44	124.56	116.40
1	A	448	PRO	CA-C-N	5.43	131.95	122.82
1	A	448	PRO	C-N-CA	5.43	131.95	122.82
1	G	802	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	G	1065	ARG	CD-NE-CZ	5.43	132.01	124.40
2	c	3968	THR	OG1-CB-CG2	-5.43	98.43	109.30
2	c	4112	ASP	CA-CB-CG	5.43	118.03	112.60
1	E	2029	LYS	CA-C-N	5.43	130.13	122.09
1	E	2029	LYS	C-N-CA	5.43	130.13	122.09
2	a	2746	SER	CA-C-N	5.43	128.00	120.29
2	a	2746	SER	C-N-CA	5.43	128.00	120.29
2	c	4258	VAL	CA-C-N	5.43	129.85	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	4258	VAL	C-N-CA	5.43	129.85	122.19
2	c	4261	ASN	OD1-CG-ND2	-5.43	117.17	122.60
2	c	4406	PRO	CA-C-O	-5.43	116.44	120.73
2	f	3603	TYR	N-CA-CB	-5.43	102.98	111.56
1	E	1719	ILE	CA-CB-CG1	5.43	119.63	110.40
1	E	2121	ILE	CA-C-O	-5.43	114.74	120.39
1	G	620	VAL	CA-CB-CG2	5.43	119.63	110.40
2	a	2684	GLY	CA-C-N	5.43	130.23	121.00
2	a	2684	GLY	C-N-CA	5.43	130.23	121.00
2	c	4468	LEU	CA-C-N	5.43	129.33	122.16
2	c	4468	LEU	C-N-CA	5.43	129.33	122.16
1	E	2123	GLU	CB-CA-C	5.43	119.84	110.45
2	b	3507	GLN	OE1-CD-NE2	-5.43	117.17	122.60
2	e	3995	LEU	CB-CA-C	5.43	119.30	109.37
1	C	1012	ASN	CB-CA-C	5.43	119.64	109.71
1	F	1682	CYS	CA-C-O	-5.43	115.08	121.16
2	c	4201	ASN	CA-CB-CG	5.43	118.03	112.60
2	e	4348	THR	CA-C-O	5.43	126.34	120.43
2	f	3426	ARG	NH1-CZ-NH2	-5.43	112.25	119.30
2	g	2343	PHE	CA-CB-CG	5.43	119.23	113.80
2	g	2355	PRO	CB-CA-C	5.43	118.04	110.17
1	A	529	PHE	CA-C-O	-5.42	114.85	121.36
1	C	1112	HIS	CB-CA-C	5.42	117.60	110.06
1	F	1517	ARG	NH1-CZ-NH2	-5.42	112.25	119.30
2	a	2679	LEU	CA-C-N	5.42	130.79	122.93
2	a	2679	LEU	C-N-CA	5.42	130.79	122.93
2	b	3732	THR	OG1-CB-CG2	-5.42	98.45	109.30
2	d	2880	ASN	OD1-CG-ND2	-5.42	117.18	122.60
2	e	4347	ILE	CA-CB-CG1	5.42	119.62	110.40
2	d	2992	THR	CA-C-O	-5.42	114.68	120.92
2	e	4143	ILE	CA-C-O	5.42	126.08	120.39
1	F	1515	GLU	CA-C-N	5.42	131.89	121.54
1	F	1515	GLU	C-N-CA	5.42	131.89	121.54
2	f	3816	ASN	O-C-N	-5.42	116.89	123.29
2	b	3731	THR	CA-CB-OG1	5.42	117.73	109.60
2	b	3778	ARG	NE-CZ-NH1	5.42	126.92	121.50
2	c	4449	PRO	N-CA-CB	5.42	106.86	103.23
2	f	3675	ILE	N-CA-C	-5.42	99.75	107.77
1	A	235	ASN	CA-C-N	5.42	131.44	121.85
1	A	235	ASN	C-N-CA	5.42	131.44	121.85
1	E	2086	TRP	CD2-CE2-CZ2	5.42	127.82	122.40
1	E	2225	GLN	OE1-CD-NE2	-5.42	117.18	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	634	LEU	N-CA-CB	-5.42	102.61	110.36
2	a	2769	ASP	CA-C-O	-5.42	116.73	120.47
2	b	3741	PRO	N-CA-CB	5.42	108.90	103.48
1	B	2206	GLN	CA-C-N	5.42	131.06	122.94
1	B	2206	GLN	C-N-CA	5.42	131.06	122.94
2	e	4038	ASP	N-CA-C	5.42	118.68	111.75
1	A	2	TRP	CE2-CD2-CE3	-5.41	113.39	118.80
2	d	2822	ARG	CD-NE-CZ	5.41	131.98	124.40
2	g	2666	ALA	CA-C-N	5.41	128.54	120.31
2	g	2666	ALA	C-N-CA	5.41	128.54	120.31
1	C	625	THR	CA-C-O	5.41	124.47	118.52
1	C	1011	ASP	CA-CB-CG	5.41	118.01	112.60
2	f	3401	GLN	CA-C-O	-5.41	114.79	120.58
1	A	113	ASP	N-CA-C	5.41	117.26	111.36
1	D	1545	ASN	CA-C-N	5.41	130.36	122.46
1	D	1545	ASN	C-N-CA	5.41	130.36	122.46
1	A	210	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	F	1578	ASN	OD1-CG-ND2	-5.41	117.19	122.60
2	a	2745	THR	CA-CB-CG2	5.41	119.69	110.50
2	b	3783	ILE	N-CA-CB	-5.41	104.95	112.52
1	B	2135	LEU	CA-C-O	-5.41	114.67	120.46
1	F	1146	ASP	CA-CB-CG	5.41	118.01	112.60
2	c	3971	TYR	O-C-N	-5.41	116.91	123.29
2	g	2301	SER	CA-C-N	5.41	131.22	122.68
2	g	2301	SER	C-N-CA	5.41	131.22	122.68
1	E	1949	GLU	CA-C-O	5.41	127.08	120.92
1	F	1528	SER	N-CA-C	5.41	121.08	113.56
2	a	2303	ARG	NE-CZ-NH1	5.41	126.91	121.50
2	a	2439	GLN	CG-CD-OE1	5.41	131.61	120.80
2	a	2722	GLU	O-C-N	-5.41	116.85	122.96
1	G	940	PRO	CA-C-O	-5.40	115.29	121.56
2	f	3890	VAL	CG1-CB-CG2	-5.40	98.91	110.80
1	C	906	LYS	N-CA-C	-5.40	106.37	113.12
1	D	1236	ASN	CB-CA-C	5.40	120.18	111.05
1	G	1057	MET	O-C-N	5.40	128.31	122.15
1	D	1274	THR	CA-CB-OG1	-5.40	101.50	109.60
1	F	1571	ASN	CA-C-N	5.40	130.63	122.91
1	F	1571	ASN	C-N-CA	5.40	130.63	122.91
1	G	888	THR	CA-CB-OG1	5.40	117.70	109.60
2	a	2453	LYS	O-C-N	-5.40	117.23	123.33
2	d	3206	ILE	CA-C-N	5.40	129.01	121.02
2	d	3206	ILE	C-N-CA	5.40	129.01	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	4190	ARG	CD-NE-CZ	5.40	131.96	124.40
1	F	1420	ILE	CB-CA-C	5.40	117.89	111.20
2	a	2761	ALA	N-CA-C	5.40	117.46	108.99
1	C	739	THR	CB-CA-C	-5.40	98.48	109.65
1	E	2137	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	F	1366	GLU	O-C-N	5.40	129.23	122.86
1	F	1413	ASN	CA-CB-CG	-5.40	107.20	112.60
1	F	1552	ILE	CB-CG1-CD1	5.39	125.13	113.80
1	G	1086	GLN	N-CA-C	5.39	118.42	109.46
2	c	3981	GLU	N-CA-C	5.39	116.45	109.65
2	d	2963	HIS	CB-CG-CD2	-5.39	124.19	131.20
2	d	3235	VAL	CA-CB-CG2	5.39	119.57	110.40
1	E	2149	ILE	CA-C-O	5.39	125.01	119.35
2	b	3485	ILE	CA-C-N	5.39	128.37	120.71
2	b	3485	ILE	C-N-CA	5.39	128.37	120.71
2	c	4293	TYR	CA-CB-CG	5.39	123.60	113.90
2	d	2868	PRO	N-CD-CG	5.39	110.27	103.80
2	g	2665	GLU	CA-C-O	5.39	125.73	119.32
1	G	1080	LEU	CA-C-O	-5.39	115.27	121.47
2	b	3451	SER	N-CA-C	5.39	117.03	108.79
2	g	2772	PHE	N-CA-C	5.39	117.84	110.24
2	c	4436	SER	CA-C-O	-5.39	115.51	121.33
1	B	1782	ASP	N-CA-C	5.39	116.87	110.19
1	D	1289	ALA	N-CA-C	5.39	119.57	112.89
1	E	1953	ASP	N-CA-C	5.39	119.11	112.54
1	F	1574	ASP	CA-CB-CG	5.39	117.99	112.60
2	b	3750	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	e	3996	TYR	N-CA-CB	-5.39	103.05	111.56
2	e	4078	THR	OG1-CB-CG2	-5.39	98.53	109.30
1	F	1351	ASN	CA-C-N	5.38	128.62	123.02
1	F	1351	ASN	C-N-CA	5.38	128.62	123.02
1	D	1651	ILE	CA-CB-CG1	5.38	119.55	110.40
1	A	135	THR	CA-C-N	5.38	131.45	122.73
1	A	135	THR	C-N-CA	5.38	131.45	122.73
1	D	1303	ILE	N-CA-C	5.38	116.05	108.36
1	F	1561	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	G	659	PRO	N-CA-CB	5.38	108.03	103.35
2	b	3505	VAL	CA-C-N	5.38	127.92	120.92
2	b	3505	VAL	C-N-CA	5.38	127.92	120.92
1	B	2061	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	2077	TYR	CA-CB-CG	5.38	123.58	113.90
1	C	568	TRP	CA-C-N	5.38	129.71	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	568	TRP	C-N-CA	5.38	129.71	122.93
1	C	675	VAL	O-C-N	-5.38	117.50	123.20
2	d	3224	GLU	CA-C-N	5.38	132.70	121.94
2	d	3224	GLU	C-N-CA	5.38	132.70	121.94
2	d	3248	THR	N-CA-CB	5.38	121.05	111.69
1	A	165	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	E	2134	VAL	N-CA-CB	5.38	119.37	111.52
2	b	3898	ARG	CA-CB-CG	5.38	124.85	114.10
1	E	1927	GLU	CA-C-N	5.38	128.91	122.03
1	E	1927	GLU	C-N-CA	5.38	128.91	122.03
2	e	4101	THR	O-C-N	-5.38	115.10	122.46
2	e	4438	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	A	312	HIS	CB-CG-ND1	5.37	130.76	122.70
2	b	3716	PRO	CA-C-N	5.37	125.07	119.64
2	b	3716	PRO	C-N-CA	5.37	125.07	119.64
2	c	4120	GLN	CA-C-N	5.37	130.72	122.93
2	c	4120	GLN	C-N-CA	5.37	130.72	122.93
2	d	3325	ASN	CB-CA-C	5.37	120.00	111.51
1	B	2095	GLU	CA-C-N	5.37	130.41	122.94
1	B	2095	GLU	C-N-CA	5.37	130.41	122.94
1	C	1000	GLY	O-C-N	-5.37	119.00	123.73
1	F	1478	ILE	O-C-N	-5.37	117.25	123.00
2	e	4441	PRO	CA-N-CD	-5.37	104.48	112.00
2	c	4346	ASN	N-CA-C	5.37	118.49	109.95
1	B	1823	ALA	CA-C-O	-5.37	115.30	121.47
1	B	2073	ALA	N-CA-CB	-5.37	102.70	110.70
1	D	1229	ARG	CA-C-N	5.37	129.85	123.19
1	D	1229	ARG	C-N-CA	5.37	129.85	123.19
1	A	306	ALA	N-CA-CB	-5.37	102.25	111.21
2	g	2287	GLN	O-C-N	-5.37	117.10	123.22
1	D	1224	LYS	CA-CB-CG	5.36	124.83	114.10
1	E	2233	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	G	1048	PHE	O-C-N	-5.36	116.68	123.01
2	d	3210	THR	CA-CB-OG1	5.36	117.64	109.60
2	a	2687	THR	CA-CB-CG2	5.36	119.62	110.50
1	E	1795	ARG	NH1-CZ-NH2	-5.36	112.33	119.30
1	E	2157	HIS	O-C-N	-5.36	115.06	122.46
1	F	1656	SER	N-CA-C	5.36	118.14	109.40
2	d	2957	ASP	CA-CB-CG	5.36	117.96	112.60
2	d	3162	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	257	TRP	CA-CB-CG	5.36	123.78	113.60
2	d	3072	THR	CA-CB-CG2	5.36	119.61	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1762	VAL	CA-C-O	5.36	126.16	120.48
1	F	1473	SER	CA-C-O	5.36	126.87	120.28
1	F	1549	THR	CA-CB-CG2	5.36	119.61	110.50
2	g	2308	ASP	CA-CB-CG	5.36	117.96	112.60
2	g	2345	THR	CA-CB-OG1	5.36	117.64	109.60
2	g	2568	ASN	O-C-N	-5.36	116.94	122.94
2	g	2677	THR	CA-C-O	5.36	126.75	120.80
1	A	376	HIS	ND1-CE1-NE2	5.36	113.75	108.40
1	E	2011	LYS	CB-CG-CD	5.36	123.62	111.30
2	f	3425	PRO	N-CA-CB	5.36	108.49	102.60
2	a	2468	SER	CA-C-N	5.35	130.99	122.74
2	a	2468	SER	C-N-CA	5.35	130.99	122.74
2	a	2516	ALA	CA-C-N	5.35	129.66	120.72
2	a	2516	ALA	C-N-CA	5.35	129.66	120.72
1	G	750	SER	CB-CA-C	-5.35	100.73	109.56
2	b	3732	THR	CA-C-N	5.35	132.54	123.01
2	b	3732	THR	C-N-CA	5.35	132.54	123.01
2	d	3274	THR	CA-CB-OG1	5.35	117.63	109.60
2	e	3958	GLN	CB-CG-CD	-5.35	103.50	112.60
2	e	4404	HIS	CE1-NE2-CD2	-5.35	103.65	109.00
2	g	2403	ASP	CA-CB-CG	5.35	117.95	112.60
2	g	2796	THR	CA-CB-CG2	5.35	119.60	110.50
1	B	2219	PHE	CA-C-N	5.35	130.69	122.93
1	B	2219	PHE	C-N-CA	5.35	130.69	122.93
2	c	4306	ILE	N-CA-C	5.35	115.56	107.80
2	e	4472	ILE	CA-C-O	-5.35	114.43	120.32
1	A	383	GLU	N-CA-C	5.35	119.64	113.38
1	B	1945	PHE	CA-CB-CG	5.35	119.15	113.80
1	C	1038	ASP	CA-CB-CG	5.35	117.95	112.60
1	G	652	ARG	NE-CZ-NH2	5.35	124.01	119.20
2	a	2762	ALA	N-CA-C	5.35	117.11	109.14
1	F	1560	PRO	N-CA-CB	5.35	108.48	102.60
2	a	2497	THR	CA-CB-CG2	5.34	119.59	110.50
2	a	2735	PRO	CB-CA-C	5.34	117.44	110.92
2	d	3233	ILE	CA-CB-CG1	5.34	119.48	110.40
2	e	4434	ARG	CA-C-N	5.34	129.88	122.77
2	e	4434	ARG	C-N-CA	5.34	129.88	122.77
2	b	3760	TRP	N-CA-C	5.34	120.81	113.97
2	c	4385	CYS	CA-C-N	5.34	127.63	120.58
2	c	4385	CYS	C-N-CA	5.34	127.63	120.58
2	d	2877	ASP	CA-C-N	5.34	130.25	122.08
2	d	2877	ASP	C-N-CA	5.34	130.25	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	3075	TRP	N-CA-CB	-5.34	102.90	110.81
1	B	1898	THR	O-C-N	-5.34	116.70	122.79
1	C	1112	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	E	2244	HIS	CA-CB-CG	-5.34	108.46	113.80
2	e	4001	VAL	CA-CB-CG1	5.34	119.48	110.40
2	f	3552	SER	CA-C-O	-5.34	113.31	119.56
1	A	242	THR	CA-CB-CG2	5.34	119.58	110.50
1	B	2010	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	E	2164	VAL	N-CA-C	5.34	115.40	108.35
2	f	3527	ILE	CA-CB-CG2	5.34	119.58	110.50
2	g	2314	LEU	N-CA-C	5.34	117.52	111.11
1	G	595	ALA	CA-C-N	5.34	127.69	120.38
1	G	595	ALA	C-N-CA	5.34	127.69	120.38
1	D	1538	PHE	CA-CB-CG	5.33	119.14	113.80
2	c	3980	GLN	CG-CD-NE2	5.33	124.40	116.40
2	c	4103	VAL	CA-C-N	5.33	129.02	121.66
2	c	4103	VAL	C-N-CA	5.33	129.02	121.66
1	B	1818	GLU	CB-CA-C	5.33	118.51	109.50
1	C	804	ASN	N-CA-C	5.33	119.37	112.86
1	D	1485	ASP	CA-CB-CG	5.33	117.93	112.60
2	c	4413	GLU	CA-C-N	5.33	129.75	120.68
2	c	4413	GLU	C-N-CA	5.33	129.75	120.68
2	d	2917	ILE	CA-CB-CG1	5.33	119.47	110.40
2	g	2601	ASN	O-C-N	-5.33	116.65	121.66
2	d	3298	LEU	CB-CG-CD1	5.33	126.69	110.70
2	b	3777	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	2103	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	2099	ALA	N-CA-CB	-5.33	103.28	110.95
1	G	766	THR	O-C-N	-5.33	116.66	122.84
2	a	2753	ARG	NE-CZ-NH1	5.33	126.83	121.50
2	g	2690	GLY	O-C-N	-5.33	117.17	123.61
1	D	1598	VAL	CA-CB-CG2	5.32	119.45	110.40
1	G	654	ASN	OD1-CG-ND2	-5.32	117.28	122.60
2	b	3528	ILE	CA-CB-CG1	5.32	119.45	110.40
2	e	4199	ASN	OD1-CG-ND2	-5.32	117.28	122.60
2	f	3811	GLN	CA-C-O	5.32	126.23	120.43
1	D	1583	ILE	CB-CA-C	5.32	118.97	111.94
1	G	702	ASP	OD1-CG-OD2	-5.32	110.13	122.90
2	c	4381	THR	N-CA-C	5.32	118.36	110.48
1	B	1808	PHE	N-CA-C	5.32	117.59	110.35
2	d	2928	ILE	O-C-N	-5.32	117.41	123.10
2	e	4265	GLN	CB-CA-C	5.32	118.96	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	4310	LYS	CA-CB-CG	5.32	124.74	114.10
2	b	3613	ASP	CA-CB-CG	5.32	117.92	112.60
2	e	4184	VAL	CA-C-O	5.32	127.21	121.36
2	e	4438	GLN	N-CA-C	5.32	117.16	108.76
2	g	2674	TYR	CA-C-O	-5.32	115.55	121.51
1	A	24	ILE	CA-CB-CG1	5.32	119.44	110.40
2	g	2420	SER	O-C-N	-5.32	117.77	121.65
1	B	1832	ALA	CA-C-O	5.31	127.74	121.58
1	C	613	GLU	CA-C-O	-5.31	114.29	120.03
1	C	848	GLU	CB-CA-C	5.31	118.80	110.19
2	f	3510	ALA	N-CA-CB	-5.31	102.78	111.66
1	A	180	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	C	991	GLU	CA-C-O	-5.31	115.17	121.60
1	F	1495	ASN	OD1-CG-ND2	-5.31	117.29	122.60
2	a	2512	LEU	CB-CA-C	5.31	117.81	110.16
2	c	4405	GLY	O-C-N	5.31	127.08	121.77
2	d	3304	GLU	CA-C-O	-5.31	114.79	120.42
2	f	3522	ARG	CB-CA-C	5.31	119.64	110.77
2	g	2663	ASP	N-CA-C	5.31	117.48	108.02
2	g	2493	VAL	CA-CB-CG2	5.31	119.43	110.40
1	G	872	ALA	N-CA-CB	-5.31	102.85	111.24
2	c	4126	GLN	O-C-N	-5.31	116.99	123.10
2	d	2942	CYS	CA-C-N	5.31	128.39	120.90
2	d	2942	CYS	C-N-CA	5.31	128.39	120.90
1	A	412	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	D	1242	PHE	CA-C-O	-5.31	115.78	121.56
1	E	1959	PHE	CA-C-O	5.31	126.09	120.36
2	c	4017	THR	CA-C-N	5.31	124.92	119.56
2	c	4017	THR	C-N-CA	5.31	124.92	119.56
2	c	4024	GLU	CA-C-O	5.31	127.39	121.40
1	E	2138	VAL	N-CA-C	5.30	116.36	108.46
1	F	1207	PHE	CA-CB-CG	5.30	119.10	113.80
1	G	577	GLU	N-CA-C	5.30	117.98	110.50
1	G	894	VAL	CA-CB-CG2	5.30	119.42	110.40
2	c	4478	THR	O-C-N	-5.30	116.60	122.86
2	e	4053	PHE	CA-CB-CG	5.30	119.11	113.80
2	f	3462	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	1996	ASN	CA-CB-CG	-5.30	107.30	112.60
1	D	1315	HIS	CB-CG-CD2	-5.30	124.31	131.20
2	a	2637	TYR	N-CA-C	5.30	118.04	109.40
2	g	2782	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	B	1839	ASN	OD1-CG-ND2	-5.30	117.30	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	2288	VAL	N-CA-C	5.30	114.00	106.53
1	B	1702	THR	CA-C-O	-5.30	114.91	121.06
1	D	1617	ILE	CA-C-O	-5.30	115.08	121.54
1	E	1754	ASN	CA-CB-CG	5.30	117.90	112.60
1	D	1244	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	F	1296	LEU	CB-CA-C	5.30	119.27	110.74
2	e	4471	CYS	CA-C-N	5.30	128.60	122.35
2	e	4471	CYS	C-N-CA	5.30	128.60	122.35
1	C	772	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	C	1007	GLU	CA-C-N	5.29	129.92	121.66
1	C	1007	GLU	C-N-CA	5.29	129.92	121.66
1	B	1850	VAL	N-CA-C	5.29	115.51	110.53
1	E	1762	VAL	CA-CB-CG1	5.29	119.40	110.40
1	G	1019	PRO	CA-C-N	5.29	130.33	122.71
1	G	1019	PRO	C-N-CA	5.29	130.33	122.71
2	c	3980	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	C	697	LYS	CB-CA-C	5.29	119.92	109.66
1	E	1942	ILE	N-CA-C	5.29	115.69	107.28
1	F	1407	GLU	O-C-N	-5.29	117.22	123.25
1	G	705	GLU	CA-C-N	5.29	126.03	120.11
1	G	705	GLU	C-N-CA	5.29	126.03	120.11
2	f	3773	PHE	CB-CA-C	5.29	118.49	109.24
2	d	3266	LYS	O-C-N	-5.29	115.22	122.46
1	F	1195	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	G	1010	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	114	VAL	N-CA-C	5.28	116.32	107.18
1	E	1804	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	100	VAL	O-C-N	-5.28	116.70	122.83
1	F	1496	PHE	CA-C-N	5.28	128.26	120.82
1	F	1496	PHE	C-N-CA	5.28	128.26	120.82
2	b	3876	ALA	CA-C-N	5.28	130.29	123.00
2	b	3876	ALA	C-N-CA	5.28	130.29	123.00
2	e	4149	ASN	CA-C-O	5.28	126.88	120.81
1	C	723	ALA	N-CA-C	5.28	119.43	113.15
1	C	942	HIS	ND1-CG-CD2	5.28	111.38	106.10
