



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 09:34 PM UTC

PDB ID : 6R7F / pdb_00006r7f
EMDB ID : EMD-4739
Title : Structural basis of Cullin-2 RING E3 ligase regulation by the COP9 signalosome
Authors : Faull, S.V.; Lau, A.M.C.; Martens, C.; Ahdash, Z.; Yebenes, H.; Schmidt, C.; Beuron, F.; Cronin, N.B.; Morris, E.P.; Politis, A.
Deposited on : 2019-03-28
Resolution : 8.20 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

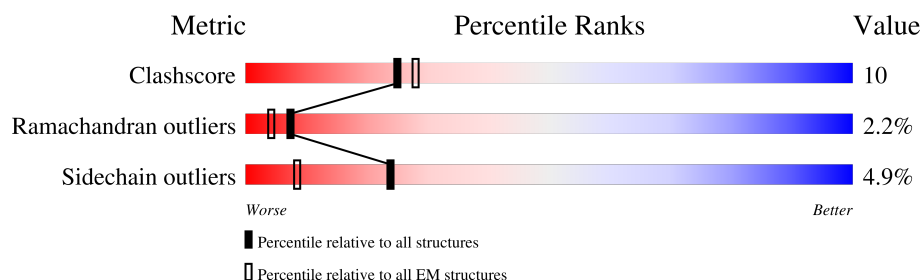
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.20 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.



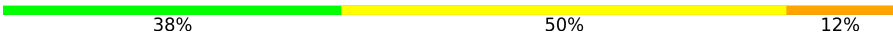
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	443	
3	C	403	
4	D	406	
5	E	311	
6	F	288	
7	H	209	
8	G	208	
9	V	160	

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Mol	Chain	Length	Quality of chain
10	P	118	 42%52%5% •
11	Q	112	 54%39%5% •
12	O	745	 39%52%9% •
13	R	90	 38%50%12%
14	N	76	 53%43%•

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	433	Total	C	N	O	S	0	0
			3450	2174	605	649	22		

- Molecule 2 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	414	Total	C	N	O	S	0	0
			3386	2149	579	643	15		

- Molecule 3 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	403	Total	C	N	O	S	0	0
			3205	2040	537	601	27		

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	406	Total	C	N	O	S	0	0
			3251	2047	566	622	16		

- Molecule 5 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	311	Total	C	N	O	S	0	0
			2472	1575	412	471	14		

- Molecule 6 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	288	Total	C	N	O	S	0	0
			2280	1452	379	434	15		

- Molecule 7 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	168	Total	C	N	O	S	0	0
			1340	859	232	245	4		

- Molecule 8 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	208	Total	C	N	O	S	0	0
			1645	1039	279	321	6		

- Molecule 9 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	160	Total	C	N	O	S	0	0
			1308	824	245	235	4		

- Molecule 10 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	118	Total	C	N	O	S	0	0
			921	575	156	185	5		

- Molecule 11 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	112	Total	C	N	O	S	0	0
			873	553	139	173	8		

- Molecule 12 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	744	Total	C	N	O	S	0	0
			6090	3869	1029	1146	46		

- Molecule 13 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	90	Total	C	N	O	S	0	0
			746	472	137	128	9		

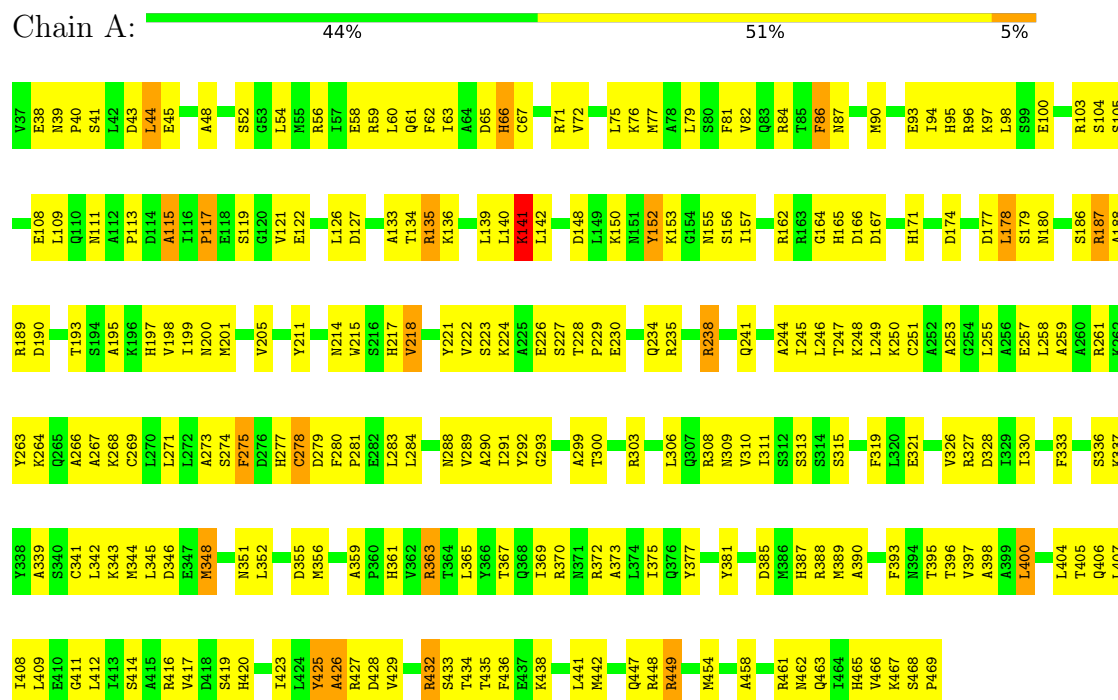
- Molecule 14 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	76	Total	C	N	O	S	0	0
			591	372	102	115	2		

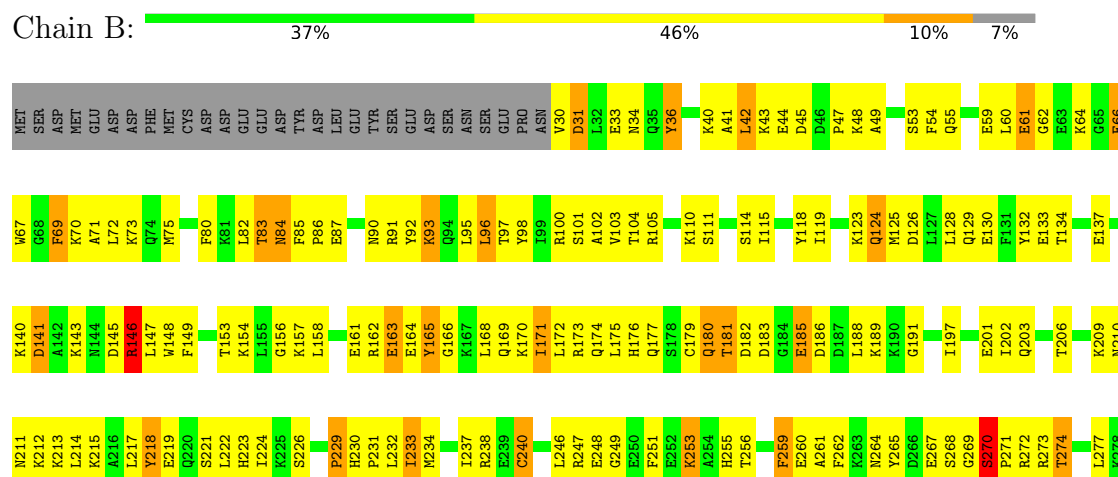
3 Residue-property plots

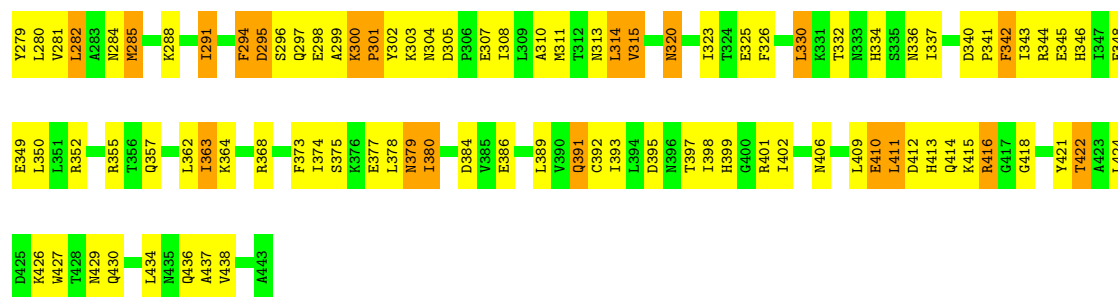
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: COP9 signalosome complex subunit 1



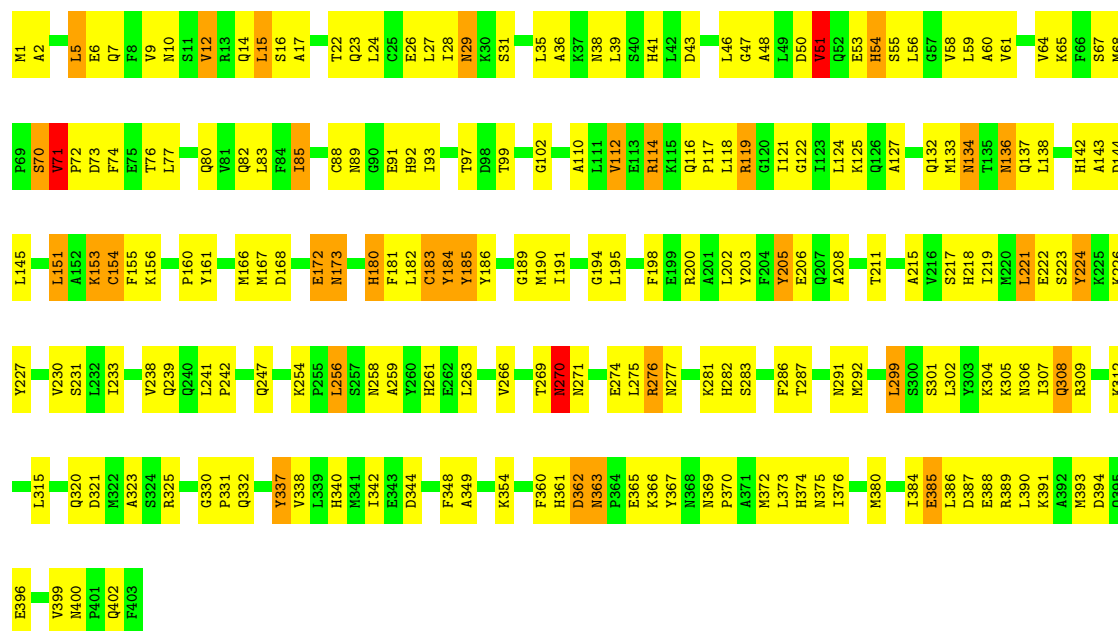
• Molecule 2: COP9 signalosome complex subunit 2





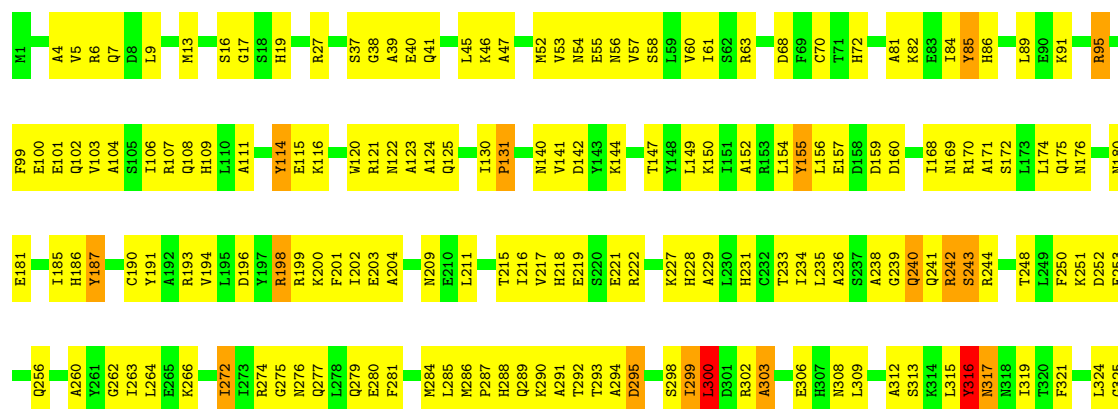
• Molecule 3: COP9 signalosome complex subunit 3

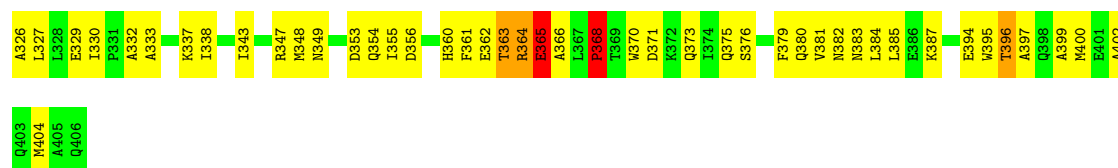
Chain C: 48% 43% 8% .



• Molecule 4: COP9 signalosome complex subunit 4

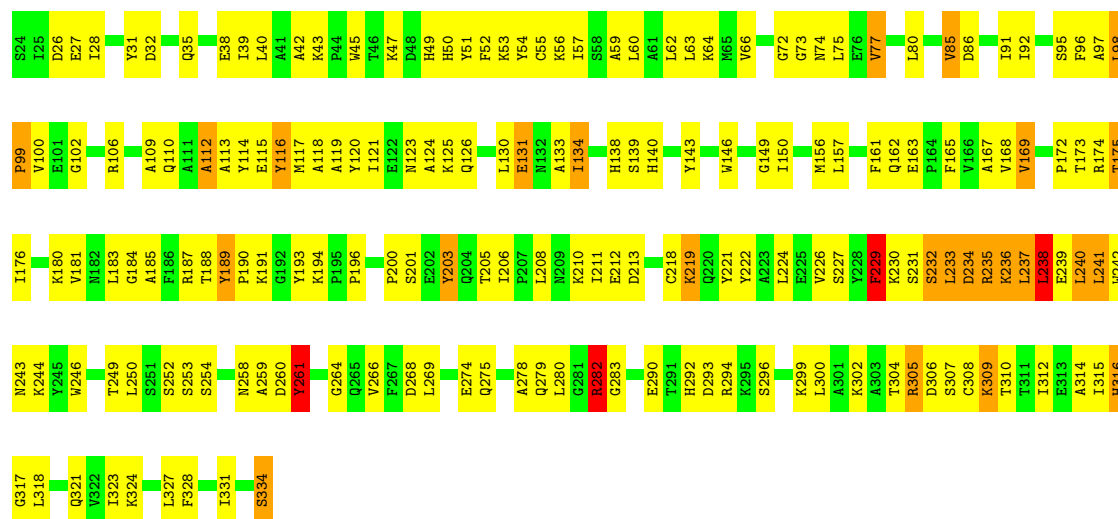
Chain D: 47% 48% . .





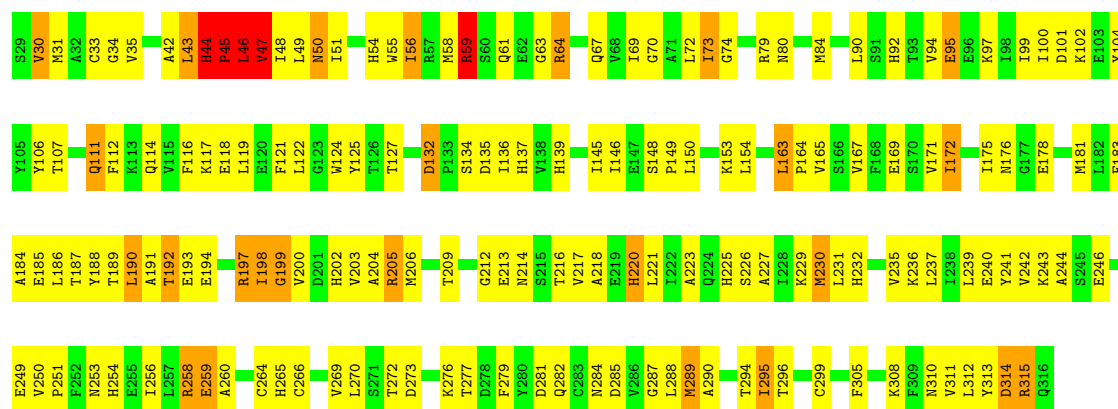
• Molecule 5: COP9 signalosome complex subunit 5

Chain E: 41% 49% 8%



• Molecule 6: COP9 signalosome complex subunit 6

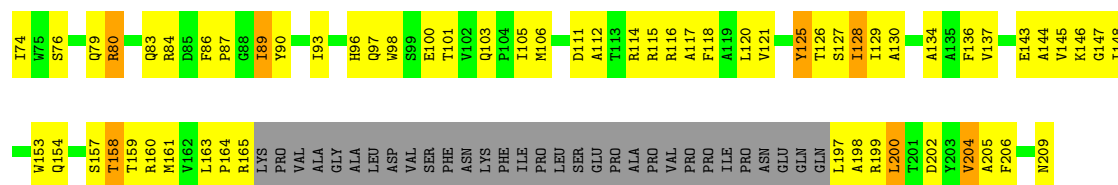
Chain F: 42% 48% 9%



• Molecule 7: COP9 signalosome complex subunit 8

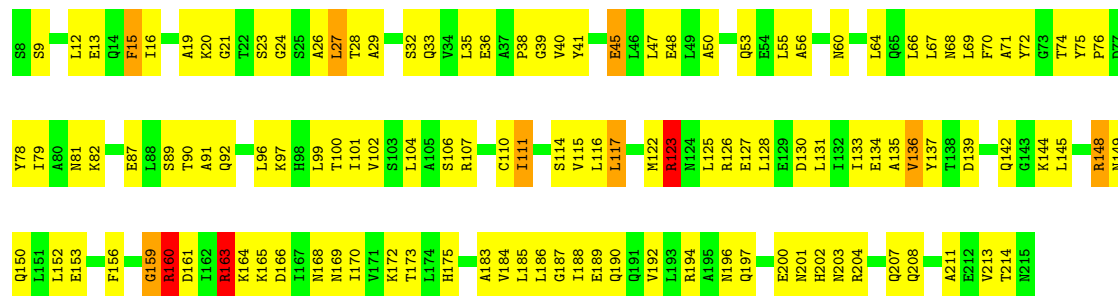
Chain H: 33% 42% 5% 20%





• Molecule 8: COP9 signalosome complex subunit 7b

Chain G: 41% 54% . .



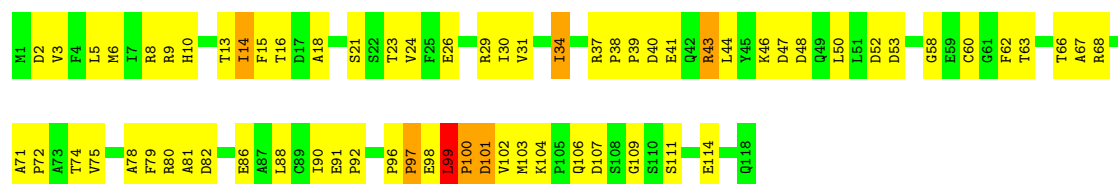
• Molecule 9: von Hippel-Lindau disease tumor suppressor

Chain V: 32% 62% 6%



• Molecule 10: Elongin-B

Chain P: 42% 52% 5%



• Molecule 11: Elongin-C

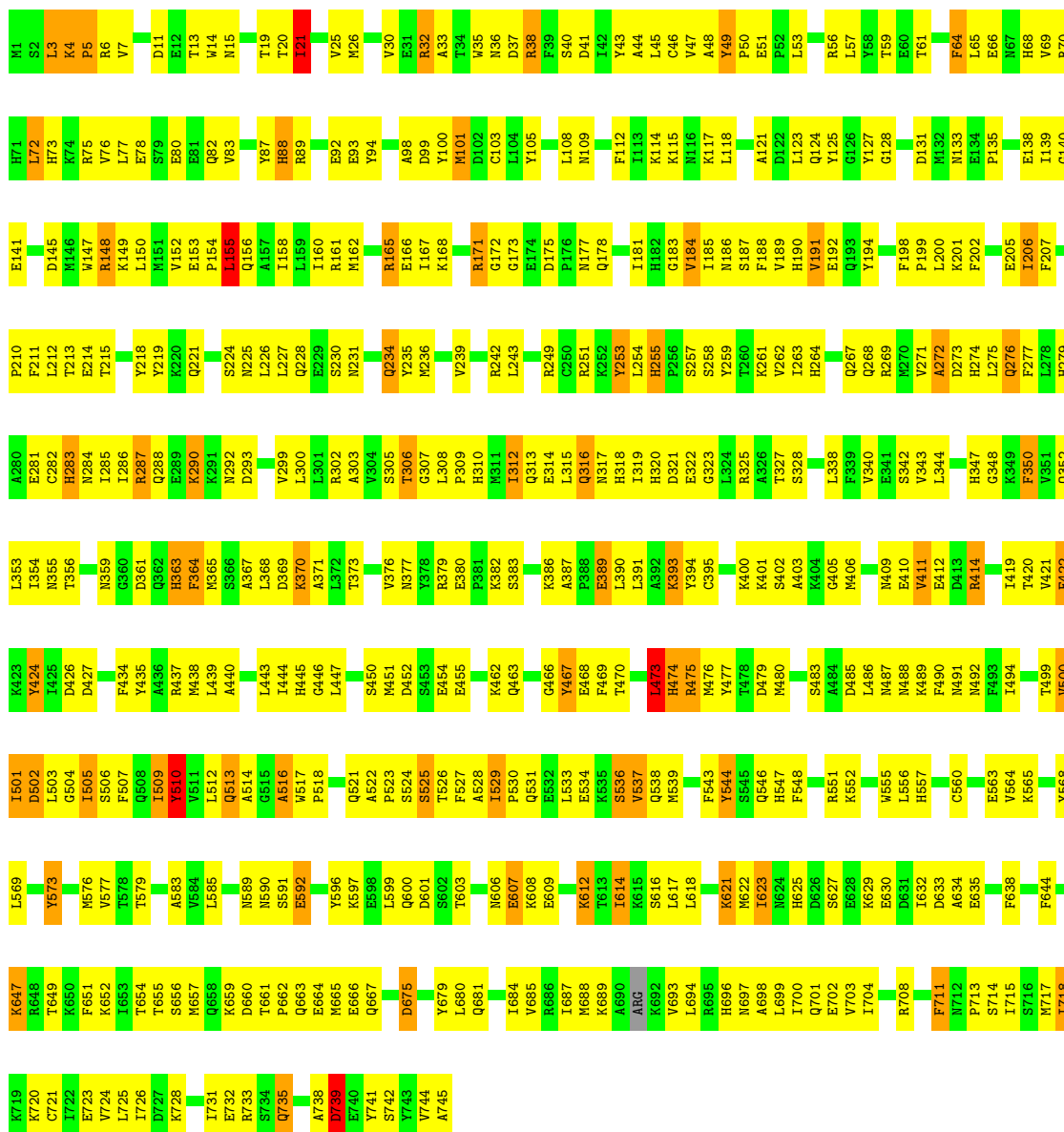
Chain Q: 54% 39% 5%





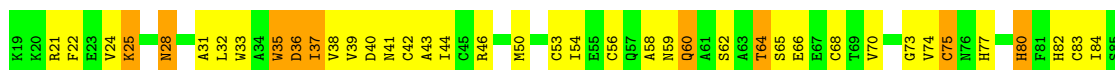
• Molecule 12: Cullin-2

Chain O: 39% 52% 9%



• Molecule 13: E3 ubiquitin-protein ligase RBX1

Chain R: 38% 50% 12%





● Molecule 14: NEDD8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.29	139/3509 (4.0%)	2.51	260/4733 (5.5%)
2	B	3.27	125/3444 (3.6%)	2.58	257/4634 (5.5%)
3	C	2.18	102/3264 (3.1%)	2.47	207/4407 (4.7%)
4	D	2.28	127/3303 (3.8%)	2.58	245/4460 (5.5%)
5	E	3.38	91/2526 (3.6%)	2.56	196/3411 (5.7%)
6	F	2.27	84/2327 (3.6%)	2.62	183/3153 (5.8%)
7	H	2.23	46/1372 (3.4%)	2.55	106/1865 (5.7%)
8	G	2.19	47/1665 (2.8%)	2.52	133/2253 (5.9%)
9	V	1.42	0/1341	1.58	10/1824 (0.5%)
10	P	2.36	41/938 (4.4%)	2.39	56/1267 (4.4%)
11	Q	2.21	24/892 (2.7%)	2.38	48/1204 (4.0%)
12	O	2.14	186/6207 (3.0%)	2.44	439/8358 (5.3%)
13	R	2.48	32/768 (4.2%)	2.52	56/1040 (5.4%)
14	N	0.45	0/596	0.87	0/800
All	All	2.42	1044/32152 (3.2%)	2.46	2196/43409 (5.1%)

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	12
2	B	0	15
3	C	0	6
4	D	0	10
5	E	0	10
6	F	0	7
7	H	0	7
8	G	0	9
10	P	0	2
11	Q	0	5
12	O	0	17