1	F	1364	VAL	CA-CB-CG2	5.28	119.37	110.40
1	F	1536	PRO	CB-CA-C	5.28	117.88	110.60
2	a	2332	ARG	NE-CZ-NH2	-5.28	114.45	119.20
2	a	2451	LYS	O-C-N	-5.28	116.53	123.02
2	g	2548	VAL	N-CA-CB	-5.28	105.64	111.66
2	g	2570	ALA	CB-CA-C	5.28	117.96	109.41
1	A	274	ILE	O-C-N	-5.28	116.99	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	3893	ILE	CA-C-N	5.28	128.97	121.42
2	b	3893	ILE	C-N-CA	5.28	128.97	121.42
2	c	4449	PRO	CB-CA-C	5.28	116.20	111.40
2	e	4375	PRO	N-CA-C	5.28	118.60	111.22
2	g	2745	THR	CA-C-O	5.28	127.67	121.87
1	A	59	THR	CA-CB-OG1	5.27	117.51	109.60
1	C	851	VAL	O-C-N	-5.27	117.46	123.10
2	f	3722	ARG	CD-NE-CZ	5.27	131.78	124.40
2	f	3846	ILE	CA-C-N	5.27	130.94	122.14
2	f	3846	ILE	C-N-CA	5.27	130.94	122.14
1	C	840	ILE	O-C-N	-5.27	116.97	123.09
1	D	1312	ARG	CA-C-N	5.27	127.87	120.28
1	D	1312	ARG	C-N-CA	5.27	127.87	120.28
2	a	2447	LYS	CA-C-O	-5.27	115.09	120.99
1	A	102	ASP	CA-C-O	5.27	127.06	121.05
1	B	2072	PRO	CA-N-CD	-5.27	104.62	112.00
2	e	4191	ALA	CB-CA-C	-5.27	100.59	109.50
1	A	337	ILE	CA-C-N	5.27	130.79	122.36
1	A	337	ILE	C-N-CA	5.27	130.79	122.36
1	B	1849	ILE	CA-C-N	5.27	127.30	120.56
1	B	1849	ILE	C-N-CA	5.27	127.30	120.56
1	F	1653	PHE	CA-CB-CG	5.27	119.07	113.80
2	c	4161	VAL	N-CA-C	5.27	115.48	108.11
2	c	3936	ARG	NE-CZ-NH2	5.26	123.94	119.20
2	d	3279	GLU	CA-C-O	5.26	126.29	120.71
2	d	3363	CYS	N-CA-C	5.26	121.47	112.99
2	c	4124	LYS	CB-CA-C	5.26	119.87	109.66
2	f	3773	PHE	CA-CB-CG	-5.26	108.54	113.80
1	E	1955	TRP	N-CA-CB	-5.26	103.59	110.59
2	b	3533	PRO	N-CD-CG	5.26	111.09	103.20
2	f	3419	PRO	N-CA-CB	5.26	108.78	103.25
1	A	241	VAL	CA-C-N	5.26	131.20	121.94
1	A	241	VAL	C-N-CA	5.26	131.20	121.94
2	f	3770	ILE	CB-CA-C	5.26	118.41	111.21
1	C	997	THR	CA-CB-CG2	5.26	119.44	110.50
2	c	3986	PHE	CA-C-O	5.26	127.48	121.28
1	B	2087	ILE	CA-C-N	5.25	130.84	122.59
1	B	2087	ILE	C-N-CA	5.25	130.84	122.59
1	C	882	ARG	NH1-CZ-NH2	-5.25	112.47	119.30
2	c	4447	VAL	N-CA-C	5.25	115.34	107.51
2	c	4250	ARG	CB-CA-C	5.25	116.27	109.28
1	D	1223	GLU	CB-CG-CD	5.25	121.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1397	SER	CA-C-N	5.25	130.10	122.28
1	F	1397	SER	C-N-CA	5.25	130.10	122.28
2	b	3514	ASP	CA-CB-CG	5.25	117.85	112.60
2	c	4180	ASP	OD1-CG-OD2	-5.25	110.29	122.90
2	e	4058	VAL	CA-CB-CG1	-5.25	101.47	110.40
2	e	4113	ARG	NE-CZ-NH1	5.25	126.75	121.50
2	e	4272	ASN	CA-CB-CG	5.25	117.85	112.60
1	G	697	LYS	O-C-N	-5.25	116.95	123.36
2	b	3519	MET	CA-C-N	5.25	129.00	120.60
2	b	3519	MET	C-N-CA	5.25	129.00	120.60
1	B	1800	ASP	CA-C-N	5.25	130.06	122.77
1	B	1800	ASP	C-N-CA	5.25	130.06	122.77
1	B	1977	GLN	N-CA-C	-5.25	105.47	111.14
1	B	2190	ALA	O-C-N	-5.25	115.40	122.43
1	E	2209	GLU	CB-CA-C	-5.25	100.06	109.24
2	g	2352	PRO	CA-C-O	5.25	125.38	118.98
1	E	1914	VAL	CA-C-O	-5.25	115.72	121.28
1	E	2138	VAL	CA-C-N	5.25	130.47	122.65
1	E	2138	VAL	C-N-CA	5.25	130.47	122.65
1	G	1017	ILE	O-C-N	-5.25	116.78	121.87
2	b	3642	ASN	OD1-CG-ND2	-5.25	117.35	122.60
2	b	3528	ILE	N-CA-C	5.25	119.56	113.42
1	D	1340	GLN	CG-CD-NE2	5.24	124.27	116.40
1	D	1537	ASP	CB-CA-C	5.24	118.08	110.79
1	F	1499	PHE	CA-CB-CG	5.24	119.04	113.80
2	b	3715	ASN	CB-CA-C	5.24	117.89	110.02
1	B	2115	THR	OG1-CB-CG2	-5.24	98.82	109.30
1	A	385	ARG	CD-NE-CZ	5.24	131.74	124.40
1	C	716	ARG	N-CA-C	5.24	117.15	109.24
1	D	1632	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	E	2214	ARG	CB-CA-C	5.24	118.74	109.89
1	D	1674	CYS	O-C-N	-5.24	116.83	123.17
2	e	4273	PRO	CA-C-N	5.24	124.56	118.85
2	e	4273	PRO	C-N-CA	5.24	124.56	118.85
1	A	142	THR	CA-C-N	5.24	129.46	120.72
1	A	142	THR	C-N-CA	5.24	129.46	120.72
1	B	2061	ASN	N-CA-C	5.24	117.64	109.52
1	E	2162	VAL	CA-CB-CG1	5.24	119.30	110.40
1	G	664	ILE	CA-CB-CG1	5.24	119.30	110.40
2	b	3876	ALA	O-C-N	-5.24	115.77	122.94
2	a	2749	GLN	CG-CD-OE1	5.23	131.27	120.80
1	A	339	PHE	CA-CB-CG	5.23	119.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2003	VAL	CA-CB-CG2	5.23	119.30	110.40
1	E	2200	SER	CB-CA-C	-5.23	100.95	110.63
2	b	3675	ILE	CA-C-N	5.23	132.59	122.07
2	b	3675	ILE	C-N-CA	5.23	132.59	122.07
2	d	3165	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	g	2763	ARG	NH1-CZ-NH2	-5.23	112.50	119.30
2	g	2782	ARG	NH1-CZ-NH2	-5.23	112.50	119.30
1	A	126	HIS	CA-CB-CG	5.23	119.03	113.80
1	E	1890	ALA	N-CA-C	5.23	117.63	109.52
2	b	3383	ILE	CB-CA-C	5.23	116.13	111.00
2	d	3343	GLY	CA-C-N	5.23	128.27	120.95
2	d	3343	GLY	C-N-CA	5.23	128.27	120.95
2	e	4151	HIS	ND1-CE1-NE2	5.23	113.63	108.40
2	c	4450	ILE	CA-CB-CG1	5.23	119.29	110.40
1	B	2145	CYS	CA-C-N	5.23	125.39	119.90
1	B	2145	CYS	C-N-CA	5.23	125.39	119.90
2	c	4017	THR	CA-C-O	-5.23	116.43	121.08
1	D	1352	ILE	O-C-N	-5.23	116.85	121.61
1	F	1378	VAL	O-C-N	-5.23	117.81	123.14
2	c	4267	GLU	CB-CA-C	5.23	118.42	109.80
2	e	4175	ARG	NE-CZ-NH2	5.23	123.90	119.20
2	g	2670	LYS	CA-C-O	5.23	126.88	120.92
1	B	1719	ILE	N-CA-CB	-5.22	104.13	112.07
1	E	1810	GLN	CA-C-N	5.22	127.28	120.28
1	E	1810	GLN	C-N-CA	5.22	127.28	120.28
1	G	856	GLU	CA-C-O	-5.22	115.86	121.56
2	e	4006	TYR	N-CA-C	5.22	117.94	109.06
2	e	4369	ASP	CA-CB-CG	5.22	117.83	112.60
2	f	3880	TYR	N-CA-C	5.22	117.60	110.55
1	F	1205	THR	CA-C-N	5.22	124.73	119.19
1	F	1205	THR	C-N-CA	5.22	124.73	119.19
2	c	4107	THR	N-CA-C	-5.22	107.08	113.50
2	d	2948	VAL	CA-C-N	5.22	128.92	121.03
2	d	2948	VAL	C-N-CA	5.22	128.92	121.03
2	f	3466	PRO	N-CA-CB	5.22	106.22	101.83
1	A	308	LYS	N-CA-C	-5.22	105.76	111.82
1	F	1220	ASN	CA-CB-CG	-5.22	107.38	112.60
2	g	2371	ILE	CB-CG1-CD1	5.22	124.77	113.80
1	D	1583	ILE	CA-C-N	5.22	129.55	122.56
1	D	1583	ILE	C-N-CA	5.22	129.55	122.56
1	F	1231	LYS	N-CA-CB	-5.22	101.87	111.37
2	a	2458	ASP	CB-CA-C	5.22	119.76	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	3830	PRO	CA-N-CD	-5.22	104.69	112.00
2	c	3958	GLN	N-CA-C	5.22	118.18	107.69
2	d	2972	GLY	N-CA-C	5.22	118.10	110.38
1	G	663	ARG	CD-NE-CZ	5.22	131.70	124.40
2	b	3563	GLN	CA-CB-CG	5.22	124.53	114.10
2	c	4462	THR	CA-C-N	5.22	129.62	122.84
2	c	4462	THR	C-N-CA	5.22	129.62	122.84
2	d	3076	ARG	NE-CZ-NH1	5.22	126.72	121.50
2	f	3390	ASN	CA-C-N	5.22	128.51	121.05
2	f	3390	ASN	C-N-CA	5.22	128.51	121.05
2	f	3515	GLU	O-C-N	-5.22	115.93	121.30
2	f	3897	ASP	CA-C-N	5.22	129.43	120.72
2	f	3897	ASP	C-N-CA	5.22	129.43	120.72
1	A	307	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	380	VAL	N-CA-C	5.21	115.88	108.42
1	D	1199	ILE	CA-CB-CG1	5.21	119.27	110.40
2	f	3580	THR	CA-CB-CG2	5.21	119.36	110.50
2	g	2507	VAL	CA-CB-CG2	5.21	119.27	110.40
1	C	839	HIS	CG-ND1-CE1	-5.21	100.44	109.30
2	b	3855	LEU	O-C-N	-5.21	115.66	122.59
2	f	3496	PHE	CA-C-N	5.21	130.86	121.06
2	f	3496	PHE	C-N-CA	5.21	130.86	121.06
1	B	2106	SER	N-CA-C	5.21	117.65	110.35
1	C	685	VAL	CA-CB-CG2	5.21	119.26	110.40
1	D	1573	GLU	CA-C-O	-5.21	115.13	121.28
1	E	1990	ASP	CA-CB-CG	5.21	117.81	112.60
1	G	867	PHE	N-CA-C	5.21	115.93	108.74
2	a	2429	THR	N-CA-C	5.21	119.86	112.93
2	f	3490	THR	CA-CB-CG2	5.21	119.36	110.50
2	f	3575	TYR	N-CA-C	5.21	117.38	111.02
1	B	1816	SER	CA-C-N	5.21	129.95	122.45
1	B	1816	SER	C-N-CA	5.21	129.95	122.45
2	f	3468	LEU	N-CA-CB	5.21	117.72	110.11
1	B	1810	GLN	O-C-N	-5.21	116.87	123.17
2	a	2368	ASN	CB-CA-C	5.21	118.22	109.89
2	a	2486	ARG	N-CA-CB	5.21	119.36	110.71
2	c	4442	PRO	O-C-N	-5.21	116.38	122.99
2	d	3224	GLU	CB-CA-C	5.21	118.71	109.65
2	f	3614	VAL	CA-C-N	5.21	128.10	120.71
2	f	3614	VAL	C-N-CA	5.21	128.10	120.71
2	g	2695	ILE	CA-CB-CG1	5.21	119.25	110.40
1	D	1180	PRO	CA-N-CD	-5.21	104.71	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	N-CA-CB	-5.20	102.29	110.30
1	B	2227	PHE	CA-CB-CG	5.20	119.00	113.80
2	a	2608	ARG	CA-C-N	5.20	130.76	122.59
2	a	2608	ARG	C-N-CA	5.20	130.76	122.59
2	d	2966	LEU	O-C-N	-5.20	117.23	123.06
2	g	2408	ARG	NH1-CZ-NH2	-5.20	112.54	119.30
1	A	74	PRO	N-CD-CG	5.20	111.00	103.20
1	A	297	LYS	CA-C-O	-5.20	114.14	120.54
1	E	2248	CYS	N-CA-C	5.20	117.00	110.24
1	G	575	LEU	N-CA-C	-5.20	101.39	109.24
1	G	610	GLY	O-C-N	-5.20	115.94	122.70
2	c	4187	ALA	N-CA-CB	-5.20	101.92	110.14
2	e	4307	ARG	NH1-CZ-NH2	-5.20	112.54	119.30
2	g	2791	THR	CA-CB-OG1	5.20	117.40	109.60
2	b	3919	ASP	CA-CB-CG	5.20	117.80	112.60
2	d	3284	ASP	CA-C-N	5.20	124.81	119.56
2	d	3284	ASP	C-N-CA	5.20	124.81	119.56
2	e	4039	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	553	ALA	O-C-N	-5.20	116.40	123.10
1	F	1405	HIS	ND1-CE1-NE2	5.20	113.60	108.40
2	f	3910	THR	O-C-N	-5.20	117.30	123.22
2	g	2325	TYR	CA-C-N	5.20	131.24	122.87
2	g	2325	TYR	C-N-CA	5.20	131.24	122.87
1	E	2005	ASN	CA-C-N	5.19	127.67	120.29
1	E	2005	ASN	C-N-CA	5.19	127.67	120.29
1	E	2053	SER	CA-C-N	5.19	131.46	121.54
1	E	2053	SER	C-N-CA	5.19	131.46	121.54
2	e	4034	GLU	CB-CA-C	5.19	119.74	109.66
2	f	3560	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	2249	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	C	763	GLY	CA-C-N	5.19	130.58	122.17
1	C	763	GLY	C-N-CA	5.19	130.58	122.17
1	E	1784	ARG	O-C-N	-5.19	116.60	122.10
1	E	1979	ASN	O-C-N	5.19	128.99	122.55
1	G	632	SER	CA-C-N	5.19	129.07	122.37
1	G	632	SER	C-N-CA	5.19	129.07	122.37
1	G	786	ILE	N-CA-C	-5.19	104.19	109.02
2	b	3455	ILE	CA-CB-CG1	5.19	119.23	110.40
2	d	2823	TRP	CE2-CD2-CE3	-5.19	113.61	118.80
2	f	3408	GLN	CA-C-O	-5.19	112.99	119.38
1	F	1372	GLU	O-C-N	-5.19	116.87	122.79
2	d	3290	HIS	CA-CB-CG	5.19	118.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	4451	THR	CA-C-N	5.19	130.22	123.06
2	e	4451	THR	C-N-CA	5.19	130.22	123.06
1	E	1909	ILE	CA-C-N	5.19	128.84	121.42
1	E	1909	ILE	C-N-CA	5.19	128.84	121.42
2	a	2467	THR	OG1-CB-CG2	-5.19	98.92	109.30
2	e	4239	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	D	1177	ILE	CA-C-O	-5.19	114.30	120.78
2	b	3415	SER	CA-CB-OG	5.19	121.47	111.10
2	e	4303	SER	CA-C-O	-5.19	113.44	119.14
1	C	1086	GLN	O-C-N	-5.19	117.14	123.10
2	c	4298	PRO	CA-C-N	5.18	128.90	120.60
2	c	4298	PRO	C-N-CA	5.18	128.90	120.60
2	e	4143	ILE	CA-C-N	5.18	129.76	122.09
2	e	4143	ILE	C-N-CA	5.18	129.76	122.09
1	D	1245	ASP	N-CA-CB	5.18	117.48	109.91
2	a	2411	TYR	O-C-N	-5.18	117.13	123.19
2	a	2646	TRP	CH2-CZ2-CE2	5.18	124.24	117.50
2	g	2482	PRO	O-C-N	-5.18	117.30	123.10
1	A	229	GLU	CA-C-N	5.18	127.66	120.92
1	A	229	GLU	C-N-CA	5.18	127.66	120.92
1	C	886	LYS	N-CA-CB	-5.18	101.13	109.94
2	d	3217	ARG	NE-CZ-NH2	5.18	123.86	119.20
2	e	4092	PRO	N-CA-CB	5.18	108.30	102.60
1	B	1716	LYS	CA-C-O	5.18	125.59	119.48
1	B	1982	ILE	O-C-N	-5.18	117.67	123.26
1	D	1204	GLU	CB-CG-CD	5.18	121.40	112.60
1	F	1268	ASP	CA-C-N	5.18	131.09	122.54
1	F	1268	ASP	C-N-CA	5.18	131.09	122.54
2	a	2373	THR	CA-C-N	5.18	130.90	121.89
2	a	2373	THR	C-N-CA	5.18	130.90	121.89
2	a	2632	SER	CA-C-O	5.18	127.92	120.51
2	f	3448	GLN	CA-C-O	-5.18	113.39	119.24
2	b	3722	ARG	N-CA-C	5.18	118.66	109.96
1	C	815	ALA	N-CA-C	5.18	119.46	113.20
2	c	4329	VAL	CA-CB-CG1	5.18	119.20	110.40
2	e	3940	ILE	N-CA-CB	5.18	114.89	110.08
2	g	2399	LYS	N-CA-CB	-5.18	102.52	110.44
1	E	1944	VAL	N-CA-C	5.17	116.17	108.46
1	F	1302	GLU	CA-C-N	5.17	128.84	122.37
1	F	1302	GLU	C-N-CA	5.17	128.84	122.37
2	f	3645	GLY	O-C-N	-5.17	116.22	122.38
1	A	488	PRO	N-CD-CG	5.17	110.01	103.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1259	THR	O-C-N	-5.17	117.42	123.27
1	G	643	LEU	O-C-N	-5.17	117.22	123.27
2	b	3489	GLU	CA-C-N	5.17	129.57	121.76
2	b	3489	GLU	C-N-CA	5.17	129.57	121.76
2	d	3038	LEU	CA-C-O	-5.17	115.54	120.97
2	g	2776	VAL	CA-CB-CG2	5.17	119.19	110.40
1	C	638	GLU	CB-CG-CD	5.17	121.39	112.60
2	b	3785	ASN	CA-CB-CG	5.17	117.77	112.60
1	E	2016	LYS	CA-C-O	-5.17	113.09	120.07
1	F	1432	ASP	CA-CB-CG	5.17	117.77	112.60
1	G	912	ILE	CA-CB-CG1	5.17	119.19	110.40
2	a	2346	THR	O-C-N	-5.17	114.96	121.21
2	b	3694	SER	CA-C-N	5.17	131.41	121.54
2	b	3694	SER	C-N-CA	5.17	131.41	121.54
2	c	4123	ILE	CA-CB-CG2	5.17	119.29	110.50
2	g	2620	ASN	N-CA-C	5.17	117.93	110.28
1	C	687	GLU	N-CA-C	5.17	117.52	110.24
2	g	2799	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	2122	SER	N-CA-CB	-5.17	103.05	110.44
2	f	3556	ARG	CD-NE-CZ	5.17	131.63	124.40
1	G	963	GLU	CB-CG-CD	-5.16	103.82	112.60
2	e	4460	SER	CB-CA-C	-5.16	101.67	109.99
2	d	2916	ILE	CB-CA-C	5.16	118.26	110.98
1	A	343	VAL	CA-CB-CG1	5.16	119.17	110.40
1	C	1047	SER	CA-C-N	5.16	130.69	122.74
1	C	1047	SER	C-N-CA	5.16	130.69	122.74
1	E	1795	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	c	4065	VAL	CA-C-N	5.16	131.02	121.94
2	c	4065	VAL	C-N-CA	5.16	131.02	121.94
2	c	4472	ILE	CA-CB-CG1	5.16	119.17	110.40
2	f	3715	ASN	CA-CB-CG	5.16	117.76	112.60
2	g	2652	ASN	CA-C-N	5.16	130.46	122.26
2	g	2652	ASN	C-N-CA	5.16	130.46	122.26
1	E	2036	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	E	2095	GLU	CA-CB-CG	5.16	124.42	114.10
2	a	2805	ASP	CA-C-O	5.16	127.23	121.40
2	b	3859	THR	CA-C-N	5.16	127.96	120.79
2	b	3859	THR	C-N-CA	5.16	127.96	120.79
2	c	4069	ASP	CA-C-O	5.16	127.18	120.11
2	d	2958	GLU	O-C-N	5.16	125.89	121.30
2	e	4213	ASN	CB-CA-C	5.16	118.65	111.63
2	c	4398	ASP	CB-CG-OD2	5.16	130.26	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	2333	GLU	O-C-N	5.16	127.60	122.08
2	g	2343	PHE	N-CA-C	5.16	117.09	108.99
1	A	314	SER	CA-CB-OG	-5.16	100.79	111.10
1	F	1577	ASP	CA-CB-CG	5.16	117.76	112.60
2	b	3738	ALA	CA-C-O	-5.16	115.20	121.28
2	d	2828	CYS	CA-C-O	5.16	127.04	121.06
2	d	2921	ASP	N-CA-CB	-5.16	102.02	110.52
2	d	3258	ASP	CA-C-N	5.16	130.99	122.33
2	d	3258	ASP	C-N-CA	5.16	130.99	122.33
2	a	2798	CYS	N-CA-C	5.15	116.13	108.86
2	c	4131	GLN	OE1-CD-NE2	-5.15	117.45	122.60
2	e	4255	THR	CA-C-N	5.15	130.83	122.53
2	e	4255	THR	C-N-CA	5.15	130.83	122.53
1	B	2191	GLU	CA-CB-CG	5.15	124.40	114.10
1	D	1523	VAL	O-C-N	-5.15	117.51	123.07
2	f	3421	VAL	CA-CB-CG1	5.15	119.16	110.40
1	E	1781	LEU	CB-CG-CD2	5.15	126.15	110.70
1	G	1120	HIS	CA-CB-CG	5.15	118.95	113.80
2	b	3450	GLU	CA-C-N	5.15	131.04	121.62
2	b	3450	GLU	C-N-CA	5.15	131.04	121.62
2	c	4161	VAL	CA-C-O	5.15	125.80	120.39
2	c	4265	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	B	2024	ILE	CB-CA-C	5.15	117.84	110.84
1	D	1444	HIS	ND1-CG-CD2	5.15	111.25	106.10
1	E	2044	ILE	CA-CB-CG2	5.15	119.25	110.50
2	e	3959	VAL	N-CA-CB	5.15	119.88	111.44
2	g	2316	TYR	CA-C-N	5.15	130.20	122.58
2	g	2316	TYR	C-N-CA	5.15	130.20	122.58
1	C	887	PRO	N-CA-CB	5.15	108.12	103.34
1	E	2249	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	B	1869	ILE	CA-C-O	-5.14	115.03	120.48
2	c	4104	ILE	CA-C-O	-5.14	114.98	120.85
2	e	4455	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	A	423	ILE	N-CA-CB	5.14	118.50	111.41
1	B	1880	GLU	CB-CA-C	5.14	118.95	110.83
2	f	3699	ALA	CA-C-N	5.14	130.66	122.94
2	f	3699	ALA	C-N-CA	5.14	130.66	122.94
1	E	2111	ASN	CA-CB-CG	-5.14	107.46	112.60
1	C	602	ILE	O-C-N	-5.14	117.90	123.14
1	C	690	ALA	CA-C-N	5.14	128.51	120.75
1	C	690	ALA	C-N-CA	5.14	128.51	120.75
1	G	1042	ASN	OD1-CG-ND2	-5.14	117.46	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	2435	THR	CA-CB-CG2	5.14	119.24	110.50
2	a	2672	GLY	CA-C-N	5.14	130.09	122.94
2	a	2672	GLY	C-N-CA	5.14	130.09	122.94
2	b	3390	ASN	CA-CB-CG	5.14	117.74	112.60
2	f	3594	HIS	CA-C-O	-5.14	114.83	120.43
1	E	1768	ARG	NE-CZ-NH2	5.14	123.82	119.20
2	g	2642	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	734	THR	CA-C-N	5.14	130.37	120.66
1	C	734	THR	C-N-CA	5.14	130.37	120.66
1	G	590	ILE	O-C-N	-5.14	116.87	122.83
2	a	2705	PHE	CA-C-N	5.14	128.71	122.85
2	a	2705	PHE	C-N-CA	5.14	128.71	122.85
2	c	3942	CYS	CA-CB-SG	-5.14	102.58	114.40
2	f	3452	PHE	CB-CG-CD2	-5.14	111.97	120.70
2	g	2583	SER	CB-CA-C	5.14	118.69	110.16
2	g	2750	ARG	CB-CA-C	5.14	118.23	109.24
1	F	1670	THR	CA-CB-OG1	5.13	117.30	109.60
2	a	2714	CYS	CA-CB-SG	-5.13	102.59	114.40
2	d	2869	ARG	NH1-CZ-NH2	-5.13	112.63	119.30
2	e	4247	ALA	N-CA-CB	-5.13	102.40	110.46
2	g	2287	GLN	CB-CA-C	5.13	118.51	110.19
1	C	797	MET	N-CA-CB	-5.13	101.84	111.13
1	C	900	LYS	O-C-N	-5.13	115.76	122.59
2	a	2531	GLY	CA-C-N	5.13	127.67	120.28
2	a	2531	GLY	C-N-CA	5.13	127.67	120.28
2	b	3462	ASP	CA-C-N	5.13	128.55	121.26
2	b	3462	ASP	C-N-CA	5.13	128.55	121.26
1	D	1467	GLU	OE1-CD-OE2	-5.13	110.59	122.90
1	E	1935	VAL	CB-CA-C	5.13	118.41	110.82
1	F	1156	ILE	CA-CB-CG1	5.13	119.12	110.40
1	F	1268	ASP	CA-C-O	5.13	126.74	120.99
1	G	759	ARG	CD-NE-CZ	5.13	131.59	124.40
1	G	1032	VAL	CA-CB-CG2	5.13	119.12	110.40
1	B	1907	VAL	CA-C-O	-5.13	114.87	120.72
1	F	1620	PRO	N-CA-CB	5.13	108.24	102.60
2	d	3108	PRO	N-CD-CG	5.13	110.89	103.20
1	C	722	PRO	CA-N-CD	-5.13	104.32	111.50
1	D	1161	ALA	O-C-N	-5.13	116.30	122.15
1	D	1537	ASP	CA-C-N	5.13	129.28	120.72
1	D	1537	ASP	C-N-CA	5.13	129.28	120.72
2	f	3390	ASN	CB-CA-C	5.13	119.63	111.48
2	g	2509	ASP	CB-CG-OD2	5.13	130.19	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ILE	O-C-N	5.13	128.26	122.67
1	D	1578	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	F	1157	HIS	ND1-CG-CD2	5.13	111.23	106.10
2	b	3632	TRP	NE1-CE2-CZ2	5.13	137.79	130.10
2	g	2491	THR	N-CA-C	5.13	116.78	109.14
1	C	739	THR	OG1-CB-CG2	-5.12	99.05	109.30
2	d	3063	THR	CA-CB-CG2	5.12	119.21	110.50
2	g	2790	VAL	CA-CB-CG2	5.12	119.11	110.40
1	F	1266	ALA	N-CA-C	5.12	116.08	108.86
2	a	2287	GLN	CA-C-N	5.12	130.54	122.70
2	a	2287	GLN	C-N-CA	5.12	130.54	122.70
2	c	4412	LEU	CA-C-N	5.12	129.28	120.72
2	c	4412	LEU	C-N-CA	5.12	129.28	120.72
1	D	1433	PHE	CA-C-N	5.12	130.74	122.29
1	D	1433	PHE	C-N-CA	5.12	130.74	122.29
1	E	2215	SER	CA-C-N	5.12	129.63	122.41
1	E	2215	SER	C-N-CA	5.12	129.63	122.41
1	F	1331	VAL	N-CA-CB	5.12	116.69	110.95
1	G	1042	ASN	CB-CG-ND2	5.12	124.08	116.40
2	d	3065	GLU	CA-C-O	-5.12	115.68	121.72
1	D	1502	ASP	N-CA-C	5.12	117.60	111.71
1	G	631	THR	CA-C-O	5.12	125.27	119.18
1	G	923	LYS	O-C-N	-5.12	116.58	122.87
1	C	1120	HIS	CA-CB-CG	5.12	118.92	113.80
1	G	755	THR	O-C-N	5.12	129.05	123.22
2	a	2697	GLN	O-C-N	5.12	129.22	122.93
1	D	1268	ASP	OD1-CG-OD2	-5.11	110.63	122.90
1	G	910	ILE	CA-C-N	5.11	130.12	122.86
1	G	910	ILE	C-N-CA	5.11	130.12	122.86
2	f	3412	ILE	O-C-N	-5.11	118.28	123.19
2	f	3731	THR	O-C-N	-5.11	117.33	123.06
2	c	4457	GLY	CA-C-O	-5.11	113.97	118.77
2	d	2869	ARG	CA-C-N	5.11	131.30	121.54
2	d	2869	ARG	C-N-CA	5.11	131.30	121.54
2	g	2752	TRP	N-CA-C	5.11	117.65	110.14
1	E	1790	LYS	O-C-N	-5.11	115.71	121.43
2	a	2364	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	5	ALA	N-CA-C	5.11	118.26	110.50
1	A	212	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	D	1182	PHE	CA-CB-CG	5.11	118.91	113.80
1	E	2222	SER	N-CA-C	5.11	117.94	109.46
1	C	784	ASP	CA-CB-CG	5.11	117.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	3136	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	e	3970	TYR	CD1-CG-CD2	5.11	125.76	118.10
2	d	2927	PRO	CA-C-O	-5.10	115.77	121.23
1	B	1844	LYS	N-CA-C	5.10	117.40	108.52
1	C	650	ASP	CA-C-O	-5.10	116.26	121.87
1	F	1456	ILE	CA-C-N	5.10	124.86	119.76
1	F	1456	ILE	C-N-CA	5.10	124.86	119.76
2	a	2552	LEU	N-CA-C	5.10	118.03	110.48
2	e	4291	ASN	N-CA-C	5.10	116.87	110.24
2	f	3503	THR	CA-C-N	5.10	128.57	121.02
2	f	3503	THR	C-N-CA	5.10	128.57	121.02
2	f	3656	ASN	O-C-N	-5.10	115.57	122.41
1	B	2093	THR	O-C-N	-5.10	116.94	122.19
1	F	1266	ALA	N-CA-CB	-5.10	102.79	111.31
2	f	3864	ARG	NH1-CZ-NH2	-5.10	112.67	119.30
1	E	2168	ASP	OD1-CG-OD2	-5.10	110.66	122.90
1	E	2241	GLU	CA-C-O	-5.10	115.47	120.98
2	c	4370	VAL	CA-C-O	-5.10	115.73	121.75
1	G	814	ASP	OD1-CG-OD2	-5.10	110.66	122.90
2	c	4131	GLN	CG-CD-NE2	5.10	124.05	116.40
2	e	3973	ILE	O-C-N	-5.10	117.39	123.05
1	F	1394	THR	CA-CB-OG1	5.10	117.24	109.60
2	e	3983	ARG	CA-C-N	5.10	129.36	122.07
2	e	3983	ARG	C-N-CA	5.10	129.36	122.07
1	B	2214	ARG	CD-NE-CZ	5.09	131.53	124.40
1	F	1166	LEU	CD1-CG-CD2	-5.09	99.59	110.80
2	a	2356	LEU	CB-CA-C	5.09	118.62	110.62
2	a	2372	PHE	CA-CB-CG	5.09	118.89	113.80
2	a	2745	THR	O-C-N	-5.09	117.23	122.94
2	d	2865	ASP	CB-CA-C	5.09	119.50	109.72
2	d	3246	THR	CA-CB-CG2	5.09	119.16	110.50
1	G	897	LYS	CA-CB-CG	5.09	124.29	114.10
2	c	4260	VAL	O-C-N	-5.09	117.54	122.99
2	c	4374	SER	N-CA-C	5.09	117.19	110.36
2	e	4357	ARG	CB-CA-C	5.09	118.64	110.29
1	D	1683	ARG	CA-C-N	5.09	128.08	120.95
1	D	1683	ARG	C-N-CA	5.09	128.08	120.95
2	b	3740	ASP	CA-C-O	-5.09	115.49	119.66
2	c	4055	ASN	OD1-CG-ND2	5.09	127.69	122.60
2	d	2931	GLU	N-CA-CB	-5.09	102.69	111.55
1	D	1259	THR	O-C-N	-5.09	116.67	122.93
1	F	1225	PRO	N-CA-CB	5.09	107.59	103.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	2514	ASN	CB-CA-C	5.09	120.68	111.06
2	a	2563	GLN	OE1-CD-NE2	-5.09	117.51	122.60
2	b	3559	ILE	O-C-N	-5.09	117.70	123.20
2	d	2958	GLU	CA-C-O	-5.09	114.97	119.75
2	g	2578	PRO	N-CD-CG	5.09	110.83	103.20
2	g	2716	PRO	O-C-N	5.09	128.33	122.17
1	E	1993	GLU	N-CA-C	5.09	118.75	112.54
1	F	1466	LYS	CA-C-O	-5.09	115.97	121.87
2	a	2416	GLN	CA-C-N	-5.09	118.42	122.85
2	a	2416	GLN	C-N-CA	-5.09	118.42	122.85
2	c	4220	VAL	CB-CA-C	5.09	115.89	110.91
1	A	300	ASP	CA-CB-CG	5.08	117.69	112.60
1	G	771	LYS	N-CA-C	5.08	117.42	110.55
2	b	3667	ASN	OD1-CG-ND2	-5.08	117.52	122.60
2	d	3234	THR	CA-CB-CG2	5.08	119.14	110.50
2	e	4072	GLU	CA-C-O	5.08	124.89	119.80
1	F	1673	VAL	CA-CB-CG1	5.08	119.04	110.40
2	f	3853	PHE	CA-CB-CG	5.08	118.88	113.80
2	g	2749	GLN	N-CA-C	5.08	119.11	113.01
1	A	378	ARG	CB-CA-C	5.08	118.67	109.37
1	G	707	ASN	CA-C-N	5.08	130.44	122.21
1	G	707	ASN	C-N-CA	5.08	130.44	122.21
2	c	4161	VAL	O-C-N	-5.08	117.77	123.26
2	d	3221	ARG	CA-C-O	5.08	125.66	119.05
2	e	4352	SER	N-CA-C	5.08	116.97	108.99
2	e	4423	TRP	NE1-CE2-CD2	-5.08	100.80	107.40
1	F	1252	GLU	N-CA-CB	-5.08	102.57	110.29
2	e	4110	GLN	CG-CD-OE1	5.08	130.96	120.80
1	D	1656	SER	CA-C-N	5.08	130.21	120.97
1	D	1656	SER	C-N-CA	5.08	130.21	120.97
1	F	1242	PHE	CA-C-N	5.08	127.50	120.29
1	F	1242	PHE	C-N-CA	5.08	127.50	120.29
1	G	721	GLU	N-CA-CB	-5.08	101.33	110.37
2	c	4014	PHE	CA-CB-CG	5.08	118.88	113.80
1	E	1810	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	e	4286	VAL	N-CA-CB	5.08	116.93	110.13
2	b	3386	SER	CA-C-O	-5.08	115.17	121.06
2	c	4133	PHE	O-C-N	5.08	129.47	122.46
1	D	1230	ILE	CA-C-O	5.07	125.86	120.48
1	G	678	GLN	OE1-CD-NE2	-5.07	117.53	122.60
2	d	2899	ALA	CA-C-O	5.07	125.79	120.36
2	b	3681	VAL	O-C-N	-5.07	117.22	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	3893	ILE	O-C-N	-5.07	117.91	123.18
2	g	2803	GLU	CG-CD-OE2	5.07	130.06	118.40
1	F	1585	PRO	CA-C-N	5.07	129.78	123.14
1	F	1585	PRO	C-N-CA	5.07	129.78	123.14
2	a	2798	CYS	CA-C-N	5.07	129.72	122.72
2	a	2798	CYS	C-N-CA	5.07	129.72	122.72
1	A	122	LEU	CA-C-N	5.07	130.19	120.97
1	A	122	LEU	C-N-CA	5.07	130.19	120.97
1	E	1796	ILE	CB-CA-C	5.07	118.17	110.62
1	E	2019	PRO	N-CA-CB	5.07	108.96	103.23
2	b	3794	ALA	O-C-N	-5.07	117.09	123.27
2	c	4119	TYR	CA-C-O	-5.07	114.05	120.28
2	f	3773	PHE	N-CA-CB	-5.07	103.07	110.47
1	D	1334	LYS	N-CA-C	5.07	116.26	109.83
2	a	2427	HIS	CA-C-N	5.07	124.68	119.56
2	a	2427	HIS	C-N-CA	5.07	124.68	119.56
2	a	2664	ARG	CB-CA-C	5.07	118.51	109.29
2	g	2479	ASP	N-CA-CB	-5.07	103.75	111.15
2	g	2637	TYR	CB-CG-CD1	-5.07	113.20	120.80
1	B	1701	ILE	CA-C-O	5.06	126.43	120.71
1	B	1816	SER	CA-C-O	-5.06	114.88	120.30
1	B	1842	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	2063	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	F	1463	LYS	CB-CA-C	5.06	118.10	109.80
2	e	4002	ASP	CA-CB-CG	5.06	117.66	112.60
2	a	2451	LYS	CA-C-N	5.06	130.68	122.68
2	a	2451	LYS	C-N-CA	5.06	130.68	122.68
1	A	318	LYS	N-CA-CB	5.06	117.32	110.59
2	e	4258	VAL	CA-CB-CG1	5.06	119.00	110.40
2	f	3707	ASP	CA-C-N	5.06	130.41	122.21
2	f	3707	ASP	C-N-CA	5.06	130.41	122.21
1	C	717	ILE	N-CA-CB	5.06	116.23	110.72
1	C	738	TYR	CA-C-O	-5.06	115.54	121.46
2	a	2382	PHE	O-C-N	-5.06	117.24	122.96
2	b	3426	ARG	CA-C-N	5.06	131.20	121.54
2	b	3426	ARG	C-N-CA	5.06	131.20	121.54
2	c	4208	THR	CA-CB-CG2	5.06	119.10	110.50
2	c	4321	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	1587	GLN	OE1-CD-NE2	-5.06	117.54	122.60
2	d	3175	THR	CA-CB-OG1	5.06	117.18	109.60
1	A	298	ASN	CA-C-N	5.05	130.52	122.74
1	A	298	ASN	C-N-CA	5.05	130.52	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2181	SER	CA-C-N	5.05	129.76	123.14
1	B	2181	SER	C-N-CA	5.05	129.76	123.14
1	C	792	LYS	CG-CD-CE	5.05	122.92	111.30
1	D	1603	LEU	N-CA-CB	-5.05	102.68	110.46
1	A	357	LYS	CB-CA-C	5.05	117.84	110.26
1	E	1920	VAL	N-CA-C	5.05	115.76	108.48
2	c	3970	TYR	CB-CA-C	5.05	118.96	109.71
2	c	4222	PRO	N-CD-CG	5.05	110.78	103.20
1	G	576	ARG	NE-CZ-NH1	5.05	126.55	121.50
2	a	2312	ARG	CA-C-N	5.05	130.49	122.61
2	a	2312	ARG	C-N-CA	5.05	130.49	122.61
2	e	4445	SER	CA-C-N	5.05	130.63	122.29
2	e	4445	SER	C-N-CA	5.05	130.63	122.29
2	g	2686	ARG	CD-NE-CZ	5.05	131.47	124.40
1	A	470	ASP	CB-CA-C	5.05	119.01	109.37
1	B	1985	LEU	CB-CA-C	5.05	118.57	110.29
1	E	2238	THR	CA-CB-CG2	5.05	119.08	110.50
1	G	958	ASP	CA-C-N	5.05	129.22	120.58
1	G	958	ASP	C-N-CA	5.05	129.22	120.58
2	a	2299	TYR	CA-C-N	5.05	131.00	122.87
2	a	2299	TYR	C-N-CA	5.05	131.00	122.87
2	a	2305	PRO	N-CA-CB	5.05	108.55	103.25
2	g	2524	ILE	N-CA-CB	5.05	116.76	111.00
1	A	112	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	B	1872	THR	O-C-N	-5.05	117.29	122.84
2	b	3918	ASN	CB-CG-ND2	5.05	123.97	116.40
2	e	4107	THR	CA-CB-CG2	5.04	119.08	110.50
1	F	1502	ASP	OD1-CG-OD2	-5.04	110.80	122.90
2	b	3654	LYS	O-C-N	5.04	129.42	122.46
2	b	3654	LYS	N-CA-CB	-5.04	102.18	110.40
2	c	3986	PHE	CA-C-N	5.04	130.14	121.87
2	c	3986	PHE	C-N-CA	5.04	130.14	121.87
2	c	4330	PHE	N-CA-CB	-5.04	104.32	110.98
2	f	3877	ARG	NH1-CZ-NH2	-5.04	112.75	119.30
1	C	1000	GLY	CA-C-N	5.04	130.90	122.73
1	C	1000	GLY	C-N-CA	5.04	130.90	122.73
1	E	1717	ASN	CA-C-O	-5.04	115.01	119.75
2	b	3809	ILE	CA-CB-CG1	5.04	118.97	110.40
1	B	2196	ALA	N-CA-CB	-5.04	103.05	111.06
2	c	4172	GLU	CA-C-N	5.04	127.73	122.14
2	c	4172	GLU	C-N-CA	5.04	127.73	122.14
2	c	4313	ASP	N-CA-C	5.04	114.10	108.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	3064	VAL	N-CA-C	5.04	115.63	108.42
2	g	2440	LEU	N-CA-CB	-5.04	104.38	110.53
1	D	1352	ILE	N-CA-CB	-5.04	104.81	111.21
1	F	1169	THR	O-C-N	-5.04	116.64	123.19
2	c	3957	GLN	CA-C-N	5.04	130.74	123.13
2	c	3957	GLN	C-N-CA	5.04	130.74	123.13
2	e	4104	ILE	CA-C-O	-5.04	115.18	120.57
2	f	3427	ASN	OD1-CG-ND2	-5.04	117.56	122.60
2	g	2299	TYR	O-C-N	5.04	129.27	123.17
2	g	2678	VAL	CA-C-O	5.04	127.12	121.28
2	b	3853	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	392	ASP	CB-CA-C	5.04	118.06	109.75
1	E	2132	GLY	O-C-N	-5.04	117.92	123.66
1	G	578	GLY	CA-C-N	5.04	131.20	122.64
1	G	578	GLY	C-N-CA	5.04	131.20	122.64
2	c	3973	ILE	CA-C-N	5.04	130.46	121.75
2	c	3973	ILE	C-N-CA	5.04	130.46	121.75
1	A	48	PRO	N-CD-CG	5.03	110.75	103.20
1	C	701	THR	CA-C-N	5.03	130.49	122.94
1	C	701	THR	C-N-CA	5.03	130.49	122.94
2	c	4051	THR	CA-CB-CG2	5.03	119.06	110.50
1	E	1885	THR	CA-CB-OG1	5.03	117.15	109.60
2	d	3205	THR	N-CA-C	5.03	117.06	109.41
2	f	3854	SER	N-CA-C	5.03	117.45	109.50
1	A	310	ALA	N-CA-C	5.03	117.02	110.43
1	A	471	LEU	CA-C-O	5.03	125.78	120.10
1	B	1762	VAL	O-C-N	5.03	128.63	123.05
1	B	1910	ARG	NE-CZ-NH1	5.03	126.53	121.50
2	g	2403	ASP	N-CA-CB	-5.03	104.65	112.30
1	C	692	HIS	CG-ND1-CE1	-5.03	100.75	109.30
1	G	590	ILE	CA-CB-CG2	-5.03	101.95	110.50
2	b	3756	ASP	O-C-N	-5.03	115.54	121.32
2	b	3864	ARG	CB-CA-C	5.03	119.40	110.85
2	e	4134	GLY	CA-C-N	5.03	127.99	120.95
2	e	4134	GLY	C-N-CA	5.03	127.99	120.95
2	e	4176	VAL	CA-CB-CG1	5.03	118.95	110.40
1	E	2037	PHE	CA-CB-CG	5.03	118.83	113.80
2	a	2347	PRO	N-CA-CB	5.03	108.34	103.51
2	d	3080	THR	CA-CB-OG1	5.03	117.14	109.60
2	g	2540	LYS	CB-CA-C	5.03	118.62	110.37
1	B	1895	GLY	CA-C-N	5.03	128.34	120.75
1	B	1895	GLY	C-N-CA	5.03	128.34	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	788	VAL	CA-C-N	5.03	130.54	122.50
1	G	788	VAL	C-N-CA	5.03	130.54	122.50
2	d	3140	SER	N-CA-C	5.03	118.00	109.76
1	C	875	ALA	CB-CA-C	5.02	117.82	109.53
1	F	1249	GLY	O-C-N	-5.02	117.73	123.51
2	e	3982	PRO	CA-C-N	5.02	128.60	121.42
2	e	3982	PRO	C-N-CA	5.02	128.60	121.42
1	B	1739	THR	O-C-N	-5.02	117.09	123.17
1	D	1452	LYS	CA-C-N	5.02	125.29	119.92
1	D	1452	LYS	C-N-CA	5.02	125.29	119.92
1	D	1466	LYS	CB-CA-C	5.02	118.70	109.46
1	F	1591	HIS	CB-CG-CD2	-5.02	124.67	131.20
2	b	3850	PRO	N-CA-CB	5.02	108.13	102.60
2	f	3881	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	G	871	VAL	CB-CA-C	5.02	118.21	110.28
2	b	3569	GLN	CA-C-O	-5.02	115.37	120.99
2	c	4344	ILE	CA-C-N	5.02	130.39	122.36
2	c	4344	ILE	C-N-CA	5.02	130.39	122.36
2	d	3035	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	D	1620	PRO	N-CD-CG	5.02	109.82	103.80
1	D	1674	CYS	N-CA-C	5.02	116.82	109.24
1	F	1179	GLU	OE1-CD-OE2	-5.02	110.86	122.90
2	d	2973	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	B	2071	LEU	N-CA-C	5.02	116.20	109.83
1	C	851	VAL	CA-C-N	5.01	130.75	122.33
1	C	851	VAL	C-N-CA	5.01	130.75	122.33
1	E	1854	PRO	N-CD-CG	5.01	109.82	103.80
1	E	2164	VAL	CA-CB-CG1	5.01	118.92	110.40
1	F	1136	THR	N-CA-CB	-5.01	102.24	110.41
1	A	204	VAL	O-C-N	-5.01	117.49	123.00
2	d	3039	PRO	N-CA-CB	5.01	107.31	103.30
2	g	2410	LYS	CB-CA-C	5.01	118.42	109.65
2	g	2608	ARG	CD-NE-CZ	5.01	131.42	124.40
1	E	1908	GLN	CG-CD-NE2	5.01	123.92	116.40
2	f	3725	GLU	N-CA-C	5.01	118.65	112.54
1	A	133	ASN	N-CA-CB	-5.01	102.16	111.13
1	C	742	VAL	N-CA-C	5.01	115.79	108.53
1	E	1763	THR	CA-CB-CG2	5.01	119.02	110.50
1	F	1587	GLN	O-C-N	-5.01	117.11	123.17
2	c	4287	GLY	CA-C-N	5.01	129.47	121.66
2	c	4287	GLY	C-N-CA	5.01	129.47	121.66
2	e	3958	GLN	N-CA-C	5.01	117.42	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	3839	ALA	CB-CA-C	5.01	118.73	109.71
2	g	2402	PRO	CB-CA-C	5.01	117.51	110.95
1	E	2076	ARG	NH1-CZ-NH2	-5.01	112.79	119.30
2	a	2763	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	D	1457	PRO	N-CD-CG	5.00	110.71	103.20
1	B	1974	THR	N-CA-CB	5.00	118.42	110.16
1	D	1542	TYR	N-CA-CB	-5.00	103.97	110.88
2	c	4433	ALA	CA-C-N	5.00	129.05	122.30
2	c	4433	ALA	C-N-CA	5.00	129.05	122.30
2	f	3518	THR	CA-C-O	-5.00	116.23	121.88
1	B	1734	ILE	CA-C-O	5.00	126.52	120.67
2	f	3721	VAL	O-C-N	-5.00	117.65	123.00