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	R	0	2
All	All	0	102

All (1044) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	294	PHE	CA-C	140.04	3.36	1.52
5	E	309	LYS	CA-CB	121.17	3.41	1.53
5	E	203	TYR	CG-CD2	16.34	1.73	1.39
13	R	106	TYR	CG-CD2	16.28	1.73	1.39
10	P	38	PRO	CA-C	16.22	1.60	1.51
5	E	203	TYR	CE1-CZ	14.67	1.73	1.38
13	R	106	TYR	CG-CD1	14.63	1.70	1.39
5	E	203	TYR	CE2-CZ	14.37	1.72	1.38
13	R	106	TYR	CE2-CZ	14.22	1.72	1.38
5	E	203	TYR	CG-CD1	14.18	1.69	1.39
5	E	234	ASP	CA-C	13.19	1.69	1.52
1	A	229	PRO	CA-CB	12.49	1.61	1.53
5	E	233	LEU	C-N	12.38	1.50	1.33
6	F	45	PRO	CA-C	12.36	1.70	1.52
13	R	106	TYR	CE1-CZ	11.87	1.66	1.38
13	R	106	TYR	CD1-CE1	10.79	1.71	1.38
7	H	164	PRO	CA-C	-10.71	1.41	1.52
5	E	203	TYR	CD1-CE1	10.50	1.70	1.38
5	E	203	TYR	CD2-CE2	9.93	1.68	1.38
13	R	106	TYR	CD2-CE2	9.93	1.68	1.38
1	A	103	ARG	CD-NE	9.90	1.60	1.46
6	F	44	HIS	CA-C	9.80	1.65	1.52
5	E	230	LYS	C-N	9.78	1.47	1.33
5	E	85	VAL	N-CA	-9.71	1.34	1.46
5	E	309	LYS	CA-C	9.60	1.65	1.52
1	A	96	ARG	CD-NE	9.52	1.59	1.46
2	B	294	PHE	CA-CB	9.30	1.68	1.53
11	Q	40	GLY	N-CA	-9.21	1.34	1.45
3	C	71	VAL	CA-C	9.16	1.62	1.52
2	B	164	GLU	CA-CB	9.13	1.65	1.53
2	B	219	GLU	N-CA	9.03	1.57	1.46
2	B	399	HIS	CA-C	-8.86	1.41	1.52
7	H	145	VAL	CA-C	-8.81	1.41	1.52
12	O	303	ALA	CA-C	-8.78	1.41	1.52
5	E	235	ARG	CA-C	-8.67	1.41	1.52
12	O	629	LYS	CA-C	-8.66	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	121	ALA	CA-C	-8.66	1.42	1.52
5	E	184	GLY	CA-C	-8.65	1.44	1.51
4	D	121	ARG	NE-CZ	8.62	1.42	1.33
13	R	91	ARG	CA-CB	8.55	1.67	1.53
11	Q	71	SER	CA-CB	8.52	1.66	1.53
1	A	428	ASP	CA-C	-8.52	1.42	1.52
1	A	426	ALA	C-N	8.50	1.45	1.33
1	A	244	ALA	CA-C	-8.49	1.41	1.52
4	D	274	ARG	NE-CZ	8.48	1.42	1.33
4	D	45	LEU	C-N	8.47	1.44	1.33
5	E	183	LEU	CA-C	-8.41	1.43	1.52
5	E	187	ARG	CD-NE	8.40	1.58	1.46
4	D	159	ASP	C-N	8.39	1.40	1.33
12	O	576	MET	CA-CB	8.39	1.64	1.53
6	F	225	HIS	ND1-CE1	8.39	1.41	1.32
2	B	345	GLU	N-CA	-8.37	1.36	1.46
1	A	100	GLU	N-CA	-8.33	1.36	1.46
1	A	165	HIS	CE1-NE2	-8.33	1.24	1.32
5	E	120	TYR	CA-CB	8.32	1.66	1.53
2	B	273	ARG	NE-CZ	8.31	1.42	1.33
1	A	449	ARG	NE-CZ	8.26	1.42	1.33
4	D	364	ARG	CD-NE	8.25	1.57	1.46
13	R	86	ARG	NE-CZ	8.25	1.42	1.33
8	G	207	GLN	N-CA	-8.24	1.35	1.46
1	A	330	ILE	C-N	8.22	1.44	1.33
7	H	130	ALA	C-N	8.20	1.45	1.34
12	O	302	ARG	CD-NE	8.18	1.57	1.46
4	D	217	VAL	CA-C	-8.14	1.42	1.52
10	P	67	ALA	CA-C	-8.13	1.42	1.52
12	O	161	ARG	CD-NE	8.13	1.57	1.46
1	A	417	VAL	CA-C	-8.11	1.42	1.52
4	D	115	GLU	CA-C	-8.11	1.42	1.52
2	B	410	GLU	CA-C	-8.06	1.44	1.53
2	B	230	HIS	ND1-CE1	8.06	1.40	1.32
6	F	281	ASP	CA-CB	8.05	1.65	1.53
2	B	310	ALA	CA-C	-8.04	1.42	1.52
4	D	201	PHE	CA-C	-8.04	1.42	1.52
4	D	302	ARG	NE-CZ	7.99	1.41	1.33
4	D	170	ARG	NE-CZ	7.96	1.41	1.33
3	C	85	ILE	CA-CB	-7.93	1.44	1.54
5	E	232	SER	C-N	7.92	1.44	1.33
12	O	302	ARG	NE-CZ	7.92	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	530	PRO	CA-C	-7.88	1.44	1.52
6	F	125	TYR	CA-C	-7.86	1.43	1.52
3	C	223	SER	CA-CB	7.83	1.65	1.53
2	B	233	ILE	C-N	7.82	1.44	1.33
2	B	255	HIS	ND1-CE1	7.82	1.40	1.32
2	B	202	ILE	C-N	7.81	1.44	1.33
4	D	120	TRP	C-N	7.81	1.44	1.33
1	A	363	ARG	CD-NE	7.78	1.57	1.46
10	P	81	ALA	CA-C	7.78	1.62	1.52
3	C	127	ALA	C-N	7.75	1.43	1.33
3	C	36	ALA	CA-C	-7.74	1.42	1.52
2	B	368	ARG	N-CA	-7.73	1.37	1.46
3	C	41	HIS	ND1-CE1	7.71	1.40	1.32
12	O	44	ALA	CA-C	-7.69	1.42	1.52
3	C	10	ASN	CA-C	7.66	1.63	1.52
4	D	363	THR	N-CA	-7.64	1.36	1.46
6	F	74	GLY	CA-C	-7.62	1.40	1.51
6	F	46	LEU	CA-C	7.61	1.63	1.52
6	F	172	ILE	N-CA	-7.58	1.36	1.46
1	A	281	PRO	N-CA	-7.56	1.42	1.47
4	D	122	ASN	CA-C	-7.55	1.43	1.52
2	B	401	ARG	CZ-NH2	7.46	1.43	1.33
8	G	160	ARG	CA-C	-7.46	1.42	1.52
3	C	7	GLN	N-CA	-7.45	1.37	1.46
5	E	56	LYS	CA-C	-7.44	1.43	1.52
7	H	97	GLN	CA-C	-7.42	1.43	1.52
12	O	480	MET	CA-C	-7.40	1.43	1.52
12	O	347	HIS	CE1-NE2	7.39	1.40	1.32
5	E	268	ASP	N-CA	-7.39	1.37	1.46
12	O	445	HIS	C-N	7.38	1.41	1.33
1	A	222	VAL	C-N	7.37	1.43	1.33
3	C	112	VAL	C-N	7.35	1.43	1.33
4	D	288	HIS	ND1-CE1	7.35	1.39	1.32
6	F	250	VAL	CA-CB	-7.34	1.44	1.54
4	D	170	ARG	CD-NE	7.33	1.56	1.46
10	P	68	ARG	NE-CZ	7.32	1.41	1.33
3	C	292	MET	CA-C	-7.30	1.43	1.52
3	C	47	GLY	C-N	7.29	1.43	1.33
1	A	387	HIS	C-N	7.29	1.43	1.33
5	E	187	ARG	CA-C	-7.29	1.43	1.52
8	G	189	GLU	CA-C	-7.29	1.43	1.52
4	D	326	ALA	CA-C	7.28	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	80	ARG	NE-CZ	7.28	1.41	1.33
6	F	107	THR	C-N	7.27	1.44	1.34
8	G	55	LEU	CA-CB	7.27	1.65	1.53
12	O	590	ASN	C-N	7.27	1.42	1.33
3	C	47	GLY	CA-C	-7.26	1.43	1.52
12	O	274	HIS	CG-CD2	7.26	1.43	1.35
1	A	467	LYS	N-CA	-7.25	1.36	1.46
2	B	437	ALA	C-N	7.25	1.43	1.33
10	P	90	ILE	CA-C	-7.23	1.43	1.52
5	E	211	ILE	CA-CB	-7.22	1.45	1.54
8	G	188	ILE	CA-C	-7.22	1.43	1.52
3	C	271	ASN	CA-CB	7.21	1.61	1.53
7	H	96	HIS	CG-CD2	7.20	1.43	1.35
6	F	135	ASP	C-N	7.19	1.43	1.33
8	G	114	SER	C-N	7.17	1.43	1.33
7	H	23	GLN	C-N	7.17	1.43	1.33
13	R	38	VAL	CA-C	-7.14	1.43	1.52
1	A	52	SER	C-N	7.14	1.42	1.33
4	D	144	LYS	N-CA	-7.14	1.37	1.46
4	D	217	VAL	C-N	7.12	1.43	1.33
1	A	156	SER	CA-CB	7.12	1.63	1.53
5	E	91	ILE	N-CA	-7.11	1.38	1.46
3	C	385	GLU	CA-CB	7.10	1.64	1.53
10	P	9	ARG	CZ-NH1	7.08	1.42	1.32
8	G	127	GLU	CA-C	-7.07	1.43	1.52
4	D	199	ARG	NE-CZ	7.07	1.40	1.33
8	G	90	THR	C-N	7.06	1.43	1.33
1	A	95	HIS	ND1-CE1	7.05	1.39	1.32
3	C	167	MET	N-CA	-7.05	1.37	1.46
1	A	299	ALA	CA-C	-7.05	1.44	1.52
1	A	416	ARG	NE-CZ	7.05	1.40	1.33
6	F	102	LYS	CA-C	-7.04	1.43	1.52
2	B	209	LYS	CA-C	-7.04	1.44	1.53
1	A	448	ARG	NE-CZ	7.03	1.40	1.33
5	E	43	LYS	C-O	7.03	1.27	1.23
3	C	211	THR	CA-C	-7.02	1.45	1.53
12	O	5	PRO	CA-C	-7.02	1.44	1.52
4	D	38	GLY	CA-C	-7.01	1.45	1.52
6	F	72	LEU	CA-C	-7.00	1.44	1.52
4	D	252	ASP	CA-C	-7.00	1.44	1.52
13	R	91	ARG	C-N	6.98	1.43	1.33
4	D	281	PHE	CA-C	-6.97	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	510	TYR	CA-C	-6.97	1.43	1.52
3	C	23	GLN	N-CA	-6.97	1.37	1.46
7	H	165	ARG	CD-NE	6.97	1.56	1.46
6	F	55	TRP	C-N	6.96	1.42	1.33
2	B	100	ARG	NE-CZ	6.95	1.40	1.33
3	C	180	HIS	ND1-CE1	6.95	1.39	1.32
3	C	92	HIS	ND1-CE1	6.94	1.39	1.32
10	P	78	ALA	N-CA	-6.94	1.36	1.45
2	B	427	TRP	C-N	6.93	1.42	1.33
10	P	40	ASP	N-CA	-6.93	1.37	1.46
12	O	131	ASP	CA-C	-6.93	1.42	1.52
13	R	54	ILE	CA-C	-6.93	1.44	1.52
5	E	27	GLU	N-CA	6.92	1.54	1.46
11	Q	75	MET	CA-C	-6.92	1.43	1.52
1	A	420	HIS	CE1-NE2	-6.91	1.25	1.32
12	O	560	CYS	CA-C	6.91	1.61	1.52
12	O	75	ARG	CA-C	6.89	1.61	1.52
8	G	123	ARG	C-N	6.89	1.42	1.33
5	E	231	SER	C-N	6.89	1.43	1.33
13	R	87	TRP	N-CA	-6.89	1.38	1.46
10	P	48	ASP	CA-C	-6.88	1.43	1.53
4	D	347	ARG	NE-CZ	6.88	1.40	1.33
6	F	59	ARG	CD-NE	6.88	1.55	1.46
12	O	368	LEU	N-CA	-6.88	1.38	1.46
1	A	429	VAL	N-CA	-6.87	1.38	1.46
1	A	414	SER	C-N	6.87	1.42	1.33
6	F	33	CYS	C-N	6.86	1.42	1.33
3	C	389	ARG	NE-CZ	6.86	1.40	1.33
8	G	194	ARG	C-N	6.85	1.42	1.33
4	D	39	ALA	N-CA	6.85	1.54	1.46
3	C	387	ASP	N-CA	-6.85	1.38	1.46
12	O	133	ASN	C-O	-6.85	1.15	1.23
1	A	385	ASP	CA-C	6.84	1.61	1.52
1	A	234	GLN	CA-C	-6.83	1.45	1.52
12	O	243	LEU	CA-CB	6.83	1.64	1.53
8	G	75	TYR	N-CA	-6.82	1.39	1.46
4	D	174	LEU	CA-C	-6.81	1.43	1.52
12	O	6	ARG	CD-NE	6.81	1.55	1.46
1	A	414	SER	CA-CB	6.81	1.61	1.53
12	O	434	PHE	CA-C	-6.79	1.44	1.52
4	D	228	HIS	N-CA	-6.79	1.38	1.46
4	D	233	THR	C-N	6.77	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	227	TYR	C-N	6.77	1.42	1.33
1	A	108	GLU	C-N	6.76	1.43	1.33
1	A	461	ARG	CZ-NH1	6.75	1.42	1.32
8	G	208	GLN	C-N	6.72	1.42	1.33
3	C	222	GLU	CA-C	-6.71	1.44	1.52
12	O	224	SER	CA-C	-6.71	1.44	1.52
6	F	206	MET	CA-CB	6.70	1.63	1.53
2	B	323	ILE	C-N	6.69	1.42	1.33
12	O	368	LEU	CA-CB	6.69	1.63	1.53
1	A	90	MET	C-N	6.68	1.42	1.33
1	A	293	GLY	CA-C	-6.68	1.43	1.51
5	E	224	LEU	C-N	6.67	1.42	1.33
6	F	94	VAL	CA-CB	6.67	1.62	1.54
1	A	427	ARG	NE-CZ	6.66	1.40	1.33
12	O	70	ARG	CD-NE	6.66	1.55	1.46
5	E	174	ARG	NE-CZ	6.66	1.40	1.33
3	C	270	ASN	CA-C	-6.66	1.43	1.52
2	B	156	GLY	CA-C	-6.64	1.44	1.52
5	E	140	HIS	CG-CD2	6.64	1.43	1.35
1	A	136	LYS	CA-CB	6.63	1.63	1.53
1	A	397	VAL	CA-C	-6.63	1.44	1.52
5	E	309	LYS	N-CA	6.63	1.54	1.46
11	Q	101	LEU	C-O	-6.63	1.16	1.24
2	B	143	LYS	CA-CB	6.62	1.63	1.53
6	F	45	PRO	N-CD	6.62	1.57	1.47
4	D	383	ASN	CA-CB	6.62	1.63	1.53
7	H	121	VAL	CA-C	6.62	1.61	1.52
1	A	217	HIS	C-N	6.61	1.42	1.33
12	O	14	TRP	CA-CB	6.60	1.63	1.53
12	O	488	ASN	C-N	6.58	1.42	1.33
4	D	27	ARG	NE-CZ	6.58	1.40	1.33
12	O	438	MET	N-CA	-6.58	1.38	1.46
5	E	47	LYS	CA-C	6.57	1.61	1.52
3	C	91	GLU	CA-C	-6.57	1.43	1.52
3	C	331	PRO	N-CD	6.57	1.56	1.47
12	O	618	LEU	C-N	6.57	1.42	1.33
5	E	77	VAL	CA-C	6.57	1.60	1.52
3	C	60	ALA	N-CA	-6.57	1.38	1.46
2	B	129	GLN	N-CA	-6.56	1.38	1.46
2	B	114	SER	CA-CB	6.56	1.63	1.53
4	D	293	THR	CB-OG1	-6.56	1.33	1.43
10	P	109	GLY	CA-C	-6.56	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	83	TYR	C-N	6.56	1.42	1.33
5	E	66	VAL	N-CA	6.55	1.54	1.46
4	D	91	LYS	C-N	6.54	1.41	1.34
5	E	72	GLY	CA-C	-6.54	1.44	1.52
2	B	325	GLU	CA-C	-6.54	1.44	1.52
12	O	105	TYR	C-N	6.54	1.42	1.33
12	O	282	CYS	CA-CB	6.54	1.63	1.53
1	A	271	LEU	CA-C	-6.54	1.44	1.52
10	P	68	ARG	CD-NE	6.53	1.55	1.46
5	E	190	PRO	CA-C	-6.52	1.44	1.52
5	E	260	ASP	C-N	6.52	1.42	1.33
2	B	215	LYS	CA-C	6.51	1.61	1.52
6	F	284	ASN	N-CA	-6.51	1.38	1.46
2	B	75	MET	C-N	6.50	1.42	1.33
5	E	47	LYS	C-N	6.50	1.42	1.33
6	F	73	ILE	CA-C	-6.49	1.45	1.52
10	P	10	HIS	ND1-CE1	6.49	1.39	1.32
12	O	370	LYS	CA-C	6.48	1.61	1.52
12	O	592	GLU	CA-CB	6.47	1.63	1.53
3	C	223	SER	C-N	6.47	1.42	1.33
6	F	218	ALA	CA-C	-6.46	1.44	1.52
2	B	267	GLU	CA-CB	6.45	1.63	1.53
3	C	373	LEU	CA-C	-6.45	1.44	1.52
12	O	249	ARG	CZ-NH1	6.45	1.41	1.32
3	C	219	ILE	CA-CB	6.45	1.64	1.54
3	C	27	LEU	CA-CB	6.43	1.63	1.53
1	A	71	ARG	CD-NE	6.43	1.55	1.46
1	A	235	ARG	CA-C	-6.43	1.45	1.52
3	C	132	GLN	C-N	6.43	1.42	1.33
5	E	280	LEU	CA-C	-6.43	1.44	1.52
4	D	399	ALA	C-N	6.41	1.42	1.33
8	G	9	SER	CA-C	-6.40	1.44	1.52
1	A	259	ALA	C-N	6.40	1.42	1.33
5	E	40	LEU	CA-CB	6.38	1.63	1.53
12	O	454	GLU	CA-C	-6.37	1.44	1.52
8	G	102	VAL	C-N	6.37	1.42	1.33
5	E	201	SER	CA-C	6.36	1.60	1.52
5	E	290	GLU	C-N	6.36	1.42	1.33
2	B	71	ALA	CA-C	-6.36	1.44	1.52
5	E	310	THR	CA-C	-6.35	1.44	1.52
12	O	290	LYS	N-CA	6.34	1.54	1.46
1	A	228	THR	N-CA	6.34	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	66	THR	C-N	6.34	1.42	1.33
1	A	228	THR	CA-C	6.33	1.59	1.52
8	G	27	LEU	C-N	6.33	1.42	1.33
2	B	272	ARG	NE-CZ	6.32	1.40	1.33
13	R	77	HIS	ND1-CE1	6.32	1.38	1.32
8	G	148	ARG	CD-NE	6.32	1.55	1.46
12	O	243	LEU	C-O	-6.31	1.16	1.24
12	O	269	ARG	NE-CZ	6.28	1.40	1.33
4	D	315	LEU	C-N	6.28	1.42	1.33
11	Q	30	ILE	CA-C	-6.28	1.44	1.52
5	E	294	ARG	NE-CZ	6.27	1.40	1.33
4	D	216	ILE	N-CA	-6.26	1.38	1.46
5	E	244	LYS	CA-CB	6.26	1.63	1.53
5	E	316	HIS	ND1-CE1	6.26	1.38	1.32
7	H	45	LEU	C-N	6.26	1.42	1.33
12	O	530	PRO	C-N	6.26	1.42	1.33
1	A	309	ASN	C-N	6.25	1.41	1.33
4	D	251	LYS	CA-C	-6.25	1.44	1.52
8	G	40	VAL	CA-CB	-6.25	1.46	1.54
2	B	91	ARG	CD-NE	6.24	1.54	1.46
2	B	357	GLN	CA-CB	6.24	1.63	1.53
2	B	175	LEU	CA-CB	6.24	1.63	1.53
12	O	347	HIS	ND1-CE1	6.24	1.38	1.32
1	A	223	SER	N-CA	-6.24	1.38	1.46
2	B	143	LYS	C-N	6.23	1.42	1.33
2	B	201	GLU	C-N	6.23	1.41	1.33
5	E	32	ASP	CA-CB	6.23	1.63	1.53
2	B	134	THR	C-N	6.22	1.42	1.33
6	F	45	PRO	N-CA	6.22	1.55	1.47
7	H	59	ARG	NE-CZ	6.22	1.39	1.33
4	D	315	LEU	N-CA	-6.22	1.38	1.46
7	H	70	GLU	N-CA	-6.22	1.38	1.46
7	H	137	VAL	C-N	6.22	1.41	1.33
4	D	338	ILE	C-N	6.21	1.41	1.33
12	O	255	HIS	CE1-NE2	-6.21	1.26	1.32
4	D	228	HIS	C-N	6.21	1.41	1.33
1	A	466	VAL	CA-C	-6.21	1.45	1.52
7	H	84	ARG	NE-CZ	6.20	1.39	1.33
2	B	36	TYR	CA-CB	6.19	1.62	1.53
4	D	242	ARG	CA-CB	6.19	1.62	1.53
12	O	494	ILE	C-O	-6.19	1.16	1.24
1	A	433	SER	CA-CB	6.19	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	367	TYR	CA-C	-6.18	1.44	1.52
8	G	45	GLU	N-CA	6.18	1.53	1.46
12	O	11	ASP	C-N	6.18	1.41	1.33
4	D	324	LEU	N-CA	-6.18	1.39	1.46
12	O	128	GLY	C-N	6.17	1.38	1.33
6	F	124	TRP	CA-C	-6.17	1.44	1.52
6	F	79	ARG	CZ-NH2	6.17	1.41	1.33
13	R	33	TRP	N-CA	-6.17	1.38	1.46
12	O	285	ILE	CA-CB	-6.16	1.46	1.54
11	Q	90	ILE	CA-C	-6.16	1.47	1.52
12	O	393	LYS	CA-C	-6.16	1.44	1.52
6	F	288	LEU	CA-C	-6.15	1.44	1.52
4	D	281	PHE	N-CA	-6.14	1.39	1.46
6	F	197	ARG	NE-CZ	6.14	1.39	1.33
6	F	149	PRO	CA-C	-6.14	1.46	1.52
13	R	59	ASN	CA-C	6.14	1.60	1.52
5	E	282	ARG	CD-NE	6.14	1.54	1.46
12	O	65	LEU	N-CA	-6.13	1.39	1.46
1	A	406	GLN	N-CA	-6.13	1.39	1.46
5	E	55	CYS	N-CA	-6.13	1.38	1.45
12	O	445	HIS	ND1-CE1	6.12	1.38	1.32
3	C	195	LEU	C-N	6.12	1.42	1.33
6	F	175	ILE	CA-C	-6.12	1.44	1.52
8	G	36	GLU	CA-CB	6.11	1.62	1.53
12	O	262	VAL	C-N	6.11	1.41	1.33
13	R	99	ARG	CZ-NH2	6.11	1.41	1.33
8	G	111	ILE	CB-CG1	6.11	1.65	1.53
4	D	317	ASN	C-N	6.11	1.41	1.33
1	A	43	ASP	CA-C	-6.09	1.44	1.52
1	A	66	HIS	CE1-NE2	-6.09	1.26	1.32
4	D	396	THR	C-N	6.09	1.42	1.33
12	O	422	PHE	C-N	6.08	1.42	1.33
12	O	443	LEU	C-N	6.08	1.41	1.33
2	B	438	VAL	C-N	6.08	1.40	1.34
8	G	201	ASN	C-N	6.08	1.42	1.33
1	A	193	THR	N-CA	-6.08	1.40	1.46
6	F	296	THR	C-N	6.08	1.41	1.33
1	A	62	PHE	CA-C	-6.07	1.44	1.52
1	A	189	ARG	CD-NE	6.07	1.54	1.46
5	E	97	ALA	C-N	6.07	1.41	1.33
12	O	287	ARG	CZ-NH2	6.07	1.41	1.33
1	A	135	ARG	C-N	6.07	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	261	TYR	CA-C	6.07	1.60	1.52
4	D	84	ILE	C-O	-6.06	1.17	1.24
7	H	98	TRP	CA-C	-6.06	1.45	1.52
5	E	233	LEU	N-CA	6.06	1.53	1.46
4	D	57	VAL	CA-C	-6.04	1.45	1.52
4	D	152	ALA	C-N	6.04	1.41	1.33
1	A	328	ASP	CA-CB	6.03	1.63	1.53
6	F	265	HIS	ND1-CE1	6.03	1.38	1.32
6	F	315	ARG	NE-CZ	6.03	1.39	1.33
12	O	414	ARG	CD-NE	6.03	1.54	1.46
2	B	315	VAL	C-O	-6.03	1.17	1.24
4	D	169	ASN	CA-C	-6.02	1.45	1.52
12	O	437	ARG	CD-NE	6.02	1.54	1.46
2	B	43	LYS	C-N	6.02	1.42	1.33
3	C	180	HIS	CA-C	-6.02	1.45	1.52
6	F	285	ASP	C-N	6.01	1.40	1.34
3	C	271	ASN	C-O	-6.01	1.20	1.25
10	P	114	GLU	CA-CB	6.01	1.63	1.53
12	O	38	ARG	NE-CZ	6.00	1.39	1.33
1	A	303	ARG	C-N	6.00	1.41	1.33
2	B	60	LEU	CA-CB	6.00	1.63	1.53
6	F	139	HIS	ND1-CE1	6.00	1.38	1.32
1	A	84	ARG	CA-CB	5.99	1.62	1.53
3	C	102	GLY	CA-C	-5.99	1.45	1.52
1	A	197	HIS	ND1-CE1	5.99	1.38	1.32
3	C	277	ASN	CA-CB	5.99	1.62	1.53
12	O	40	SER	C-N	5.99	1.41	1.33
8	G	131	LEU	CA-CB	5.99	1.62	1.53
5	E	124	ALA	C-O	-5.98	1.17	1.24
6	F	185	GLU	C-N	5.98	1.42	1.33
5	E	32	ASP	CA-C	5.97	1.59	1.52
2	B	402	ILE	CA-C	-5.97	1.45	1.52
3	C	344	ASP	CA-C	-5.96	1.45	1.52
6	F	97	LYS	N-CA	5.96	1.53	1.45
4	D	395	TRP	CA-C	-5.95	1.44	1.52
3	C	218	HIS	ND1-CE1	5.95	1.38	1.32
11	Q	60	VAL	CA-C	-5.95	1.45	1.52
4	D	198	ARG	CD-NE	5.95	1.54	1.46
1	A	41	SER	CA-C	-5.95	1.44	1.52
5	E	35	GLN	C-N	5.95	1.42	1.33
7	H	145	VAL	C-N	5.95	1.41	1.33
12	O	600	GLN	CA-CB	5.95	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	97	THR	C-N	5.94	1.41	1.33
3	C	286	PHE	CA-C	-5.94	1.45	1.52
1	A	84	ARG	CD-NE	5.93	1.54	1.46
1	A	56	ARG	CZ-NH1	5.93	1.41	1.32
1	A	133	ALA	N-CA	-5.93	1.39	1.46
3	C	190	MET	N-CA	-5.93	1.39	1.46
12	O	320	HIS	CG-CD2	5.93	1.42	1.35
12	O	259	TYR	C-O	-5.93	1.17	1.24
12	O	409	ASN	CA-CB	5.93	1.61	1.54
1	A	372	ARG	NE-CZ	5.92	1.39	1.33
2	B	105	ARG	CD-NE	5.92	1.54	1.46
5	E	169	VAL	CA-C	-5.92	1.45	1.52
12	O	83	VAL	N-CA	-5.92	1.39	1.46
11	Q	68	HIS	CA-C	-5.92	1.44	1.52
3	C	68	MET	CA-C	-5.92	1.47	1.53
3	C	299	LEU	CA-C	-5.92	1.45	1.52
5	E	234	ASP	N-CA	5.92	1.53	1.46
6	F	153	LYS	CA-CB	5.92	1.64	1.53
7	H	49	ASP	C-N	5.92	1.42	1.34
7	H	165	ARG	CZ-NH1	5.91	1.41	1.32
10	P	82	ASP	CA-C	-5.91	1.44	1.52
12	O	231	ASN	N-CA	-5.91	1.38	1.45
3	C	349	ALA	CA-C	-5.90	1.45	1.52
1	A	281	PRO	CA-CB	5.90	1.60	1.53
2	B	436	GLN	CA-C	-5.90	1.45	1.52
12	O	293	ASP	CA-C	5.89	1.60	1.52
12	O	205	GLU	C-N	5.89	1.41	1.33
2	B	422	THR	N-CA	5.89	1.53	1.46
10	P	63	THR	C-N	5.89	1.42	1.33
12	O	573	TYR	N-CA	5.89	1.53	1.46
12	O	310	HIS	ND1-CE1	5.89	1.38	1.32
4	D	292	THR	CA-C	-5.88	1.45	1.52
4	D	17	GLY	C-N	5.88	1.41	1.33
5	E	234	ASP	C-N	5.88	1.41	1.33
7	H	118	PHE	N-CA	-5.87	1.39	1.46
1	A	218	VAL	CA-CB	-5.87	1.47	1.54
1	A	58	GLU	CA-C	-5.86	1.45	1.52
1	A	428	ASP	CA-CB	5.86	1.61	1.53
6	F	232	HIS	ND1-CE1	5.86	1.38	1.32
13	R	22	PHE	CA-C	-5.86	1.45	1.52
1	A	369	ILE	CA-CB	-5.86	1.47	1.54
6	F	197	ARG	CA-CB	5.86	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	556	LEU	CA-C	-5.86	1.44	1.53
8	G	53	GLN	C-N	5.86	1.41	1.34
3	C	2	ALA	N-CA	-5.85	1.38	1.45
12	O	409	ASN	N-CA	-5.85	1.38	1.46
1	A	396	THR	C-N	5.85	1.41	1.33
10	P	104	LYS	CA-C	-5.85	1.47	1.53
13	R	86	ARG	CZ-NH1	5.85	1.41	1.32
7	H	164	PRO	N-CA	-5.85	1.40	1.47
5	E	328	PHE	CA-CB	5.84	1.63	1.53
11	Q	98	GLU	C-N	5.84	1.41	1.33
4	D	222	ARG	CZ-NH1	5.84	1.41	1.32
2	B	45	ASP	CA-CB	5.84	1.62	1.53
12	O	596	TYR	C-N	5.84	1.41	1.33
7	H	148	ILE	CA-CB	-5.83	1.47	1.54
2	B	247	ARG	NE-CZ	5.83	1.39	1.33
4	D	256	GLN	CA-C	5.83	1.60	1.52
3	C	372	MET	C-N	5.83	1.41	1.33
4	D	203	GLU	CA-CB	5.83	1.62	1.53
4	D	221	GLU	C-N	5.83	1.41	1.34
7	H	98	TRP	CD2-CE3	-5.83	1.30	1.40
3	C	114	ARG	CZ-NH2	5.82	1.41	1.33
12	O	547	HIS	ND1-CE1	5.82	1.38	1.32
3	C	325	ARG	CA-C	5.82	1.60	1.52
4	D	234	ILE	C-O	-5.82	1.17	1.24
12	O	283	HIS	CG-ND1	5.82	1.44	1.38
8	G	20	LYS	CA-C	-5.82	1.44	1.52
13	R	91	ARG	CA-C	-5.82	1.45	1.52
4	D	302	ARG	CD-NE	5.81	1.54	1.46
1	A	119	SER	CA-CB	5.81	1.63	1.53
1	A	135	ARG	CZ-NH1	5.81	1.40	1.32
2	B	377	GLU	CA-CB	5.81	1.62	1.53
3	C	136	ASN	C-N	5.81	1.41	1.33
12	O	342	SER	CA-C	-5.80	1.45	1.52
1	A	126	LEU	N-CA	-5.80	1.38	1.46
1	A	103	ARG	NE-CZ	5.80	1.39	1.33
5	E	121	ILE	N-CA	5.80	1.53	1.46
12	O	264	HIS	ND1-CE1	5.80	1.38	1.32
3	C	180	HIS	CD2-NE2	5.80	1.44	1.37
10	P	88	LEU	CA-C	-5.80	1.45	1.52
12	O	489	LYS	CA-C	-5.80	1.45	1.52
2	B	429	ASN	C-N	5.79	1.42	1.34
8	G	115	VAL	CA-C	-5.79	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	287	ARG	CD-NE	5.79	1.54	1.46
1	A	59	ARG	CA-C	-5.79	1.45	1.52
13	R	70	VAL	C-N	5.79	1.41	1.33
2	B	399	HIS	ND1-CE1	5.78	1.38	1.32
3	C	6	GLU	N-CA	5.78	1.53	1.46
2	B	43	LYS	CA-CB	5.78	1.63	1.53
3	C	399	VAL	CA-CB	-5.78	1.47	1.54
7	H	147	GLY	CA-C	-5.78	1.45	1.52
2	B	284	ASN	C-N	5.77	1.41	1.33
12	O	281	GLU	CA-CB	5.77	1.62	1.53
8	G	21	GLY	C-N	5.77	1.41	1.33
10	P	16	THR	CA-C	-5.77	1.45	1.52
6	F	279	PHE	C-N	5.77	1.41	1.33
12	O	525	SER	C-N	5.77	1.42	1.33
2	B	434	LEU	CA-C	-5.77	1.45	1.52
13	R	59	ASN	C-N	5.77	1.41	1.33
5	E	323	ILE	CB-CG1	5.76	1.65	1.53
6	F	295	ILE	CA-C	-5.76	1.45	1.52
12	O	318	HIS	CA-CB	5.76	1.62	1.53
12	O	47	VAL	C-N	5.76	1.41	1.33
4	D	263	ILE	C-N	5.76	1.40	1.33
12	O	325	ARG	N-CA	-5.76	1.39	1.46
13	R	98	ASN	CA-C	5.76	1.60	1.52
5	E	185	ALA	CA-C	-5.75	1.45	1.52
12	O	447	LEU	CA-C	-5.75	1.45	1.52
5	E	118	ALA	CA-C	-5.75	1.45	1.52
12	O	255	HIS	CA-C	-5.75	1.46	1.53
1	A	127	ASP	CA-C	-5.74	1.45	1.52
1	A	153	LYS	CA-C	-5.74	1.45	1.52
12	O	406	MET	CA-C	-5.73	1.45	1.52
4	D	172	SER	CA-C	-5.73	1.45	1.52
8	G	117	LEU	N-CA	-5.73	1.39	1.46
12	O	612	LYS	C-N	5.73	1.41	1.33
4	D	219	GLU	CA-C	-5.72	1.45	1.52
8	G	122	MET	CA-CB	5.72	1.62	1.53
3	C	238	VAL	CA-C	5.72	1.59	1.52
7	H	160	ARG	NE-CZ	5.72	1.39	1.33
12	O	625	HIS	C-N	5.72	1.41	1.34
3	C	202	LEU	CA-CB	5.71	1.62	1.53
4	D	218	HIS	ND1-CE1	5.71	1.38	1.32
6	F	239	LEU	C-N	5.71	1.41	1.34
3	C	376	ILE	C-N	5.71	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	251	PRO	CA-C	-5.71	1.46	1.52
12	O	100	TYR	CA-C	-5.71	1.45	1.52
2	B	209	LYS	C-N	5.70	1.41	1.33
2	B	392	CYS	CA-C	-5.70	1.45	1.52
4	D	95	ARG	CZ-NH1	5.70	1.40	1.32
1	A	164	GLY	CA-C	-5.70	1.45	1.52
4	D	63	ARG	CA-CB	5.70	1.62	1.53
2	B	237	ILE	CA-C	-5.69	1.45	1.52
13	R	105	LYS	C-O	-5.69	1.16	1.24
4	D	285	LEU	N-CA	-5.69	1.38	1.45
2	B	119	ILE	C-N	5.69	1.41	1.33
8	G	38	PRO	CA-C	-5.69	1.45	1.52
3	C	388	GLU	C-N	5.68	1.41	1.33
4	D	95	ARG	C-N	5.68	1.41	1.34
4	D	244	ARG	CZ-NH2	5.68	1.40	1.33
12	O	591	SER	C-N	5.68	1.41	1.33
12	O	504	GLY	N-CA	5.68	1.53	1.45
13	R	96	LEU	C-N	5.67	1.41	1.34
4	D	327	LEU	C-N	5.67	1.41	1.33
12	O	15	ASN	C-N	5.67	1.41	1.33
2	B	260	GLU	CA-CB	5.67	1.62	1.53
8	G	187	GLY	C-N	5.66	1.41	1.33
12	O	165	ARG	N-CA	-5.66	1.39	1.46
12	O	300	LEU	C-O	5.66	1.30	1.24
2	B	355	ARG	CA-C	-5.65	1.45	1.52
4	D	364	ARG	C-N	5.65	1.41	1.33
3	C	83	LEU	N-CA	5.65	1.53	1.46
6	F	134	SER	N-CA	-5.65	1.39	1.46
11	Q	15	ASP	CA-C	5.65	1.60	1.52
12	O	258	SER	C-N	5.65	1.41	1.33
4	D	343	ILE	CA-CB	5.65	1.61	1.54
10	P	60	CYS	CA-CB	5.65	1.63	1.53
12	O	608	LYS	CA-C	-5.65	1.45	1.52
13	R	44	ILE	N-CA	5.64	1.54	1.46
6	F	118	GLU	C-N	5.64	1.40	1.33
11	Q	72	LYS	C-N	5.64	1.41	1.33
10	P	111	SER	N-CA	-5.64	1.39	1.46
1	A	255	LEU	C-N	5.63	1.41	1.33
12	O	455	GLU	C-N	5.63	1.41	1.33
12	O	506	SER	CA-CB	5.63	1.62	1.53
1	A	458	ALA	C-N	5.63	1.41	1.33
12	O	314	GLU	CA-CB	5.63	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	TYR	C-N	5.63	1.41	1.33
3	C	281	LYS	C-N	5.63	1.42	1.33
5	E	210	LYS	N-CA	-5.63	1.38	1.46
4	D	284	MET	C-N	5.62	1.41	1.33
7	H	96	HIS	CA-C	-5.62	1.45	1.52
12	O	325	ARG	CZ-NH1	5.62	1.40	1.32
2	B	395	ASP	C-N	5.62	1.41	1.33
4	D	108	GLN	CA-C	-5.62	1.45	1.52
1	A	178	LEU	N-CA	-5.62	1.39	1.46
3	C	354	LYS	N-CA	-5.61	1.39	1.46
4	D	196	ASP	C-N	5.61	1.41	1.33
10	P	6	MET	C-N	5.61	1.40	1.33
12	O	225	ASN	CA-C	-5.61	1.45	1.52
1	A	300	THR	CA-C	5.60	1.59	1.52
12	O	462	LYS	C-N	5.60	1.41	1.33
12	O	315	LEU	C-N	5.60	1.41	1.33
10	P	47	ASP	CA-C	-5.60	1.46	1.53
10	P	101	ASP	CA-CB	5.60	1.62	1.53
12	O	516	ALA	CA-CB	5.60	1.63	1.53
1	A	197	HIS	CE1-NE2	-5.60	1.26	1.32
4	D	321	PHE	C-N	5.60	1.41	1.33
12	O	251	ARG	CD-NE	5.59	1.54	1.46
5	E	264	GLY	C-N	5.59	1.41	1.33
6	F	43	LEU	N-CA	5.59	1.52	1.46
2	B	375	SER	CA-C	-5.59	1.45	1.52
1	A	267	ALA	C-N	5.59	1.41	1.33
12	O	454	GLU	CA-CB	5.59	1.62	1.53
1	A	135	ARG	CD-NE	5.59	1.54	1.46
7	H	59	ARG	CA-C	5.59	1.60	1.52
4	D	316	TYR	CA-C	5.58	1.60	1.52
12	O	299	VAL	C-N	5.58	1.41	1.33
6	F	169	GLU	N-CA	-5.58	1.39	1.45
12	O	479	ASP	C-N	5.58	1.41	1.33
6	F	314	ASP	CA-CB	-5.58	1.44	1.53
12	O	273	ASP	N-CA	-5.58	1.39	1.46
12	O	443	LEU	N-CA	5.58	1.53	1.46
3	C	194	GLY	CA-C	-5.58	1.45	1.52
12	O	638	PHE	N-CA	-5.58	1.39	1.46
12	O	506	SER	C-N	5.57	1.41	1.33
1	A	48	ALA	CA-C	-5.57	1.45	1.52
6	F	163	LEU	C-O	-5.57	1.17	1.24
1	A	465	HIS	N-CA	-5.57	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	436	GLN	C-N	5.57	1.41	1.33
10	P	92	PRO	C-N	5.57	1.41	1.33
4	D	108	GLN	C-O	-5.56	1.17	1.24
10	P	10	HIS	CB-CG	-5.56	1.42	1.50
12	O	66	GLU	CA-C	-5.56	1.45	1.52
1	A	308	ARG	CZ-NH1	5.55	1.40	1.32
12	O	354	ILE	C-N	5.54	1.41	1.33
8	G	142	GLN	N-CA	-5.54	1.39	1.46
2	B	154	LYS	C-N	5.54	1.41	1.33
6	F	64	ARG	CZ-NH2	5.54	1.40	1.33
2	B	189	LYS	CA-C	-5.54	1.45	1.52
4	D	186	HIS	ND1-CE1	5.54	1.38	1.32
1	A	43	ASP	CA-CB	5.54	1.59	1.52
7	H	200	LEU	CA-CB	5.54	1.61	1.53
2	B	158	LEU	N-CA	-5.53	1.39	1.46
5	E	175	THR	N-CA	-5.53	1.39	1.46
8	G	131	LEU	CA-C	-5.53	1.45	1.52
11	Q	75	MET	N-CA	-5.53	1.39	1.46
3	C	375	ASN	CA-C	5.53	1.59	1.52
8	G	32	SER	C-N	5.53	1.41	1.33
11	Q	102	GLU	C-O	-5.53	1.17	1.24
12	O	165	ARG	CZ-NH2	5.53	1.40	1.33
13	R	74	VAL	N-CA	5.53	1.53	1.46
13	R	73	GLY	N-CA	-5.52	1.38	1.45
2	B	119	ILE	CA-CB	-5.52	1.47	1.54
4	D	244	ARG	NE-CZ	5.51	1.39	1.33
11	Q	67	SER	CA-CB	5.51	1.61	1.53
4	D	353	ASP	N-CA	-5.51	1.39	1.46
12	O	563	GLU	CA-C	-5.51	1.46	1.52
12	O	585	LEU	CA-C	5.51	1.59	1.52
3	C	301	SER	C-N	5.51	1.41	1.33
5	E	39	ILE	N-CA	-5.51	1.40	1.46
2	B	153	THR	C-N	5.50	1.41	1.33
5	E	109	ALA	C-N	5.50	1.41	1.34
6	F	61	GLN	C-N	5.50	1.41	1.33
6	F	299	CYS	CA-C	-5.50	1.45	1.52
4	D	222	ARG	C-N	5.50	1.41	1.33
2	B	177	GLN	C-N	5.49	1.40	1.33
2	B	146	ARG	CD-NE	5.49	1.53	1.46
4	D	82	LYS	CA-CB	5.49	1.61	1.53
10	P	21	SER	C-N	5.49	1.41	1.33
3	C	363	ASN	CA-CB	5.48	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	242	ARG	CA-C	5.48	1.59	1.52
13	R	50	MET	SD-CE	5.48	1.93	1.79
1	A	343	LYS	C-N	5.48	1.41	1.33
2	B	176	HIS	ND1-CE1	5.48	1.38	1.32
2	B	212	LYS	N-CA	-5.48	1.39	1.46
11	Q	79	TYR	CA-CB	5.48	1.61	1.53
5	E	234	ASP	CA-CB	5.47	1.61	1.53
6	F	145	ILE	CA-C	5.47	1.59	1.52
2	B	47	PRO	CA-C	-5.47	1.45	1.52
4	D	111	ALA	CA-C	-5.47	1.45	1.52
2	B	429	ASN	CA-C	5.47	1.59	1.52
4	D	240	GLN	CA-C	-5.47	1.45	1.52
5	E	188	THR	CA-CB	5.47	1.62	1.53
4	D	298	SER	C-N	5.46	1.41	1.33
2	B	132	TYR	CA-C	-5.46	1.45	1.52
4	D	400	MET	N-CA	-5.46	1.39	1.46
3	C	116	GLN	CA-CB	5.46	1.61	1.53
7	H	45	LEU	N-CA	5.46	1.52	1.46
1	A	40	PRO	C-N	5.46	1.39	1.33
4	D	279	GLN	CD-NE2	5.46	1.44	1.33
2	B	133	GLU	C-N	5.45	1.41	1.34
11	Q	54	GLU	CA-CB	5.45	1.61	1.53
13	R	107	GLY	C-N	5.45	1.41	1.33
1	A	261	ARG	NE-CZ	5.45	1.39	1.33
10	P	72	PRO	CA-CB	5.45	1.61	1.53
12	O	72	LEU	CA-C	-5.44	1.45	1.52
2	B	140	LYS	C-O	-5.44	1.17	1.24
4	D	360	HIS	ND1-CE1	5.44	1.38	1.32
10	P	74	THR	CA-C	5.44	1.59	1.52
11	Q	8	TYR	N-CA	-5.44	1.39	1.46
12	O	133	ASN	CA-CB	5.44	1.62	1.53
3	C	144	ASP	N-CA	-5.44	1.39	1.46
12	O	536	SER	C-N	5.44	1.40	1.33
1	A	199	ILE	CA-C	-5.43	1.46	1.52
12	O	124	GLN	CD-NE2	5.43	1.44	1.33
2	B	389	LEU	CA-C	-5.43	1.45	1.52
5	E	293	ASP	CA-C	-5.43	1.45	1.52
1	A	187	ARG	CZ-NH2	5.43	1.40	1.33
4	D	279	GLN	CA-CB	5.43	1.61	1.53
5	E	60	LEU	N-CA	-5.43	1.39	1.46
1	A	408	ILE	C-N	5.42	1.40	1.33
3	C	304	LYS	CA-C	-5.42	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	38	ARG	CZ-NH1	5.42	1.40	1.32
10	P	79	PHE	N-CA	-5.42	1.38	1.45
6	F	226	SER	N-CA	-5.42	1.39	1.46
7	H	125	TYR	C-N	5.42	1.41	1.33
12	O	476	MET	CA-C	5.42	1.59	1.52
2	B	201	GLU	N-CA	-5.42	1.39	1.46
3	C	31	SER	CA-CB	5.42	1.61	1.54
4	D	227	LYS	CA-C	5.42	1.59	1.52
4	D	199	ARG	CD-NE	5.41	1.53	1.46
2	B	234	MET	N-CA	-5.41	1.39	1.46
2	B	129	GLN	C-N	5.41	1.41	1.33
2	B	179	CYS	CA-C	-5.41	1.46	1.52
4	D	289	GLN	C-N	5.41	1.40	1.33
6	F	56	ILE	C-N	5.41	1.40	1.33
6	F	237	LEU	C-N	5.41	1.40	1.33
12	O	350	PHE	N-CA	-5.41	1.39	1.46
2	B	173	ARG	CD-NE	5.40	1.53	1.46
5	E	95	SER	N-CA	-5.40	1.39	1.45
1	A	38	GLU	C-O	-5.40	1.17	1.23
1	A	281	PRO	CA-C	-5.40	1.47	1.52
7	H	147	GLY	C-N	5.40	1.40	1.33
3	C	26	GLU	C-N	5.39	1.41	1.33
12	O	325	ARG	C-N	5.39	1.41	1.33
7	H	39	GLN	CA-C	-5.39	1.45	1.52
12	O	165	ARG	CD-NE	5.39	1.53	1.46
3	C	365	GLU	CA-C	-5.39	1.46	1.52
4	D	114	TYR	C-N	5.39	1.40	1.33
6	F	165	VAL	CA-C	-5.39	1.46	1.52
1	A	226	GLU	CA-CB	5.38	1.61	1.53
2	B	256	THR	CA-C	5.38	1.59	1.52
2	B	368	ARG	CD-NE	5.38	1.53	1.46
10	P	41	GLU	CA-CB	5.38	1.62	1.53
2	B	161	GLU	CA-CB	5.38	1.61	1.53
2	B	412	ASP	CA-C	-5.38	1.46	1.52
3	C	189	GLY	CA-C	-5.38	1.46	1.52
3	C	254	LYS	N-CA	-5.38	1.41	1.46
5	E	229	PHE	C-N	5.38	1.40	1.33
6	F	221	LEU	C-N	5.38	1.40	1.33
3	C	315	LEU	CA-C	-5.38	1.46	1.53
4	D	233	THR	CA-C	5.38	1.59	1.52
1	A	277	HIS	ND1-CE1	5.37	1.38	1.32
3	C	60	ALA	C-N	5.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	70	ARG	NE-CZ	5.37	1.39	1.33
12	O	212	LEU	CA-C	-5.37	1.46	1.52
3	C	239	GLN	C-N	5.37	1.40	1.33
4	D	376	SER	C-N	5.37	1.40	1.33
7	H	70	GLU	CA-C	-5.36	1.45	1.52
12	O	402	SER	N-CA	-5.36	1.39	1.46
12	O	564	VAL	C-O	-5.36	1.18	1.24
2	B	296	SER	C-N	5.36	1.40	1.33
12	O	249	ARG	CD-NE	5.36	1.53	1.46
12	O	350	PHE	CA-C	-5.36	1.45	1.52
1	A	141	LYS	N-CA	-5.36	1.39	1.46
1	A	241	GLN	CA-C	-5.36	1.46	1.52
3	C	215	ALA	CA-C	-5.35	1.46	1.52
10	P	24	VAL	N-CA	-5.35	1.40	1.46
2	B	145	ASP	CA-C	-5.35	1.45	1.52
12	O	181	ILE	CA-C	-5.35	1.46	1.52
12	O	323	GLY	CA-C	-5.34	1.46	1.52
12	O	523	PRO	N-CD	-5.34	1.40	1.47
13	R	58	ALA	CA-CB	5.34	1.61	1.53
3	C	14	GLN	CA-C	-5.34	1.46	1.52
6	F	139	HIS	CB-CG	-5.34	1.42	1.50
10	P	46	LYS	CA-C	-5.33	1.46	1.52
1	A	79	LEU	C-N	5.33	1.41	1.33
1	A	97	LYS	CA-CB	5.33	1.61	1.53
7	H	120	LEU	CA-C	-5.33	1.46	1.52
2	B	42	LEU	C-N	5.33	1.41	1.33
3	C	119	ARG	NE-CZ	5.33	1.39	1.33
4	D	102	GLN	CA-C	-5.33	1.46	1.52
7	H	83	GLN	CA-C	5.33	1.59	1.52
5	E	134	ILE	C-N	5.33	1.38	1.33
12	O	235	TYR	CA-CB	5.33	1.61	1.53
1	A	289	VAL	C-N	5.33	1.41	1.33
7	H	165	ARG	NE-CZ	5.33	1.39	1.33
1	A	199	ILE	N-CA	-5.32	1.40	1.46
2	B	304	ASN	CA-CB	5.32	1.62	1.53
12	O	178	GLN	CA-CB	5.32	1.61	1.53
3	C	282	HIS	CB-CG	-5.32	1.42	1.50
12	O	283	HIS	ND1-CE1	5.32	1.37	1.32
12	O	621	LYS	CA-CB	5.32	1.60	1.52
3	C	276	ARG	CZ-NH2	5.32	1.40	1.33
4	D	272	ILE	CA-CB	5.32	1.59	1.54
12	O	507	PHE	N-CA	-5.32	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	LEU	C-N	5.31	1.41	1.33
6	F	243	LYS	CA-C	-5.31	1.45	1.52
7	H	126	THR	C-N	5.31	1.40	1.33
3	C	233	ILE	N-CA	-5.31	1.40	1.46
8	G	91	ALA	C-O	-5.31	1.18	1.24
4	D	295	ASP	C-N	5.30	1.41	1.33
13	R	83	CYS	N-CA	-5.30	1.40	1.46
6	F	44	HIS	CG-CD2	5.30	1.41	1.35
4	D	84	ILE	N-CA	-5.30	1.40	1.46
6	F	114	GLN	N-CA	-5.30	1.40	1.46
1	A	166	ASP	C-O	-5.30	1.18	1.24
1	A	454	MET	C-N	5.29	1.41	1.33
6	F	266	CYS	C-O	-5.29	1.17	1.24
3	C	221	LEU	C-O	5.29	1.30	1.24
4	D	53	VAL	CA-C	-5.29	1.46	1.52
6	F	256	ILE	CA-C	5.29	1.59	1.52
12	O	422	PHE	CA-CB	5.29	1.61	1.53
2	B	59	GLU	CA-CB	5.28	1.61	1.53
11	Q	45	MET	CA-CB	5.28	1.61	1.53
4	D	6	ARG	NE-CZ	5.28	1.38	1.33
2	B	98	TYR	C-N	5.28	1.40	1.33
2	B	206	THR	CA-C	5.28	1.59	1.52
3	C	29	ASN	C-N	5.28	1.41	1.33
7	H	59	ARG	C-N	5.28	1.39	1.33
12	O	56	ARG	CZ-NH1	5.28	1.40	1.32
12	O	211	PHE	CA-C	-5.28	1.46	1.52
6	F	203	VAL	CA-CB	-5.28	1.47	1.54
1	A	188	ALA	N-CA	-5.27	1.39	1.46
5	E	294	ARG	CD-NE	5.27	1.53	1.46
7	H	116	ARG	CZ-NH2	5.27	1.40	1.33
12	O	551	ARG	NE-CZ	5.27	1.38	1.33
1	A	121	VAL	N-CA	-5.27	1.39	1.46
1	A	180	ASN	N-CA	-5.27	1.39	1.46
2	B	294	PHE	C-N	5.27	1.41	1.33
1	A	280	PHE	N-CA	5.26	1.51	1.46
6	F	48	ILE	CA-CB	-5.26	1.47	1.54
4	D	107	ARG	C-N	5.26	1.40	1.33
3	C	307	ILE	CA-CB	-5.26	1.48	1.54
2	B	393	ILE	C-N	5.25	1.40	1.33
12	O	212	LEU	N-CA	-5.25	1.40	1.46
12	O	576	MET	N-CA	-5.25	1.39	1.46
4	D	86	HIS	CB-CG	5.25	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	41	HIS	N-CA	-5.24	1.39	1.46
10	P	43	ARG	CZ-NH2	5.24	1.40	1.33
1	A	315	SER	CA-CB	5.24	1.61	1.53
2	B	342	PHE	C-N	5.24	1.40	1.33
6	F	80	ASN	C-N	5.24	1.40	1.33
5	E	208	LEU	CA-CB	5.24	1.61	1.53
4	D	116	LYS	C-N	5.24	1.41	1.33
6	F	114	GLN	CA-C	-5.24	1.46	1.52
12	O	191	VAL	CA-CB	5.23	1.61	1.54
3	C	61	VAL	C-N	5.23	1.40	1.33
4	D	285	LEU	CB-CG	5.23	1.64	1.53
2	B	430	GLN	N-CA	5.22	1.52	1.46
12	O	100	TYR	C-N	5.22	1.41	1.33
10	P	50	LEU	CA-CB	5.22	1.61	1.53
6	F	121	PHE	CA-CB	5.22	1.60	1.53
5	E	49	HIS	N-CA	-5.22	1.39	1.46
1	A	133	ALA	CA-C	-5.21	1.46	1.52
4	D	332	ALA	CA-C	-5.21	1.45	1.52
5	E	213	ASP	C-N	5.21	1.40	1.33
6	F	132	ASP	C-N	5.21	1.40	1.33
11	Q	38	THR	C-N	5.21	1.40	1.33
4	D	291	ALA	CA-CB	5.21	1.61	1.53
8	G	160	ARG	CD-NE	5.21	1.53	1.46
12	O	33	ALA	CA-C	-5.21	1.46	1.52
12	O	475	ARG	CZ-NH1	5.21	1.40	1.32
3	C	29	ASN	CA-C	5.21	1.59	1.52
2	B	415	LYS	CA-C	-5.21	1.46	1.53
4	D	373	GLN	CA-CB	5.21	1.61	1.53
12	O	172	GLY	C-N	5.21	1.41	1.33
7	H	68	ASN	CA-CB	5.21	1.61	1.53
10	P	14	ILE	C-N	5.20	1.40	1.33
2	B	262	PHE	CA-CB	5.20	1.61	1.53
11	Q	97	PRO	CA-CB	-5.20	1.46	1.53
12	O	525	SER	CA-CB	5.20	1.62	1.53
1	A	438	LYS	CA-CB	5.20	1.61	1.53
5	E	42	ALA	N-CA	-5.20	1.40	1.46
6	F	209	THR	CA-C	-5.20	1.46	1.52
12	O	198	PHE	CA-C	-5.20	1.47	1.53
12	O	516	ALA	C-N	5.20	1.38	1.33
3	C	184	TYR	CA-C	5.20	1.59	1.52
2	B	429	ASN	CA-CB	5.20	1.61	1.53
12	O	249	ARG	NE-CZ	5.19	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	332	GLN	C-O	5.19	1.30	1.24
6	F	189	THR	C-N	5.19	1.40	1.33
4	D	103	VAL	CA-CB	-5.19	1.48	1.54
1	A	423	ILE	CA-C	-5.19	1.46	1.52
8	G	214	THR	CA-C	-5.19	1.46	1.52
12	O	474	HIS	CB-CG	-5.19	1.42	1.50
1	A	72	VAL	CA-CB	5.19	1.60	1.54
10	P	9	ARG	C-N	5.19	1.41	1.33
12	O	287	ARG	NE-CZ	5.18	1.38	1.33
12	O	426	ASP	N-CA	-5.18	1.39	1.46
1	A	59	ARG	NE-CZ	5.18	1.38	1.33
10	P	96	PRO	CA-C	5.18	1.56	1.52
1	A	187	ARG	CD-NE	5.18	1.53	1.46
4	D	106	ILE	CA-C	-5.17	1.46	1.52
10	P	98	GLU	CA-C	5.17	1.59	1.52
12	O	30	VAL	N-CA	-5.17	1.40	1.46
2	B	40	LYS	CA-CB	5.17	1.61	1.53
2	B	170	LYS	CA-C	-5.17	1.46	1.52
1	A	292	TYR	CA-CB	5.17	1.61	1.53
12	O	509	ILE	CA-CB	5.17	1.61	1.54
2	B	34	ASN	C-N	5.16	1.40	1.33
5	E	323	ILE	CA-C	-5.16	1.46	1.52
6	F	50	ASN	C-O	-5.16	1.18	1.24
1	A	319	PHE	CG-CD1	5.15	1.49	1.38
1	A	326	VAL	N-CA	5.15	1.52	1.46
2	B	168	LEU	CA-CB	5.15	1.61	1.53
2	B	341	PRO	CA-CB	-5.15	1.46	1.53
7	H	198	ALA	C-N	5.15	1.40	1.33
6	F	63	GLY	C-N	5.15	1.39	1.33
2	B	380	ILE	CA-CB	-5.15	1.47	1.54
12	O	394	TYR	CA-C	5.15	1.59	1.52
1	A	200	ASN	CA-C	-5.14	1.46	1.52
5	E	52	PHE	CA-C	-5.14	1.46	1.53
5	E	243	ASN	C-N	5.14	1.41	1.33
12	O	228	GLN	N-CA	-5.14	1.40	1.46
5	E	45	TRP	C-N	5.14	1.40	1.34
8	G	90	THR	N-CA	-5.14	1.40	1.46
4	D	63	ARG	C-N	5.14	1.40	1.33
5	E	266	VAL	C-N	5.14	1.41	1.33
12	O	30	VAL	CA-CB	5.13	1.61	1.54
4	D	101	GLU	C-N	5.13	1.41	1.33
4	D	319	ILE	C-N	5.13	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	283	HIS	CB-CG	5.13	1.57	1.50
1	A	469	PRO	N-CD	5.13	1.54	1.47
7	H	127	SER	C-N	5.13	1.40	1.33
4	D	275	GLY	CA-C	5.13	1.57	1.51
12	O	528	ALA	C-O	-5.13	1.18	1.24
13	R	59	ASN	CA-CB	5.13	1.61	1.53
2	B	47	PRO	N-CA	-5.12	1.41	1.47
3	C	325	ARG	CD-NE	5.12	1.53	1.46
4	D	7	GLN	CA-C	-5.12	1.46	1.52
7	H	96	HIS	ND1-CE1	5.12	1.37	1.32
8	G	135	ALA	C-N	5.12	1.40	1.33
3	C	261	HIS	ND1-CE1	5.12	1.37	1.32
6	F	70	GLY	N-CA	-5.12	1.40	1.45
4	D	180	ASN	N-CA	-5.12	1.40	1.46
12	O	35	TRP	N-CA	-5.12	1.40	1.46
10	P	86	GLU	CD-OE1	5.12	1.35	1.25
1	A	197	HIS	CA-CB	5.11	1.61	1.53
3	C	374	HIS	ND1-CE1	5.11	1.37	1.32
2	B	416	ARG	CA-CB	5.11	1.62	1.53
6	F	44	HIS	CA-CB	5.11	1.61	1.53
12	O	187	SER	C-N	5.11	1.40	1.33
2	B	264	ASN	CA-CB	5.10	1.61	1.53
4	D	288	HIS	C-N	5.10	1.41	1.33
5	E	254	SER	CA-C	-5.10	1.45	1.52
4	D	384	LEU	C-N	5.10	1.40	1.33
7	H	114	ARG	CZ-NH1	5.10	1.39	1.32
12	O	364	PHE	CA-C	-5.10	1.46	1.52
1	A	432	ARG	NE-CZ	5.09	1.38	1.33
2	B	238	ARG	NE-CZ	5.09	1.38	1.33
6	F	226	SER	CA-CB	5.09	1.61	1.53
7	H	111	ASP	C-N	5.09	1.40	1.33
2	B	334	HIS	CG-CD2	-5.09	1.30	1.35
8	G	99	LEU	C-N	5.09	1.41	1.33
1	A	348	MET	N-CA	-5.09	1.39	1.46
1	A	171	HIS	N-CA	5.09	1.52	1.46
2	B	393	ILE	CA-C	-5.09	1.46	1.52
2	B	238	ARG	CZ-NH2	5.09	1.40	1.33
2	B	413	HIS	ND1-CE1	5.09	1.37	1.32
6	F	79	ARG	CD-NE	5.09	1.53	1.46
12	O	316	GLN	C-N	5.08	1.40	1.33
8	G	170	ILE	CA-C	-5.08	1.46	1.52
12	O	49	TYR	CA-C	5.08	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	190	HIS	CE1-NE2	5.08	1.37	1.32
1	A	432	ARG	CD-NE	5.08	1.53	1.46
4	D	204	ALA	CA-C	-5.08	1.46	1.52
1	A	155	ASN	C-N	5.08	1.41	1.33
3	C	360	PHE	CA-CB	5.08	1.61	1.53
6	F	258	ARG	CD-NE	5.08	1.53	1.46
12	O	521	GLN	CA-C	-5.08	1.46	1.52
1	A	447	GLN	CD-NE2	5.07	1.44	1.33
8	G	131	LEU	C-N	5.07	1.40	1.33
12	O	446	GLY	C-N	5.07	1.41	1.33
1	A	94	ILE	C-N	5.07	1.40	1.33
4	D	141	VAL	C-N	5.07	1.40	1.33
4	D	215	THR	CA-C	-5.07	1.46	1.52
8	G	150	GLN	C-N	-5.07	1.26	1.33
3	C	1	MET	SD-CE	5.07	1.92	1.79
3	C	307	ILE	N-CA	-5.07	1.40	1.46
3	C	374	HIS	CB-CG	5.07	1.57	1.50
4	D	290	LYS	CA-CB	5.07	1.59	1.52
12	O	190	HIS	CA-CB	-5.07	1.45	1.53
12	O	651	PHE	C-N	5.07	1.40	1.33
5	E	235	ARG	CA-CB	5.06	1.61	1.53
12	O	251	ARG	CZ-NH1	5.06	1.39	1.32
1	A	248	LYS	C-N	5.06	1.40	1.33
1	A	400	LEU	CA-CB	5.06	1.61	1.53
3	C	80	GLN	C-N	5.06	1.40	1.33
3	C	231	SER	CA-CB	5.06	1.62	1.53
4	D	303	ALA	C-O	-5.06	1.18	1.24
5	E	119	ALA	CA-CB	5.06	1.61	1.53
12	O	133	ASN	CG-ND2	5.06	1.43	1.33
12	O	322	GLU	CA-C	-5.06	1.46	1.52
6	F	254	HIS	C-N	5.06	1.40	1.33
11	Q	100	ALA	C-N	5.06	1.40	1.33
12	O	166	GLU	CA-C	-5.06	1.46	1.52
2	B	308	ILE	C-N	5.05	1.40	1.33
7	H	206	PHE	CA-CB	5.05	1.61	1.53
2	B	282	LEU	N-CA	-5.05	1.40	1.46
4	D	330	ILE	N-CA	-5.05	1.40	1.46
5	E	110	GLN	N-CA	-5.05	1.40	1.46
1	A	381	TYR	C-N	5.04	1.40	1.33
4	D	155	TYR	CA-CB	5.04	1.61	1.53
6	F	184	ALA	C-N	5.04	1.40	1.33
12	O	313	GLN	C-N	5.04	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	411	GLY	CA-C	5.04	1.58	1.52
4	D	85	TYR	C-N	5.04	1.40	1.33
12	O	148	ARG	NE-CZ	5.04	1.38	1.33
2	B	96	LEU	CA-CB	5.04	1.61	1.53
12	O	405	GLY	N-CA	5.04	1.50	1.45
2	B	272	ARG	CZ-NH2	5.04	1.40	1.33
2	B	33	GLU	C-N	5.04	1.40	1.33
5	E	309	LYS	C-N	5.04	1.40	1.33
8	G	100	THR	C-N	5.04	1.40	1.33
11	Q	31	VAL	N-CA	-5.04	1.40	1.46
1	A	44	LEU	CA-C	-5.03	1.46	1.52
3	C	186	TYR	C-O	-5.03	1.18	1.24
6	F	311	VAL	CA-CB	-5.03	1.48	1.54
6	F	54	HIS	ND1-CE1	5.03	1.37	1.32
8	G	101	ILE	CA-C	-5.03	1.46	1.52
1	A	308	ARG	NE-CZ	5.02	1.38	1.33
4	D	376	SER	CA-CB	5.02	1.61	1.53
12	O	218	TYR	CA-C	-5.02	1.46	1.52
2	B	217	LEU	CA-C	-5.02	1.46	1.52
8	G	169	ASN	CA-CB	5.02	1.61	1.53
2	B	277	LEU	CA-C	5.02	1.59	1.52
2	B	90	ASN	N-CA	-5.02	1.40	1.46
4	D	253	GLU	CA-C	5.02	1.59	1.52
7	H	72	GLY	N-CA	-5.01	1.39	1.45
7	H	73	GLY	CA-C	-5.01	1.46	1.52
8	G	163	ARG	CZ-NH1	5.01	1.39	1.32
1	A	257	GLU	N-CA	-5.01	1.40	1.46
3	C	309	ARG	CZ-NH1	5.01	1.39	1.32
5	E	53	LYS	CA-CB	5.01	1.61	1.53
6	F	204	ALA	N-CA	-5.01	1.40	1.46
8	G	116	LEU	CA-CB	5.01	1.61	1.53
1	A	271	LEU	CA-CB	5.01	1.61	1.53
5	E	146	TRP	NE1-CE2	-5.01	1.31	1.37
12	O	390	LEU	C-N	5.01	1.40	1.33
3	C	195	LEU	CB-CG	5.01	1.63	1.53
12	O	309	PRO	C-N	5.01	1.40	1.33
1	A	244	ALA	CA-CB	5.01	1.59	1.53
2	B	314	LEU	CA-C	-5.01	1.46	1.52
4	D	150	LYS	C-N	5.01	1.40	1.33
3	C	354	LYS	CA-CB	5.00	1.61	1.53
11	Q	81	VAL	C-N	5.00	1.40	1.33
12	O	228	GLN	CA-C	-5.00	1.46	1.52

All (2196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	45	PRO	N-CA-C	19.84	153.33	112.47
6	F	44	HIS	CA-CB-CG	19.16	132.96	113.80
5	E	234	ASP	N-CA-C	16.32	129.14	111.36
6	F	44	HIS	O-C-N	-14.65	104.47	121.32
6	F	46	LEU	N-CA-C	13.89	127.69	111.71
2	B	191	GLY	N-CA-C	-13.43	96.67	112.79
12	O	487	ASN	CA-CB-CG	13.41	126.02	112.60
4	D	317	ASN	N-CA-C	12.52	129.28	112.13
6	F	44	HIS	N-CA-CB	-12.49	88.14	110.37
5	E	309	LYS	N-CA-C	-12.47	97.72	111.07
2	B	294	PHE	O-C-N	-12.40	107.24	122.24
5	E	233	LEU	N-CA-C	12.31	129.05	112.68
1	A	81	PHE	CA-CB-CG	-12.25	101.55	113.80
5	E	232	SER	N-CA-C	12.19	130.11	114.75
12	O	211	PHE	CA-CB-CG	11.84	125.64	113.80
2	B	295	ASP	N-CA-C	-11.56	98.60	113.17
12	O	99	ASP	CA-CB-CG	11.44	124.04	112.60
5	E	233	LEU	CA-C-N	11.32	136.36	120.29
5	E	233	LEU	C-N-CA	11.32	136.36	120.29
3	C	247	GLN	CA-C-N	11.02	135.56	120.46
3	C	247	GLN	C-N-CA	11.02	135.56	120.46
2	B	414	GLN	N-CA-C	-10.81	99.54	113.17
2	B	176	HIS	CA-C-N	10.80	134.75	120.28
2	B	176	HIS	C-N-CA	10.80	134.75	120.28
2	B	210	ASN	CA-CB-CG	10.78	123.38	112.60
8	G	203	ASN	OD1-CG-ND2	10.77	133.37	122.60
2	B	294	PHE	N-CA-CB	-10.60	94.61	110.61
4	D	303	ALA	N-CA-CB	10.42	125.58	110.16
3	C	218	HIS	CA-CB-CG	-10.36	103.44	113.80
12	O	149	LYS	N-CA-C	10.29	123.54	111.71
2	B	304	ASN	CA-CB-CG	-10.27	102.33	112.60
2	B	234	MET	CA-C-O	-10.25	109.69	120.55
12	O	3	LEU	CA-C-N	10.22	135.32	120.51
12	O	3	LEU	C-N-CA	10.22	135.32	120.51
4	D	306	GLU	N-CA-C	10.21	122.48	111.36
5	E	309	LYS	N-CA-CB	10.11	124.67	110.01
7	H	15	LYS	CA-C-N	10.10	133.82	120.28
7	H	15	LYS	C-N-CA	10.10	133.82	120.28
12	O	608	LYS	CA-C-N	10.05	134.56	120.29
12	O	608	LYS	C-N-CA	10.05	134.56	120.29
4	D	321	PHE	CA-CB-CG	-10.02	103.78	113.80
6	F	84	MET	N-CA-C	9.92	123.89	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	42	ALA	CA-C-N	9.86	137.74	122.94
6	F	42	ALA	C-N-CA	9.86	137.74	122.94
2	B	336	ASN	CA-CB-CG	9.81	122.41	112.60
5	E	309	LYS	CB-CA-C	9.81	126.28	110.88
7	H	93	ILE	N-CA-C	-9.76	100.66	110.62
1	A	40	PRO	N-CA-C	-9.73	102.22	114.68
2	B	294	PHE	CB-CA-C	9.63	126.44	110.17
10	P	24	VAL	CA-C-N	9.58	133.12	120.28
10	P	24	VAL	C-N-CA	9.58	133.12	120.28
6	F	205	ARG	NE-CZ-NH1	-9.57	111.93	121.50
13	R	94	CYS	CA-C-N	9.55	128.90	118.97
13	R	94	CYS	C-N-CA	9.55	128.90	118.97
4	D	243	SER	N-CA-CB	9.55	124.29	110.16
5	E	174	ARG	CA-C-O	9.54	130.88	120.10
5	E	309	LYS	CA-CB-CG	9.53	133.17	114.10
5	E	212	GLU	CA-C-N	9.50	133.78	120.29
5	E	212	GLU	C-N-CA	9.50	133.78	120.29
1	A	279	ASP	CA-CB-CG	9.46	122.06	112.60
3	C	182	LEU	CA-C-O	-9.45	110.41	120.42
8	G	15	PHE	N-CA-C	9.43	122.75	111.82
8	G	126	ARG	CA-C-O	-9.38	110.48	120.42
7	H	209	ASN	CA-CB-CG	9.36	121.96	112.60
4	D	387	LYS	CA-C-N	9.35	133.27	120.46
4	D	387	LYS	C-N-CA	9.35	133.27	120.46
6	F	54	HIS	CA-C-N	9.35	133.56	120.29
6	F	54	HIS	C-N-CA	9.35	133.56	120.29
2	B	104	THR	CA-C-N	9.29	132.52	120.44
2	B	104	THR	C-N-CA	9.29	132.52	120.44
11	Q	83	TYR	CA-C-O	-9.28	110.58	120.42
1	A	275	PHE	CA-CB-CG	-9.27	104.53	113.80
11	Q	99	ILE	CA-C-N	9.27	133.07	120.38
11	Q	99	ILE	C-N-CA	9.27	133.07	120.38
6	F	45	PRO	O-C-N	-9.25	110.15	122.64
1	A	214	ASN	CA-C-N	9.23	134.34	120.31
1	A	214	ASN	C-N-CA	9.23	134.34	120.31
3	C	155	PHE	CA-CB-CG	-9.19	104.61	113.80
4	D	125	GLN	CA-C-N	9.19	132.14	120.56
4	D	125	GLN	C-N-CA	9.19	132.14	120.56
2	B	92	TYR	CA-C-O	9.16	130.26	120.55
7	H	129	ILE	CA-C-N	9.14	132.53	120.28
7	H	129	ILE	C-N-CA	9.14	132.53	120.28
7	H	34	PRO	N-CA-C	9.12	121.82	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	248	THR	CA-C-N	9.07	132.44	120.28
4	D	248	THR	C-N-CA	9.07	132.44	120.28
5	E	237	LEU	N-CA-CB	9.07	123.45	110.12
1	A	359	ALA	N-CA-C	9.04	125.00	113.25
1	A	72	VAL	N-CA-CB	9.03	120.46	110.62
1	A	289	VAL	N-CA-CB	8.98	122.76	110.54
4	D	365	GLU	N-CA-C	8.97	129.91	110.80
6	F	205	ARG	NE-CZ-NH2	8.94	127.24	119.20
11	Q	108	ASN	CA-C-N	8.91	132.02	120.44
11	Q	108	ASN	C-N-CA	8.91	132.02	120.44
4	D	68	ASP	CA-C-N	8.90	132.55	120.54
4	D	68	ASP	C-N-CA	8.90	132.55	120.54
5	E	185	ALA	N-CA-C	-8.90	95.27	109.59
12	O	616	SER	CA-C-N	8.87	132.17	120.28
12	O	616	SER	C-N-CA	8.87	132.17	120.28
9	V	91	PHE	CA-CB-CG	-8.87	104.93	113.80
1	A	435	THR	CA-C-O	-8.87	111.02	120.42
2	B	343	ILE	N-CA-C	-8.86	101.77	110.72
6	F	45	PRO	N-CA-CB	-8.85	93.96	103.25
8	G	116	LEU	CA-C-N	8.83	132.11	120.28
8	G	116	LEU	C-N-CA	8.83	132.11	120.28
2	B	260	GLU	CA-C-N	8.82	132.10	120.28
2	B	260	GLU	C-N-CA	8.82	132.10	120.28
1	A	434	THR	CA-C-O	-8.78	111.11	120.42
4	D	302	ARG	CA-C-O	-8.76	111.68	120.70
1	A	152	TYR	O-C-N	8.75	131.39	122.12
12	O	546	GLN	CA-C-N	8.74	132.51	120.63
12	O	546	GLN	C-N-CA	8.74	132.51	120.63
2	B	126	ASP	CA-CB-CG	-8.70	103.90	112.60
3	C	206	GLU	N-CA-CB	8.68	122.88	110.12
5	E	189	TYR	CA-C-O	-8.66	111.71	120.63
3	C	271	ASN	CA-C-N	8.65	128.36	119.19
3	C	271	ASN	C-N-CA	8.65	128.36	119.19
7	H	87	PRO	CA-C-N	8.65	131.21	120.22
7	H	87	PRO	C-N-CA	8.65	131.21	120.22
2	B	90	ASN	N-CA-CB	8.64	122.83	110.12
4	D	190	CYS	N-CA-C	8.64	120.70	111.28
4	D	242	ARG	N-CA-C	8.63	120.31	111.07
12	O	269	ARG	NE-CZ-NH2	8.63	126.97	119.20
12	O	114	LYS	N-CA-C	-8.61	102.78	113.28
12	O	283	HIS	CA-CB-CG	8.60	122.40	113.80
11	Q	98	GLU	O-C-N	8.57	131.92	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	24	LEU	CA-C-N	8.56	131.75	120.28
3	C	24	LEU	C-N-CA	8.56	131.75	120.28
6	F	47	VAL	N-CA-C	8.56	119.35	110.62
3	C	190	MET	N-CA-CB	8.54	122.67	110.12
2	B	75	MET	O-C-N	8.51	131.14	122.12
6	F	260	ALA	CA-C-N	8.50	131.49	120.44
6	F	260	ALA	C-N-CA	8.50	131.49	120.44
12	O	186	ASN	CA-CB-CG	8.50	121.10	112.60
11	Q	61	ASN	CA-CB-CG	-8.49	104.11	112.60
2	B	307	GLU	O-C-N	8.49	130.81	122.07
1	A	395	THR	N-CA-C	-8.48	96.84	109.81
3	C	56	LEU	CA-C-N	8.47	130.72	120.14
3	C	56	LEU	C-N-CA	8.47	130.72	120.14
2	B	305	ASP	CA-C-N	8.46	128.19	119.56
2	B	305	ASP	C-N-CA	8.46	128.19	119.56
6	F	312	LEU	N-CA-C	8.43	120.39	111.03
8	G	134	GLU	CA-C-O	-8.43	111.62	120.55
8	G	207	GLN	CB-CG-CD	-8.42	98.29	112.60
1	A	152	TYR	CA-C-O	-8.39	111.66	120.55
4	D	302	ARG	O-C-N	-8.35	113.07	122.09
3	C	5	LEU	N-CA-C	8.35	120.38	111.28
12	O	190	HIS	N-CA-CB	8.35	122.52	110.16
11	Q	68	HIS	CG-CD2-NE2	8.33	115.53	107.20
4	D	300	LEU	N-CA-C	8.32	128.52	110.80
7	H	33	THR	CA-C-O	-8.30	111.24	120.87
7	H	103	GLN	CA-C-O	-8.30	110.59	118.73
1	A	218	VAL	N-CA-CB	8.27	121.78	110.54
2	B	31	ASP	CA-C-N	8.26	131.35	120.28
2	B	31	ASP	C-N-CA	8.26	131.35	120.28
3	C	348	PHE	CA-CB-CG	-8.25	105.55	113.80
4	D	364	ARG	N-CA-C	8.24	128.35	110.80
5	E	237	LEU	CB-CA-C	-8.23	97.12	110.79
11	Q	12	GLU	N-CA-C	-8.22	96.00	109.40
1	A	205	VAL	CA-C-N	8.21	131.71	120.46
1	A	205	VAL	C-N-CA	8.21	131.71	120.46
3	C	17	ALA	N-CA-C	-8.21	102.29	113.30
7	H	69	SER	CA-C-N	8.21	131.95	120.29
7	H	69	SER	C-N-CA	8.21	131.95	120.29
12	O	82	GLN	N-CA-C	-8.21	101.74	112.41
2	B	308	ILE	CA-C-N	8.18	131.59	120.38
2	B	308	ILE	C-N-CA	8.18	131.59	120.38
2	B	345	GLU	N-CA-C	8.17	120.19	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	200	LYS	CA-C-N	8.16	131.88	120.29
4	D	200	LYS	C-N-CA	8.16	131.88	120.29
3	C	97	THR	N-CA-CB	8.14	122.27	110.06
7	H	70	GLU	CA-C-N	8.14	131.19	120.28
7	H	70	GLU	C-N-CA	8.14	131.19	120.28
4	D	241	GLN	CA-C-N	-8.13	109.87	120.44
4	D	241	GLN	C-N-CA	-8.13	109.87	120.44
10	P	31	VAL	N-CA-CB	8.13	121.60	110.54
11	Q	101	LEU	N-CA-CB	8.13	121.86	110.07
4	D	264	LEU	CA-C-N	8.11	130.98	120.44
4	D	264	LEU	C-N-CA	8.11	130.98	120.44
3	C	185	TYR	CA-C-N	8.11	130.98	120.44
3	C	185	TYR	C-N-CA	8.11	130.98	120.44
12	O	189	VAL	CA-C-O	-8.11	112.52	120.95
5	E	66	VAL	N-CA-C	8.10	118.88	110.62
10	P	23	THR	CA-C-N	8.09	131.91	120.42
10	P	23	THR	C-N-CA	8.09	131.91	120.42
1	A	223	SER	CA-C-N	8.08	130.95	120.44
1	A	223	SER	C-N-CA	8.08	130.95	120.44
5	E	232	SER	CA-C-O	-8.06	109.28	118.47
7	H	163	LEU	CA-C-O	-8.05	111.82	119.55
12	O	68	HIS	CA-CB-CG	8.04	121.84	113.80
6	F	194	GLU	CA-C-N	8.03	131.04	120.28
6	F	194	GLU	C-N-CA	8.03	131.04	120.28
5	E	51	TYR	CA-C-O	-8.03	112.39	120.82
7	H	159	THR	CA-C-N	8.02	134.47	122.68
7	H	159	THR	C-N-CA	8.02	134.47	122.68
2	B	281	VAL	CB-CA-C	-8.02	101.16	112.22
4	D	312	ALA	N-CA-C	8.00	121.10	111.82
12	O	421	VAL	CA-C-N	7.99	130.99	120.28
12	O	421	VAL	C-N-CA	7.99	130.99	120.28
2	B	183	ASP	CA-CB-CG	7.98	120.58	112.60
1	A	60	LEU	CA-C-N	7.98	130.98	120.28
1	A	60	LEU	C-N-CA	7.98	130.98	120.28
6	F	284	ASN	CA-CB-CG	-7.98	104.62	112.60
3	C	92	HIS	CE1-NE2-CD2	-7.98	101.02	109.00
4	D	274	ARG	CA-C-N	7.97	129.00	119.99
4	D	274	ARG	C-N-CA	7.97	129.00	119.99
11	Q	27	HIS	CB-CG-CD2	-7.97	120.84	131.20
1	A	171	HIS	CB-CG-CD2	-7.97	120.84	131.20
2	B	294	PHE	N-CA-C	7.96	123.97	113.30
1	A	291	ILE	N-CA-C	-7.95	103.05	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	318	HIS	N-CA-C	7.95	119.58	111.07
8	G	79	ILE	CA-C-N	7.95	130.93	120.28
8	G	79	ILE	C-N-CA	7.95	130.93	120.28
12	O	627	SER	CA-C-N	7.93	130.91	120.28
12	O	627	SER	C-N-CA	7.93	130.91	120.28
1	A	420	HIS	ND1-CE1-NE2	7.92	116.32	108.40
1	A	309	ASN	CA-C-O	-7.92	110.41	120.31
12	O	310	HIS	CA-C-N	7.91	130.88	120.28
12	O	310	HIS	C-N-CA	7.91	130.88	120.28
12	O	263	ILE	CA-C-N	7.91	130.88	120.28
12	O	263	ILE	C-N-CA	7.91	130.88	120.28
3	C	173	ASN	CA-CB-CG	7.88	120.48	112.60
12	O	386	LYS	CA-C-N	7.88	130.82	120.26
12	O	386	LYS	C-N-CA	7.88	130.82	120.26
6	F	55	TRP	CB-CG-CD2	-7.86	115.79	126.80
5	E	258	ASN	CA-C-N	7.84	130.79	120.28
5	E	258	ASN	C-N-CA	7.84	130.79	120.28
12	O	440	ALA	CA-C-N	7.81	130.59	120.44
12	O	440	ALA	C-N-CA	7.81	130.59	120.44
4	D	306	GLU	CA-C-N	7.80	130.74	120.28
4	D	306	GLU	C-N-CA	7.80	130.74	120.28
13	R	87	TRP	CA-C-N	7.80	130.73	120.28
13	R	87	TRP	C-N-CA	7.80	130.73	120.28
12	O	409	ASN	OD1-CG-ND2	7.79	130.39	122.60
4	D	6	ARG	NE-CZ-NH2	-7.76	112.22	119.20
2	B	298	GLU	CA-C-N	7.75	136.35	121.54
2	B	298	GLU	C-N-CA	7.75	136.35	121.54
2	B	110	LYS	CA-C-N	7.74	130.50	120.44
2	B	110	LYS	C-N-CA	7.74	130.50	120.44
6	F	69	ILE	N-CA-C	-7.74	97.34	108.48
5	E	123	ASN	CA-C-O	7.73	128.75	120.55
2	B	374	ILE	CA-C-O	-7.73	112.66	120.85
3	C	287	THR	N-CA-C	7.73	119.78	111.36
12	O	609	GLU	N-CA-C	-7.71	102.95	111.36
13	R	87	TRP	CB-CG-CD2	-7.70	116.02	126.80
5	E	95	SER	CA-C-O	-7.70	113.02	121.33
4	D	252	ASP	CA-CB-CG	7.69	120.29	112.60
5	E	316	HIS	CE1-NE2-CD2	-7.69	101.31	109.00
4	D	239	GLY	CA-C-N	7.68	130.57	120.28
4	D	239	GLY	C-N-CA	7.68	130.57	120.28
3	C	198	PHE	CA-C-N	7.67	130.42	120.44
3	C	198	PHE	C-N-CA	7.67	130.42	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	300	LEU	CA-C-N	7.66	130.88	120.54
4	D	300	LEU	C-N-CA	7.66	130.88	120.54
5	E	174	ARG	CA-C-N	7.63	130.50	120.28
5	E	174	ARG	C-N-CA	7.63	130.50	120.28
4	D	324	LEU	CA-C-N	7.63	128.41	119.94
4	D	324	LEU	C-N-CA	7.63	128.41	119.94
1	A	115	ALA	N-CA-CB	7.61	123.36	110.49
3	C	183	CYS	N-CA-CB	7.60	121.41	110.16
6	F	44	HIS	CE1-NE2-CD2	-7.60	101.40	109.00
12	O	264	HIS	CB-CG-CD2	-7.60	121.31	131.20
8	G	107	ARG	N-CA-C	7.60	120.67	111.40
5	E	306	ASP	CA-CB-CG	-7.60	105.00	112.60
4	D	147	THR	CA-C-O	-7.59	112.88	120.70
2	B	124	GLN	CA-C-N	7.59	131.21	120.28
2	B	124	GLN	C-N-CA	7.59	131.21	120.28
5	E	117	MET	CA-C-N	7.59	130.45	120.28
5	E	117	MET	C-N-CA	7.59	130.45	120.28
4	D	114	TYR	CA-C-N	7.59	130.30	120.44
4	D	114	TYR	C-N-CA	7.59	130.30	120.44
6	F	44	HIS	CA-C-O	-7.55	109.81	120.16
12	O	140	GLY	CA-C-N	7.55	131.01	120.29
12	O	140	GLY	C-N-CA	7.55	131.01	120.29
2	B	143	LYS	N-CA-C	-7.55	104.11	112.72
7	H	136	PHE	N-CA-C	7.54	119.14	111.07
8	G	166	ASP	CA-C-N	7.54	132.99	120.62
8	G	166	ASP	C-N-CA	7.54	132.99	120.62
1	A	253	ALA	CA-C-N	7.54	128.30	120.00
1	A	253	ALA	C-N-CA	7.54	128.30	120.00
6	F	137	HIS	ND1-CE1-NE2	7.54	115.94	108.40
12	O	409	ASN	CA-C-N	7.54	130.69	120.44
12	O	409	ASN	C-N-CA	7.54	130.69	120.44
1	A	171	HIS	CB-CG-ND1	7.52	133.98	122.70
2	B	424	LEU	CB-CA-C	-7.52	98.31	110.79
4	D	364	ARG	CA-C-N	7.51	135.89	121.54
4	D	364	ARG	C-N-CA	7.51	135.89	121.54
5	E	275	GLN	CA-C-N	7.51	130.96	120.29
5	E	275	GLN	C-N-CA	7.51	130.96	120.29
2	B	221	SER	CA-C-N	7.51	131.09	120.28
2	B	221	SER	C-N-CA	7.51	131.09	120.28
1	A	281	PRO	N-CA-C	-7.50	105.08	114.68
12	O	88	HIS	CE1-NE2-CD2	-7.50	101.50	109.00
1	A	311	ILE	N-CA-C	7.49	117.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	487	ASN	CA-C-N	7.49	130.31	120.28
12	O	487	ASN	C-N-CA	7.49	130.31	120.28
12	O	363	HIS	CE1-NE2-CD2	-7.49	101.52	109.00
1	A	321	GLU	CA-C-N	7.47	130.29	120.28
1	A	321	GLU	C-N-CA	7.47	130.29	120.28
12	O	155	LEU	CA-C-N	7.46	130.60	120.38
12	O	155	LEU	C-N-CA	7.46	130.60	120.38
6	F	51	ILE	CA-C-N	7.46	130.13	120.44
6	F	51	ILE	C-N-CA	7.46	130.13	120.44
1	A	40	PRO	N-CA-CB	7.45	108.09	101.83
13	R	43	ALA	N-CA-C	7.45	121.28	111.75
1	A	180	ASN	CA-C-N	7.44	130.25	120.28
1	A	180	ASN	C-N-CA	7.44	130.25	120.28
2	B	248	GLU	CB-CG-CD	-7.43	99.97	112.60
12	O	279	HIS	CA-C-N	7.43	130.23	120.28
12	O	279	HIS	C-N-CA	7.43	130.23	120.28
8	G	123	ARG	NE-CZ-NH2	-7.42	112.52	119.20
7	H	86	PHE	CA-CB-CG	-7.41	106.39	113.80
8	G	165	LYS	N-CA-C	-7.41	102.37	111.40
1	A	284	LEU	CA-C-O	7.40	129.01	119.98
2	B	98	TYR	CB-CG-CD2	-7.40	109.70	120.80
12	O	322	GLU	CA-C-N	7.39	128.13	120.00
12	O	322	GLU	C-N-CA	7.39	128.13	120.00
12	O	470	THR	CA-C-N	7.39	130.52	120.54
12	O	470	THR	C-N-CA	7.39	130.52	120.54
12	O	462	LYS	CA-C-N	7.39	130.04	120.44
12	O	462	LYS	C-N-CA	7.39	130.04	120.44
7	H	50	MET	N-CA-C	7.38	120.39	111.82
2	B	53	SER	N-CA-CB	7.38	121.08	110.16
3	C	291	ASN	CA-CB-CG	7.38	119.98	112.60
7	H	22	ASN	CA-CB-CG	-7.38	105.22	112.60
8	G	149	ASN	CA-CB-CG	-7.37	105.23	112.60
1	A	122	GLU	CA-C-O	-7.37	111.70	119.22
12	O	427	ASP	CA-C-N	7.36	131.50	120.31
12	O	427	ASP	C-N-CA	7.36	131.50	120.31
12	O	473	LEU	CA-C-O	7.35	128.21	120.42
4	D	144	LYS	O-C-N	7.35	130.03	122.09
13	R	36	ASP	CB-CA-C	7.35	124.06	110.10
12	O	718	ILE	CB-CA-C	-7.33	102.58	111.97
2	B	48	LYS	CA-C-N	7.33	135.53	121.54
2	B	48	LYS	C-N-CA	7.33	135.53	121.54
5	E	268	ASP	CA-C-N	7.31	130.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	268	ASP	C-N-CA	7.31	130.07	120.28
3	C	74	PHE	CA-C-O	-7.30	112.02	120.20
12	O	201	LYS	O-C-N	7.30	129.86	122.12
12	O	529	ILE	N-CA-CB	7.30	121.43	111.21
2	B	334	HIS	CE1-NE2-CD2	-7.30	101.70	109.00
4	D	219	GLU	N-CA-C	7.29	119.86	111.11
12	O	139	ILE	N-CA-C	7.29	117.42	110.42
3	C	282	HIS	CA-C-N	7.29	130.38	120.54
3	C	282	HIS	C-N-CA	7.29	130.38	120.54
2	B	185	GLU	CA-C-N	7.29	135.45	121.54
2	B	185	GLU	C-N-CA	7.29	135.45	121.54
7	H	145	VAL	CA-C-N	7.28	130.04	120.28
7	H	145	VAL	C-N-CA	7.28	130.04	120.28
2	B	364	LYS	CA-C-N	7.28	126.95	119.82
2	B	364	LYS	C-N-CA	7.28	126.95	119.82
8	G	67	LEU	CA-C-N	7.28	129.90	120.44
8	G	67	LEU	C-N-CA	7.28	129.90	120.44
11	Q	15	ASP	CA-CB-CG	-7.27	105.33	112.60
2	B	212	LYS	N-CA-C	7.26	118.83	111.07
3	C	184	TYR	N-CA-C	-7.25	103.31	111.07
12	O	505	ILE	N-CA-C	7.25	124.43	109.34
6	F	187	THR	CA-C-O	-7.25	113.69	121.88
2	B	64	LYS	CA-C-N	7.25	134.74	121.70
2	B	64	LYS	C-N-CA	7.25	134.74	121.70
5	E	234	ASP	CA-C-O	7.25	128.10	120.42
12	O	305	SER	CA-C-N	7.25	133.18	122.74
12	O	305	SER	C-N-CA	7.25	133.18	122.74
12	O	56	ARG	CA-C-N	7.25	129.99	120.28
12	O	56	ARG	C-N-CA	7.25	129.99	120.28
4	D	317	ASN	CA-CB-CG	7.23	119.83	112.60
2	B	261	ALA	N-CA-C	7.23	119.16	111.28
4	D	218	HIS	CA-C-N	7.23	130.30	120.54
4	D	218	HIS	C-N-CA	7.23	130.30	120.54
5	E	62	LEU	N-CA-C	7.23	119.16	111.28
7	H	42	ALA	CA-C-N	7.22	129.95	120.28
7	H	42	ALA	C-N-CA	7.22	129.95	120.28
3	C	390	LEU	CB-CA-C	-7.21	98.82	110.79
6	F	47	VAL	N-CA-CB	7.20	120.33	110.54
13	R	36	ASP	N-CA-CB	7.20	122.74	110.50
1	A	284	LEU	O-C-N	-7.19	114.34	123.26
12	O	533	LEU	CA-C-N	7.19	129.79	120.44
12	O	533	LEU	C-N-CA	7.19	129.79	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	7	VAL	N-CA-C	-7.19	98.04	108.11
12	O	524	SER	N-CA-C	-7.19	103.38	111.14
6	F	134	SER	CA-C-O	-7.19	111.71	119.97
1	A	157	ILE	N-CA-C	-7.18	97.39	107.80
3	C	323	ALA	N-CA-C	7.18	119.10	111.28
11	Q	68	HIS	CE1-NE2-CD2	-7.17	101.83	109.00
8	G	66	LEU	N-CA-C	7.16	119.17	111.36
3	C	366	LYS	N-CA-C	-7.16	104.42	113.72
1	A	211	TYR	N-CA-CB	7.15	120.74	110.16
5	E	218	CYS	N-CA-C	7.15	119.07	111.28
2	B	285	MET	CG-SD-CE	-7.14	85.19	100.90
3	C	110	ALA	N-CA-C	7.14	119.14	111.36
10	P	101	ASP	CA-CB-CG	-7.13	105.47	112.60
6	F	55	TRP	CB-CG-CD1	7.13	137.59	126.90
4	D	140	ASN	CA-C-N	7.13	129.79	120.60
4	D	140	ASN	C-N-CA	7.13	129.79	120.60
12	O	606	ASN	CA-C-O	-7.12	114.00	121.55
5	E	50	HIS	CA-C-N	7.10	129.67	120.44
5	E	50	HIS	C-N-CA	7.10	129.67	120.44
3	C	93	ILE	N-CA-C	7.09	119.92	111.05
3	C	258	ASN	CA-C-N	7.09	129.79	120.28
3	C	258	ASN	C-N-CA	7.09	129.79	120.28
4	D	229	ALA	CA-C-N	7.09	129.66	120.44
4	D	229	ALA	C-N-CA	7.09	129.66	120.44
12	O	327	THR	CA-C-N	7.08	130.48	120.28
12	O	327	THR	C-N-CA	7.08	130.48	120.28
8	G	169	ASN	CA-C-N	7.08	130.16	120.46
8	G	169	ASN	C-N-CA	7.08	130.16	120.46
12	O	622	MET	N-CA-C	-7.08	103.64	111.36
8	G	134	GLU	O-C-N	7.07	129.62	122.12
5	E	66	VAL	N-CA-CB	7.07	120.16	110.54
4	D	363	THR	CA-C-N	7.06	135.02	121.54
4	D	363	THR	C-N-CA	7.06	135.02	121.54
6	F	136	ILE	CA-C-N	7.05	129.61	120.44
6	F	136	ILE	C-N-CA	7.05	129.61	120.44
2	B	269	GLY	N-CA-C	-7.05	102.87	112.52
13	R	75	CYS	CA-C-O	-7.04	113.03	120.63
1	A	222	VAL	N-CA-CB	7.04	120.11	110.54
4	D	379	PHE	CA-CB-CG	7.04	120.84	113.80
1	A	229	PRO	CA-C-O	-7.04	115.96	121.38
3	C	73	ASP	CA-C-N	7.03	130.65	120.38
3	C	73	ASP	C-N-CA	7.03	130.65	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	38	GLU	O-C-N	-7.03	114.50	122.09
5	E	324	LYS	CA-C-N	7.03	129.58	120.44
5	E	324	LYS	C-N-CA	7.03	129.58	120.44
12	O	155	LEU	CA-C-O	7.03	127.35	119.41
4	D	303	ALA	CA-C-O	-7.02	112.97	120.42
2	B	348	GLU	CA-C-O	7.02	128.00	120.55
13	R	21	ARG	CD-NE-CZ	-7.02	114.57	124.40
8	G	78	TYR	N-CA-C	7.02	118.58	111.07
12	O	395	CYS	CA-C-N	7.02	129.68	120.28
12	O	395	CYS	C-N-CA	7.02	129.68	120.28
3	C	50	ASP	CA-C-N	7.02	134.60	121.97
3	C	50	ASP	C-N-CA	7.02	134.60	121.97
3	C	134	ASN	OD1-CG-ND2	7.02	129.62	122.60
3	C	97	THR	CB-CA-C	-7.01	98.76	110.68
4	D	241	GLN	N-CA-C	7.01	118.57	111.07
3	C	119	ARG	CA-C-N	7.01	129.12	120.22
3	C	119	ARG	C-N-CA	7.01	129.12	120.22
3	C	143	ALA	CA-C-N	7.01	130.96	120.31
3	C	143	ALA	C-N-CA	7.01	130.96	120.31
9	V	119	PHE	CA-CB-CG	-7.01	106.79	113.80
12	O	527	PHE	O-C-N	-6.99	114.27	122.87
12	O	557	HIS	CB-CG-CD2	-6.99	122.12	131.20
5	E	316	HIS	ND1-CE1-NE2	6.99	115.39	108.40
3	C	117	PRO	CA-C-N	6.98	129.52	120.44
3	C	117	PRO	C-N-CA	6.98	129.52	120.44
5	E	66	VAL	O-C-N	6.98	128.64	121.87
1	A	44	LEU	CA-C-N	6.97	129.50	120.44
1	A	44	LEU	C-N-CA	6.97	129.50	120.44
3	C	136	ASN	CA-CB-CG	-6.96	105.64	112.60
2	B	334	HIS	ND1-CE1-NE2	6.96	115.36	108.40
1	A	65	ASP	CA-C-O	-6.96	113.05	120.42
10	P	34	ILE	N-CA-C	6.96	117.57	110.82
7	H	47	HIS	ND1-CE1-NE2	6.95	115.35	108.40
1	A	86	PHE	CA-CB-CG	-6.95	106.85	113.80
4	D	193	ARG	O-C-N	-6.95	114.23	122.15
4	D	219	GLU	CA-C-N	6.95	129.59	120.28
4	D	219	GLU	C-N-CA	6.95	129.59	120.28
5	E	304	THR	CA-C-N	6.95	130.15	120.29
5	E	304	THR	C-N-CA	6.95	130.15	120.29
1	A	39	ASN	CA-CB-CG	6.94	119.54	112.60
5	E	249	THR	CA-CB-OG1	6.94	120.01	109.60
6	F	64	ARG	O-C-N	-6.94	116.42	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	412	GLU	CA-C-N	6.93	130.14	120.29
12	O	412	GLU	C-N-CA	6.93	130.14	120.29
3	C	238	VAL	CA-C-O	-6.93	113.82	121.23
5	E	27	GLU	CA-C-N	6.93	129.95	120.46
5	E	27	GLU	C-N-CA	6.93	129.95	120.46
2	B	45	ASP	CA-CB-CG	6.92	119.53	112.60
5	E	112	ALA	CA-C-N	6.92	132.28	120.72
5	E	112	ALA	C-N-CA	6.92	132.28	120.72
4	D	227	LYS	O-C-N	6.91	129.19	122.07
6	F	116	PHE	CA-CB-CG	-6.91	106.89	113.80
12	O	526	THR	CB-CA-C	6.91	121.12	111.86
5	E	66	VAL	CA-C-O	-6.91	113.77	120.95
5	E	125	LYS	O-C-N	6.91	129.44	122.12
7	H	79	GLN	CB-CA-C	-6.91	99.33	110.79
2	B	410	GLU	N-CA-CB	6.90	118.08	110.35
6	F	139	HIS	CG-CD2-NE2	6.90	114.10	107.20
12	O	273	ASP	CA-CB-CG	6.90	119.50	112.60
3	C	384	ILE	N-CA-CB	6.89	119.91	110.54
4	D	394	GLU	N-CA-CB	6.89	120.00	110.01
3	C	369	ASN	OD1-CG-ND2	6.89	129.49	122.60
5	E	31	TYR	N-CA-C	-6.89	99.00	109.95
4	D	99	PHE	CA-CB-CG	-6.88	106.92	113.80
13	R	35	TRP	CA-C-N	6.88	134.09	121.70
13	R	35	TRP	C-N-CA	6.88	134.09	121.70
6	F	31	MET	CA-C-N	6.88	132.20	120.71
6	F	31	MET	C-N-CA	6.88	132.20	120.71
2	B	320	ASN	N-CA-CB	6.88	121.81	110.39
12	O	21	ILE	CA-C-O	-6.88	113.80	120.95
2	B	189	LYS	CA-C-O	6.88	130.34	120.51
1	A	82	VAL	CA-C-O	6.88	127.93	120.57
1	A	355	ASP	CA-C-O	-6.87	112.91	120.81
10	P	15	PHE	N-CA-C	-6.87	98.05	109.24
12	O	69	VAL	CA-C-O	-6.87	113.57	120.85
6	F	44	HIS	N-CA-C	6.86	124.96	109.81
3	C	60	ALA	CA-C-O	-6.86	113.62	120.82
4	D	362	GLU	N-CA-C	-6.85	96.44	108.23
2	B	62	GLY	N-CA-C	-6.85	96.94	113.18
12	O	206	ILE	N-CA-C	6.85	116.97	110.53
7	H	100	GLU	CA-C-N	6.85	132.29	120.58
7	H	100	GLU	C-N-CA	6.85	132.29	120.58
6	F	171	VAL	N-CA-C	-6.84	97.70	108.86
12	O	557	HIS	CA-CB-CG	6.84	120.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	332	THR	N-CA-C	6.83	118.52	111.14
3	C	172	GLU	N-CA-CB	6.83	122.04	110.49
12	O	155	LEU	N-CA-C	-6.83	105.08	113.41
11	Q	52	PHE	CA-CB-CG	-6.83	106.97	113.80
12	O	268	GLN	CA-C-N	6.82	129.97	120.29
12	O	268	GLN	C-N-CA	6.82	129.97	120.29
12	O	14	TRP	CA-C-O	-6.82	113.32	120.55
12	O	43	TYR	CA-C-N	6.82	129.41	120.28
12	O	43	TYR	C-N-CA	6.82	129.41	120.28
3	C	136	ASN	N-CA-CB	6.82	122.01	110.49
13	R	65	SER	O-C-N	-6.81	114.39	122.15
2	B	211	ASN	CA-CB-CG	6.81	119.41	112.60
6	F	229	LYS	CA-C-N	6.81	129.29	120.44
6	F	229	LYS	C-N-CA	6.81	129.29	120.44
6	F	230	MET	CA-C-O	-6.81	113.67	120.82
1	A	425	TYR	CA-C-N	6.80	133.94	121.70
1	A	425	TYR	C-N-CA	6.80	133.94	121.70
6	F	101	ASP	CA-C-N	6.80	129.95	120.29
6	F	101	ASP	C-N-CA	6.80	129.95	120.29
12	O	267	GLN	OE1-CD-NE2	6.80	129.40	122.60
3	C	340	HIS	CA-C-N	6.79	130.64	120.31
3	C	340	HIS	C-N-CA	6.79	130.64	120.31
4	D	360	HIS	CB-CA-C	-6.79	99.05	110.19
13	R	80	HIS	CG-CD2-NE2	6.79	113.99	107.20
3	C	390	LEU	N-CA-C	6.78	118.67	111.28
5	E	188	THR	CA-C-O	-6.78	113.39	121.66
6	F	44	HIS	ND1-CE1-NE2	6.78	115.18	108.40
12	O	373	THR	N-CA-CB	6.78	120.09	110.12
12	O	344	LEU	N-CA-CB	6.78	120.79	110.28
13	R	80	HIS	CE1-NE2-CD2	-6.78	102.22	109.00
10	P	13	THR	CA-C-N	6.77	132.01	123.14
10	P	13	THR	C-N-CA	6.77	132.01	123.14
12	O	355	ASN	N-CA-C	6.77	118.31	111.07
2	B	237	ILE	CA-C-N	6.77	129.35	120.28
2	B	237	ILE	C-N-CA	6.77	129.35	120.28
11	Q	96	ALA	CA-C-O	-6.76	113.33	120.70
12	O	468	GLU	CA-C-N	6.76	129.23	120.44
12	O	468	GLU	C-N-CA	6.76	129.23	120.44
4	D	332	ALA	CA-C-N	6.76	129.34	120.28
4	D	332	ALA	C-N-CA	6.76	129.34	120.28
1	A	462	ASN	CA-CB-CG	6.76	119.36	112.60
2	B	153	THR	CA-C-N	6.74	129.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	THR	C-N-CA	6.74	129.31	120.28
12	O	483	SER	CA-C-N	6.74	129.20	120.44
12	O	483	SER	C-N-CA	6.74	129.20	120.44
4	D	360	HIS	CA-C-N	6.73	134.99	122.74
4	D	360	HIS	C-N-CA	6.73	134.99	122.74
12	O	243	LEU	N-CA-CB	6.73	120.02	110.12
11	Q	55	ASN	CA-CB-CG	-6.73	105.87	112.60
1	A	266	ALA	CA-C-N	6.73	129.18	120.44
1	A	266	ALA	C-N-CA	6.73	129.18	120.44
2	B	174	GLN	CB-CA-C	-6.73	99.42	110.85
2	B	340	ASP	CA-C-O	-6.72	114.29	119.46
12	O	387	ALA	O-C-N	-6.72	114.50	120.48
10	P	107	ASP	N-CA-C	-6.71	98.86	109.07
13	R	95	PRO	CA-C-O	-6.71	110.29	120.03
5	E	26	ASP	CA-C-O	-6.71	111.66	119.24
5	E	100	VAL	CA-CB-CG1	6.71	121.81	110.40
7	H	96	HIS	CA-C-O	6.71	128.38	120.66
12	O	438	MET	N-CA-CB	6.71	120.09	110.16
3	C	12	VAL	CA-C-N	6.71	130.50	120.31
3	C	12	VAL	C-N-CA	6.71	130.50	120.31
3	C	121	ILE	CA-C-N	6.70	127.37	120.00
3	C	121	ILE	C-N-CA	6.70	127.37	120.00
6	F	181	MET	N-CA-C	-6.70	97.81	108.73
8	G	71	ALA	CA-C-O	-6.70	113.80	120.70
5	E	55	CYS	O-C-N	-6.70	115.00	123.24
12	O	255	HIS	CB-CG-CD2	6.70	139.91	131.20
6	F	102	LYS	N-CA-C	6.70	118.66	111.36
12	O	625	HIS	CA-C-N	6.69	129.92	120.28
12	O	625	HIS	C-N-CA	6.69	129.92	120.28
1	A	441	LEU	N-CA-C	6.69	118.57	111.28
2	B	111	SER	N-CA-C	-6.69	103.91	111.07
4	D	325	GLY	CA-C-O	-6.68	113.78	121.00
3	C	112	VAL	O-C-N	-6.68	115.39	121.87
6	F	106	TYR	N-CA-CB	6.68	119.94	110.12
2	B	391	GLN	CA-CB-CG	6.68	127.45	114.10
3	C	391	LYS	CB-CA-C	-6.67	100.40	110.88
12	O	411	VAL	O-C-N	-6.67	115.40	121.87
4	D	381	VAL	N-CA-CB	6.67	118.35	110.55
12	O	589	ASN	N-CA-CB	6.67	120.06	110.06
4	D	287	PRO	N-CA-CB	6.66	110.41	103.15
8	G	60	ASN	N-CA-C	-6.66	102.28	112.99
1	A	113	PRO	CA-C-N	6.65	131.58	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	PRO	C-N-CA	6.65	131.58	122.07
9	V	143	ASP	CA-C-N	6.65	128.51	120.13
9	V	143	ASP	C-N-CA	6.65	128.51	120.13
8	G	175	HIS	ND1-CE1-NE2	6.64	115.04	108.40
2	B	344	ARG	CA-C-N	6.64	129.17	120.28
2	B	344	ARG	C-N-CA	6.64	129.17	120.28
1	A	230	GLU	CB-CG-CD	-6.62	101.34	112.60
2	B	415	LYS	CA-C-O	-6.62	114.58	121.87
4	D	60	VAL	CA-C-N	6.62	128.80	120.72
4	D	60	VAL	C-N-CA	6.62	128.80	120.72
5	E	42	ALA	CA-C-N	6.62	129.46	123.10
5	E	42	ALA	C-N-CA	6.62	129.46	123.10
4	D	354	GLN	N-CA-C	-6.62	104.78	112.92
10	P	37	ARG	CA-C-N	6.62	124.49	119.66
10	P	37	ARG	C-N-CA	6.62	124.49	119.66
7	H	89	ILE	CB-CA-C	-6.61	103.51	111.97
12	O	548	PHE	CA-CB-CG	-6.61	107.19	113.80
5	E	118	ALA	CA-C-O	-6.60	113.56	120.55
3	C	238	VAL	O-C-N	6.59	129.80	122.61
12	O	350	PHE	CA-CB-CG	-6.59	107.21	113.80
12	O	118	LEU	CA-C-O	6.59	127.74	120.82
11	Q	90	ILE	CA-C-N	6.59	128.03	120.98
11	Q	90	ILE	C-N-CA	6.59	128.03	120.98
4	D	199	ARG	NE-CZ-NH2	6.58	125.12	119.20
6	F	139	HIS	CA-C-O	-6.58	113.57	120.55
6	F	149	PRO	N-CA-CB	6.58	110.29	102.85
6	F	227	ALA	CA-C-N	6.58	128.85	120.56
6	F	227	ALA	C-N-CA	6.58	128.85	120.56
3	C	82	GLN	N-CA-C	-6.58	104.19	111.82
6	F	51	ILE	O-C-N	6.58	128.61	121.83
1	A	417	VAL	CB-CA-C	-6.58	102.75	110.91
3	C	142	HIS	ND1-CE1-NE2	6.58	114.98	108.40
2	B	165	TYR	N-CA-C	6.58	121.59	112.45
4	D	291	ALA	N-CA-C	-6.58	98.48	109.07
12	O	467	TYR	CA-C-N	6.58	129.09	120.28
12	O	467	TYR	C-N-CA	6.58	129.09	120.28
1	A	377	TYR	O-C-N	-6.57	114.99	122.09
12	O	234	GLN	CA-C-N	6.57	129.38	120.44
12	O	234	GLN	C-N-CA	6.57	129.38	120.44
4	D	61	ILE	N-CA-C	-6.57	104.25	110.42
5	E	183	LEU	N-CA-C	-6.57	96.84	108.13
7	H	86	PHE	N-CA-C	6.56	121.67	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	139	ILE	CA-C-O	-6.56	114.22	121.17
4	D	52	MET	N-CA-CB	6.56	119.86	110.16
6	F	59	ARG	N-CA-C	6.55	118.50	111.36
12	O	284	ASN	CA-CB-CG	6.54	119.14	112.60
1	A	277	HIS	CA-C-N	6.53	134.02	121.54
1	A	277	HIS	C-N-CA	6.53	134.02	121.54
12	O	632	ILE	N-CA-C	-6.53	98.87	108.54
4	D	46	LYS	CB-CA-C	-6.53	100.64	110.88
8	G	175	HIS	CE1-NE2-CD2	-6.53	102.47	109.00
3	C	256	LEU	N-CA-C	6.52	120.34	112.38
5	E	296	SER	CA-C-N	6.52	131.10	122.30
5	E	296	SER	C-N-CA	6.52	131.10	122.30
3	C	281	LYS	CA-C-N	6.52	134.97	121.94
3	C	281	LYS	C-N-CA	6.52	134.97	121.94
9	V	143	ASP	N-CA-C	-6.52	104.43	112.38
3	C	271	ASN	CA-C-O	-6.51	112.78	119.49
10	P	38	PRO	N-CA-CB	6.51	106.84	103.19
3	C	230	VAL	N-CA-C	6.51	117.30	110.72
6	F	139	HIS	CE1-NE2-CD2	-6.51	102.49	109.00
10	P	62	PHE	N-CA-CB	6.51	119.34	110.42
4	D	72	HIS	N-CA-C	-6.51	104.82	112.89
8	G	164	LYS	CA-C-O	6.50	126.91	119.18
12	O	184	VAL	CA-CB-CG1	6.50	121.45	110.40
12	O	306	THR	CA-C-N	6.50	127.15	120.00
12	O	306	THR	C-N-CA	6.50	127.15	120.00
1	A	113	PRO	N-CA-CB	6.50	110.04	102.76
12	O	6	ARG	NE-CZ-NH1	6.50	128.00	121.50
7	H	106	MET	CA-C-N	6.49	128.98	120.28
7	H	106	MET	C-N-CA	6.49	128.98	120.28
10	P	58	GLY	CA-C-N	6.49	129.62	120.28
10	P	58	GLY	C-N-CA	6.49	129.62	120.28
3	C	200	ARG	NE-CZ-NH1	-6.48	115.02	121.50
4	D	316	TYR	CA-C-O	-6.48	111.24	120.51
4	D	185	ILE	CB-CA-C	-6.47	103.29	112.22
12	O	738	ALA	N-CA-C	-6.47	101.38	110.50
1	A	257	GLU	N-CA-C	6.47	118.33	111.28
1	A	407	LEU	N-CA-CB	6.46	120.30	110.28
8	G	76	PRO	CA-C-N	6.46	130.13	120.31
8	G	76	PRO	C-N-CA	6.46	130.13	120.31
1	A	356	MET	O-C-N	-6.46	115.17	122.08
2	B	84	ASN	N-CA-CB	6.45	121.39	110.49
3	C	51	VAL	N-CA-CB	6.45	121.87	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	354	LYS	CA-C-O	6.45	127.34	120.70
6	F	232	HIS	CE1-NE2-CD2	-6.44	102.56	109.00
3	C	9	VAL	N-CA-C	6.43	116.60	110.42
3	C	43	ASP	CA-CB-CG	-6.43	106.17	112.60
3	C	180	HIS	CE1-NE2-CD2	-6.43	102.56	109.00
5	E	317	GLY	N-CA-C	-6.43	104.71	112.49
5	E	323	ILE	CB-CA-C	6.43	120.82	112.14
13	R	84	ILE	CA-C-N	6.43	128.90	120.28
13	R	84	ILE	C-N-CA	6.43	128.90	120.28
3	C	330	GLY	N-CA-C	-6.43	99.22	112.34
4	D	327	LEU	CA-C-O	-6.43	113.61	120.42
12	O	318	HIS	CA-CB-CG	6.43	120.23	113.80
2	B	294	PHE	CA-C-O	6.43	126.97	119.32
2	B	320	ASN	CA-CB-CG	6.43	119.03	112.60
2	B	251	PHE	CA-C-O	6.42	127.40	120.20
4	D	181	GLU	CB-CG-CD	-6.42	101.68	112.60
12	O	323	GLY	CA-C-N	6.42	128.89	120.28
12	O	323	GLY	C-N-CA	6.42	128.89	120.28
2	B	67	TRP	O-C-N	6.42	128.92	122.12
8	G	117	LEU	CA-C-O	6.42	127.35	120.55
2	B	362	LEU	CA-C-N	6.41	130.60	120.47
2	B	362	LEU	C-N-CA	6.41	130.60	120.47
2	B	128	LEU	N-CA-C	6.41	119.08	111.71
1	A	277	HIS	CE1-NE2-CD2	-6.41	102.59	109.00
7	H	96	HIS	ND1-CE1-NE2	6.40	114.80	108.40
1	A	341	CYS	CA-C-N	6.40	128.85	120.28
1	A	341	CYS	C-N-CA	6.40	128.85	120.28
2	B	140	LYS	CA-C-N	6.39	133.75	121.54
2	B	140	LYS	C-N-CA	6.39	133.75	121.54
2	B	297	GLN	OE1-CD-NE2	6.39	128.99	122.60
8	G	64	LEU	N-CA-CB	6.39	119.73	110.20
1	A	171	HIS	CG-CD2-NE2	6.39	113.59	107.20
12	O	625	HIS	CE1-NE2-CD2	-6.39	102.61	109.00
12	O	494	ILE	CA-CB-CG2	6.39	121.36	110.50
1	A	375	ILE	CA-C-N	6.38	129.47	120.28
1	A	375	ILE	C-N-CA	6.38	129.47	120.28
2	B	67	TRP	CA-C-N	6.38	127.02	120.00
2	B	67	TRP	C-N-CA	6.38	127.02	120.00
4	D	371	ASP	CA-C-N	6.38	130.01	120.31
4	D	371	ASP	C-N-CA	6.38	130.01	120.31
4	D	130	ILE	N-CA-CB	6.38	119.12	111.08
11	Q	31	VAL	N-CA-C	-6.38	98.42	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	9	LEU	CA-C-N	6.37	128.82	120.28
4	D	9	LEU	C-N-CA	6.37	128.82	120.28
3	C	223	SER	CA-C-N	6.37	129.33	120.29
3	C	223	SER	C-N-CA	6.37	129.33	120.29
6	F	74	GLY	N-CA-C	-6.37	101.81	111.42
10	P	26	GLU	CA-C-N	6.37	128.81	120.28
10	P	26	GLU	C-N-CA	6.37	128.81	120.28
4	D	329	GLU	CA-C-O	-6.36	114.20	121.65
5	E	246	TRP	N-CA-C	6.36	120.61	112.34
10	P	30	ILE	CA-C-N	6.36	129.17	120.46
10	P	30	ILE	C-N-CA	6.36	129.17	120.46
12	O	226	LEU	CA-C-O	-6.35	113.69	120.42
5	E	162	GLN	N-CA-C	6.34	120.76	112.89
4	D	86	HIS	CE1-NE2-CD2	-6.34	102.66	109.00
4	D	354	GLN	O-C-N	-6.34	114.73	122.34
13	R	74	VAL	CB-CA-C	-6.34	103.58	112.14
3	C	28	ILE	CA-C-N	6.34	128.68	120.44
3	C	28	ILE	C-N-CA	6.34	128.68	120.44
8	G	130	ASP	CA-CB-CG	-6.33	106.27	112.60
12	O	485	ASP	CA-CB-CG	-6.33	106.27	112.60
12	O	51	GLU	CA-C-O	-6.33	115.18	119.29