There are no chirality outliers.

All (168) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	40	TYR	Sidechain
1	A	416	TYR	Sidechain
1	A	429	ARG	Sidechain
1	A	474	HIS	Sidechain
1	A	477	SER	Peptide
1	A	551	ARG	Sidechain
1	B	1704	PRO	Peptide,Mainchain
1	B	1779	TYR	Sidechain
1	B	1799	LEU	Peptide
1	B	1856	TYR	Sidechain
1	B	1862	LEU	Peptide
1	B	1884	TYR	Sidechain
1	B	1910	ARG	Sidechain
1	B	2014	ARG	Sidechain
1	B	2045	TYR	Sidechain
1	B	2077	TYR	Sidechain
1	B	2127	ARG	Sidechain
1	B	2154	THR	Peptide
1	B	2161	TYR	Sidechain
1	B	2191	GLU	Mainchain
1	C	1029	TYR	Sidechain
1	C	1082	ARG	Sidechain
1	C	604	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	636	ARG	Sidechain
1	C	647	TYR	Sidechain
1	C	715	TYR	Sidechain
1	C	746	ARG	Sidechain
1	C	759	ARG	Sidechain
1	C	905	PHE	Sidechain
1	C	951	ARG	Sidechain
1	C	976	TYR	Sidechain
1	C	982	TYR	Sidechain
1	C	993	TYR	Sidechain
1	D	1138	PRO	Peptide
1	D	1172	TYR	Sidechain
1	D	1295	TYR	Sidechain
1	D	1304	TYR	Sidechain
1	D	1318	TYR	Sidechain
1	D	1352	ILE	Mainchain
1	D	1403	TYR	Sidechain
1	D	1436	ILE	Mainchain
1	D	1451	TYR	Sidechain
1	D	1508	HIS	Sidechain
1	D	1608	ASN	Mainchain
1	D	1612	PHE	Mainchain
1	D	1614	PHE	Sidechain
1	D	1659	GLN	Peptide
1	D	1683	ARG	Mainchain
1	E	1736	TYR	Sidechain
1	E	1748	PHE	Sidechain
1	E	1753	PHE	Sidechain
1	E	1774	PHE	Sidechain
1	E	1778	GLY	Mainchain
1	E	1861	TYR	Sidechain
1	E	1932	GLU	Sidechain
1	E	2009	PHE	Mainchain
1	E	2010	HIS	Peptide,Sidechain
1	E	2013	ILE	Peptide
1	E	2014	ARG	Mainchain
1	E	2052	ARG	Sidechain
1	E	2108	TYR	Sidechain
1	E	2114	TYR	Sidechain
1	E	2127	ARG	Sidechain
1	E	2161	TYR	Peptide
1	E	2219	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	F	1138	PRO	Peptide
1	F	1172	TYR	Sidechain
1	F	1195	ASN	Mainchain
1	F	1290	TYR	Sidechain
1	F	1294	PHE	Sidechain
1	F	1318	TYR	Sidechain
1	F	1443	PHE	Sidechain
1	F	1486	ARG	Sidechain
1	F	1511	TYR	Sidechain
1	F	1628	LYS	Mainchain
1	F	1645	LYS	Mainchain
1	F	1678	HIS	Sidechain
1	G	606	TYR	Sidechain
1	G	616	PHE	Sidechain
1	G	652	ARG	Sidechain
1	G	724	TYR	Sidechain
1	G	746	ARG	Sidechain
1	G	752	TYR	Sidechain
1	G	930	PHE	Peptide
1	G	943	ALA	Mainchain
1	G	982	TYR	Sidechain
2	a	2284	PHE	Sidechain
2	a	2296	TYR	Sidechain
2	a	2308	ASP	Peptide
2	a	2315	PHE	Sidechain
2	a	2316	TYR	Sidechain
2	a	2333	GLU	Sidechain
2	a	2350	TYR	Sidechain
2	a	2386	ARG	Sidechain
2	a	2402	PRO	Mainchain
2	a	2408	ARG	Sidechain
2	a	2442	ARG	Sidechain
2	a	2462	PHE	Sidechain
2	a	2475	ASP	Peptide
2	a	2620	ASN	Peptide
2	a	2750	ARG	Sidechain
2	b	3395	PHE	Sidechain
2	b	3525	TYR	Sidechain
2	b	3575	TYR	Sidechain
2	b	3633	ARG	Sidechain
2	b	3636	TYR	Sidechain
2	b	3736	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	b	3751	TYR	Sidechain
2	b	3769	SER	Mainchain
2	b	3788	TYR	Sidechain
2	b	3833	SER	Peptide
2	b	3880	TYR	Sidechain
2	c	3979	ASP	Peptide
2	c	4035	ASP	Peptide
2	c	4040	TYR	Sidechain
2	c	4048	TYR	Sidechain
2	c	4131	GLN	Sidechain
2	c	4132	TYR	Sidechain
2	c	4160	TYR	Sidechain
2	c	4220	VAL	Mainchain
2	c	4279	ARG	Mainchain
2	c	4293	TYR	Sidechain
2	c	4455	ARG	Sidechain
2	d	2853	TYR	Sidechain
2	d	2857	TYR	Sidechain
2	d	2889	ARG	Sidechain
2	d	3043	ARG	Sidechain
2	d	3187	ARG	Sidechain
2	e	3941	PRO	Peptide
2	e	3955	PHE	Sidechain
2	e	4006	TYR	Sidechain
2	e	4034	GLU	Peptide
2	e	4040	TYR	Sidechain
2	e	4192	ASN	Peptide
2	e	4261	ASN	Mainchain
2	e	4264	ASP	Peptide
2	e	4296	TYR	Peptide
2	e	4301	ARG	Sidechain
2	e	4307	ARG	Sidechain
2	e	4434	ARG	Sidechain
2	f	3379	ARG	Sidechain
2	f	3398	PHE	Sidechain
2	f	3410	TYR	Sidechain
2	f	3414	TYR	Sidechain
2	f	3442	ARG	Sidechain
2	f	3483	TYR	Sidechain
2	f	3513	LYS	Peptide
2	f	3636	TYR	Sidechain
2	f	3764	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	f	3853	PHE	Sidechain
2	f	3880	TYR	Sidechain
2	g	2284	PHE	Mainchain
2	g	2386	ARG	Sidechain
2	g	2412	SER	Peptide
2	g	2442	ARG	Sidechain
2	g	2443	GLU	Sidechain
2	g	2461	TYR	Sidechain
2	g	2574	ARG	Sidechain
2	g	2579	ARG	Sidechain
2	g	2660	ARG	Sidechain
2	g	2766	TYR	Sidechain
2	g	2775	TYR	Sidechain
2	g	2789	SER	Peptide
2	g	2795	VAL	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4355	4294	4294	11	0
1	B	4355	4294	4291	8	0
1	C	4355	4294	4291	6	0
1	D	4355	4294	4291	17	0
1	E	4355	4294	4291	58	0
1	F	4355	4294	4291	13	0
1	G	4355	4294	4291	9	0
2	a	4268	4154	4151	26	0
2	b	4268	4154	4150	20	0
2	c	4268	4154	4151	18	0
2	d	4268	4154	4151	9	0
2	e	4268	4154	4151	12	0
2	f	4268	4154	4151	16	0
2	g	4268	4154	4151	19	0
All	All	60361	59136	59096	236	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 (236) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2010:HIS:CG	1:E:2010:HIS:ND1	1.76	1.54
1:E:2010:HIS:N	1:E:2010:HIS:CA	1.73	1.51
1:E:2011:LYS:C	1:E:2012:SER:N	1.70	1.47
2:b:3691:SER:OG	2:b:3692:PRO:CD	1.65	1.44
2:f:3691:SER:OG	2:f:3692:PRO:CD	1.69	1.38
1:E:1769:GLU:CG	1:E:1835:ALA:HB1	1.51	1.38
2:a:2333:GLU:O	2:a:2333:GLU:CD	1.66	1.35
1:E:1769:GLU:HG2	1:E:1835:ALA:CB	1.60	1.31
1:E:2010:HIS:ND1	1:E:2010:HIS:CE1	1.99	1.31
2:a:2333:GLU:CD	2:a:2333:GLU:C	2.02	1.26
1:D:1444:HIS:CE1	1:D:1445:LYS:HG2	1.71	1.26
2:g:2577:SER:HB3	2:g:2578:PRO:CD	1.62	1.25
2:b:3691:SER:OG	2:b:3692:PRO:HD3	1.04	1.17
2:a:2577:SER:HB3	2:a:2578:PRO:CD	1.74	1.16
2:g:2577:SER:HB3	2:g:2578:PRO:HD2	1.18	1.12
2:a:2577:SER:HB3	2:a:2578:PRO:HD2	1.19	1.12
2:g:2577:SER:CB	2:g:2578:PRO:CD	2.30	1.09
1:E:2010:HIS:ND1	1:E:2010:HIS:CA	2.16	1.08
1:E:2010:HIS:ND1	1:E:2010:HIS:HA	1.61	1.05
1:E:1804:ASN:ND2	1:E:1835:ALA:HB3	1.74	1.02
2:a:2577:SER:CB	2:a:2578:PRO:CD	2.38	0.99
2:f:3691:SER:OG	2:f:3692:PRO:HD2	0.80	0.97
1:E:1802:ASN:HA	1:E:1836:ASP:OD1	1.65	0.96
2:a:2333:GLU:OE1	2:a:2334:GLN:CG	2.14	0.95
1:E:1804:ASN:CG	1:E:1835:ALA:HB3	1.91	0.95
2:f:3691:SER:HG	2:f:3692:PRO:HD2	1.13	0.95
2:g:2577:SER:CB	2:g:2578:PRO:HD3	1.97	0.93
2:b:3691:SER:OG	2:b:3692:PRO:HD2	1.67	0.91
1:E:2012:SER:H	1:E:2013:ILE:HB	1.33	0.89
2:a:2333:GLU:OE1	2:a:2334:GLN:HG3	1.74	0.87
1:E:2011:LYS:C	1:E:2012:SER:CA	2.47	0.87
1:E:1769:GLU:HG2	1:E:1835:ALA:HB1	0.87	0.87
2:g:2577:SER:OG	2:g:2578:PRO:HD3	1.73	0.86
2:a:2333:GLU:C	2:a:2333:GLU:OE1	2.19	0.84
2:a:2333:GLU:O	2:a:2333:GLU:OE2	1.95	0.84
2:b:3447:GLU:CD	2:b:3447:GLU:O	2.19	0.84
2:a:2333:GLU:OE1	2:a:2334:GLN:HG2	1.78	0.83
2:g:2333:GLU:CD	2:g:2399:LYS:HG3	2.03	0.83
1:D:1444:HIS:ND1	1:D:1445:LYS:HG2	1.95	0.81
1:E:1709:GLU:OE1	1:E:1803:ASP:OD2	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:2577:SER:CB	2:a:2578:PRO:HD2	2.07	0.80
1:D:1444:HIS:HE1	1:D:1445:LYS:HG2	1.39	0.80
1:E:1804:ASN:ND2	1:E:1835:ALA:CB	2.46	0.79
2:b:3691:SER:CB	2:b:3692:PRO:CD	2.62	0.78
2:f:3691:SER:CB	2:f:3692:PRO:HD2	2.12	0.75
1:E:2012:SER:N	1:E:2013:ILE:CA	2.42	0.75
1:E:2010:HIS:ND1	1:E:2010:HIS:NE2	2.34	0.74
2:b:3690:ALA:O	2:b:3691:SER:HB3	1.85	0.74
2:a:2333:GLU:HG2	2:a:2399:LYS:HE2	1.68	0.74
1:E:2010:HIS:N	1:E:2010:HIS:CB	2.48	0.73
2:a:2333:GLU:O	2:a:2333:GLU:OE1	2.02	0.72
2:c:4248:SER:HB3	2:c:4249:PRO:HD3	1.71	0.72
2:f:3445:ASP:OD1	2:f:3447:GLU:HB3	1.90	0.72
1:E:2010:HIS:ND1	1:E:2010:HIS:CD2	2.49	0.71
1:E:1802:ASN:OD1	1:E:1836:ASP:OD2	2.08	0.71
1:B:1819:GLU:HG3	1:B:1914:VAL:HG22	1.73	0.71
2:a:2577:SER:CB	2:a:2578:PRO:HD3	2.20	0.71
1:E:2009:PHE:C	1:E:2010:HIS:CA	2.61	0.70
1:E:1769:GLU:CD	1:E:1804:ASN:ND2	2.49	0.69
2:b:3690:ALA:O	2:b:3691:SER:CB	2.40	0.68
2:d:2890:GLU:OE2	2:d:2956:LYS:HD3	1.94	0.68
1:E:2012:SER:H	1:E:2013:ILE:CA	2.07	0.68
2:a:2577:SER:OG	2:a:2578:PRO:HD3	1.95	0.66
1:E:2010:HIS:ND1	1:E:2010:HIS:CB	2.57	0.66
1:D:1444:HIS:CG	1:D:1445:LYS:H	2.14	0.65
1:E:2012:SER:H	1:E:2013:ILE:CB	2.09	0.65
1:A:99:LYS:HE2	1:A:101:LEU:HD21	1.79	0.64
1:E:1769:GLU:CD	1:E:1835:ALA:HB1	2.20	0.64
1:F:1596:VAL:HG12	1:F:1627:TRP:CZ3	2.33	0.64
2:b:3497:GLU:HG3	2:b:3591:VAL:HG22	1.79	0.63
2:c:4423:TRP:CH2	2:c:4466:VAL:HG11	2.33	0.63
1:E:1769:GLU:HG2	1:E:1835:ALA:HB2	1.75	0.63
2:d:2982:SER:HB2	2:d:2993:THR:HG21	1.82	0.62
1:C:1014:PRO:HG2	1:C:1089:ILE:HG22	1.83	0.61
2:d:3134:SER:HB3	2:d:3135:PRO:HD3	1.82	0.60
1:F:1254:LEU:HD13	1:F:1444:HIS:CE1	2.36	0.60
1:E:2012:SER:N	1:E:2013:ILE:HB	2.13	0.60
1:E:1709:GLU:OE1	1:E:1803:ASP:CG	2.44	0.59
1:E:1802:ASN:CA	1:E:1836:ASP:OD1	2.47	0.58
2:a:2379:PHE:CE1	2:a:2392:GLY:HA3	2.38	0.58
2:b:3447:GLU:O	2:b:3447:GLU:OE2	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2011:LYS:C	1:E:2012:SER:C	2.73	0.57
1:F:1393:PHE:CE2	1:F:1437:VAL:HG12	2.40	0.57
1:E:1915:ASN:CG	1:E:1954:ASN:HB3	2.31	0.56
2:d:2890:GLU:OE2	2:d:2890:GLU:O	2.23	0.56
2:f:3528:ILE:HD11	2:f:3567:LYS:HD3	1.88	0.56
2:e:3965:GLN:CD	2:e:3965:GLN:H	2.14	0.56
2:c:4376:PHE:CE1	2:c:4397:VAL:HG23	2.41	0.56
1:C:727:VAL:HG23	1:C:728:PHE:CD2	2.40	0.55
1:D:1444:HIS:ND1	1:D:1445:LYS:CG	2.68	0.55
1:D:1444:HIS:ND1	1:D:1445:LYS:N	2.52	0.55
1:D:1595:TYR:HB3	1:D:1638:LEU:HD11	1.89	0.55
1:E:1769:GLU:HG3	1:E:1835:ALA:HB1	1.75	0.55
2:a:2484:PHE:CE1	2:a:2566:VAL:HG12	2.43	0.54
1:E:1802:ASN:HA	1:E:1836:ASP:CG	2.32	0.54
2:d:2890:GLU:O	2:d:2890:GLU:CD	2.51	0.53
2:b:3493:PHE:CD1	2:b:3506:GLY:HA3	2.44	0.53
2:b:3497:GLU:CG	2:b:3591:VAL:HG22	2.39	0.53
1:E:2010:HIS:CD2	1:E:2011:LYS:N	2.73	0.52
1:G:1033:THR:HG22	1:G:1070:SER:HB3	1.91	0.52
1:A:340:LYS:HE3	1:A:367:PHE:CE1	2.45	0.52
1:D:1444:HIS:CG	1:D:1445:LYS:N	2.77	0.52
1:A:99:LYS:HE2	1:A:101:LEU:CD2	2.39	0.52
1:E:1769:GLU:CD	1:E:1804:ASN:HD21	2.18	0.52
1:E:1775:LEU:C	1:E:1776:LEU:HD12	2.35	0.51
1:E:1801:ILE:O	1:E:1836:ASP:OD1	2.28	0.51
1:D:1630:ALA:HB2	1:D:1640:GLN:HB2	1.92	0.51
2:g:2624:ALA:C	2:g:2625:TYR:CG	2.89	0.51
2:g:2751:MET:HE2	2:g:2752:TRP:CZ2	2.45	0.51
2:a:2503:LEU:HD12	2:a:2504:ARG:H	1.75	0.51
1:A:554:HIS:CB	1:B:2050:MET:HG2	2.41	0.50
2:d:2929:PHE:CE2	2:d:3011:VAL:HG12	2.46	0.50
1:E:1804:ASN:OD1	1:E:1835:ALA:HB3	2.09	0.50
1:B:2119:VAL:HG12	1:B:2131:THR:HG22	1.93	0.50
2:a:2331:ASP:OD2	2:a:2333:GLU:HB3	2.11	0.50
1:D:1475:VAL:HG23	1:D:1567:THR:HB	1.95	0.49
2:d:2890:GLU:OE2	2:d:2956:LYS:CD	2.60	0.49
2:c:4052:ILE:HG21	2:c:4062:VAL:HA	1.94	0.49
2:g:2333:GLU:OE1	2:g:2333:GLU:O	2.30	0.49
2:c:4155:PHE:CE1	2:c:4237:VAL:HG12	2.47	0.49
1:B:1819:GLU:CG	1:B:1914:VAL:HG22	2.42	0.49
2:g:2333:GLU:OE2	2:g:2399:LYS:HG3	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1885:THR:HG22	1:B:1886:LEU:N	2.28	0.49
1:E:1915:ASN:OD1	1:E:1948:ASP:OD2	2.30	0.49
1:F:1319:THR:C	1:F:1320:LEU:HD12	2.38	0.48
2:g:2330:VAL:HG21	2:g:2362:ILE:HD12	1.95	0.48
2:e:4386:LYS:N	2:e:4387:PRO:HD2	2.27	0.48
2:f:3445:ASP:OD2	2:f:3447:GLU:HB2	2.13	0.48
2:g:2577:SER:HG	2:g:2578:PRO:HD3	1.71	0.48
1:A:423:ILE:N	1:A:423:ILE:HD12	2.28	0.47
2:c:4016:THR:HG22	2:c:4017:THR:H	1.80	0.47
1:A:553:ALA:HB1	1:B:2227:PHE:CD1	2.49	0.47
1:C:1051:ILE:HG22	1:C:1053:LYS:H	1.79	0.47
2:b:3832:MET:HG3	2:b:3834:SER:H	1.78	0.47
2:e:4144:ASN:C	2:e:4145:ILE:HD13	2.40	0.47
1:E:1802:ASN:CG	1:E:1836:ASP:OD2	2.58	0.47
2:e:4296:TYR:CE2	2:e:4301:ARG:NH2	2.83	0.47
2:f:3915:ILE:O	2:f:3916:THR:HG23	2.15	0.47
1:D:1177:ILE:HD11	1:D:1194:LEU:HD11	1.97	0.46
1:E:1819:GLU:HG3	1:E:1914:VAL:HG22	1.97	0.46
2:b:3621:VAL:HG11	2:b:3680:VAL:HG11	1.96	0.46
1:G:605:LYS:HA	1:G:621:PHE:CE1	2.51	0.46
2:g:2369:TYR:CZ	2:g:2464:LEU:HD22	2.51	0.46
1:C:955:ILE:HG22	1:C:966:LEU:HA	1.97	0.46
1:D:1472:LYS:HE3	1:D:1499:PHE:CG	2.50	0.46
1:E:1804:ASN:HD21	1:E:1835:ALA:CB	2.26	0.46
1:D:1135:ILE:CD1	2:b:3403:GLN:H	2.29	0.46
2:f:3686:PHE:CE2	2:f:3694:SER:HB3	2.51	0.46
2:g:2642:ASP:CG	2:g:2676:ILE:HG22	2.40	0.45
1:E:1915:ASN:HD21	1:E:1954:ASN:HA	1.81	0.45
2:f:3691:SER:CB	2:f:3692:PRO:CD	2.78	0.45
2:a:2747:GLU:CD	2:a:2750:ARG:HH12	2.24	0.45
1:C:783:ASN:HD21	1:C:873:ASN:HB2	1.82	0.45
1:E:1915:ASN:ND2	1:E:1954:ASN:HA	2.32	0.44
1:E:1746:PRO:HA	1:E:1747:PRO:C	2.41	0.44
1:B:1775:LEU:HD23	1:B:1776:LEU:N	2.32	0.44
2:e:4296:TYR:CD2	2:e:4301:ARG:NH2	2.85	0.44
1:F:1366:GLU:HB2	1:F:1465:VAL:HG22	1.99	0.44
1:F:1517:ARG:HB3	1:F:1542:TYR:CD2	2.52	0.44
2:c:4406:PRO:HA	2:c:4407:PRO:C	2.41	0.44
1:G:792:LYS:C	1:G:793:VAL:HG13	2.43	0.44
1:E:1804:ASN:HD21	1:E:1835:ALA:HB3	1.71	0.44
2:c:4017:THR:HG21	2:c:4021:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:2646:TRP:CH2	2:a:2669:ILE:HD11	2.53	0.43
2:b:3838:VAL:HG22	2:b:3875:ALA:HB2	2.00	0.43
2:c:4016:THR:HG22	2:c:4017:THR:N	2.32	0.43
1:A:47:GLU:HB3	1:A:48:PRO:HD2	2.01	0.43
2:c:3952:PHE:HA	2:c:3953:PRO:C	2.44	0.43
1:E:1914:VAL:HB	1:E:2010:HIS:HB2	2.00	0.43
2:g:2356:LEU:HA	2:g:2357:PRO:HD2	1.92	0.43
2:a:2331:ASP:CG	2:a:2333:GLU:HB3	2.43	0.43
1:A:379:TYR:CE1	1:A:396:SER:HB3	2.54	0.43
1:F:1515:GLU:CD	1:F:1517:ARG:HH12	2.27	0.43
1:F:1286:LEU:HD12	1:F:1287:GLU:H	1.84	0.43
2:g:2713:ILE:HB	2:g:2797:LEU:HD23	2.00	0.43
1:E:1724:SER:HG	2:c:3936:ARG:N	2.17	0.43
1:E:1819:GLU:CG	1:E:1914:VAL:HG22	2.49	0.43
2:e:4004:GLU:OE2	2:e:4070:LYS:HE2	2.18	0.43
2:f:3841:ASP:HA	2:f:3842:PRO:HD3	1.97	0.43
1:B:1732:LEU:HD23	1:B:1732:LEU:HA	1.88	0.43
1:D:1452:LYS:HA	1:D:1453:PRO:HD3	1.93	0.43
2:g:2310:GLU:HA	2:g:2311:PRO:C	2.44	0.42
1:F:1180:PRO:HA	1:F:1181:PRO:C	2.44	0.42
1:G:796:GLY:HA2	1:G:808:THR:HB	2.00	0.42
2:e:4164:VAL:HG11	2:e:4223:LEU:HD12	2.01	0.42
2:f:3395:PHE:HA	2:f:3396:PRO:C	2.44	0.42
1:G:790:GLU:HB2	1:G:811:LYS:HE2	2.00	0.42
2:c:4061:THR:HA	2:c:4105:THR:HG22	2.02	0.42
2:e:4308:TYR:CD1	2:e:4351:ALA:HB2	2.54	0.42
2:a:2333:GLU:CG	2:a:2399:LYS:HE2	2.43	0.42
2:c:4178:VAL:HG11	2:c:4237:VAL:HG11	2.01	0.42
1:A:427:TYR:CD1	1:A:427:TYR:C	2.97	0.42
2:b:3395:PHE:HA	2:b:3396:PRO:C	2.45	0.42
1:A:340:LYS:HE3	1:A:367:PHE:CZ	2.55	0.42
2:f:3541:HIS:HA	2:f:3542:PRO:HD3	1.83	0.42
2:g:2480:HIS:CD2	2:g:2510:LYS:H	2.38	0.42
1:F:1247:PHE:CD2	1:F:1264:ILE:HG22	2.55	0.42
2:d:2873:TYR:HE2	2:e:4093:THR:OG1	2.02	0.42
1:E:1922:GLU:OE1	1:E:1943:LYS:HE2	2.20	0.42
1:C:1047:SER:O	1:C:1089:ILE:HG23	2.20	0.41
2:a:2706:ILE:N	2:a:2706:ILE:HD12	2.35	0.41
2:b:3415:SER:HB2	2:b:3457:PHE:CZ	2.55	0.41
2:c:4133:PHE:CD2	2:c:4133:PHE:N	2.88	0.41
2:f:3740:ASP:HA	2:f:3741:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:3829:LYS:HE3	2:f:3886:PHE:CD1	2.55	0.41
1:E:2013:ILE:HG23	1:E:2017:TYR:HB3	2.02	0.41
1:E:2104:PHE:CD1	1:E:2104:PHE:C	2.98	0.41
2:b:3493:PHE:CE1	2:b:3506:GLY:HA3	2.54	0.41
2:c:4164:VAL:HG21	2:c:4168:THR:HG21	2.01	0.41
1:D:1444:HIS:CE1	1:D:1445:LYS:CG	2.67	0.41
2:a:2379:PHE:CB	2:a:2391:VAL:HG12	2.51	0.41
2:b:3806:LEU:C	2:b:3806:LEU:HD13	2.45	0.41
2:e:4398:ASP:HA	2:e:4399:PRO:HD3	1.88	0.41
1:G:1075:GLN:HB3	1:G:1078:LYS:H	1.85	0.41
1:E:2012:SER:N	1:E:2013:ILE:CB	2.77	0.41
2:f:3723:MET:HE2	2:f:3727:ALA:CB	2.50	0.41
1:D:1160:LEU:HB2	1:D:1168:ILE:HD11	2.03	0.41
1:F:1484:MET:H	1:F:1484:MET:HG3	1.71	0.41
2:d:3272:LYS:N	2:d:3273:PRO:CD	2.84	0.41
2:a:2735:PRO:HA	2:a:2736:PRO:C	2.45	0.41
2:c:4377:ILE:CD1	2:c:4450:ILE:HD11	2.51	0.41
1:A:257:TRP:CZ2	1:A:281:ASN:HB2	2.56	0.41
2:g:2715:LYS:HB3	2:g:2716:PRO:HD3	2.03	0.41
1:E:1709:GLU:OE1	1:E:1803:ASP:OD1	2.39	0.41
1:G:1082:ARG:HA	1:G:1105:LEU:O	2.20	0.41
2:e:4297:ASP:HA	2:e:4298:PRO:HD2	1.98	0.41
1:E:1959:PHE:CE2	1:E:2003:VAL:HG23	2.56	0.41
1:E:1991:TYR:CD2	1:E:1991:TYR:C	2.99	0.41
1:G:793:VAL:C	1:G:794:LEU:HD23	2.46	0.40
2:e:4282:GLU:HG3	2:e:4370:VAL:HG22	2.02	0.40
1:D:1135:ILE:HD12	2:b:3403:GLN:HB2	2.04	0.40
1:G:614:PRO:HB3	1:G:616:PHE:CE1	2.57	0.40
2:c:4040:TYR:CE1	2:c:4135:LEU:HB3	2.57	0.40
2:c:4423:TRP:HH2	2:c:4466:VAL:HG11	1.84	0.40
1:F:1583:ILE:HD13	1:F:1583:ILE:HG21	1.83	0.40
1:F:1520:TRP:CD1	1:F:1548:TYR:CZ	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	552/554 (100%)	513 (93%)	39 (7%)	0	100	100
1	B	552/554 (100%)	512 (93%)	38 (7%)	2 (0%)	30	67
1	C	552/554 (100%)	516 (94%)	32 (6%)	4 (1%)	18	56
1	D	552/554 (100%)	516 (94%)	34 (6%)	2 (0%)	30	67
1	E	552/554 (100%)	510 (92%)	32 (6%)	10 (2%)	6	34
1	F	552/554 (100%)	516 (94%)	33 (6%)	3 (0%)	24	63
1	G	552/554 (100%)	517 (94%)	33 (6%)	2 (0%)	30	67
2	a	542/544 (100%)	505 (93%)	33 (6%)	4 (1%)	18	56
2	b	542/544 (100%)	505 (93%)	31 (6%)	6 (1%)	11	46
2	c	542/544 (100%)	499 (92%)	42 (8%)	1 (0%)	43	78
2	d	542/544 (100%)	493 (91%)	47 (9%)	2 (0%)	30	67
2	e	542/544 (100%)	501 (92%)	38 (7%)	3 (1%)	21	59
2	f	542/544 (100%)	498 (92%)	39 (7%)	5 (1%)	14	51
2	g	542/544 (100%)	499 (92%)	40 (7%)	3 (1%)	21	59
All	All	7658/7686 (100%)	7100 (93%)	511 (7%)	47 (1%)	23	59

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	992	ASP
1	E	1783	ALA
1	E	2010	HIS
1	E	2011	LYS
1	E	2013	ILE
2	a	2577	SER
2	b	3427	ASN
2	b	3691	SER
2	d	2864	VAL
2	e	4242	PRO
2	f	3498	ASN
2	f	3691	SER
2	g	2577	SER
1	B	2124	ASP
1	C	741	SER

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Mol	Chain	Res	Type
1	D	1402	GLY
1	F	1489	LYS
1	G	1025	HIS
2	a	2367	ASP
2	d	3070	VAL
2	g	2759	ASP
1	B	2015	SER
1	E	2015	SER
1	E	2244	HIS
1	F	1217	ALA
2	b	3689	GLU
2	b	3855	LEU
2	g	2367	ASP
1	C	795	GLU
1	E	1902	VAL
1	F	1516	ASP
2	c	4166	GLU
2	e	4474	GLU
2	f	3480	ASN
1	E	2124	ASP
1	G	880	SER
2	a	2511	ASP
2	f	3419	PRO
1	C	783	ASN
2	b	3447	GLU
1	E	2188	GLY
2	e	4314	PRO
2	b	3885	PRO
1	D	1177	ILE
1	E	1788	VAL
2	f	3384	PRO
2	a	2282	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/492 (100%)	479 (97%)	13 (3%)	40	62
1	B	492/492 (100%)	485 (99%)	7 (1%)	59	72
1	C	492/492 (100%)	478 (97%)	14 (3%)	38	60
1	D	492/492 (100%)	477 (97%)	15 (3%)	36	57
1	E	492/492 (100%)	475 (96%)	17 (4%)	32	53
1	F	492/492 (100%)	481 (98%)	11 (2%)	45	64
1	G	492/492 (100%)	475 (96%)	17 (4%)	32	53
2	a	494/494 (100%)	476 (96%)	18 (4%)	31	52
2	b	494/494 (100%)	479 (97%)	15 (3%)	36	57
2	c	494/494 (100%)	473 (96%)	21 (4%)	26	47
2	d	494/494 (100%)	481 (97%)	13 (3%)	40	62
2	e	494/494 (100%)	477 (97%)	17 (3%)	32	54
2	f	494/494 (100%)	480 (97%)	14 (3%)	38	60
2	g	494/494 (100%)	483 (98%)	11 (2%)	45	64
All	All	6902/6902 (100%)	6699 (97%)	203 (3%)	38	58