1	A	179	SER	CA-C-O	-6.33	114.18	120.70
6	F	99	ILE	N-CA-C	-6.32	99.01	108.12
12	O	400	LYS	CA-C-O	-6.32	113.77	121.36
5	E	323	ILE	N-CA-CB	-6.32	101.94	110.54
2	B	255	HIS	CE1-NE2-CD2	-6.32	102.68	109.00
3	C	65	LYS	N-CA-C	6.32	118.17	111.28
3	C	390	LEU	O-C-N	6.32	128.81	122.12
4	D	387	LYS	O-C-N	-6.32	114.95	122.15
8	G	139	ASP	CA-CB-CG	6.31	118.91	112.60
2	B	80	PHE	CA-CB-CG	6.31	120.11	113.80
6	F	30	VAL	CA-C-O	6.31	125.83	120.22
7	H	148	ILE	CA-CB-CG2	-6.31	99.78	110.50
4	D	109	HIS	CB-CA-C	-6.30	100.33	110.79
1	A	436	PHE	O-C-N	6.30	128.80	122.12
11	Q	41	THR	O-C-N	6.30	128.80	122.12
12	O	118	LEU	N-CA-C	6.30	117.81	111.07
7	H	202	ASP	CA-CB-CG	6.29	118.89	112.60
12	O	41	ASP	N-CA-CB	6.29	119.13	110.01
5	E	269	LEU	N-CA-C	-6.29	104.43	111.28
6	F	198	ILE	CA-C-N	6.29	126.79	119.94
6	F	198	ILE	C-N-CA	6.29	126.79	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	THR	N-CA-C	-6.28	104.19	113.61
7	H	22	ASN	O-C-N	6.28	129.31	122.15
4	D	228	HIS	N-CA-C	6.28	118.12	111.28
7	H	158	THR	N-CA-CB	6.28	121.10	110.49
3	C	370	PRO	CA-C-N	6.28	128.69	120.28
3	C	370	PRO	C-N-CA	6.28	128.69	120.28
12	O	272	ALA	N-CA-CB	6.28	121.09	110.49
3	C	286	PHE	CB-CG-CD1	6.27	131.36	120.70
5	E	59	ALA	N-CA-C	-6.27	104.44	111.28
13	R	105	LYS	N-CA-CB	6.27	121.09	110.49
1	A	224	LYS	CA-C-N	6.27	128.68	120.28
1	A	224	LYS	C-N-CA	6.27	128.68	120.28
1	A	264	LYS	CA-C-N	6.27	129.84	120.31
1	A	264	LYS	C-N-CA	6.27	129.84	120.31
5	E	56	LYS	N-CA-CB	6.26	121.33	110.81
6	F	167	VAL	CB-CA-C	-6.26	101.30	110.81
12	O	264	HIS	CB-CG-ND1	6.26	132.09	122.70
12	O	468	GLU	N-CA-C	6.26	118.10	111.28
1	A	199	ILE	N-CA-CB	6.25	117.87	110.55
12	O	583	ALA	N-CA-C	6.25	118.09	111.28
7	H	205	ALA	CA-C-N	6.25	128.94	120.44
7	H	205	ALA	C-N-CA	6.25	128.94	120.44
12	O	474	HIS	CE1-NE2-CD2	-6.25	102.75	109.00
2	B	75	MET	CA-C-O	-6.24	113.94	120.55
7	H	101	THR	N-CA-C	-6.24	104.02	111.69
1	A	306	LEU	N-CA-CB	6.24	119.05	110.01
8	G	56	ALA	CA-C-N	6.23	130.97	122.19
8	G	56	ALA	C-N-CA	6.23	130.97	122.19
2	B	154	LYS	N-CA-CB	6.22	119.27	110.12
12	O	161	ARG	CA-C-N	6.22	129.13	120.29
12	O	161	ARG	C-N-CA	6.22	129.13	120.29
3	C	28	ILE	N-CA-C	6.22	116.97	110.62
1	A	404	LEU	CA-C-N	6.22	128.53	120.44
1	A	404	LEU	C-N-CA	6.22	128.53	120.44
5	E	309	LYS	CA-C-O	-6.22	114.29	120.82
6	F	146	ILE	N-CA-C	-6.22	98.74	108.81
8	G	185	LEU	CB-CA-C	-6.22	100.47	110.79
1	A	105	SER	CA-C-N	6.21	128.89	120.44
1	A	105	SER	C-N-CA	6.21	128.89	120.44
2	B	169	GLN	CB-CG-CD	-6.21	102.04	112.60
12	O	101	MET	N-CA-C	6.21	118.13	111.36
10	P	31	VAL	CA-C-N	6.21	128.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	31	VAL	C-N-CA	6.21	128.59	120.28
5	E	316	HIS	CB-CG-CD2	6.20	139.26	131.20
1	A	409	LEU	N-CA-C	6.20	117.91	111.03
3	C	203	TYR	CA-C-N	6.20	128.50	120.44
3	C	203	TYR	C-N-CA	6.20	128.50	120.44
3	C	312	LYS	N-CA-CB	6.20	119.24	110.12
8	G	192	VAL	N-CA-CB	-6.20	102.11	110.54
2	B	232	LEU	CB-CA-C	-6.20	100.31	110.85
12	O	101	MET	O-C-N	6.20	129.22	122.15
1	A	299	ALA	N-CA-C	6.20	117.83	111.14
5	E	66	VAL	CB-CA-C	-6.20	103.78	112.14
12	O	263	ILE	N-CA-C	6.19	116.94	110.62
6	F	172	ILE	CA-C-O	-6.18	113.91	120.53
4	D	266	LYS	N-CA-CB	6.18	119.21	110.12
2	B	146	ARG	CA-C-N	6.18	128.56	120.28
2	B	146	ARG	C-N-CA	6.18	128.56	120.28
4	D	366	ALA	N-CA-CB	6.18	120.93	110.49
12	O	210	PRO	CA-C-N	6.18	129.06	120.29
12	O	210	PRO	C-N-CA	6.18	129.06	120.29
1	A	148	ASP	CA-C-N	6.18	128.56	120.28
1	A	148	ASP	C-N-CA	6.18	128.56	120.28
3	C	259	ALA	CA-C-O	6.18	127.10	120.55
12	O	414	ARG	CA-C-O	6.17	127.10	120.55
1	A	227	SER	CA-C-N	6.17	130.10	120.97
1	A	227	SER	C-N-CA	6.17	130.10	120.97
6	F	295	ILE	CA-C-N	6.17	128.54	120.28
6	F	295	ILE	C-N-CA	6.17	128.54	120.28
8	G	136	VAL	CA-CB-CG1	6.17	120.89	110.40
12	O	87	TYR	CB-CG-CD2	-6.17	111.55	120.80
1	A	111	ASN	CA-C-O	6.17	126.77	119.56
2	B	66	GLU	N-CA-C	6.16	119.64	111.75
12	O	343	VAL	CA-C-N	6.16	129.68	120.31
12	O	343	VAL	C-N-CA	6.16	129.68	120.31
1	A	58	GLU	CA-C-N	6.16	129.04	120.29
1	A	58	GLU	C-N-CA	6.16	129.04	120.29
1	A	393	PHE	CA-CB-CG	-6.16	107.64	113.80
4	D	86	HIS	ND1-CE1-NE2	6.16	114.56	108.40
4	D	157	GLU	O-C-N	6.15	128.64	122.12
5	E	282	ARG	NE-CZ-NH1	-6.15	115.35	121.50
12	O	139	ILE	CA-CB-CG2	6.15	120.96	110.50
4	D	242	ARG	CA-C-N	-6.15	111.56	120.29
4	D	242	ARG	C-N-CA	-6.15	111.56	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	ALA	CB-CA-C	-6.15	101.28	110.50
2	B	98	TYR	CA-C-N	6.14	130.86	120.29
2	B	98	TYR	C-N-CA	6.14	130.86	120.29
12	O	6	ARG	NE-CZ-NH2	-6.14	113.67	119.20
13	R	56	CYS	CA-C-N	6.14	129.01	120.29
13	R	56	CYS	C-N-CA	6.14	129.01	120.29
8	G	200	GLU	CB-CG-CD	6.14	123.04	112.60
12	O	450	SER	CA-C-N	6.14	129.64	120.31
12	O	450	SER	C-N-CA	6.14	129.64	120.31
1	A	346	ASP	O-C-N	-6.13	115.16	122.15
2	B	296	SER	N-CA-CB	6.13	116.51	108.96
5	E	40	LEU	CA-C-N	6.13	129.00	120.29
5	E	40	LEU	C-N-CA	6.13	129.00	120.29
1	A	94	ILE	CA-C-N	6.13	129.00	120.29
1	A	94	ILE	C-N-CA	6.13	129.00	120.29
3	C	110	ALA	O-C-N	6.13	129.14	122.15
1	A	142	LEU	N-CA-CB	6.13	119.13	110.12
12	O	410	GLU	CA-C-N	6.12	128.85	120.46
12	O	410	GLU	C-N-CA	6.12	128.85	120.46
5	E	200	PRO	CA-C-N	6.12	132.26	122.10
5	E	200	PRO	C-N-CA	6.12	132.26	122.10
12	O	93	GLU	N-CA-C	-6.12	104.61	111.28
1	A	82	VAL	O-C-N	-6.12	115.69	121.87
10	P	31	VAL	CB-CA-C	-6.12	103.88	112.14
12	O	88	HIS	ND1-CE1-NE2	6.12	114.52	108.40
12	O	37	ASP	CA-CB-CG	6.11	118.71	112.60
13	R	97	ASP	O-C-N	6.11	129.37	122.22
5	E	323	ILE	CA-C-O	-6.11	114.60	120.95
2	B	270	SER	CA-C-O	-6.10	111.80	120.16
6	F	235	VAL	CA-C-N	6.10	128.38	120.44
6	F	235	VAL	C-N-CA	6.10	128.38	120.44
1	A	171	HIS	CE1-NE2-CD2	-6.10	102.90	109.00
3	C	206	GLU	CB-CA-C	-6.10	100.67	110.79
4	D	233	THR	CA-C-N	6.10	128.81	120.46
4	D	233	THR	C-N-CA	6.10	128.81	120.46
11	Q	71	SER	CA-C-N	6.10	128.45	120.28
11	Q	71	SER	C-N-CA	6.10	128.45	120.28
12	O	192	GLU	N-CA-C	-6.10	100.07	109.52
2	B	349	GLU	CA-C-N	6.09	128.94	120.29
2	B	349	GLU	C-N-CA	6.09	128.94	120.29
3	C	41	HIS	N-CA-C	6.09	118.89	111.82
3	C	191	ILE	CA-C-O	-6.09	114.71	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	90	ASN	OD1-CG-ND2	6.09	128.69	122.60
3	C	132	GLN	N-CA-C	6.09	118.63	110.35
10	P	2	ASP	CA-CB-CG	-6.08	106.52	112.60
2	B	350	LEU	CA-C-N	6.08	128.93	120.29
2	B	350	LEU	C-N-CA	6.08	128.93	120.29
4	D	38	GLY	CA-C-N	6.08	129.04	120.28
4	D	38	GLY	C-N-CA	6.08	129.04	120.28
6	F	61	GLN	N-CA-CB	6.08	118.80	109.98
12	O	150	LEU	CA-C-N	6.08	129.55	120.31
12	O	150	LEU	C-N-CA	6.08	129.55	120.31
10	P	91	GLU	CA-C-O	-6.08	114.35	119.76
4	D	355	ILE	CB-CA-C	-6.07	104.10	112.24
1	A	461	ARG	N-CA-CB	6.07	119.14	110.16
3	C	133	MET	CA-C-N	6.07	133.14	121.54
3	C	133	MET	C-N-CA	6.07	133.14	121.54
5	E	236	LYS	N-CA-CB	6.07	119.69	110.28
1	A	417	VAL	N-CA-CB	6.07	117.33	110.72
6	F	33	CYS	N-CA-CB	6.07	120.74	110.49
5	E	259	ALA	CA-C-N	6.06	128.41	120.28
5	E	259	ALA	C-N-CA	6.06	128.41	120.28
12	O	269	ARG	NE-CZ-NH1	-6.06	115.44	121.50
3	C	242	PRO	O-C-N	6.06	130.37	122.86
2	B	274	THR	CA-C-O	-6.06	114.46	120.82
4	D	7	GLN	CA-C-N	6.06	128.31	120.44
4	D	7	GLN	C-N-CA	6.06	128.31	120.44
3	C	182	LEU	O-C-N	6.06	129.05	122.15
9	V	154	PRO	CA-C-N	-6.06	114.80	122.43
9	V	154	PRO	C-N-CA	-6.06	114.80	122.43
5	E	229	PHE	CA-C-O	-6.05	114.79	121.33
12	O	352	GLN	CA-C-N	6.05	128.31	120.44
12	O	352	GLN	C-N-CA	6.05	128.31	120.44
2	B	268	SER	N-CA-CB	-6.05	101.30	110.07
4	D	353	ASP	CA-C-O	-6.05	113.98	120.46
4	D	56	ASN	N-CA-C	-6.05	105.55	113.17
5	E	73	GLY	N-CA-C	-6.05	98.84	113.18
7	H	114	ARG	O-C-N	6.05	128.53	122.12
12	O	338	LEU	CA-C-N	6.05	128.31	120.44
12	O	338	LEU	C-N-CA	6.05	128.31	120.44
4	D	176	ASN	N-CA-C	6.05	118.83	111.82
5	E	234	ASP	CA-CB-CG	6.05	118.65	112.60
7	H	20	CYS	N-CA-C	6.04	117.87	111.28
1	A	245	ILE	CA-C-N	6.04	128.30	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ILE	C-N-CA	6.04	128.30	120.44
4	D	149	LEU	CB-CA-C	-6.04	101.39	110.88
4	D	4	ALA	CA-C-N	6.04	128.17	120.56
4	D	4	ALA	C-N-CA	6.04	128.17	120.56
12	O	184	VAL	CA-C-N	6.04	128.29	120.56
12	O	184	VAL	C-N-CA	6.04	128.29	120.56
4	D	404	MET	CA-C-N	6.04	129.49	120.31
4	D	404	MET	C-N-CA	6.04	129.49	120.31
12	O	215	THR	N-CA-C	-6.04	104.70	111.28
12	O	556	LEU	CA-C-N	6.04	128.37	120.28
12	O	556	LEU	C-N-CA	6.04	128.37	120.28
12	O	141	GLU	CA-C-N	6.03	128.37	120.28
12	O	141	GLU	C-N-CA	6.03	128.37	120.28
12	O	308	LEU	CA-C-O	-6.03	111.89	120.16
5	E	237	LEU	N-CA-C	-6.03	104.71	111.28
8	G	128	LEU	CA-C-N	6.03	129.47	120.31
8	G	128	LEU	C-N-CA	6.03	129.47	120.31
2	B	281	VAL	CA-C-N	6.02	128.27	120.44
2	B	281	VAL	C-N-CA	6.02	128.27	120.44
7	H	83	GLN	CA-C-N	6.02	131.30	122.63
7	H	83	GLN	C-N-CA	6.02	131.30	122.63
2	B	137	GLU	O-C-N	6.02	128.27	122.07
5	E	283	GLY	CA-C-O	-6.02	118.08	122.23
2	B	54	PHE	CA-CB-CG	-6.02	107.78	113.80
4	D	302	ARG	CA-C-N	-6.02	111.75	120.29
4	D	302	ARG	C-N-CA	-6.02	111.75	120.29
12	O	361	ASP	CA-C-N	6.02	128.34	120.28
12	O	361	ASP	C-N-CA	6.02	128.34	120.28
12	O	579	THR	N-CA-C	-6.01	104.84	111.82
13	R	86	ARG	CA-C-N	6.01	128.34	120.28
13	R	86	ARG	C-N-CA	6.01	128.34	120.28
2	B	125	MET	CA-C-N	6.01	128.25	120.44
2	B	125	MET	C-N-CA	6.01	128.25	120.44
3	C	92	HIS	CG-CD2-NE2	6.01	113.21	107.20
5	E	269	LEU	CA-C-N	6.01	128.34	120.28
5	E	269	LEU	C-N-CA	6.01	128.34	120.28
5	E	118	ALA	N-CA-C	-6.01	104.73	111.28
6	F	92	HIS	ND1-CE1-NE2	6.01	114.41	108.40
12	O	171	ARG	NE-CZ-NH2	6.01	124.61	119.20
12	O	486	LEU	CA-C-O	-6.01	114.18	120.55
2	B	174	GLN	N-CA-CB	6.00	119.05	110.16
2	B	413	HIS	N-CA-C	-6.00	104.17	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	139	ASP	N-CA-C	6.00	117.93	110.91
1	A	66	HIS	ND1-CE1-NE2	6.00	114.40	108.40
1	A	280	PHE	CA-C-O	-6.00	113.50	120.34
12	O	59	THR	N-CA-C	-6.00	104.75	111.28
4	D	171	ALA	CA-C-N	5.99	128.91	120.28
4	D	171	ALA	C-N-CA	5.99	128.91	120.28
6	F	273	ASP	CA-C-N	5.99	128.80	120.29
6	F	273	ASP	C-N-CA	5.99	128.80	120.29
12	O	274	HIS	CB-CG-CD2	-5.99	123.41	131.20
7	H	71	LEU	CA-C-N	5.98	127.82	120.22
7	H	71	LEU	C-N-CA	5.98	127.82	120.22
2	B	44	GLU	N-CA-CB	5.98	120.60	110.49
2	B	410	GLU	CB-CA-C	-5.98	103.22	112.07
6	F	95	GLU	O-C-N	5.98	130.54	122.59
6	F	135	ASP	CB-CA-C	-5.98	100.69	110.85
4	D	100	GLU	CA-C-N	5.97	128.21	120.44
4	D	100	GLU	C-N-CA	5.97	128.21	120.44
12	O	236	MET	CA-C-O	-5.97	114.55	120.70
1	A	365	LEU	CA-C-N	5.97	128.28	120.28
1	A	365	LEU	C-N-CA	5.97	128.28	120.28
6	F	119	LEU	O-C-N	-5.97	115.98	122.79
7	H	129	ILE	O-C-N	-5.97	115.68	122.72
7	H	117	ALA	N-CA-C	5.97	117.86	111.36
1	A	333	PHE	CA-C-N	5.96	128.27	120.28
1	A	333	PHE	C-N-CA	5.96	128.27	120.28
11	Q	31	VAL	CA-C-N	5.96	129.75	120.75
11	Q	31	VAL	C-N-CA	5.96	129.75	120.75
3	C	122	GLY	CA-C-O	-5.96	114.34	120.66
2	B	84	ASN	CA-CB-CG	5.96	118.56	112.60
8	G	70	PHE	CA-C-O	-5.96	114.24	120.55
1	A	71	ARG	N-CA-C	5.96	117.77	111.28
3	C	391	LYS	N-CA-CB	5.95	118.64	110.01
12	O	486	LEU	O-C-N	5.95	128.43	122.12
1	A	398	ALA	N-CA-C	5.95	117.76	111.28
2	B	265	TYR	N-CA-CB	5.95	120.27	110.39
4	D	315	LEU	N-CA-CB	5.95	119.16	110.47
12	O	200	LEU	CA-C-N	5.95	128.53	120.38
12	O	200	LEU	C-N-CA	5.95	128.53	120.38
1	A	186	SER	O-C-N	5.95	129.58	122.27
5	E	173	THR	CB-CA-C	5.95	121.35	110.11
6	F	282	GLN	OE1-CD-NE2	-5.94	116.66	122.60
12	O	190	HIS	CE1-NE2-CD2	-5.94	103.06	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	15	LEU	N-CA-CB	5.94	120.08	110.40
12	O	711	PHE	CA-CB-CG	-5.94	107.86	113.80
12	O	147	TRP	N-CA-C	5.93	118.70	111.82
5	E	77	VAL	N-CA-C	-5.93	99.25	108.44
5	E	96	PHE	CA-C-N	5.93	133.77	121.32
5	E	96	PHE	C-N-CA	5.93	133.77	121.32
5	E	125	LYS	CA-C-O	-5.93	114.27	120.55
12	O	214	GLU	O-C-N	5.93	128.91	122.15
1	A	66	HIS	CA-C-O	-5.92	112.80	119.79
3	C	55	SER	CA-C-O	5.92	126.80	120.10
6	F	289	MET	CA-C-N	5.92	128.70	120.29
6	F	289	MET	C-N-CA	5.92	128.70	120.29
6	F	308	LYS	CA-C-N	5.92	128.22	120.28
6	F	308	LYS	C-N-CA	5.92	128.22	120.28
12	O	19	THR	CA-C-N	5.92	128.70	120.29
12	O	19	THR	C-N-CA	5.92	128.70	120.29
2	B	119	ILE	CA-C-O	-5.92	114.57	120.85
6	F	277	THR	CA-CB-OG1	5.92	118.48	109.60
12	O	444	ILE	N-CA-C	5.92	116.66	110.62
6	F	95	GLU	CA-C-O	-5.92	112.05	120.51
1	A	419	SER	CA-C-N	5.92	128.13	120.44
1	A	419	SER	C-N-CA	5.92	128.13	120.44
13	R	104	GLN	N-CA-C	-5.91	98.21	110.80
4	D	89	LEU	CA-C-O	-5.91	114.28	120.55
3	C	110	ALA	CA-C-O	-5.91	114.16	120.42
3	C	134	ASN	CA-CB-CG	5.91	118.50	112.60
5	E	38	GLU	CA-C-O	5.91	126.78	120.70
13	R	28	ASN	N-CA-CB	5.90	121.07	111.21
3	C	202	LEU	CA-C-O	5.90	127.02	120.82
1	A	77	MET	CA-C-N	5.90	128.46	120.44
1	A	77	MET	C-N-CA	5.90	128.46	120.44
3	C	92	HIS	ND1-CE1-NE2	5.90	114.30	108.40
3	C	186	TYR	N-CA-C	-5.90	104.76	111.07
3	C	291	ASN	N-CA-C	-5.90	103.42	111.56
3	C	340	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	199	ILE	CA-C-O	-5.89	114.92	121.17
3	C	218	HIS	CG-CD2-NE2	5.89	113.09	107.20
5	E	38	GLU	CA-C-N	5.89	127.99	120.56
5	E	38	GLU	C-N-CA	5.89	127.99	120.56
6	F	229	LYS	CA-C-O	-5.89	114.30	120.55
5	E	43	LYS	CA-C-O	-5.89	116.41	120.47
5	E	278	ALA	N-CA-C	5.89	117.78	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	20	CYS	CA-C-N	5.89	128.17	120.28
7	H	20	CYS	C-N-CA	5.89	128.17	120.28
1	A	66	HIS	CE1-NE2-CD2	-5.89	103.11	109.00
3	C	14	GLN	N-CA-C	5.89	117.78	111.36
4	D	16	SER	CA-C-O	-5.88	114.40	121.34
8	G	126	ARG	O-C-N	5.88	128.86	122.15
1	A	179	SER	O-C-N	5.88	128.44	122.09
2	B	203	GLN	CG-CD-NE2	-5.88	107.58	116.40
4	D	384	LEU	CA-C-N	5.88	128.16	120.28
4	D	384	LEU	C-N-CA	5.88	128.16	120.28
6	F	132	ASP	CA-C-N	5.88	125.74	119.28
6	F	132	ASP	C-N-CA	5.88	125.74	119.28
11	Q	48	GLY	N-CA-C	-5.88	100.35	112.34
12	O	494	ILE	N-CA-CB	5.88	117.81	110.47
12	O	739	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	108	GLU	O-C-N	-5.87	115.29	122.34
12	O	635	GLU	N-CA-C	-5.87	105.77	113.17
1	A	141	LYS	O-C-N	-5.87	115.90	122.12
1	A	462	ASN	CA-C-N	5.87	131.31	122.68
1	A	462	ASN	C-N-CA	5.87	131.31	122.68
5	E	49	HIS	CB-CG-CD2	-5.87	123.57	131.20
5	E	233	LEU	CA-C-O	-5.87	111.91	120.13
8	G	19	ALA	CA-C-O	5.87	126.77	120.55
12	O	221	GLN	N-CA-CB	5.87	118.84	110.16
8	G	194	ARG	N-CA-C	5.87	117.67	111.28
3	C	320	GLN	CA-C-N	5.86	128.14	120.28
3	C	320	GLN	C-N-CA	5.86	128.14	120.28
5	E	60	LEU	CA-C-N	5.86	128.06	120.44
5	E	60	LEU	C-N-CA	5.86	128.06	120.44
6	F	270	LEU	O-C-N	-5.86	114.79	122.59
1	A	63	ILE	N-CA-C	-5.86	104.80	110.72
2	B	85	PHE	CA-C-N	5.86	125.40	119.19
2	B	85	PHE	C-N-CA	5.86	125.40	119.19
3	C	29	ASN	CA-CB-CG	5.86	118.46	112.60
3	C	261	HIS	N-CA-CB	5.86	118.74	110.12
4	D	293	THR	N-CA-C	-5.86	105.79	113.17
12	O	25	VAL	N-CA-CB	5.86	118.29	110.26
5	E	233	LEU	CB-CA-C	-5.86	100.45	110.24
5	E	226	VAL	CA-C-O	-5.86	113.82	120.67
12	O	380	GLU	N-CA-C	5.86	122.76	109.81
6	F	122	LEU	N-CA-CB	5.85	119.11	110.33
6	F	259	GLU	CA-C-O	-5.85	114.22	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	499	THR	O-C-N	-5.85	114.80	122.59
7	H	36	VAL	CB-CA-C	-5.85	104.24	112.14
13	R	33	TRP	N-CA-CB	5.85	121.72	111.13
2	B	291	ILE	N-CA-C	5.85	117.27	109.37
4	D	279	GLN	OE1-CD-NE2	5.85	128.45	122.60
2	B	285	MET	CA-C-N	5.85	128.70	120.28
2	B	285	MET	C-N-CA	5.85	128.70	120.28
3	C	386	LEU	CA-C-N	5.85	128.12	120.28
3	C	386	LEU	C-N-CA	5.85	128.12	120.28
8	G	13	GLU	N-CA-CB	5.85	118.81	110.16
11	Q	67	SER	N-CA-C	5.85	117.65	111.28
1	A	211	TYR	CB-CA-C	-5.84	100.92	110.85
2	B	259	PHE	CA-CB-CG	5.84	119.64	113.80
4	D	204	ALA	CA-C-N	5.84	128.38	120.38
4	D	204	ALA	C-N-CA	5.84	128.38	120.38
7	H	154	GLN	CB-CA-C	5.84	119.16	109.53
1	A	63	ILE	CA-C-N	5.84	128.10	120.28
1	A	63	ILE	C-N-CA	5.84	128.10	120.28
3	C	144	ASP	CA-C-N	5.83	128.03	120.44
3	C	144	ASP	C-N-CA	5.83	128.03	120.44
1	A	387	HIS	ND1-CE1-NE2	5.83	114.23	108.40
2	B	294	PHE	CA-CB-CG	5.83	119.63	113.80
12	O	201	LYS	CA-C-N	5.83	128.02	120.44
12	O	201	LYS	C-N-CA	5.83	128.02	120.44
6	F	202	HIS	CB-CG-ND1	5.83	131.44	122.70
7	H	13	PHE	CA-CB-CG	-5.83	107.97	113.80
12	O	242	ARG	N-CA-C	-5.83	104.93	111.28
7	H	204	VAL	CB-CA-C	-5.82	104.28	112.14
8	G	196	ASN	CA-C-N	5.82	128.08	120.28
8	G	196	ASN	C-N-CA	5.82	128.08	120.28
1	A	139	LEU	CA-C-N	5.82	128.56	120.29
1	A	139	LEU	C-N-CA	5.82	128.56	120.29
12	O	36	ASN	CA-C-N	5.82	128.08	120.28
12	O	36	ASN	C-N-CA	5.82	128.08	120.28
4	D	315	LEU	CB-CA-C	-5.82	99.06	109.24
13	R	46	ARG	N-CA-C	-5.82	106.18	113.28
4	D	354	GLN	CA-C-O	5.82	126.37	119.56
5	E	323	ILE	O-C-N	5.82	127.51	121.87
12	O	32	ARG	CA-C-N	5.82	128.35	120.44
12	O	32	ARG	C-N-CA	5.82	128.35	120.44
12	O	356	THR	CA-C-N	5.82	128.01	120.56
12	O	356	THR	C-N-CA	5.82	128.01	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	VAL	CA-C-N	5.81	127.89	120.56
1	A	198	VAL	C-N-CA	5.81	127.89	120.56
12	O	517	TRP	N-CA-C	-5.81	99.48	108.55
1	A	117	PRO	O-C-N	-5.81	114.79	122.64
4	D	131	PRO	CA-C-O	-5.81	114.40	121.03
6	F	117	LYS	N-CA-C	-5.81	106.04	114.12
8	G	172	LYS	N-CA-CB	5.81	118.43	110.01
4	D	107	ARG	CA-C-O	-5.81	114.39	120.55
12	O	387	ALA	CA-C-N	5.81	125.50	119.05
12	O	387	ALA	C-N-CA	5.81	125.50	119.05
5	E	307	SER	N-CA-CB	5.81	118.65	110.12
6	F	50	ASN	CA-C-N	5.80	128.66	120.42
6	F	50	ASN	C-N-CA	5.80	128.66	120.42
12	O	43	TYR	N-CA-C	5.80	117.28	111.07
7	H	115	ARG	CA-C-N	5.80	128.05	120.28
7	H	115	ARG	C-N-CA	5.80	128.05	120.28
1	A	61	GLN	CA-C-O	-5.80	114.41	120.55
2	B	406	ASN	O-C-N	-5.80	114.88	122.59
7	H	47	HIS	CE1-NE2-CD2	-5.79	103.20	109.00
13	R	31	ALA	CA-C-N	5.79	131.63	122.36
13	R	31	ALA	C-N-CA	5.79	131.63	122.36
1	A	397	VAL	CA-C-O	-5.79	115.03	121.17
3	C	400	ASN	CA-C-O	-5.79	114.00	120.25
5	E	242	TRP	CB-CG-CD1	5.79	135.58	126.90
6	F	254	HIS	ND1-CE1-NE2	5.79	114.19	108.40
12	O	92	GLU	CA-C-N	5.79	128.04	120.28
12	O	92	GLU	C-N-CA	5.79	128.04	120.28
1	A	227	SER	O-C-N	-5.79	115.84	122.09
5	E	180	LYS	N-CA-CB	5.79	119.65	110.57
10	P	39	PRO	CA-C-N	5.79	129.10	120.31
10	P	39	PRO	C-N-CA	5.79	129.10	120.31
12	O	371	ALA	CA-C-N	5.79	128.51	120.29
12	O	371	ALA	C-N-CA	5.79	128.51	120.29
5	E	60	LEU	N-CA-C	5.78	117.58	111.28
1	A	41	SER	CA-C-N	5.78	131.51	123.07
1	A	41	SER	C-N-CA	5.78	131.51	123.07
13	R	77	HIS	ND1-CE1-NE2	5.78	114.18	108.40
6	F	150	LEU	CB-CA-C	-5.78	99.73	109.50
11	Q	83	TYR	O-C-N	5.78	128.74	122.15
12	O	516	ALA	CA-C-O	5.78	126.11	119.35
2	B	246	LEU	CA-C-N	5.78	128.02	120.28
2	B	246	LEU	C-N-CA	5.78	128.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	280	LEU	N-CA-C	5.78	117.25	111.07
2	B	295	ASP	CA-CB-CG	5.78	118.38	112.60
12	O	320	HIS	N-CA-C	5.78	117.58	111.28
1	A	397	VAL	CA-C-N	5.77	128.02	120.28
1	A	397	VAL	C-N-CA	5.77	128.02	120.28
4	D	325	GLY	N-CA-C	-5.77	105.80	112.50
7	H	19	GLN	OE1-CD-NE2	5.77	128.37	122.60
12	O	88	HIS	CA-C-O	-5.77	114.76	120.82
1	A	134	THR	CA-C-N	5.77	128.01	120.28
1	A	134	THR	C-N-CA	5.77	128.01	120.28
4	D	47	ALA	CA-C-O	-5.77	114.44	120.55
6	F	231	LEU	CA-C-O	-5.77	113.58	120.10
1	A	436	PHE	CA-C-O	-5.76	114.44	120.55
5	E	244	LYS	CA-C-N	5.76	129.82	120.60
5	E	244	LYS	C-N-CA	5.76	129.82	120.60
6	F	289	MET	CG-SD-CE	-5.76	88.22	100.90
7	H	48	ASN	OD1-CG-ND2	5.76	128.36	122.60
5	E	51	TYR	O-C-N	5.76	128.00	122.07
4	D	86	HIS	N-CA-C	5.76	117.23	111.07
6	F	127	THR	N-CA-C	-5.76	100.40	109.50
4	D	70	CYS	N-CA-CB	5.76	118.58	110.12
10	P	53	ASP	O-C-N	-5.76	115.14	122.34
4	D	209	ASN	OD1-CG-ND2	5.75	128.35	122.60
4	D	353	ASP	CA-CB-CG	-5.75	106.85	112.60
5	E	250	LEU	CB-CA-C	-5.75	98.50	109.95
8	G	196	ASN	OD1-CG-ND2	-5.75	116.85	122.60
11	Q	79	TYR	N-CA-CB	-5.75	101.67	110.01
12	O	649	THR	O-C-N	-5.75	116.62	123.06
5	E	334	SER	N-CA-CB	5.75	120.27	110.50
1	A	367	THR	N-CA-CB	5.75	118.34	110.01
12	O	312	ILE	N-CA-C	5.74	116.48	110.62
10	P	78	ALA	N-CA-CB	5.74	121.54	111.55
12	O	230	SER	CA-C-N	5.74	132.80	122.64
12	O	230	SER	C-N-CA	5.74	132.80	122.64
8	G	87	GLU	N-CA-C	5.74	123.02	110.80
12	O	251	ARG	CA-C-N	5.74	128.44	120.63
12	O	251	ARG	C-N-CA	5.74	128.44	120.63
2	B	378	LEU	N-CA-C	5.73	118.47	111.82
3	C	41	HIS	CA-C-N	5.73	128.43	120.29
3	C	41	HIS	C-N-CA	5.73	128.43	120.29
2	B	240	CYS	CA-C-N	5.73	126.34	119.98
2	B	240	CYS	C-N-CA	5.73	126.34	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	224	TYR	N-CA-C	5.73	117.61	111.36
12	O	276	GLN	CA-CB-CG	5.73	125.56	114.10
1	A	277	HIS	CG-CD2-NE2	5.73	112.93	107.20
8	G	101	ILE	CB-CA-C	-5.73	104.31	112.22
4	D	5	VAL	CA-C-O	-5.72	115.10	121.17
4	D	280	GLU	CA-C-O	-5.72	114.81	120.70
5	E	240	LEU	O-C-N	5.72	128.67	122.15
8	G	202	HIS	CB-CG-CD2	-5.72	123.77	131.20
13	R	37	ILE	N-CA-C	-5.72	99.41	108.90
2	B	281	VAL	N-CA-CB	5.72	119.16	110.58
2	B	427	TRP	CA-C-N	5.71	127.87	120.44
2	B	427	TRP	C-N-CA	5.71	127.87	120.44
1	A	432	ARG	CA-C-O	-5.71	114.82	120.70
2	B	197	ILE	CB-CA-C	-5.71	104.34	112.22
5	E	294	ARG	N-CA-C	-5.71	100.26	108.60
12	O	555	TRP	CA-C-N	5.71	132.74	123.37
12	O	555	TRP	C-N-CA	5.71	132.74	123.37
12	O	124	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	390	ALA	CA-C-N	5.71	128.39	120.29
1	A	390	ALA	C-N-CA	5.71	128.39	120.29
12	O	310	HIS	CE1-NE2-CD2	-5.71	103.29	109.00
2	B	262	PHE	CA-C-O	-5.70	114.51	120.55
5	E	238	LEU	N-CA-C	5.70	117.49	111.28
7	H	100	GLU	CB-CG-CD	-5.70	102.92	112.60
5	E	331	ILE	CB-CA-C	-5.69	104.36	112.22
12	O	286	ILE	N-CA-CB	5.69	119.12	110.58
2	B	176	HIS	ND1-CE1-NE2	5.69	114.09	108.40
5	E	266	VAL	N-CA-C	5.69	116.47	110.72
3	C	12	VAL	N-CA-C	5.69	118.20	111.09
3	C	172	GLU	O-C-N	5.69	130.16	122.59
5	E	211	ILE	O-C-N	5.69	127.39	121.87
12	O	147	TRP	CA-C-N	5.69	128.47	120.28
12	O	147	TRP	C-N-CA	5.69	128.47	120.28
8	G	60	ASN	CA-C-N	5.69	128.95	120.31
8	G	60	ASN	C-N-CA	5.69	128.95	120.31
1	A	387	HIS	O-C-N	-5.68	116.09	122.12
3	C	70	SER	O-C-N	5.68	130.15	122.59
4	D	140	ASN	CA-C-O	-5.68	115.53	121.55
4	D	263	ILE	CA-C-N	5.68	128.69	120.79
4	D	263	ILE	C-N-CA	5.68	128.69	120.79
6	F	202	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	A	174	ASP	CA-CB-CG	5.68	118.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	161	MET	CG-SD-CE	-5.68	88.40	100.90
4	D	154	LEU	CA-C-O	-5.68	114.53	120.55
7	H	34	PRO	CA-C-O	-5.68	112.33	120.56
1	A	167	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	162	ARG	NH1-CZ-NH2	-5.68	111.92	119.30
2	B	149	PHE	O-C-N	-5.68	116.22	122.07
1	A	342	LEU	CA-C-O	-5.67	114.53	120.55
3	C	53	GLU	CA-C-N	5.67	127.88	120.28
3	C	53	GLU	C-N-CA	5.67	127.88	120.28
2	B	234	MET	O-C-N	5.67	128.13	122.12
4	D	327	LEU	O-C-N	5.67	128.61	122.15
6	F	242	VAL	N-CA-CB	5.67	117.18	110.55
8	G	186	LEU	N-CA-C	-5.67	105.19	111.71
12	O	184	VAL	CA-CB-CG2	-5.67	100.76	110.40
1	A	385	ASP	CA-CB-CG	5.67	118.27	112.60
5	E	26	ASP	CA-C-N	5.66	127.87	120.28
5	E	26	ASP	C-N-CA	5.66	127.87	120.28
6	F	136	ILE	CA-C-O	-5.66	115.06	120.95
1	A	441	LEU	CA-C-N	5.66	128.33	120.29
1	A	441	LEU	C-N-CA	5.66	128.33	120.29
3	C	190	MET	CB-CA-C	-5.66	101.39	110.79
5	E	242	TRP	CB-CG-CD2	-5.66	118.88	126.80
13	R	59	ASN	CA-C-O	-5.66	114.88	120.82
3	C	161	TYR	CA-CB-CG	-5.66	103.72	113.90
3	C	222	GLU	CA-C-N	5.65	127.85	120.28
3	C	222	GLU	C-N-CA	5.65	127.85	120.28
4	D	275	GLY	N-CA-C	5.65	119.48	112.64
4	D	329	GLU	CB-CA-C	-5.65	104.28	111.86
12	O	185	ILE	CA-C-O	-5.65	114.78	121.05
4	D	82	LYS	CA-C-N	5.65	127.78	120.44
4	D	82	LYS	C-N-CA	5.65	127.78	120.44
6	F	51	ILE	CA-C-O	-5.64	114.87	120.85
11	Q	59	GLU	O-C-N	-5.64	116.95	123.33
12	O	53	LEU	N-CA-C	-5.64	105.65	112.54
12	O	53	LEU	CA-C-N	5.64	126.37	119.99
12	O	53	LEU	C-N-CA	5.64	126.37	119.99
13	R	58	ALA	CA-C-N	5.64	127.78	120.44
13	R	58	ALA	C-N-CA	5.64	127.78	120.44
3	C	92	HIS	N-CA-C	-5.64	105.71	112.59
4	D	58	SER	CA-C-N	5.64	128.40	120.28
4	D	58	SER	C-N-CA	5.64	128.40	120.28
5	E	221	TYR	CA-C-N	5.64	131.60	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	221	TYR	C-N-CA	5.64	131.60	122.29
12	O	123	LEU	N-CA-C	-5.64	104.62	113.02
12	O	573	TYR	CA-C-N	-5.64	115.44	123.11
12	O	573	TYR	C-N-CA	-5.64	115.44	123.11
1	A	373	ALA	CA-C-N	5.63	128.29	120.29
1	A	373	ALA	C-N-CA	5.63	128.29	120.29
1	A	388	ARG	NE-CZ-NH2	5.63	124.27	119.20
12	O	160	ILE	N-CA-CB	5.63	117.14	110.55
12	O	328	SER	O-C-N	5.63	128.81	122.22
7	H	112	ALA	CA-C-O	-5.63	114.58	120.55
5	E	74	ASN	CA-CB-CG	-5.63	106.97	112.60
5	E	86	ASP	CA-C-O	5.63	127.25	120.27
2	B	269	GLY	CA-C-N	5.62	135.53	121.80
2	B	269	GLY	C-N-CA	5.62	135.53	121.80
8	G	39	GLY	N-CA-C	-5.62	107.88	115.36
1	A	352	LEU	CA-C-N	5.62	128.38	120.28
1	A	352	LEU	C-N-CA	5.62	128.38	120.28
1	A	190	ASP	N-CA-CB	5.62	116.65	110.35
2	B	342	PHE	CA-C-N	5.62	128.40	120.42
2	B	342	PHE	C-N-CA	5.62	128.40	120.42
12	O	557	HIS	CB-CG-ND1	5.62	131.13	122.70
2	B	386	GLU	O-C-N	5.62	128.08	122.12
8	G	159	GLY	CA-C-N	5.62	132.27	121.54
8	G	159	GLY	C-N-CA	5.62	132.27	121.54
13	R	28	ASN	CA-C-O	5.62	127.31	121.36
1	A	361	HIS	CA-C-O	-5.62	112.34	119.31
1	A	201	MET	CB-CA-C	-5.62	101.30	110.85
2	B	176	HIS	CG-CD2-NE2	5.62	112.82	107.20
8	G	127	GLU	CA-C-N	5.62	128.08	120.44
8	G	127	GLU	C-N-CA	5.62	128.08	120.44
10	P	38	PRO	O-C-N	-5.62	118.73	121.31
12	O	518	PRO	CA-C-N	5.61	129.33	121.02
12	O	518	PRO	C-N-CA	5.61	129.33	121.02
2	B	181	THR	CA-CB-OG1	5.61	118.02	109.60
4	D	54	ASN	CA-C-N	5.61	132.29	121.18
4	D	54	ASN	C-N-CA	5.61	132.29	121.18
5	E	167	ALA	CA-C-O	-5.61	114.63	121.36
12	O	254	LEU	CA-C-O	5.61	128.60	121.82
2	B	313	ASN	CA-C-N	5.61	128.25	120.29
2	B	313	ASN	C-N-CA	5.61	128.25	120.29
4	D	375	GLN	CA-C-N	5.61	127.73	120.44
4	D	375	GLN	C-N-CA	5.61	127.73	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	241	TYR	CA-C-O	-5.61	114.93	120.82
1	A	290	ALA	CA-C-N	5.60	127.73	120.56
1	A	290	ALA	C-N-CA	5.60	127.73	120.56
5	E	302	LYS	CA-C-N	5.60	128.25	120.29
5	E	302	LYS	C-N-CA	5.60	128.25	120.29
12	O	199	PRO	CA-C-N	5.60	132.24	121.54
12	O	199	PRO	C-N-CA	5.60	132.24	121.54
1	A	249	LEU	CA-C-N	5.60	128.24	120.29
1	A	249	LEU	C-N-CA	5.60	128.24	120.29
4	D	333	ALA	CA-C-O	-5.60	114.61	120.55
8	G	153	GLU	CB-CA-C	-5.60	101.66	110.79
8	G	168	ASN	CA-CB-CG	5.60	118.20	112.60
5	E	99	PRO	N-CA-C	-5.60	100.94	112.47
12	O	492	ASN	CA-C-N	5.60	129.56	120.60
12	O	492	ASN	C-N-CA	5.60	129.56	120.60
13	R	87	TRP	CB-CG-CD1	5.60	135.29	126.90
11	Q	6	LYS	CA-C-N	5.60	127.72	120.44
11	Q	6	LYS	C-N-CA	5.60	127.72	120.44
12	O	255	HIS	CA-C-N	5.60	125.70	119.32
12	O	255	HIS	C-N-CA	5.60	125.70	119.32
7	H	129	ILE	N-CA-C	-5.59	101.60	109.21
8	G	145	LEU	N-CA-C	-5.59	100.58	109.76
12	O	64	PHE	CA-C-N	5.59	127.78	120.28
12	O	64	PHE	C-N-CA	5.59	127.78	120.28
6	F	137	HIS	O-C-N	5.59	127.83	122.07
4	D	286	MET	N-CA-C	-5.59	102.08	110.24
4	D	262	GLY	CA-C-N	5.59	127.60	120.56
4	D	262	GLY	C-N-CA	5.59	127.60	120.56
10	P	72	PRO	N-CD-CG	5.59	111.58	103.20
13	R	108	HIS	ND1-CE1-NE2	5.59	113.99	108.40
2	B	218	TYR	O-C-N	5.58	128.04	122.12
2	B	285	MET	CB-CA-C	-5.58	102.11	110.88
3	C	9	VAL	CA-C-O	-5.58	115.25	121.17
6	F	244	ALA	CA-C-O	-5.58	114.50	120.42
9	V	105	THR	CA-C-N	5.58	127.10	121.35
9	V	105	THR	C-N-CA	5.58	127.10	121.35
1	A	45	GLU	N-CA-C	-5.58	105.10	111.07
5	E	176	ILE	CA-C-N	5.58	128.03	120.44
5	E	176	ILE	C-N-CA	5.58	128.03	120.44
12	O	367	ALA	CA-C-N	5.58	127.69	120.44
12	O	367	ALA	C-N-CA	5.58	127.69	120.44
1	A	288	ASN	CA-C-O	-5.58	113.55	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	293	THR	CA-C-N	5.58	132.19	121.54
4	D	293	THR	C-N-CA	5.58	132.19	121.54
6	F	42	ALA	O-C-N	5.58	129.94	123.30
13	R	24	VAL	N-CA-CB	5.58	120.62	111.58
1	A	54	LEU	N-CA-C	5.58	117.44	111.36
1	A	141	LYS	CA-C-O	5.58	126.46	120.55
1	A	261	ARG	NE-CZ-NH2	5.58	124.22	119.20
11	Q	68	HIS	ND1-CE1-NE2	5.58	113.98	108.40
5	E	86	ASP	O-C-N	-5.57	117.10	123.40
2	B	176	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
12	O	279	HIS	N-CA-C	-5.57	105.29	111.36
3	C	156	LYS	CA-C-N	5.57	125.41	119.28
3	C	156	LYS	C-N-CA	5.57	125.41	119.28
8	G	97	LYS	N-CA-CB	5.57	118.40	110.16
3	C	332	GLN	CB-CG-CD	5.57	122.07	112.60
12	O	308	LEU	CA-C-N	5.57	125.93	119.47
12	O	308	LEU	C-N-CA	5.57	125.93	119.47
3	C	221	LEU	CA-C-O	5.57	126.43	120.70
8	G	50	ALA	CA-C-N	5.57	127.74	120.28
8	G	50	ALA	C-N-CA	5.57	127.74	120.28
2	B	176	HIS	N-CA-C	5.56	118.11	111.71
7	H	204	VAL	CA-C-N	5.56	127.73	120.28
7	H	204	VAL	C-N-CA	5.56	127.73	120.28
8	G	128	LEU	CB-CA-C	-5.56	102.11	110.90
2	B	60	LEU	CA-C-N	5.56	132.16	121.54
2	B	60	LEU	C-N-CA	5.56	132.16	121.54
11	Q	81	VAL	CA-C-O	-5.56	114.88	121.05
12	O	435	TYR	CA-CB-CG	-5.56	103.89	113.90
2	B	255	HIS	ND1-CE1-NE2	5.56	113.96	108.40
4	D	313	SER	N-CA-CB	5.56	118.78	110.22
5	E	200	PRO	N-CA-C	5.56	119.95	111.34
13	R	56	CYS	N-CA-C	5.56	117.14	111.14
12	O	568	TYR	N-CA-C	-5.55	105.86	113.30
1	A	197	HIS	ND1-CE1-NE2	5.55	113.95	108.40
4	D	86	HIS	CB-CG-CD2	-5.55	123.98	131.20
12	O	145	ASP	N-CA-C	5.55	117.33	111.28
3	C	270	ASN	CA-CB-CG	-5.55	107.05	112.60
6	F	51	ILE	N-CA-C	5.55	116.33	110.72
7	H	57	TRP	CD2-CE2-CZ2	-5.55	116.85	122.40
8	G	68	ASN	CA-C-O	5.55	126.65	120.82
6	F	217	VAL	CB-CA-C	-5.55	104.56	112.22
4	D	260	ALA	CA-C-N	5.55	127.71	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	260	ALA	C-N-CA	5.55	127.71	120.28
2	B	103	VAL	N-CA-C	-5.55	100.43	108.36
12	O	212	LEU	CB-CA-C	-5.55	102.14	110.90
2	B	226	SER	N-CA-C	5.54	117.32	111.28
3	C	156	LYS	CA-C-O	-5.54	113.30	118.73
4	D	211	LEU	CA-C-O	5.54	126.43	120.55
1	A	465	HIS	N-CA-C	-5.54	100.70	108.96
5	E	157	LEU	CA-C-N	5.54	127.70	120.28
5	E	157	LEU	C-N-CA	5.54	127.70	120.28
4	D	41	GLN	CB-CG-CD	-5.54	103.18	112.60
13	R	104	GLN	CA-C-N	5.54	132.12	121.54
13	R	104	GLN	C-N-CA	5.54	132.12	121.54
4	D	70	CYS	N-CA-C	5.54	117.32	111.28
2	B	305	ASP	O-C-N	-5.54	115.60	121.30
1	A	65	ASP	CA-CB-CG	5.54	118.14	112.60
2	B	379	ASN	CA-CB-CG	-5.53	107.07	112.60
1	A	426	ALA	N-CA-CB	5.53	118.70	110.40
3	C	282	HIS	CA-CB-CG	-5.53	108.27	113.80
9	V	92	ASP	CA-CB-CG	-5.53	107.07	112.60
12	O	569	LEU	O-C-N	-5.53	116.74	123.10
13	R	108	HIS	CE1-NE2-CD2	-5.53	103.47	109.00
12	O	359	ASN	CA-C-N	5.53	130.40	121.00
12	O	359	ASN	C-N-CA	5.53	130.40	121.00
12	O	371	ALA	CB-CA-C	-5.53	101.45	110.85
5	E	314	ALA	N-CA-C	5.53	117.11	111.14
10	P	52	ASP	N-CA-C	-5.53	101.73	109.69
4	D	72	HIS	CA-CB-CG	-5.53	108.28	113.80
11	Q	76	TYR	CA-C-N	5.53	127.68	120.28
11	Q	76	TYR	C-N-CA	5.53	127.68	120.28
12	O	523	PRO	CA-C-O	-5.53	115.47	121.27
3	C	156	LYS	O-C-N	-5.52	115.57	120.48
5	E	52	PHE	CA-C-O	-5.52	115.47	121.87
1	A	328	ASP	CA-CB-CG	-5.52	107.08	112.60
2	B	149	PHE	CA-C-N	5.52	127.61	120.44
2	B	149	PHE	C-N-CA	5.52	127.61	120.44
1	A	420	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
2	B	157	LYS	CA-C-O	5.51	126.39	120.55
13	R	102	GLU	CA-C-O	-5.51	114.93	121.16
8	G	144	LYS	CA-C-O	5.51	127.55	121.11
1	A	361	HIS	CG-CD2-NE2	5.51	112.71	107.20