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	161	VAL
1	A	163	TYR
1	A	164	LEU
1	A	204	VAL
1	A	265	SER
1	A	349	SER
1	A	364	PHE
1	A	387	ASN
1	A	389	ILE
1	A	395	THR
1	A	423	ILE
1	A	519	ILE
1	B	1839	ASN
1	B	1884	TYR
1	B	1978	THR
1	B	2062	PHE
1	B	2124	ASP
1	B	2230	PRO

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Mol	Chain	Res	Type
1	B	2237	LEU
1	C	629	ASN
1	C	639	THR
1	C	673	GLU
1	C	718	VAL
1	C	739	THR
1	C	753	THR
1	C	828	THR
1	C	851	VAL
1	C	919	ASP
1	C	946	VAL
1	C	956	SER
1	C	983	THR
1	C	1006	VAL
1	C	1022	THR
1	D	1135	ILE
1	D	1158	SER
1	D	1233	LEU
1	D	1237	ASP
1	D	1258	HIS
1	D	1363	MET
1	D	1482	GLU
1	D	1484	MET
1	D	1496	PHE
1	D	1523	VAL
1	D	1545	ASN
1	D	1572	VAL
1	D	1599	THR
1	D	1604	ASP
1	D	1616	VAL
1	E	1702	THR
1	E	1768	ARG
1	E	1769	GLU
1	E	1807	VAL
1	E	1876	LEU
1	E	1878	ARG
1	E	1883	SER
1	E	1901	PRO
1	E	1942	ILE
1	E	2062	PHE
1	E	2093	THR
1	E	2100	LYS

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Mol	Chain	Res	Type
1	E	2131	THR
1	E	2138	VAL
1	E	2157	HIS
1	E	2183	ILE
1	E	2220	LEU
1	F	1235	ILE
1	F	1241	VAL
1	F	1337	LYS
1	F	1435	VAL
1	F	1437	VAL
1	F	1460	VAL
1	F	1497	GLN
1	F	1597	ASN
1	F	1650	GLU
1	F	1677	LEU
1	F	1678	HIS
1	G	639	THR
1	G	685	VAL
1	G	719	SER
1	G	760	ASP
1	G	775	VAL
1	G	777	ILE
1	G	822	ASN
1	G	851	VAL
1	G	862	MET
1	G	927	ILE
1	G	942	HIS
1	G	955	ILE
1	G	957	VAL
1	G	964	ILE
1	G	1006	VAL
1	G	1025	HIS
1	G	1071	VAL
2	a	2292	THR
2	a	2297	THR
2	a	2302	ILE
2	a	2332	ARG
2	a	2333	GLU
2	a	2354	LEU
2	a	2381	ILE
2	a	2442	ARG
2	a	2465	GLN

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Mol	Chain	Res	Type
2	a	2487	THR
2	a	2489	TYR
2	a	2546	LEU
2	a	2577	SER
2	a	2586	THR
2	a	2629	THR
2	a	2668	THR
2	a	2785	LEU
2	a	2795	VAL
2	b	3462	ASP
2	b	3480	ASN
2	b	3495	ILE
2	b	3498	ASN
2	b	3536	THR
2	b	3556	ARG
2	b	3588	ILE
2	b	3619	VAL
2	b	3692	PRO
2	b	3705	VAL
2	b	3778	ARG
2	b	3801	THR
2	b	3817	SER
2	b	3831	THR
2	b	3904	VAL
2	c	3963	THR
2	c	3970	TYR
2	c	3972	SER
2	c	3985	LEU
2	c	4004	GLU
2	c	4009	PHE
2	c	4012	ILE
2	c	4052	ILE
2	c	4107	THR
2	c	4120	GLN
2	c	4133	PHE
2	c	4156	THR
2	c	4183	LEU
2	c	4233	LEU
2	c	4290	SER
2	c	4308	TYR
2	c	4312	THR
2	c	4340	ILE

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Mol	Chain	Res	Type
2	c	4430	ASP
2	c	4451	THR
2	c	4462	THR
2	d	2870	ASN
2	d	2889	ARG
2	d	2919	ILE
2	d	2947	THR
2	d	2951	VAL
2	d	2999	ARG
2	d	3132	GLU
2	d	3139	MET
2	d	3221	ARG
2	d	3235	VAL
2	d	3256	VAL
2	d	3351	ASP
2	d	3355	CYS
2	e	3940	ILE
2	e	4061	THR
2	e	4083	SER
2	e	4096	SER
2	e	4107	THR
2	e	4123	ILE
2	e	4135	LEU
2	e	4150	ASP
2	e	4168	THR
2	e	4200	GLU
2	e	4233	LEU
2	e	4275	ILE
2	e	4311	LEU
2	e	4324	THR
2	e	4367	LEU
2	e	4381	THR
2	e	4452	VAL
2	f	3459	THR
2	f	3466	PRO
2	f	3524	LYS
2	f	3536	THR
2	f	3550	THR
2	f	3606	SER
2	f	3619	VAL
2	f	3697	SER
2	f	3769	SER

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Mol	Chain	Res	Type
2	f	3824	THR
2	f	3846	ILE
2	f	3857	SER
2	f	3874	THR
2	f	3895	VAL
2	g	2297	THR
2	g	2308	ASP
2	g	2333	GLU
2	g	2359	ILE
2	g	2429	THR
2	g	2518	TRP
2	g	2575	GLU
2	g	2577	SER
2	g	2662	LEU
2	g	2681	SER
2	g	2731	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	219	ASN
1	A	225	ASN
1	A	554	HIS
1	B	1802	ASN
1	B	1810	GLN
1	B	1842	ASN
1	B	1934	GLN
1	B	1965	ASN
1	B	2030	ASN
1	B	2061	ASN
1	C	591	HIS
1	C	655	ASN
1	C	804	ASN
1	C	1005	ASN
1	C	1074	GLN
1	D	1236	ASN
1	D	1340	GLN
1	D	1342	GLN
1	D	1464	ASN
1	D	1578	ASN
1	D	1686	HIS

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Mol	Chain	Res	Type
1	E	1804	ASN
1	E	1915	ASN
1	E	1917	ASN
1	E	2010	HIS
1	E	2030	ASN
1	E	2085	ASN
1	E	2163	ASN
1	E	2174	ASN
1	F	1221	ASN
1	F	1368	GLN
1	F	1399	ASN
1	F	1470	HIS
1	F	1545	ASN
1	F	1571	ASN
1	F	1640	GLN
1	G	655	ASN
1	G	678	GLN
1	G	707	ASN
1	G	898	ASN
1	G	904	HIS
1	G	1086	GLN
2	a	2276	ASN
2	a	2478	ASN
2	a	2563	GLN
2	a	2620	ASN
2	a	2702	ASN
2	b	3403	GLN
2	b	3498	ASN
2	b	3594	HIS
2	b	3644	ASN
2	b	3656	ASN
2	b	3667	ASN
2	b	3704	ASN
2	b	3708	GLN
2	c	4087	GLN
2	c	4110	GLN
2	c	4120	GLN
2	c	4144	ASN
2	c	4201	ASN
2	c	4224	ASN
2	c	4230	GLN
2	c	4475	ASN

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Mol	Chain	Res	Type
2	d	2846	GLN
2	d	2852	ASN
2	d	2941	ASN
2	d	3053	ASN
2	d	3116	GLN
2	d	3147	ASN
2	d	3232	ASN
2	e	3958	GLN
2	e	3994	ASN
2	e	4039	ASN
2	e	4144	ASN
2	e	4149	ASN
2	e	4167	ASN
2	e	4192	ASN
2	e	4224	ASN
2	e	4230	GLN
2	e	4439	ASN
2	f	3401	GLN
2	f	3498	ASN
2	f	3563	GLN
2	f	3587	ASN
2	f	3667	ASN
2	f	3673	GLN
2	f	3677	GLN
2	f	3789	ASN
2	f	3814	ASN
2	f	3918	ASN
2	g	2276	ASN
2	g	2334	GLN
2	g	2368	ASN
2	g	2406	HIS
2	g	2416	GLN
2	g	2449	GLN
2	g	2480	HIS
2	g	2496	ASN
2	g	2559	GLN
2	g	2590	ASN
2	g	2675	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	2011:LYS	C	2012:SER	N	1.70

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11678. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

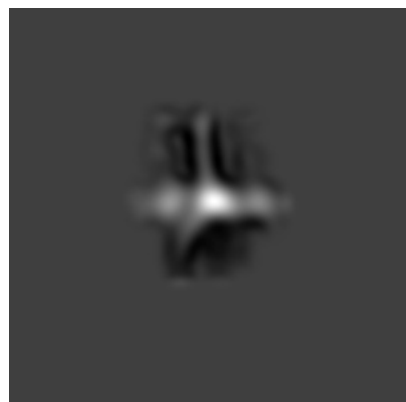


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 62



Y Index: 66

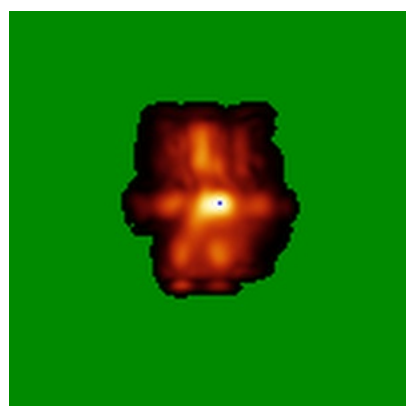


Z Index: 66

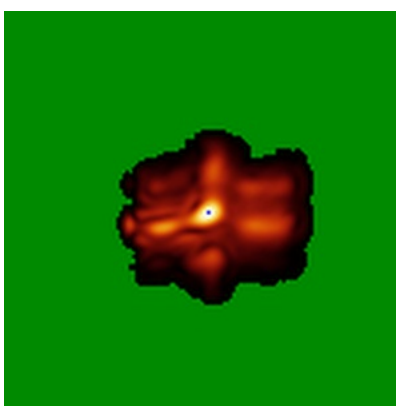
The images above show the largest variance slices of the map in three orthogonal directions.

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

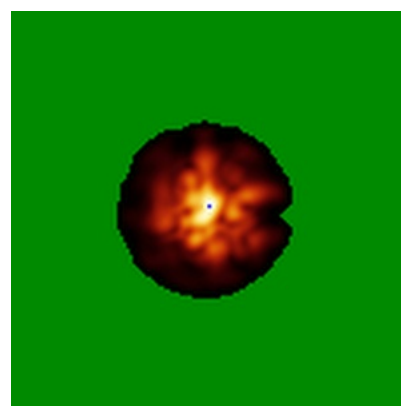
6.4.1 Primary map



X



Y

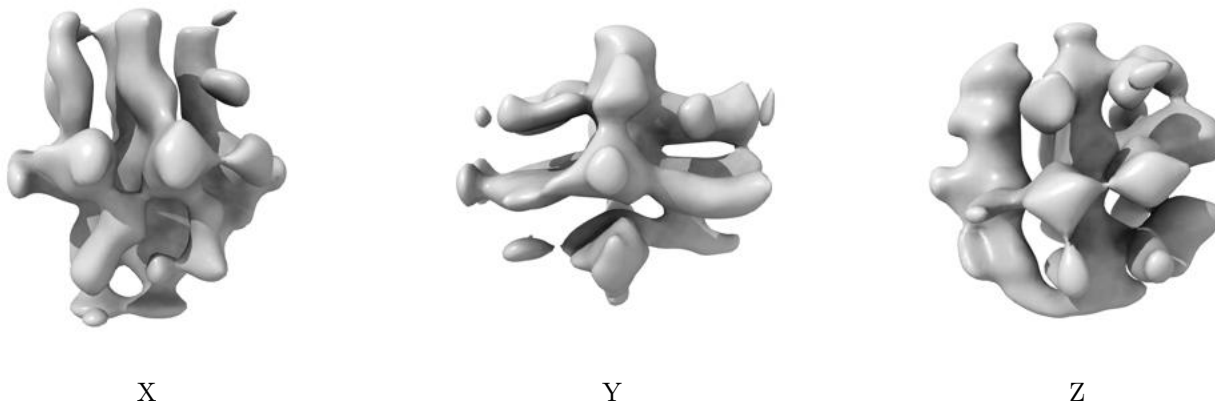


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0133. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

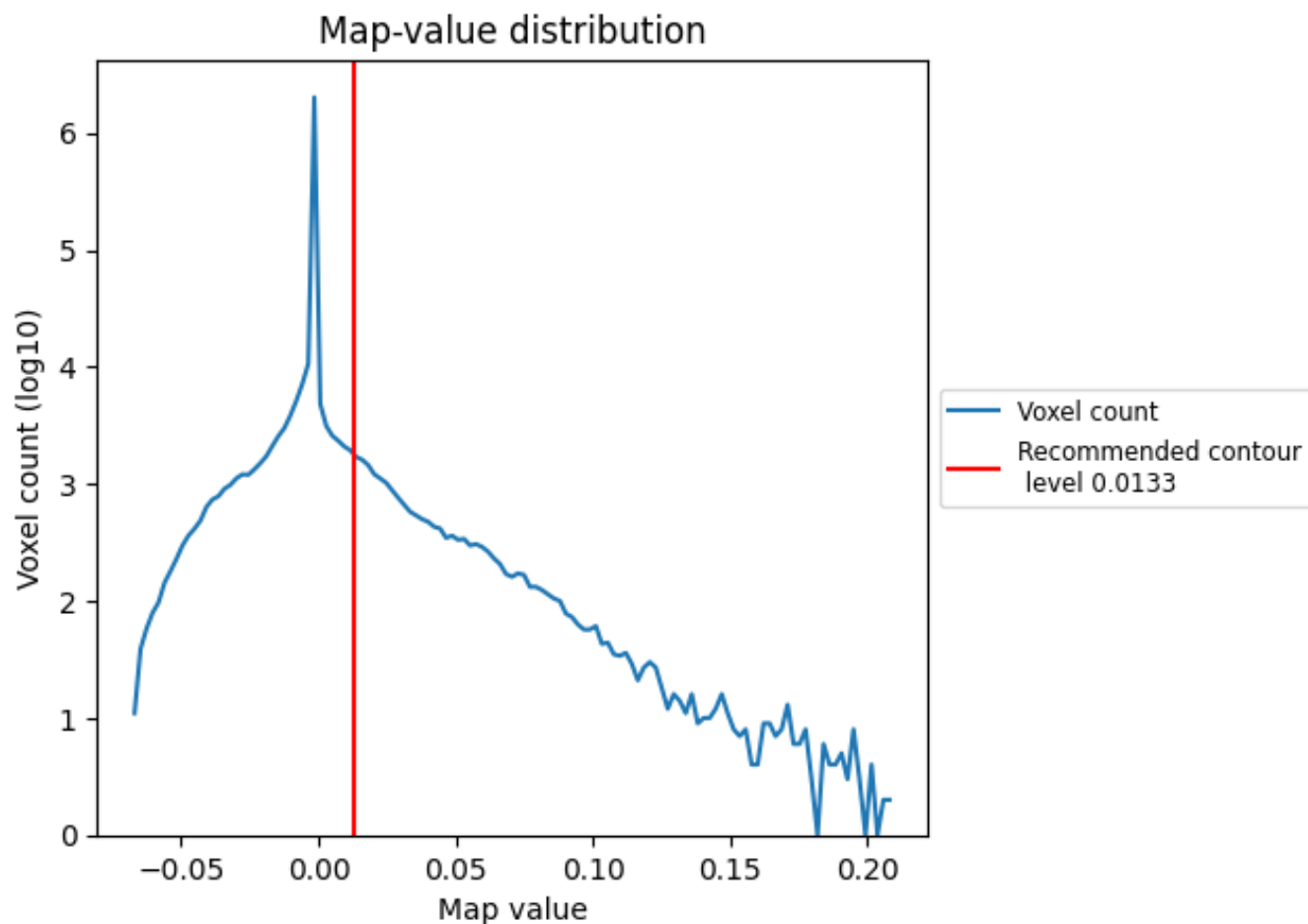
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

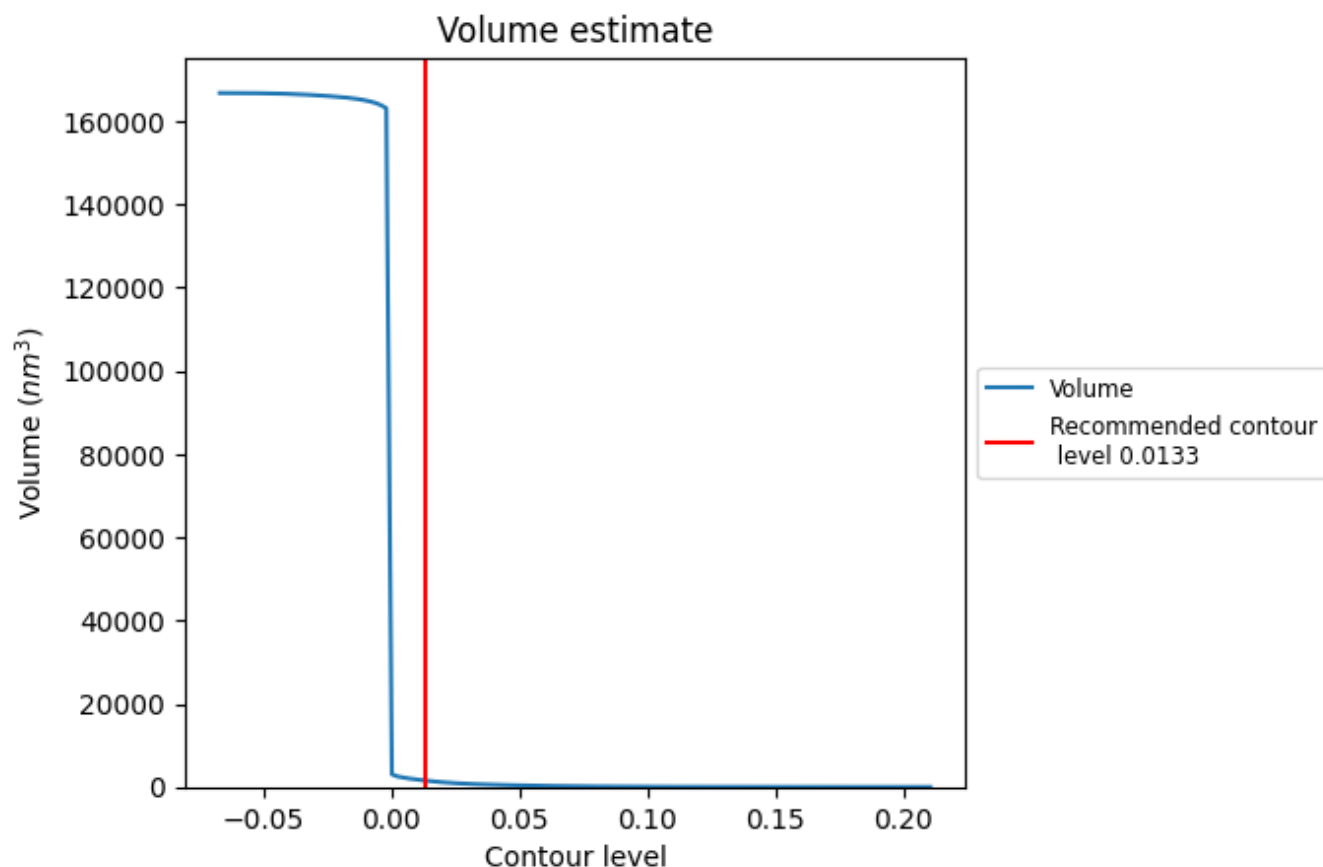
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