2	B	398	ILE	N-CA-C	-5.51	100.30	108.45
6	F	310	ASN	CA-CB-CG	5.50	118.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	106	ILE	CA-C-O	-5.50	115.23	120.95
4	D	343	ILE	N-CA-C	-5.50	105.14	110.42
12	O	149	LYS	CA-C-N	5.50	127.65	120.28
12	O	149	LYS	C-N-CA	5.50	127.65	120.28
1	A	339	ALA	CA-C-O	-5.50	114.72	120.55
5	E	57	ILE	N-CA-C	-5.50	100.27	108.46
12	O	502	ASP	CA-CB-CG	5.50	118.10	112.60
12	O	546	GLN	CB-CG-CD	-5.50	103.25	112.60
5	E	131	GLU	N-CA-C	5.50	118.29	110.10
4	D	363	THR	N-CA-C	5.49	122.50	110.80
6	F	287	GLY	CA-C-O	-5.49	114.84	120.66
10	P	101	ASP	O-C-N	5.49	127.94	122.12
12	O	491	ASN	CA-C-N	5.49	128.19	120.28
12	O	491	ASN	C-N-CA	5.49	128.19	120.28
1	A	303	ARG	N-CA-C	5.49	117.26	111.28
4	D	235	LEU	CA-C-N	5.49	132.02	121.54
4	D	235	LEU	C-N-CA	5.49	132.02	121.54
7	H	147	GLY	CA-C-N	5.49	127.98	120.46
7	H	147	GLY	C-N-CA	5.49	127.98	120.46
5	E	168	VAL	CA-C-O	-5.48	114.73	120.76
3	C	338	VAL	CA-C-N	5.48	127.62	120.28
3	C	338	VAL	C-N-CA	5.48	127.62	120.28
8	G	202	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
4	D	40	GLU	CA-C-N	5.48	127.56	120.44
4	D	40	GLU	C-N-CA	5.48	127.56	120.44
3	C	99	THR	N-CA-CB	5.48	118.27	110.16
12	O	98	ALA	CB-CA-C	-5.48	101.70	110.79
5	E	299	LYS	N-CA-C	5.48	117.25	111.28
12	O	625	HIS	ND1-CE1-NE2	5.48	113.88	108.40
2	B	69	PHE	O-C-N	5.47	128.00	122.09
8	G	207	GLN	N-CA-CB	5.47	118.76	110.28
3	C	308	GLN	N-CA-C	5.47	118.17	111.82
5	E	28	ILE	N-CA-C	5.47	116.20	110.62
7	H	126	THR	N-CA-C	-5.47	105.33	112.23
12	O	364	PHE	CA-CB-CG	-5.47	108.33	113.80
2	B	221	SER	CB-CA-C	-5.47	100.17	110.67
6	F	45	PRO	CA-N-CD	-5.47	104.34	112.00
12	O	288	GLN	CA-C-O	-5.47	115.65	121.94
5	E	318	LEU	N-CA-CB	5.47	118.16	110.12
12	O	61	THR	N-CA-CB	5.47	118.16	110.12
5	E	126	GLN	CA-C-O	-5.47	114.62	120.42
3	C	394	ASP	CA-C-N	5.46	127.60	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	394	ASP	C-N-CA	5.46	127.60	120.28
7	H	89	ILE	N-CA-CB	5.46	116.94	110.55
12	O	440	ALA	N-CA-C	5.46	116.92	111.07
6	F	30	VAL	N-CA-C	-5.46	97.73	107.18
6	F	178	GLU	N-CA-C	-5.46	100.80	109.59
12	O	221	GLN	CA-C-N	5.46	127.60	120.28
12	O	221	GLN	C-N-CA	5.46	127.60	120.28
8	G	91	ALA	CB-CA-C	-5.46	101.73	110.79
13	R	60	GLN	OE1-CD-NE2	-5.46	117.14	122.60
3	C	315	LEU	N-CA-C	-5.46	104.18	112.04
7	H	11	PHE	CA-CB-CG	-5.46	108.34	113.80
8	G	106	SER	N-CA-CB	5.46	118.74	110.28
12	O	239	VAL	CA-CB-CG1	5.46	119.68	110.40
12	O	634	ALA	N-CA-C	-5.46	106.29	113.17
2	B	246	LEU	CB-CA-C	-5.45	101.74	110.79
3	C	82	GLN	CA-C-N	5.45	128.03	120.29
3	C	82	GLN	C-N-CA	5.45	128.03	120.29
2	B	91	ARG	CA-C-N	5.45	127.58	120.28
2	B	91	ARG	C-N-CA	5.45	127.58	120.28
8	G	16	ILE	CA-C-N	5.45	127.58	120.28
8	G	16	ILE	C-N-CA	5.45	127.58	120.28
12	O	255	HIS	ND1-CE1-NE2	5.45	113.85	108.40
1	A	90	MET	CA-C-N	5.45	127.58	120.28
1	A	90	MET	C-N-CA	5.45	127.58	120.28
3	C	361	HIS	CE1-NE2-CD2	-5.45	103.55	109.00
5	E	254	SER	N-CA-C	5.45	118.72	111.75
6	F	239	LEU	CB-CA-C	-5.44	102.33	110.88
1	A	273	ALA	CA-C-O	-5.44	115.06	121.16
10	P	3	VAL	CA-C-N	5.44	130.23	122.72
10	P	3	VAL	C-N-CA	5.44	130.23	122.72
12	O	293	ASP	CA-C-N	5.44	128.58	120.31
12	O	293	ASP	C-N-CA	5.44	128.58	120.31
4	D	19	HIS	CB-CA-C	-5.44	102.58	110.96
4	D	349	ASN	CB-CG-ND2	-5.44	108.24	116.40
12	O	13	THR	CA-C-N	5.44	127.57	120.28
12	O	13	THR	C-N-CA	5.44	127.57	120.28
12	O	112	PHE	N-CA-C	-5.44	101.30	109.95
2	B	111	SER	N-CA-CB	5.44	117.90	110.01
1	A	251	CYS	N-CA-C	-5.44	105.43	111.36
5	E	321	GLN	N-CA-CB	5.44	118.30	110.20
6	F	199	GLY	O-C-N	-5.44	116.97	122.19
7	H	128	ILE	CA-C-O	-5.44	115.52	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	71	ALA	CA-C-N	5.43	125.64	120.31
10	P	71	ALA	C-N-CA	5.43	125.64	120.31
10	P	81	ALA	N-CA-C	-5.43	104.23	111.24
12	O	347	HIS	ND1-CG-CD2	5.43	111.53	106.10
12	O	21	ILE	O-C-N	5.43	127.14	121.87
12	O	188	PHE	N-CA-CB	5.43	118.20	110.16
13	R	40	ASP	N-CA-CB	5.43	120.99	112.46
12	O	589	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	93	GLU	CA-C-O	5.43	126.29	120.70
6	F	186	LEU	CA-C-N	5.43	132.08	121.66
6	F	186	LEU	C-N-CA	5.43	132.08	121.66
8	G	168	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	A	356	MET	N-CA-C	5.43	117.64	111.02
1	A	205	VAL	CB-CA-C	-5.42	104.82	112.14
2	B	130	GLU	CA-C-N	5.42	127.55	120.28
2	B	130	GLU	C-N-CA	5.42	127.55	120.28
12	O	537	VAL	CB-CA-C	5.42	119.15	112.04
1	A	389	MET	CA-C-O	5.42	126.28	120.70
3	C	266	VAL	CA-C-N	5.42	127.55	120.28
3	C	266	VAL	C-N-CA	5.42	127.55	120.28
6	F	190	LEU	CA-C-O	-5.42	115.04	121.16
4	D	124	ALA	O-C-N	5.42	127.65	122.07
10	P	52	ASP	CA-CB-CG	-5.42	107.18	112.60
12	O	253	TYR	CB-CG-CD2	-5.42	112.68	120.80
6	F	183	PHE	CA-CB-CG	-5.42	108.39	113.80
2	B	209	LYS	N-CA-C	5.41	119.30	111.56
3	C	291	ASN	CA-C-N	5.41	128.56	120.87
3	C	291	ASN	C-N-CA	5.41	128.56	120.87
4	D	142	ASP	N-CA-C	5.41	117.18	111.28
2	B	123	LYS	CA-C-O	-5.41	115.66	121.45
4	D	57	VAL	CA-C-O	-5.41	114.55	120.72
2	B	64	LYS	CA-C-O	-5.41	114.69	120.42
2	B	163	GLU	N-CA-CB	5.41	119.63	110.49
3	C	142	HIS	N-CA-CB	5.41	118.07	110.12
12	O	369	ASP	O-C-N	5.41	127.64	122.07
6	F	232	HIS	CG-CD2-NE2	5.41	112.61	107.20
12	O	419	ILE	CA-C-O	-5.40	115.33	120.95
7	H	76	SER	N-CA-C	5.40	118.08	111.82
6	F	175	ILE	CA-C-N	5.40	130.23	122.40
6	F	175	ILE	C-N-CA	5.40	130.23	122.40
13	R	90	THR	CA-C-N	5.40	130.38	122.77
13	R	90	THR	C-N-CA	5.40	130.38	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	46	LYS	N-CA-CB	5.40	117.83	110.01
8	G	28	THR	CA-C-N	5.40	127.51	120.28
8	G	28	THR	C-N-CA	5.40	127.51	120.28
1	A	104	SER	N-CA-C	5.39	117.65	110.53
6	F	240	GLU	CA-C-N	5.39	127.45	120.44
6	F	240	GLU	C-N-CA	5.39	127.45	120.44
11	Q	73	VAL	CA-C-N	5.39	127.51	120.28
11	Q	73	VAL	C-N-CA	5.39	127.51	120.28
12	O	275	LEU	CA-C-N	5.39	127.51	120.28
12	O	275	LEU	C-N-CA	5.39	127.51	120.28
12	O	318	HIS	CB-CA-C	-5.39	102.41	110.88
12	O	451	MET	CA-C-N	5.39	127.51	120.28
12	O	451	MET	C-N-CA	5.39	127.51	120.28
12	O	89	ARG	CA-C-O	-5.39	114.70	120.42
12	O	534	GLU	N-CA-C	5.39	116.84	111.07
6	F	236	LYS	N-CA-C	5.39	116.84	111.07
3	C	137	GLN	N-CA-C	-5.39	100.62	109.40
7	H	21	GLU	CA-C-N	5.38	127.94	120.29
7	H	21	GLU	C-N-CA	5.38	127.94	120.29
6	F	264	CYS	O-C-N	5.38	128.28	122.15
2	B	210	ASN	CA-C-O	5.38	126.06	120.30
12	O	618	LEU	N-CA-C	5.38	117.22	111.36
1	A	313	SER	CA-C-N	5.38	127.93	120.29
1	A	313	SER	C-N-CA	5.38	127.93	120.29
3	C	361	HIS	ND1-CE1-NE2	5.38	113.78	108.40
5	E	149	GLY	CA-C-N	5.38	128.06	120.42
5	E	149	GLY	C-N-CA	5.38	128.06	120.42
6	F	265	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
1	A	195	ALA	CA-C-N	5.38	127.48	120.28
1	A	195	ALA	C-N-CA	5.38	127.48	120.28
2	B	288	LYS	CA-C-N	5.38	131.38	121.70
2	B	288	LYS	C-N-CA	5.38	131.38	121.70
12	O	202	PHE	CA-CB-CG	-5.38	108.42	113.80
12	O	601	ASP	N-CA-C	-5.38	105.33	111.14
12	O	109	ASN	O-C-N	5.38	128.28	122.15
4	D	371	ASP	N-CA-C	5.37	117.22	111.36
12	O	269	ARG	N-CA-CB	5.37	118.11	110.16
12	O	57	LEU	CA-C-N	5.37	127.42	120.44
12	O	57	LEU	C-N-CA	5.37	127.42	120.44
12	O	445	HIS	ND1-CE1-NE2	5.37	113.77	108.40
13	R	64	THR	CA-C-N	5.37	127.92	120.29
13	R	64	THR	C-N-CA	5.37	127.92	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	134	ALA	CB-CA-C	-5.37	101.88	110.79
2	B	55	GLN	O-C-N	5.37	127.81	122.12
5	E	40	LEU	CA-C-O	-5.37	114.03	120.10
2	B	288	LYS	N-CA-C	5.37	117.73	111.02
4	D	276	ASN	CA-C-N	5.37	127.91	120.29
4	D	276	ASN	C-N-CA	5.37	127.91	120.29
12	O	614	ILE	CB-CA-C	5.36	119.38	112.14
4	D	329	GLU	N-CA-CB	5.36	120.06	111.91
1	A	269	CYS	N-CA-CB	5.36	118.09	110.16
12	O	274	HIS	CB-CG-ND1	5.36	130.74	122.70
12	O	391	LEU	CA-C-N	5.36	127.73	120.44
12	O	391	LEU	C-N-CA	5.36	127.73	120.44
12	O	435	TYR	CA-C-O	-5.36	114.05	120.10
1	A	327	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	104	SER	CA-C-N	5.35	132.02	122.06
1	A	104	SER	C-N-CA	5.35	132.02	122.06
12	O	310	HIS	ND1-CE1-NE2	5.35	113.75	108.40
3	C	76	THR	CA-CB-OG1	5.35	117.63	109.60
8	G	133	ILE	N-CA-CB	5.35	117.82	110.54
11	Q	68	HIS	CA-CB-CG	5.35	119.15	113.80
12	O	225	ASN	CA-C-N	5.35	127.89	120.29
12	O	225	ASN	C-N-CA	5.35	127.89	120.29
3	C	46	LEU	N-CA-C	-5.35	105.89	112.90
4	D	356	ASP	N-CA-CB	5.35	119.81	110.98
2	B	253	LYS	O-C-N	5.35	128.25	122.15
2	B	343	ILE	CA-C-N	5.35	127.44	120.28
2	B	343	ILE	C-N-CA	5.35	127.44	120.28
3	C	393	MET	N-CA-C	5.35	117.19	111.36
4	D	368	PRO	CB-CA-C	5.35	120.55	112.21
12	O	320	HIS	ND1-CE1-NE2	5.35	113.75	108.40
3	C	306	ASN	N-CA-CB	5.34	118.56	110.28
7	H	144	ALA	CA-C-O	-5.34	115.20	120.70
8	G	190	GLN	OE1-CD-NE2	5.34	127.94	122.60
5	E	274	GLU	CB-CG-CD	-5.34	103.52	112.60
7	H	153	TRP	CA-C-N	5.34	130.00	122.09
7	H	153	TRP	C-N-CA	5.34	130.00	122.09
1	A	215	TRP	O-C-N	-5.34	115.70	122.27
5	E	98	LEU	CB-CA-C	-5.34	100.59	108.87
2	B	148	TRP	CA-C-N	5.34	127.38	120.44
2	B	148	TRP	C-N-CA	5.34	127.38	120.44
12	O	466	GLY	N-CA-C	-5.34	100.53	113.18
4	D	325	GLY	CA-C-N	5.33	127.87	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	325	GLY	C-N-CA	5.33	127.87	120.29
6	F	242	VAL	CA-C-N	5.33	127.43	120.28
6	F	242	VAL	C-N-CA	5.33	127.43	120.28
12	O	45	LEU	CA-C-N	5.33	127.87	120.29
12	O	45	LEU	C-N-CA	5.33	127.87	120.29
5	E	219	LYS	CB-CG-CD	5.33	123.57	111.30
11	Q	60	VAL	CA-C-O	-5.33	114.70	120.67
12	O	177	ASN	OD1-CG-ND2	-5.33	117.27	122.60
2	B	177	GLN	CA-C-N	5.33	129.31	120.94
2	B	177	GLN	C-N-CA	5.33	129.31	120.94
3	C	71	VAL	O-C-N	-5.33	115.02	121.10
12	O	321	ASP	CA-C-N	5.33	127.42	120.28
12	O	321	ASP	C-N-CA	5.33	127.42	120.28
2	B	215	LYS	CB-CG-CD	5.33	123.55	111.30
2	B	298	GLU	O-C-N	5.33	129.67	122.59
5	E	156	MET	CA-CB-CG	-5.32	103.45	114.10
6	F	315	ARG	N-CA-C	-5.32	106.17	113.30
4	D	316	TYR	N-CA-C	5.32	122.14	110.80
12	O	651	PHE	CA-CB-CG	-5.32	108.48	113.80
12	O	32	ARG	CB-CA-C	-5.32	101.81	110.85
12	O	395	CYS	N-CA-C	-5.32	105.56	111.36
2	B	307	GLU	N-CA-C	5.32	116.76	111.07
4	D	361	PHE	CA-CB-CG	-5.32	108.48	113.80
5	E	253	SER	CA-C-N	5.32	128.14	120.38
5	E	253	SER	C-N-CA	5.32	128.14	120.38
1	A	330	ILE	N-CA-CB	5.31	117.37	110.57
1	A	435	THR	O-C-N	5.31	128.21	122.15
2	B	166	GLY	O-C-N	5.31	127.29	122.19
3	C	22	THR	CA-C-N	5.31	127.93	120.28
3	C	22	THR	C-N-CA	5.31	127.93	120.28
4	D	402	ALA	N-CA-C	5.31	117.82	111.71
10	P	10	HIS	N-CA-C	5.31	122.11	110.80
6	F	118	GLU	N-CA-C	-5.31	105.57	111.36
3	C	308	GLN	CG-CD-NE2	-5.31	108.44	116.40
4	D	279	GLN	CB-CG-CD	-5.31	103.58	112.60
6	F	45	PRO	CB-CA-C	-5.31	102.80	111.56
3	C	321	ASP	CA-CB-CG	-5.31	107.29	112.60
4	D	363	THR	CA-CB-OG1	5.31	117.56	109.60
6	F	34	GLY	CA-C-N	5.30	128.50	120.75
6	F	34	GLY	C-N-CA	5.30	128.50	120.75
12	O	299	VAL	N-CA-C	5.30	116.08	110.72
12	O	523	PRO	N-CA-CB	5.30	107.89	103.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
10	P	111	SER	CA-C-N	5.30	128.24	120.71
10	P	111	SER	C-N-CA	5.30	128.24	120.71
4	D	176	ASN	CA-CB-CG	5.30	117.90	112.60
8	G	48	GLU	CA-CB-CG	5.30	124.70	114.10
8	G	152	LEU	N-CA-C	-5.30	100.54	109.07
11	Q	35	HIS	CA-C-N	5.30	128.36	120.31
11	Q	35	HIS	C-N-CA	5.30	128.36	120.31
12	O	274	HIS	ND1-CE1-NE2	5.30	113.70	108.40
4	D	68	ASP	N-CA-CB	5.30	117.83	109.94
12	O	389	GLU	N-CA-C	5.30	117.13	111.36
12	O	563	GLU	N-CA-C	5.30	118.19	109.72
2	B	85	PHE	CA-CB-CG	-5.29	108.50	113.80
12	O	633	ASP	N-CA-C	-5.29	101.07	108.96
1	A	336	SER	N-CA-CB	5.29	119.44	110.49
3	C	23	GLN	N-CA-C	5.29	117.80	111.71
2	B	237	ILE	N-CA-CB	5.29	118.52	110.58
12	O	307	GLY	O-C-N	-5.29	117.06	122.19
2	B	255	HIS	CA-C-O	-5.29	115.27	120.82
4	D	263	ILE	N-CA-C	-5.29	105.34	110.42
11	Q	62	PHE	CA-CB-CG	-5.29	108.51	113.80
12	O	592	GLU	CA-CB-CG	5.29	124.68	114.10
10	P	5	LEU	CA-C-N	5.29	130.22	122.77
10	P	5	LEU	C-N-CA	5.29	130.22	122.77
1	A	97	LYS	N-CA-CB	5.29	117.98	110.16
6	F	35	VAL	N-CA-C	-5.29	102.77	109.80
6	F	80	ASN	CA-CB-CG	-5.29	107.31	112.60
12	O	20	THR	CA-C-N	5.29	127.70	120.46
12	O	20	THR	C-N-CA	5.29	127.70	120.46
7	H	44	TYR	CB-CA-C	-5.28	101.87	110.85
12	O	463	GLN	CA-C-N	5.28	127.62	120.44
12	O	463	GLN	C-N-CA	5.28	127.62	120.44
13	R	77	HIS	CG-CD2-NE2	5.28	112.48	107.20
3	C	88	CYS	CA-C-O	-5.28	115.28	120.82
3	C	154	CYS	CA-C-O	5.28	128.06	120.51
12	O	78	GLU	N-CA-C	5.28	117.04	111.28
12	O	105	TYR	N-CA-C	5.28	119.47	113.19
12	O	607	GLU	CA-C-N	5.28	127.30	120.44
12	O	607	GLU	C-N-CA	5.28	127.30	120.44
6	F	100	ILE	N-CA-C	-5.28	100.85	108.71
12	O	292	ASN	CA-CB-CG	5.28	117.88	112.60
5	E	264	GLY	N-CA-C	5.27	118.87	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	163	GLU	O-C-N	-5.27	115.58	122.59
2	B	302	TYR	CA-C-N	5.27	127.87	120.28
2	B	302	TYR	C-N-CA	5.27	127.87	120.28
4	D	101	GLU	N-CA-CB	5.27	117.66	110.01
6	F	35	VAL	CA-C-N	5.27	128.36	120.87
6	F	35	VAL	C-N-CA	5.27	128.36	120.87
13	R	77	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
8	G	40	VAL	N-CA-CB	5.27	117.38	111.21
2	B	398	ILE	CA-CB-CG1	5.27	119.36	110.40
12	O	504	GLY	CA-C-N	5.27	131.45	121.97
12	O	504	GLY	C-N-CA	5.27	131.45	121.97
7	H	52	ASN	N-CA-C	-5.26	105.71	111.82
10	P	99	LEU	CD1-CG-CD2	5.26	122.37	110.80
12	O	490	PHE	CA-CB-CG	-5.26	108.54	113.80
2	B	348	GLU	O-C-N	-5.26	116.54	122.12
5	E	292	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
8	G	33	GLN	CB-CG-CD	-5.26	103.66	112.60
12	O	518	PRO	N-CA-C	-5.26	107.17	114.27
1	A	126	LEU	N-CA-CB	5.26	117.77	110.04
1	A	197	HIS	N-CA-CB	5.26	117.94	110.16
1	A	423	ILE	N-CA-C	-5.26	100.91	108.48
2	B	272	ARG	CA-C-O	-5.26	114.16	120.10
2	B	280	LEU	CB-CA-C	-5.26	102.63	110.88
4	D	81	ALA	CA-C-O	-5.26	115.30	120.82
12	O	316	GLN	CA-C-N	5.26	127.75	120.29
12	O	316	GLN	C-N-CA	5.26	127.75	120.29
2	B	111	SER	CA-C-N	5.25	127.88	120.42
2	B	111	SER	C-N-CA	5.25	127.88	120.42
8	G	200	GLU	CB-CA-C	-5.25	102.63	110.88
1	A	351	ASN	CB-CA-C	-5.25	102.63	110.88
5	E	139	SER	N-CA-C	5.25	117.24	108.99
3	C	362	ASP	O-C-N	-5.25	115.60	122.59
6	F	61	GLN	CB-CA-C	-5.25	102.81	110.95
8	G	213	VAL	CA-C-N	5.25	127.27	120.44
8	G	213	VAL	C-N-CA	5.25	127.27	120.44
2	B	264	ASN	CB-CA-C	-5.25	101.92	110.85
1	A	246	LEU	CA-C-N	5.25	127.74	120.29
1	A	246	LEU	C-N-CA	5.25	127.74	120.29
4	D	382	ASN	CA-C-N	5.25	127.31	120.28
4	D	382	ASN	C-N-CA	5.25	127.31	120.28
5	E	232	SER	O-C-N	-5.25	115.19	121.64
8	G	87	GLU	CA-C-N	5.25	131.62	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	87	GLU	C-N-CA	5.25	131.62	122.81
12	O	526	THR	CA-C-N	5.24	128.15	120.71
12	O	526	THR	C-N-CA	5.24	128.15	120.71
1	A	344	MET	CA-C-N	5.24	127.30	120.28
1	A	344	MET	C-N-CA	5.24	127.30	120.28
3	C	208	ALA	O-C-N	-5.24	115.41	122.43
4	D	47	ALA	CA-C-N	5.24	127.25	120.44
4	D	47	ALA	C-N-CA	5.24	127.25	120.44
6	F	97	LYS	CA-C-N	5.24	129.86	123.10
6	F	97	LYS	C-N-CA	5.24	129.86	123.10
5	E	252	SER	CA-C-O	5.24	126.09	120.70
8	G	188	ILE	N-CA-C	5.23	116.00	110.72
10	P	97	PRO	N-CA-C	5.23	118.81	111.33
12	O	536	SER	N-CA-CB	5.23	119.33	110.49
10	P	18	ALA	N-CA-CB	5.23	120.40	111.66
12	O	488	ASN	N-CA-CB	5.23	117.81	110.12
6	F	288	LEU	N-CA-C	5.23	117.06	111.36
2	B	82	LEU	N-CA-C	-5.23	101.92	109.29
7	H	70	GLU	N-CA-CB	5.23	117.90	110.16
8	G	89	SER	CA-CB-OG	5.23	121.55	111.10
7	H	21	GLU	CB-CA-C	-5.23	102.11	110.79
1	A	150	LYS	CA-C-N	5.22	127.71	120.29
1	A	150	LYS	C-N-CA	5.22	127.71	120.29
2	B	334	HIS	CA-C-N	5.22	127.28	120.28
2	B	334	HIS	C-N-CA	5.22	127.28	120.28
4	D	337	LYS	N-CA-C	5.22	116.66	111.07
7	H	143	GLU	CA-C-N	5.22	127.55	120.44
7	H	143	GLU	C-N-CA	5.22	127.55	120.44
12	O	450	SER	N-CA-C	-5.22	98.76	107.80
8	G	197	GLN	OE1-CD-NE2	5.22	127.82	122.60
12	O	158	ILE	N-CA-CB	5.22	117.26	110.57
12	O	255	HIS	O-C-N	-5.22	115.01	121.64
2	B	224	ILE	CA-C-N	5.22	128.00	120.38
2	B	224	ILE	C-N-CA	5.22	128.00	120.38
2	B	256	THR	CA-CB-CG2	-5.22	101.63	110.50
8	G	130	ASP	CA-C-O	-5.22	115.02	120.55
10	P	100	PRO	CA-C-O	-5.22	115.26	122.15
12	O	48	ALA	O-C-N	5.22	129.35	122.93
2	B	424	LEU	N-CA-CB	5.22	117.79	110.12
6	F	250	VAL	CA-C-O	-5.22	112.96	119.95
12	O	348	GLY	CA-C-O	-5.22	115.38	120.75
1	A	387	HIS	CE1-NE2-CD2	-5.21	103.78	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213	LYS	CA-C-O	5.21	126.08	120.55
10	P	90	ILE	CA-C-O	5.21	126.11	120.53
13	R	41	ASN	CA-C-O	-5.21	115.79	121.84
4	D	193	ARG	CA-C-O	5.21	125.95	120.42
5	E	305	ARG	N-CA-CB	5.21	117.87	110.16
8	G	184	VAL	CA-C-O	-5.21	115.27	121.05
4	D	121	ARG	N-CA-C	5.21	116.77	111.14
8	G	183	ALA	CA-C-N	5.21	127.23	120.56
8	G	183	ALA	C-N-CA	5.21	127.23	120.56
2	B	156	GLY	O-C-N	-5.20	117.19	122.19
6	F	235	VAL	N-CA-C	-5.20	105.47	110.72
12	O	53	LEU	N-CA-CB	5.20	119.03	110.39
1	A	177	ASP	CA-C-N	5.20	127.68	120.29
1	A	177	ASP	C-N-CA	5.20	127.68	120.29
1	A	96	ARG	CA-C-N	5.20	127.67	120.29
1	A	96	ARG	C-N-CA	5.20	127.67	120.29
6	F	312	LEU	O-C-N	-5.20	116.41	122.03
7	H	67	ALA	CA-C-O	5.20	125.93	120.42
12	O	630	GLU	CA-C-O	-5.20	115.17	120.89
3	C	51	VAL	CB-CA-C	-5.20	102.76	111.29
7	H	72	GLY	CA-C-N	5.20	125.72	120.00
7	H	72	GLY	C-N-CA	5.20	125.72	120.00
12	O	452	ASP	CA-C-N	5.20	127.20	120.44
12	O	452	ASP	C-N-CA	5.20	127.20	120.44
12	O	735	GLN	CA-C-N	-5.20	115.28	123.13
12	O	735	GLN	C-N-CA	-5.20	115.28	123.13
2	B	73	LYS	CA-C-N	5.20	127.67	120.29
2	B	73	LYS	C-N-CA	5.20	127.67	120.29
3	C	43	ASP	N-CA-C	5.19	117.68	111.71
11	Q	101	LEU	CB-CA-C	-5.19	102.69	110.90
11	Q	27	HIS	CB-CG-ND1	5.19	130.49	122.70
12	O	162	MET	CA-C-N	5.19	127.66	120.29
12	O	162	MET	C-N-CA	5.19	127.66	120.29
12	O	80	GLU	O-C-N	5.19	128.96	122.63
12	O	488	ASN	OD1-CG-ND2	5.19	127.79	122.60
8	G	29	ALA	CA-C-O	-5.19	115.05	120.55
4	D	231	HIS	ND1-CG-CD2	-5.19	100.91	106.10
8	G	12	LEU	CB-CA-C	-5.19	102.18	110.79
12	O	117	LYS	N-CA-C	-5.19	98.85	108.24
1	A	405	THR	CA-C-N	5.18	127.23	120.28
1	A	405	THR	C-N-CA	5.18	127.23	120.28
4	D	46	LYS	CA-C-O	5.18	126.27	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	124	TRP	N-CA-C	5.18	116.86	109.14
6	F	148	SER	O-C-N	-5.18	116.70	121.37
12	O	148	ARG	NE-CZ-NH2	-5.18	114.53	119.20
4	D	370	TRP	CE2-CD2-CE3	5.18	123.98	118.80
1	A	268	LYS	N-CA-C	5.18	116.93	111.28
3	C	396	GLU	CA-C-N	5.18	127.78	120.42
3	C	396	GLU	C-N-CA	5.18	127.78	120.42
4	D	397	ALA	CA-C-N	5.18	127.22	120.28
4	D	397	ALA	C-N-CA	5.18	127.22	120.28
5	E	194	LYS	CB-CG-CD	5.18	123.21	111.30
8	G	36	GLU	CA-C-N	5.18	127.69	120.65
8	G	36	GLU	C-N-CA	5.18	127.69	120.65
12	O	255	HIS	CG-CD2-NE2	5.18	112.38	107.20
2	B	93	LYS	N-CA-CB	5.18	119.12	110.32
2	B	146	ARG	N-CA-CB	5.18	117.82	110.16
6	F	256	ILE	CA-C-N	5.18	127.64	120.29
6	F	256	ILE	C-N-CA	5.18	127.64	120.29
10	P	75	VAL	CB-CA-C	-5.17	103.42	110.77
3	C	308	GLN	N-CA-CB	5.17	118.30	110.28
8	G	126	ARG	CB-CG-CD	5.17	123.20	111.30
13	R	99	ARG	CB-CG-CD	5.17	123.20	111.30
1	A	95	HIS	CB-CG-CD2	-5.17	124.48	131.20
4	D	156	LEU	CA-C-N	5.17	127.21	120.28
4	D	156	LEU	C-N-CA	5.17	127.21	120.28
7	H	26	GLU	CA-C-O	-5.17	115.38	120.70
2	B	223	HIS	CA-C-N	5.17	128.78	120.30
2	B	223	HIS	C-N-CA	5.17	128.78	120.30
2	B	342	PHE	N-CA-C	5.17	116.72	111.14
1	A	250	LYS	N-CA-CB	5.17	117.81	110.16
4	D	380	GLN	CA-C-N	5.17	127.07	120.56
4	D	380	GLN	C-N-CA	5.17	127.07	120.56
6	F	246	GLU	CA-C-N	5.17	127.47	120.44
6	F	246	GLU	C-N-CA	5.17	127.47	120.44
12	O	161	ARG	CA-C-O	-5.17	115.40	120.82
12	O	377	ASN	CB-CG-OD1	5.17	131.13	120.80
5	E	47	LYS	CA-C-O	-5.17	115.38	120.70
2	B	314	LEU	CA-C-N	5.16	127.75	120.42
2	B	314	LEU	C-N-CA	5.16	127.75	120.42
2	B	401	ARG	O-C-N	-5.16	116.45	122.96
7	H	60	ILE	CB-CA-C	5.16	120.76	111.36
12	O	40	SER	CA-C-N	5.16	127.15	120.44
12	O	40	SER	C-N-CA	5.16	127.15	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	LEU	O-C-N	-5.16	116.11	122.25
5	E	35	GLN	O-C-N	-5.16	116.65	122.12
3	C	133	MET	N-CA-C	5.16	116.59	111.07
7	H	199	ARG	O-C-N	5.16	127.59	122.12
8	G	35	LEU	N-CA-CB	-5.16	102.28	110.28
12	O	194	TYR	O-C-N	-5.16	116.87	123.06
12	O	264	HIS	ND1-CE1-NE2	5.16	113.56	108.40
5	E	64	LYS	CA-C-O	-5.16	115.08	120.55
2	B	311	MET	N-CA-C	5.16	116.90	111.28
4	D	13	MET	N-CA-C	5.16	119.88	111.37
6	F	216	THR	CA-CB-CG2	5.16	119.26	110.50
8	G	213	VAL	CB-CA-C	-5.16	105.18	112.14
4	D	160	ASP	CB-CA-C	5.15	117.36	110.81
5	E	294	ARG	CA-C-O	-5.15	115.92	121.38
6	F	64	ARG	NE-CZ-NH2	-5.15	114.56	119.20
1	A	397	VAL	O-C-N	5.15	126.96	121.91
2	B	49	ALA	O-C-N	-5.15	115.74	122.59
1	A	250	LYS	CA-C-N	5.15	127.60	120.29
1	A	250	LYS	C-N-CA	5.15	127.60	120.29
3	C	145	LEU	CA-C-N	5.15	127.18	120.28
3	C	145	LEU	C-N-CA	5.15	127.18	120.28
8	G	142	GLN	N-CA-C	-5.15	100.06	108.76
5	E	75	LEU	N-CA-C	-5.15	100.65	109.24
1	A	67	CYS	CA-C-N	-5.14	113.41	119.84
1	A	67	CYS	C-N-CA	-5.14	113.41	119.84
1	A	98	LEU	N-CA-C	-5.14	105.67	111.28
2	B	249	GLY	N-CA-C	-5.14	107.70	114.95
4	D	123	ALA	CA-C-N	5.14	127.13	120.44
4	D	123	ALA	C-N-CA	5.14	127.13	120.44
4	D	343	ILE	CB-CA-C	-5.14	105.38	111.97
6	F	226	SER	CA-C-N	5.14	127.17	120.28
6	F	226	SER	C-N-CA	5.14	127.17	120.28
12	O	26	MET	CA-C-N	5.14	129.44	122.19
12	O	26	MET	C-N-CA	5.14	129.44	122.19
4	D	54	ASN	CA-CB-CG	-5.14	107.46	112.60
5	E	161	PHE	N-CA-C	5.14	117.67	111.40
8	G	110	CYS	N-CA-C	-5.14	101.02	109.40
12	O	340	VAL	N-CA-CB	5.14	116.56	110.55
8	G	153	GLU	CA-C-O	5.13	125.95	120.46
12	O	424	TYR	CB-CG-CD2	-5.13	113.10	120.80
6	F	232	HIS	O-C-N	5.13	127.36	122.07
8	G	26	ALA	N-CA-C	5.13	116.95	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	292	HIS	CA-C-N	5.13	131.33	121.54
5	E	292	HIS	C-N-CA	5.13	131.33	121.54
7	H	146	LYS	CA-C-O	-5.13	115.11	120.55
11	Q	82	ARG	O-C-N	-5.13	116.79	122.07
12	O	521	GLN	CB-CG-CD	-5.13	103.88	112.60
2	B	86	PRO	N-CA-C	-5.13	106.85	113.57
3	C	181	PHE	N-CA-C	-5.13	105.58	111.07
6	F	191	ALA	CA-C-N	5.13	131.33	121.54
6	F	191	ALA	C-N-CA	5.13	131.33	121.54
8	G	81	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	72	VAL	CA-C-N	5.12	127.15	120.28
1	A	72	VAL	C-N-CA	5.12	127.15	120.28
12	O	365	MET	N-CA-CB	5.12	117.65	110.12
1	A	346	ASP	CA-C-N	5.12	127.56	120.29
1	A	346	ASP	C-N-CA	5.12	127.56	120.29
2	B	147	LEU	CA-C-N	5.12	127.56	120.29
2	B	147	LEU	C-N-CA	5.12	127.56	120.29
4	D	102	GLN	OE1-CD-NE2	5.12	127.72	122.60
4	D	104	ALA	N-CA-C	5.12	116.55	111.07
5	E	308	CYS	CA-C-N	5.12	127.09	120.44
5	E	308	CYS	C-N-CA	5.12	127.09	120.44
6	F	270	LEU	CA-C-O	5.12	127.83	120.51
12	O	523	PRO	CA-C-N	5.12	127.40	120.44
12	O	523	PRO	C-N-CA	5.12	127.40	120.44
1	A	319	PHE	CA-CB-CG	-5.12	108.69	113.80
1	A	345	LEU	N-CA-C	5.12	116.86	111.28
3	C	205	TYR	CA-C-O	-5.12	115.13	120.55
3	C	274	GLU	N-CA-CB	5.12	117.73	110.16
5	E	296	SER	CA-C-O	5.12	124.83	119.51
12	O	370	LYS	N-CA-C	-5.12	105.70	111.28
2	B	61	GLU	CA-C-N	5.11	131.43	121.41
2	B	61	GLU	C-N-CA	5.11	131.43	121.41
12	O	316	GLN	CA-C-O	-5.11	115.45	120.82
12	O	156	GLN	CA-C-O	-5.11	115.11	120.63
1	A	390	ALA	CB-CA-C	-5.11	102.31	110.79
6	F	220	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
8	G	53	GLN	CA-C-N	5.11	127.64	120.28
8	G	53	GLN	C-N-CA	5.11	127.64	120.28
3	C	38	ASN	N-CA-C	5.11	118.29	111.75
5	E	133	ALA	CA-C-N	5.11	128.74	120.82
5	E	133	ALA	C-N-CA	5.11	128.74	120.82
5	E	274	GLU	CA-C-O	-5.11	115.00	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	74	ILE	CB-CG1-CD1	5.11	124.53	113.80
8	G	125	LEU	CA-C-N	5.11	127.54	120.29
8	G	125	LEU	C-N-CA	5.11	127.54	120.29
12	O	505	ILE	CB-CA-C	-5.11	102.91	111.29
4	D	37	SER	N-CA-C	-5.11	101.61	109.52
6	F	176	ASN	CA-CB-CG	5.11	117.71	112.60
7	H	103	GLN	N-CA-C	5.11	119.69	112.75
2	B	34	ASN	N-CA-C	-5.10	105.72	111.28
1	A	273	ALA	O-C-N	5.10	129.12	122.89
3	C	342	ILE	CB-CA-C	-5.10	105.18	112.22
4	D	376	SER	CA-C-O	5.10	126.18	120.82
5	E	279	GLN	CB-CA-C	-5.10	102.87	110.88
4	D	292	THR	CA-C-O	5.09	126.83	121.33
5	E	174	ARG	N-CA-C	5.09	117.57	111.71
12	O	528	ALA	CA-C-N	5.09	131.56	122.13
12	O	528	ALA	C-N-CA	5.09	131.56	122.13
10	P	68	ARG	CA-C-O	-5.09	115.60	120.64
12	O	211	PHE	CA-C-N	5.09	127.36	120.44
12	O	211	PHE	C-N-CA	5.09	127.36	120.44
2	B	41	ALA	CA-C-N	5.09	129.22	120.72
2	B	41	ALA	C-N-CA	5.09	129.22	120.72
4	D	376	SER	CA-C-N	5.09	127.06	120.44
4	D	376	SER	C-N-CA	5.09	127.06	120.44
1	A	142	LEU	N-CA-C	-5.09	105.73	111.28
3	C	254	LYS	CA-C-O	-5.09	113.74	118.73
4	D	308	ASN	N-CA-CB	5.09	117.69	110.16
1	A	241	GLN	OE1-CD-NE2	5.09	127.69	122.60
10	P	60	CYS	CA-C-N	5.09	129.65	122.63
10	P	60	CYS	C-N-CA	5.09	129.65	122.63
11	Q	25	ASP	N-CA-C	-5.09	106.66	112.92
2	B	421	TYR	CA-C-O	-5.08	115.03	120.42
4	D	317	ASN	CB-CA-C	-5.08	102.80	110.83
6	F	111	GLN	CA-C-N	-5.08	112.58	120.31
6	F	111	GLN	C-N-CA	-5.08	112.58	120.31
8	G	160	ARG	CA-C-N	5.08	131.25	121.54
8	G	160	ARG	C-N-CA	5.08	131.25	121.54
8	G	185	LEU	CA-C-O	-5.08	115.16	120.55
10	P	75	VAL	N-CA-CB	5.08	118.25	111.64
12	O	227	LEU	CA-C-N	5.08	127.35	120.44
12	O	227	LEU	C-N-CA	5.08	127.35	120.44
12	O	501	ILE	CB-CA-C	5.08	119.63	111.29
12	O	510	TYR	N-CA-CB	5.08	119.08	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	577	VAL	O-C-N	-5.08	117.40	123.04
2	B	330	LEU	CA-C-N	5.08	127.35	120.44
2	B	330	LEU	C-N-CA	5.08	127.35	120.44
2	B	426	LYS	CB-CG-CD	5.08	122.99	111.30
5	E	163	GLU	N-CA-C	5.08	121.04	109.81
8	G	96	LEU	N-CA-C	5.08	116.90	111.36
12	O	213	THR	CA-C-N	5.08	127.50	120.29
12	O	213	THR	C-N-CA	5.08	127.50	120.29
12	O	317	ASN	OD1-CG-ND2	5.08	127.68	122.60
1	A	197	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
11	Q	111	ASP	CA-C-O	5.08	127.44	121.40
5	E	117	MET	N-CA-CB	5.08	117.37	110.01
8	G	90	THR	CA-C-N	5.08	127.08	120.28
8	G	90	THR	C-N-CA	5.08	127.08	120.28
12	O	255	HIS	ND1-CG-CD2	-5.08	101.03	106.10
12	O	262	VAL	CA-C-O	-5.08	115.79	121.17
2	B	373	PHE	N-CA-CB	5.07	117.43	110.07
3	C	118	LEU	CA-C-N	5.07	128.02	120.31
3	C	118	LEU	C-N-CA	5.07	128.02	120.31
12	O	597	LYS	CA-C-N	5.07	127.08	120.28
12	O	597	LYS	C-N-CA	5.07	127.08	120.28
1	A	165	HIS	ND1-CE1-NE2	5.07	113.47	108.40
6	F	134	SER	O-C-N	5.07	128.51	122.27
6	F	305	PHE	CB-CA-C	-5.07	102.89	110.90
8	G	104	LEU	CA-C-N	5.07	127.58	120.28
8	G	104	LEU	C-N-CA	5.07	127.58	120.28
10	P	29	ARG	N-CA-CB	5.07	117.67	110.16
12	O	630	GLU	CB-CG-CD	-5.07	103.98	112.60
2	B	141	ASP	N-CA-C	-5.07	100.00	110.80
5	E	226	VAL	N-CA-C	5.07	115.78	108.48
6	F	188	TYR	CA-C-N	5.07	130.47	122.36
6	F	188	TYR	C-N-CA	5.07	130.47	122.36
8	G	74	THR	CA-C-N	5.07	126.42	120.09
8	G	74	THR	C-N-CA	5.07	126.42	120.09
6	F	253	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	463	GLN	N-CA-C	5.06	118.23	111.24
12	O	167	ILE	CA-C-O	-5.06	115.48	120.85
12	O	447	LEU	O-C-N	-5.06	115.64	122.22
3	C	151	LEU	O-C-N	5.06	127.56	122.09
8	G	211	ALA	CA-C-N	5.06	129.17	120.72
8	G	211	ALA	C-N-CA	5.06	129.17	120.72
1	A	269	CYS	CB-CA-C	-5.06	102.25	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	120	TYR	CA-C-N	5.06	127.60	120.42
5	E	120	TYR	C-N-CA	5.06	127.60	120.42
8	G	156	PHE	CA-CB-CG	5.06	118.86	113.80
2	B	222	LEU	N-CA-CB	5.05	118.00	110.22
12	O	4	LYS	CB-CA-C	-5.05	101.27	109.56
12	O	513	GLN	OE1-CD-NE2	5.05	127.66	122.60
2	B	171	ILE	CB-CG1-CD1	-5.05	103.19	113.80
7	H	130	ALA	CA-C-N	5.05	127.55	120.28
7	H	130	ALA	C-N-CA	5.05	127.55	120.28
12	O	46	CYS	CB-CA-C	-5.05	102.26	110.85
5	E	327	LEU	CB-CA-C	-5.05	102.95	110.88
6	F	58	MET	CB-CA-C	-5.05	102.27	110.85
12	O	192	GLU	N-CA-CB	5.05	120.33	111.55
3	C	283	SER	N-CA-C	5.05	117.17	111.11
6	F	314	ASP	CA-C-N	5.05	130.31	122.49
6	F	314	ASP	C-N-CA	5.05	130.31	122.49
1	A	96	ARG	NE-CZ-NH1	5.04	126.55	121.50
6	F	294	THR	CA-CB-OG1	5.04	117.17	109.60
13	R	104	GLN	CB-CG-CD	-5.04	104.03	112.60
6	F	165	VAL	CA-C-O	5.04	125.82	120.48
3	C	54	HIS	CB-CA-C	-5.04	102.42	110.79
4	D	277	GLN	O-C-N	-5.04	116.41	122.15
4	D	379	PHE	CA-C-N	5.04	127.03	120.28
4	D	379	PHE	C-N-CA	5.04	127.03	120.28
8	G	92	GLN	CA-C-N	5.04	127.45	120.29
8	G	92	GLN	C-N-CA	5.04	127.45	120.29
12	O	544	TYR	CA-C-N	5.04	128.66	120.60
12	O	544	TYR	C-N-CA	5.04	128.66	120.60
1	A	337	LYS	CA-C-N	5.04	127.28	120.38
1	A	337	LYS	C-N-CA	5.04	127.28	120.38
1	A	363	ARG	CA-C-N	5.04	127.03	120.28
1	A	363	ARG	C-N-CA	5.04	127.03	120.28
5	E	99	PRO	CA-C-N	5.04	129.48	122.23
5	E	99	PRO	C-N-CA	5.04	129.48	122.23
12	O	500	VAL	N-CA-C	-5.04	107.94	113.43
1	A	278	CYS	N-CA-CB	5.03	119.00	110.49
4	D	115	GLU	CB-CG-CD	-5.03	104.04	112.60
4	D	231	HIS	CG-CD2-NE2	5.03	112.23	107.20
6	F	281	ASP	CA-CB-CG	-5.03	107.57	112.60
7	H	117	ALA	CA-C-N	5.03	127.44	120.29
7	H	117	ALA	C-N-CA	5.03	127.44	120.29
8	G	33	GLN	CA-C-O	-5.03	115.52	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	142	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	A	346	ASP	CA-C-O	5.03	125.75	120.42
3	C	337	TYR	CA-C-O	-5.03	115.09	120.42
12	O	259	TYR	N-CA-C	-5.03	105.07	111.11
12	O	277	PHE	N-CA-CB	5.03	117.36	110.07
12	O	603	THR	N-CA-C	5.03	117.66	111.82
3	C	348	PHE	CB-CA-C	5.03	118.83	110.74
4	D	9	LEU	N-CA-C	5.03	116.76	111.28
5	E	292	HIS	CA-CB-CG	5.03	118.83	113.80
6	F	223	ALA	N-CA-CB	5.03	117.51	110.12
8	G	66	LEU	CA-C-N	5.03	127.43	120.29
8	G	66	LEU	C-N-CA	5.03	127.43	120.29
11	Q	25	ASP	CB-CA-C	5.03	119.06	110.56
12	O	230	SER	N-CA-CB	5.03	118.06	110.42
12	O	434	PHE	CA-C-O	5.03	125.88	120.70
12	O	644	PHE	N-CA-CB	5.03	117.36	109.97
2	B	169	GLN	CA-C-N	5.03	127.43	120.29
2	B	169	GLN	C-N-CA	5.03	127.43	120.29
12	O	543	PHE	CA-C-O	5.02	125.88	120.55
12	O	94	TYR	N-CA-CB	5.02	117.59	110.16
12	O	135	PRO	N-CA-CB	5.02	108.11	103.39
7	H	111	ASP	N-CA-CB	5.02	117.59	110.16
12	O	555	TRP	CD2-CE2-CZ2	-5.02	117.38	122.40
1	A	425	TYR	N-CA-C	-5.02	102.46	109.69
3	C	5	LEU	CB-CA-C	-5.02	102.46	110.79
3	C	16	SER	N-CA-C	-5.02	106.84	113.17
3	C	160	PRO	N-CD-CG	5.02	110.73	103.20
12	O	401	LYS	CA-C-O	5.02	126.78	121.16
12	O	675	ASP	CA-CB-CG	-5.02	107.58	112.60
4	D	191	TYR	CA-C-O	-5.02	115.55	120.82
2	B	424	LEU	CA-C-O	-5.01	115.23	120.55
5	E	117	MET	CB-CA-C	-5.01	103.01	110.88
12	O	190	HIS	CB-CA-C	-5.01	102.33	110.85
5	E	234	ASP	CA-C-N	5.01	126.96	120.44
5	E	234	ASP	C-N-CA	5.01	126.96	120.44
1	A	367	THR	N-CA-C	-5.01	105.71	111.07
4	D	125	GLN	CB-CG-CD	-5.01	104.08	112.60
4	D	130	ILE	CA-C-O	-5.01	116.19	119.15
7	H	157	SER	N-CA-C	-5.01	101.58	109.50
6	F	272	THR	N-CA-CB	5.01	117.40	110.04
3	C	325	ARG	NE-CZ-NH1	5.01	126.51	121.50
3	C	338	VAL	CA-C-O	-5.01	115.06	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	276	LYS	N-CA-CB	5.01	117.27	110.01
12	O	352	GLN	CG-CD-NE2	-5.01	108.89	116.40
12	O	447	LEU	N-CA-C	-5.01	105.90	112.41
1	A	469	PRO	N-CA-CB	5.00	108.51	103.00
3	C	166	MET	CA-C-N	5.00	130.84	122.73
3	C	166	MET	C-N-CA	5.00	130.84	122.73
6	F	44	HIS	CG-CD2-NE2	5.00	112.20	107.20
6	F	112	PHE	CA-C-N	5.00	128.61	120.60
6	F	112	PHE	C-N-CA	5.00	128.61	120.60
12	O	403	ALA	N-CA-C	5.00	116.73	111.28
7	H	46	LEU	CA-C-N	5.00	129.07	120.72
7	H	46	LEU	C-N-CA	5.00	129.07	120.72

There are no chirality outliers.

All (102) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ARG	Sidechain
1	A	152	TYR	Sidechain
1	A	187	ARG	Sidechain
1	A	221	TYR	Sidechain
1	A	238	ARG	Sidechain
1	A	263	TYR	Sidechain
1	A	363	ARG	Sidechain
1	A	370	ARG	Sidechain
1	A	425	TYR	Peptide
1	A	432	ARG	Sidechain
1	A	449	ARG	Sidechain
1	A	66	HIS	Sidechain
2	B	118	TYR	Sidechain
2	B	146	ARG	Sidechain
2	B	162	ARG	Sidechain
2	B	165	TYR	Sidechain
2	B	180	GLN	Peptide
2	B	218	TYR	Sidechain
2	B	259	PHE	Sidechain
2	B	279	TYR	Sidechain
2	B	342	PHE	Sidechain
2	B	352	ARG	Sidechain
2	B	36	TYR	Sidechain
2	B	410	GLU	Peptide,Mainchain
2	B	416	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	83	THR	Mainchain
3	C	114	ARG	Sidechain
3	C	119	ARG	Sidechain
3	C	185	TYR	Sidechain
3	C	224	TYR	Sidechain
3	C	276	ARG	Sidechain
3	C	337	TYR	Sidechain
4	D	114	TYR	Sidechain
4	D	155	TYR	Sidechain
4	D	187	TYR	Sidechain
4	D	198	ARG	Sidechain
4	D	242	ARG	Sidechain
4	D	250	PHE	Sidechain
4	D	299	ILE	Peptide
4	D	300	LEU	Mainchain
4	D	85	TYR	Sidechain
4	D	95	ARG	Sidechain
5	E	114	TYR	Sidechain
5	E	116	TYR	Sidechain
5	E	143	TYR	Sidechain
5	E	189	TYR	Sidechain
5	E	193	TYR	Sidechain
5	E	222	TYR	Sidechain
5	E	229	PHE	Sidechain
5	E	261	TYR	Sidechain
5	E	282	ARG	Sidechain
5	E	54	TYR	Sidechain
6	F	104	TYR	Sidechain
6	F	205	ARG	Sidechain
6	F	212	GLY	Peptide
6	F	313	TYR	Sidechain
6	F	43	LEU	Mainchain
6	F	44	HIS	Peptide
6	F	59	ARG	Sidechain
8	G	123	ARG	Sidechain
8	G	137	TYR	Sidechain
8	G	15	PHE	Sidechain
8	G	160	ARG	Sidechain,Peptide
8	G	163	ARG	Sidechain
8	G	204	ARG	Sidechain
8	G	41	TYR	Sidechain
8	G	72	TYR	Sidechain