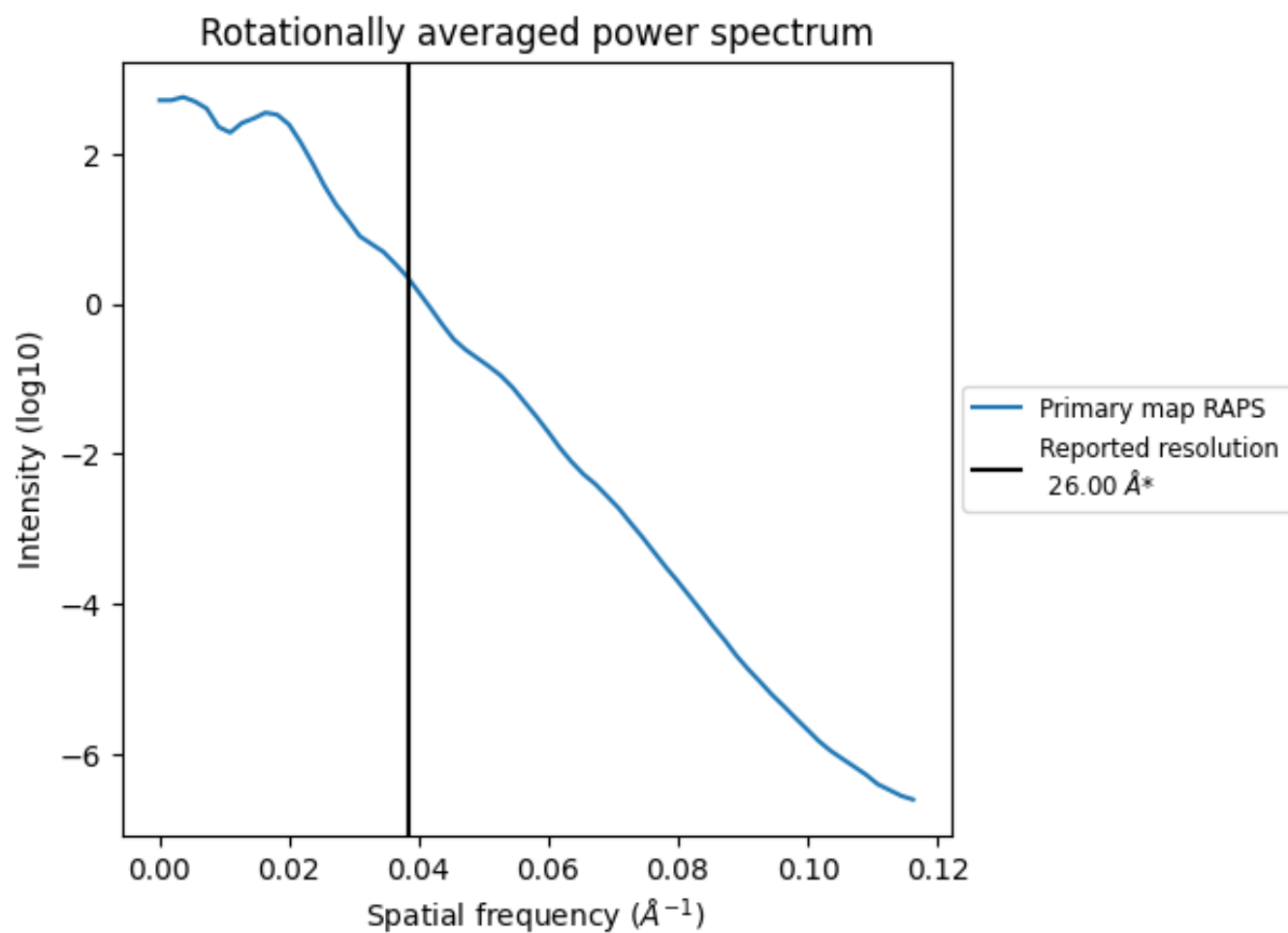
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1526 nm^3 ; this corresponds to an approximate mass of 1378 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 ⓘ

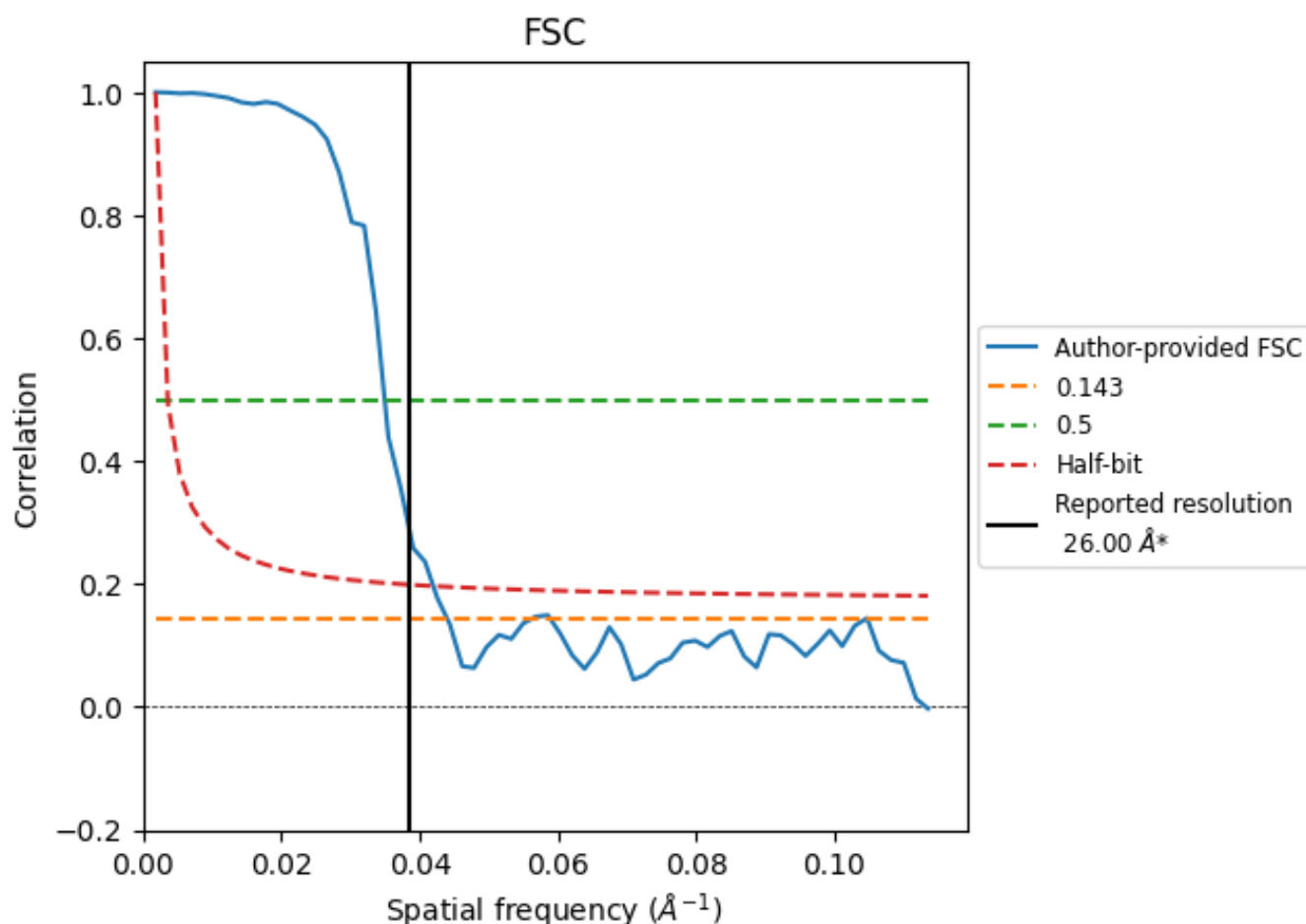


*Reported resolution corresponds to spatial frequency of 0.038 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.038 Å⁻¹

8.2 Resolution estimates [i](#)

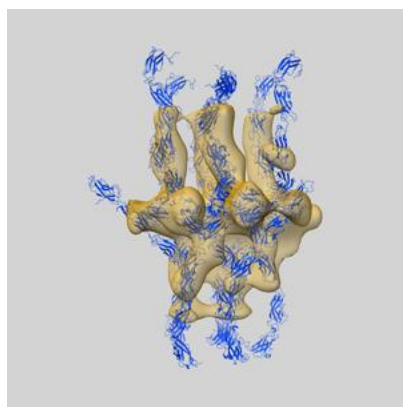
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	26.00	-
Author-provided FSC curve	22.73	28.57	23.81
Unmasked-calculated*	-	-	-

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

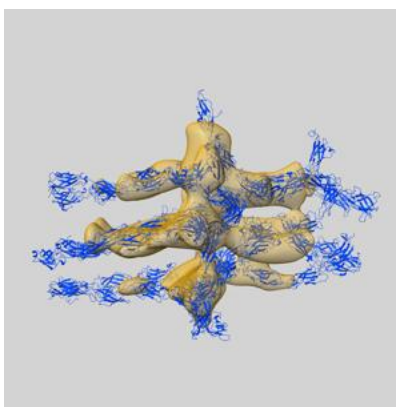
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11678 and PDB model 7A7D. Per-residue inclusion information can be found in section [3](#) on page [6](#).

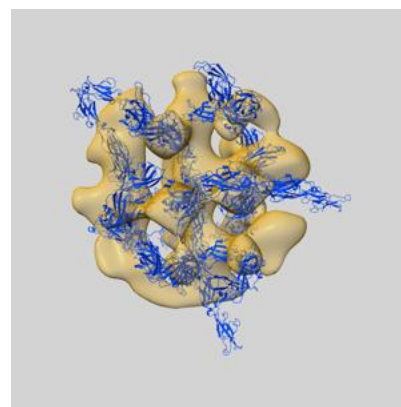
9.1 Map-model overlay [i](#)



X



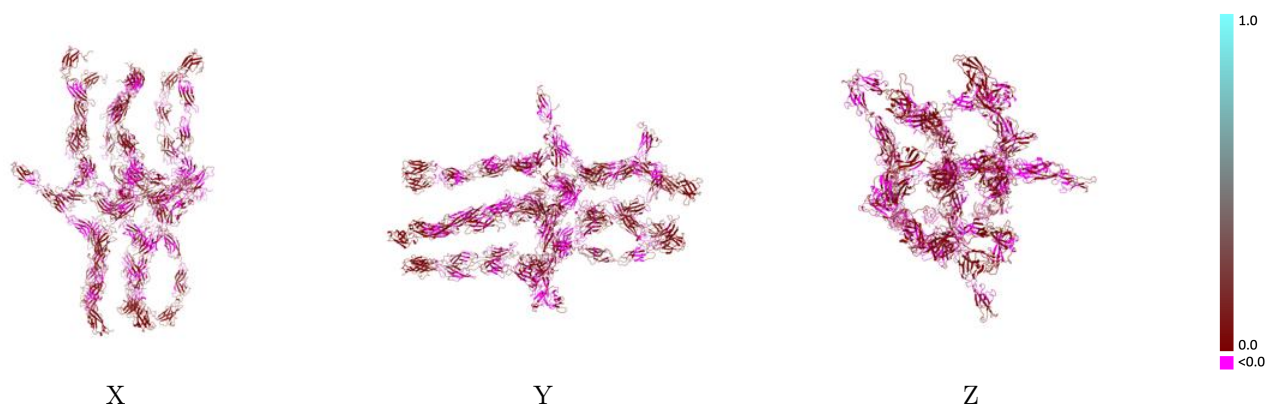
Y



Z

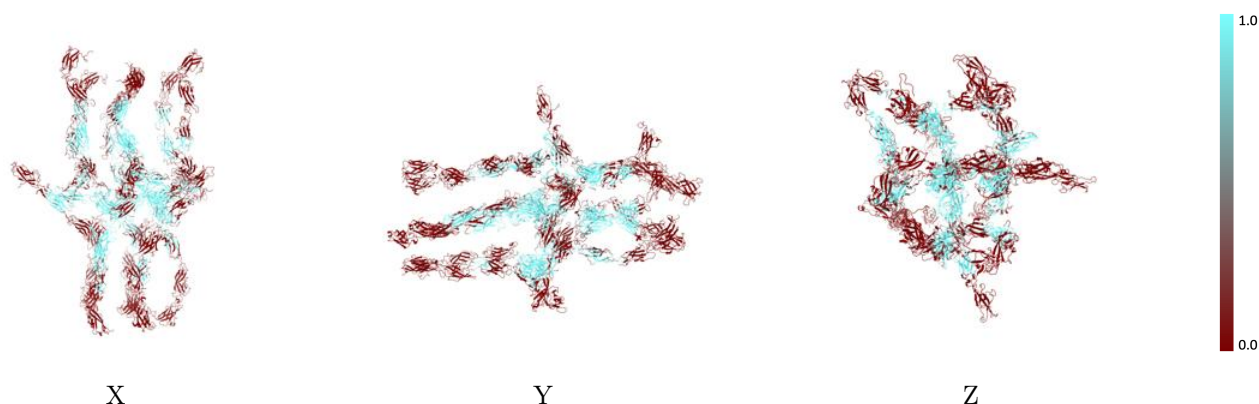
The images above show the 3D surface view of the map at the recommended contour level 0.0133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



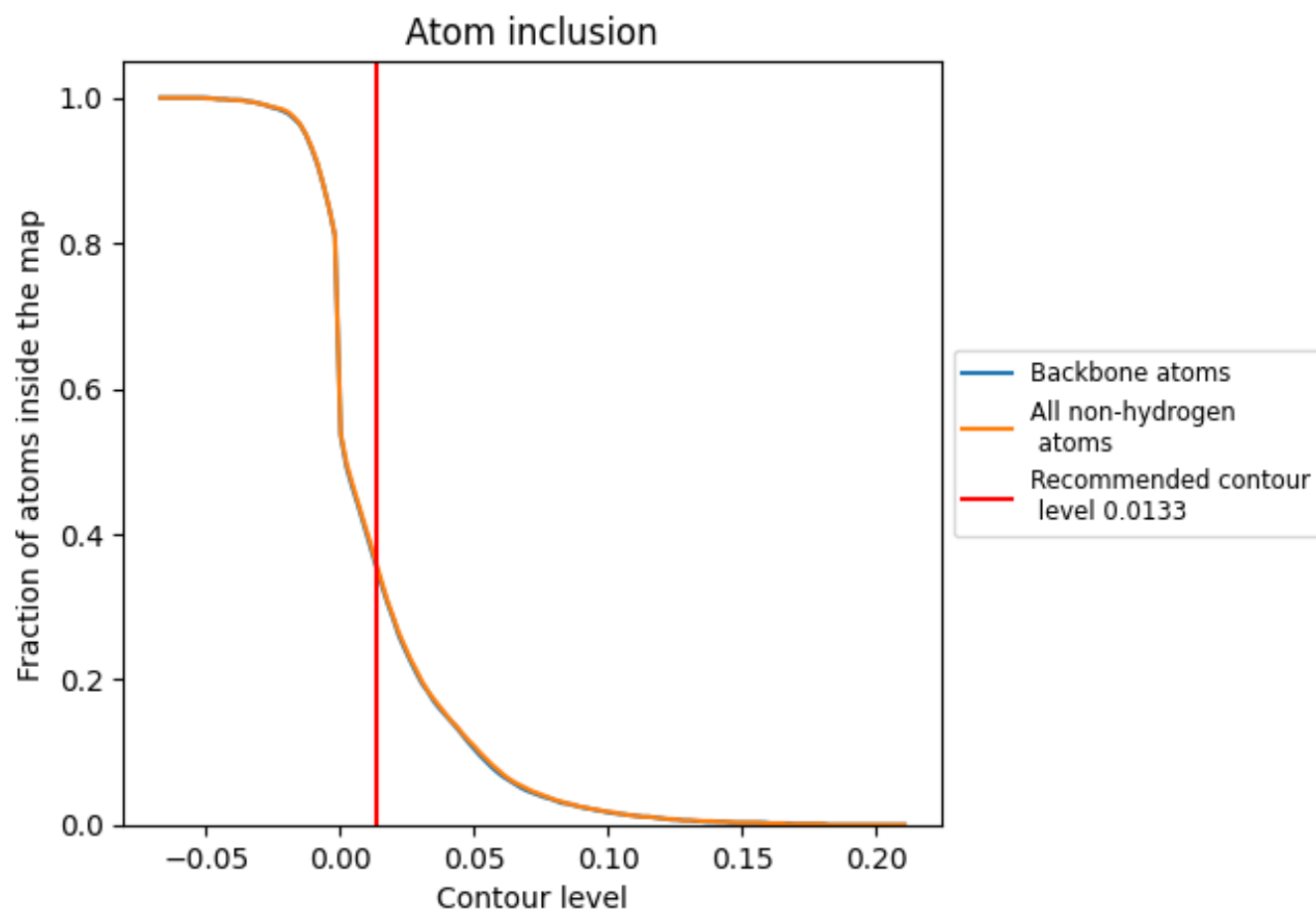
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0133).

9.4 Atom inclusion [i](#)



At the recommended contour level, 36% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3610	 0.0190
A	 0.5620	 0.0360
B	 0.2970	 0.0080
C	 0.2210	 0.0050
D	 0.3270	 0.0090
E	 0.3840	 0.0380
F	 0.2940	 0.0200
G	 0.3450	 0.0280
a	 0.4010	 0.0340
b	 0.1990	 0.0090
c	 0.4870	 0.0250
d	 0.6420	 0.0160
e	 0.3780	 0.0050
f	 0.1100	 0.0080
g	 0.4450	 0.0270