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Mol	Chain	Res	Type	Group
7	H	125	TYR	Sidechain
7	H	37	TYR	Sidechain
7	H	44	TYR	Sidechain
7	H	55	TYR	Sidechain
7	H	59	ARG	Sidechain
7	H	80	ARG	Sidechain
7	H	90	TYR	Sidechain
12	O	125	TYR	Sidechain
12	O	127	TYR	Sidechain
12	O	152	VAL	Peptide
12	O	165	ARG	Sidechain
12	O	207	PHE	Sidechain
12	O	219	TYR	Sidechain
12	O	253	TYR	Sidechain
12	O	364	PHE	Sidechain
12	O	38	ARG	Sidechain
12	O	382	LYS	Peptide
12	O	414	ARG	Sidechain
12	O	422	PHE	Sidechain
12	O	467	TYR	Sidechain
12	O	469	PHE	Sidechain
12	O	544	TYR	Sidechain
12	O	573	TYR	Sidechain
12	O	64	PHE	Sidechain
10	P	43	ARG	Sidechain
10	P	8	ARG	Sidechain
11	Q	18	TYR	Sidechain
11	Q	33	ARG	Sidechain
11	Q	76	TYR	Sidechain
11	Q	77	PHE	Sidechain
11	Q	83	TYR	Sidechain
13	R	25	LYS	Peptide
13	R	35	TRP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3450	0	3482	3	0
2	B	3386	0	3424	38	0
3	C	3205	0	3225	16	0
4	D	3251	0	3253	14	0
5	E	2472	0	2444	78	0
6	F	2280	0	2263	41	0
7	H	1340	0	1324	2	0
8	G	1645	0	1667	4	0
9	V	1308	0	1299	329	0
10	P	921	0	908	92	0
11	Q	873	0	845	91	0
12	O	6090	0	6071	183	0
13	R	746	0	705	29	0
14	N	591	0	616	48	0
All	All	31558	0	31526	660	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 10.

All (660) 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)
9:V:178:LEU:CD2	10:P:103:MET:HG3	1.06	1.53
9:V:178:LEU:CD1	10:P:103:MET:HE3	1.32	1.53
9:V:171:LYS:NZ	10:P:106:GLN:CB	1.70	1.52
9:V:178:LEU:CD2	10:P:103:MET:CG	1.75	1.50
9:V:178:LEU:HD21	10:P:103:MET:CG	1.27	1.50
9:V:178:LEU:HD13	10:P:103:MET:CE	1.32	1.50
9:V:171:LYS:NZ	10:P:106:GLN:HB3	1.19	1.47
9:V:178:LEU:HD21	10:P:103:MET:CB	1.43	1.46
9:V:174:ASN:HB3	10:P:102:VAL:CA	1.48	1.42
9:V:178:LEU:CG	10:P:103:MET:HG3	1.49	1.40
9:V:180:ILE:CG1	11:Q:101:LEU:HD23	1.13	1.40
9:V:180:ILE:N	11:Q:101:LEU:HD22	1.38	1.36
12:O:612:LYS:HB3	12:O:657:MET:CE	1.57	1.34
9:V:180:ILE:HG12	11:Q:101:LEU:CD2	1.22	1.32
5:E:203:TYR:CG	5:E:309:LYS:HA	1.63	1.30
12:O:654:THR:HG1	12:O:655:THR:N	1.28	1.28
9:V:182:ARG:H	12:O:5:PRO:CD	1.44	1.28
9:V:178:LEU:HA	10:P:100:PRO:CG	1.62	1.28
12:O:370:LYS:HG3	14:N:32:GLU:O	1.18	1.27
9:V:163:LEU:CD2	11:Q:104:LEU:CD1	2.14	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:163:LEU:CD2	11:Q:104:LEU:HD11	1.64	1.24
9:V:163:LEU:CD2	11:Q:104:LEU:CD2	2.16	1.24
2:B:294:PHE:HA	13:R:106:TYR:CG	1.73	1.24
9:V:163:LEU:CD2	11:Q:104:LEU:HD21	1.67	1.23
9:V:174:ASN:CB	10:P:102:VAL:O	1.87	1.22
9:V:159:LYS:HD3	11:Q:104:LEU:CD1	1.68	1.22
9:V:171:LYS:CE	10:P:106:GLN:HB3	1.73	1.19
12:O:389:GLU:OE2	12:O:665:MET:HB3	1.04	1.19
9:V:174:ASN:HB2	10:P:102:VAL:O	1.35	1.18
12:O:654:THR:OG1	12:O:655:THR:N	1.77	1.18
9:V:159:LYS:HD3	11:Q:104:LEU:HD12	1.21	1.16
9:V:181:VAL:HG21	12:O:3:LEU:HB3	1.23	1.15
5:E:115:GLU:HG3	12:O:693:VAL:HB	1.16	1.15
12:O:680:LEU:HD21	12:O:718:ILE:HA	1.18	1.15
12:O:612:LYS:CB	12:O:657:MET:HE2	1.77	1.13
12:O:389:GLU:OE2	12:O:665:MET:CB	1.97	1.13
9:V:163:LEU:HD21	11:Q:104:LEU:HD11	1.20	1.12
9:V:142:VAL:HG23	9:V:144:GLY:H	1.10	1.12
9:V:174:ASN:HB3	10:P:102:VAL:HA	1.16	1.12
12:O:654:THR:C	12:O:655:THR:HB	1.72	1.12
12:O:685:VAL:HG12	12:O:689:LYS:HE3	1.29	1.12
9:V:174:ASN:HB3	10:P:102:VAL:C	1.75	1.11
12:O:370:LYS:CG	14:N:32:GLU:O	1.96	1.11
9:V:182:ARG:N	12:O:5:PRO:HD3	1.40	1.11
9:V:178:LEU:HA	10:P:100:PRO:HG2	1.29	1.11
9:V:163:LEU:HD21	11:Q:104:LEU:HD21	1.33	1.10
9:V:178:LEU:CD1	10:P:103:MET:HG3	1.80	1.10
2:B:294:PHE:CA	13:R:106:TYR:CZ	2.34	1.10
9:V:171:LYS:CD	10:P:106:GLN:HB3	1.82	1.09
9:V:170:VAL:HG21	10:P:103:MET:HG2	1.26	1.09
9:V:178:LEU:CD1	10:P:103:MET:CG	2.31	1.08
12:O:654:THR:C	12:O:655:THR:CB	2.24	1.08
5:E:203:TYR:CZ	5:E:309:LYS:CA	2.37	1.08
12:O:702:GLU:OE2	14:N:74:ARG:HD3	1.53	1.08
5:E:203:TYR:CD1	5:E:309:LYS:CA	2.37	1.08
2:B:294:PHE:CA	13:R:106:TYR:CD1	2.37	1.07
5:E:203:TYR:CD2	5:E:309:LYS:CA	2.38	1.07
2:B:294:PHE:HA	13:R:106:TYR:CD2	1.90	1.06
12:O:370:LYS:HG2	14:N:33:LYS:HA	1.10	1.06
5:E:203:TYR:CE2	5:E:309:LYS:CA	2.39	1.06
12:O:654:THR:CA	12:O:655:THR:HB	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:681:GLN:HG3	12:O:725:LEU:HD21	1.10	1.06
2:B:294:PHE:CA	13:R:106:TYR:CE2	2.39	1.05
2:B:294:PHE:C	13:R:106:TYR:CE1	2.34	1.05
9:V:163:LEU:HD21	11:Q:104:LEU:CD1	1.81	1.05
9:V:178:LEU:HD22	10:P:103:MET:CG	1.78	1.05
5:E:203:TYR:CG	5:E:309:LYS:CA	2.40	1.05
12:O:316:GLN:CD	14:N:32:GLU:OE1	2.00	1.04
5:E:203:TYR:CE1	5:E:309:LYS:CA	2.40	1.04
2:B:294:PHE:CA	13:R:106:TYR:CE1	2.41	1.04
2:B:294:PHE:CA	13:R:106:TYR:CG	2.41	1.04
2:B:294:PHE:CA	13:R:106:TYR:CD2	2.41	1.03
12:O:688:MET:HG3	12:O:731:ILE:HD13	1.38	1.03
5:E:203:TYR:CE1	5:E:309:LYS:CB	2.42	1.02
5:E:203:TYR:CE2	5:E:309:LYS:CB	2.43	1.02
5:E:115:GLU:HG3	12:O:693:VAL:CB	1.89	1.02
9:V:171:LYS:NZ	10:P:106:GLN:HB2	1.71	1.02
9:V:178:LEU:CB	11:Q:101:LEU:HD21	1.90	1.01
2:B:294:PHE:C	13:R:106:TYR:CG	2.39	1.01
2:B:294:PHE:C	13:R:106:TYR:CZ	2.39	1.01
9:V:178:LEU:CD1	10:P:103:MET:CE	2.09	1.01
9:V:178:LEU:HB3	11:Q:101:LEU:HD21	1.42	1.01
5:E:203:TYR:CZ	5:E:309:LYS:CB	2.44	1.01
9:V:159:LYS:NZ	11:Q:108:ASN:HB2	1.75	1.00
12:O:717:MET:HA	12:O:717:MET:HE2	1.44	1.00
5:E:203:TYR:CG	5:E:309:LYS:CB	2.45	1.00
2:B:294:PHE:C	13:R:106:TYR:CD2	2.40	1.00
2:B:294:PHE:C	13:R:106:TYR:CE2	2.40	1.00
9:V:163:LEU:CG	11:Q:104:LEU:HD11	1.92	0.99
9:V:178:LEU:HD21	10:P:103:MET:CA	1.92	0.99
5:E:203:TYR:CD1	5:E:309:LYS:CB	2.45	0.99
2:B:294:PHE:C	13:R:106:TYR:CD1	2.41	0.99
5:E:203:TYR:CD2	5:E:309:LYS:CB	2.46	0.98
9:V:181:VAL:HG21	12:O:3:LEU:CB	1.93	0.98
9:V:178:LEU:CD2	10:P:103:MET:CB	2.18	0.97
9:V:162:CYS:SG	11:Q:95:ILE:HD13	2.03	0.97
9:V:181:VAL:HA	12:O:4:LYS:HA	1.47	0.97
9:V:184:LEU:HD21	11:Q:105:MET:N	1.79	0.97
9:V:163:LEU:HD21	11:Q:104:LEU:CD2	1.89	0.97
9:V:163:LEU:HD23	11:Q:104:LEU:CD2	1.90	0.97
9:V:178:LEU:HD23	10:P:100:PRO:HG2	1.46	0.96
9:V:179:ASP:H	10:P:100:PRO:HG3	1.25	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:203:TYR:CD2	5:E:309:LYS:HA	2.00	0.95
9:V:174:ASN:CB	10:P:102:VAL:HA	1.95	0.95
9:V:159:LYS:CD	11:Q:104:LEU:HD12	1.97	0.94
9:V:174:ASN:CB	10:P:102:VAL:CA	2.45	0.94
9:V:175:TYR:C	10:P:102:VAL:HG11	1.90	0.94
9:V:177:ARG:O	10:P:100:PRO:HB2	1.67	0.94
9:V:178:LEU:HD11	10:P:103:MET:CG	1.96	0.93
9:V:179:ASP:N	10:P:100:PRO:HG3	1.82	0.93
12:O:370:LYS:CG	14:N:33:LYS:HA	1.97	0.93
9:V:177:ARG:HB3	10:P:102:VAL:H	1.33	0.93
5:E:115:GLU:CG	12:O:693:VAL:HB	1.99	0.92
12:O:612:LYS:CB	12:O:657:MET:CE	2.43	0.92
9:V:74:VAL:HG22	9:V:147:ILE:CG2	1.99	0.92
9:V:181:VAL:HG22	12:O:4:LYS:N	1.84	0.92
9:V:171:LYS:NZ	10:P:106:GLN:CG	2.33	0.92
9:V:177:ARG:HB2	10:P:102:VAL:CA	1.65	0.92
9:V:181:VAL:CG1	12:O:3:LEU:O	2.17	0.92
9:V:178:LEU:HA	10:P:100:PRO:HG3	1.49	0.91
12:O:660:ASP:HA	12:O:663:GLN:HG2	1.49	0.91
12:O:680:LEU:CD2	12:O:718:ILE:HA	2.00	0.91
12:O:370:LYS:HG2	14:N:33:LYS:CA	1.99	0.91
9:V:171:LYS:NZ	10:P:106:GLN:CD	2.29	0.90
9:V:163:LEU:HD23	11:Q:104:LEU:CD1	2.01	0.90
9:V:159:LYS:HZ1	11:Q:108:ASN:CB	1.85	0.89
9:V:178:LEU:CD2	10:P:103:MET:HB2	2.03	0.89
9:V:163:LEU:HD21	11:Q:104:LEU:CG	2.03	0.88
12:O:694:LEU:HD13	14:N:74:ARG:NH1	1.86	0.88
9:V:178:LEU:HD11	10:P:103:MET:HG2	1.56	0.87
9:V:180:ILE:N	11:Q:101:LEU:CD2	2.33	0.87
9:V:159:LYS:CD	11:Q:104:LEU:CD1	2.50	0.87
9:V:159:LYS:HZ1	11:Q:108:ASN:HB2	1.34	0.86
9:V:159:LYS:HD3	11:Q:104:LEU:HD11	1.53	0.86
9:V:184:LEU:HD23	11:Q:104:LEU:HD23	1.55	0.86
9:V:163:LEU:CD2	11:Q:104:LEU:CG	2.52	0.86
12:O:680:LEU:HD23	12:O:721:CYS:SG	2.14	0.86
12:O:681:GLN:CG	12:O:725:LEU:HD21	2.03	0.86
9:V:142:VAL:HG23	9:V:144:GLY:N	1.91	0.86
9:V:112:TYR:HB2	9:V:115:HIS:CE1	2.11	0.85
9:V:181:VAL:CG2	12:O:3:LEU:CB	2.53	0.85
9:V:181:VAL:HG11	12:O:3:LEU:O	1.75	0.85
9:V:180:ILE:CA	11:Q:101:LEU:HD22	1.96	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:180:ILE:CD1	11:Q:101:LEU:HD23	2.07	0.84
9:V:177:ARG:CB	10:P:102:VAL:N	2.40	0.84
9:V:159:LYS:NZ	11:Q:108:ASN:CB	2.39	0.84
12:O:316:GLN:NE2	14:N:32:GLU:OE1	2.11	0.83
9:V:76:PHE:CE2	9:V:109:ILE:HG12	2.13	0.83
9:V:203:GLN:O	9:V:206:ILE:HG13	1.79	0.83
9:V:178:LEU:HD22	10:P:103:MET:SD	2.19	0.83
9:V:108:ARG:C	9:V:109:ILE:HD12	2.04	0.83
5:E:203:TYR:CD1	5:E:309:LYS:HA	2.08	0.82
9:V:163:LEU:HG	11:Q:104:LEU:CD1	2.09	0.82
9:V:178:LEU:CA	10:P:100:PRO:CG	2.52	0.81
12:O:654:THR:HA	12:O:655:THR:HB	1.60	0.81
5:E:106:ARG:NH1	14:N:76:GLY:C	2.38	0.81
9:V:180:ILE:HD13	11:Q:101:LEU:HG	1.63	0.80
9:V:159:LYS:NZ	11:Q:108:ASN:CG	2.38	0.80
9:V:179:ASP:C	11:Q:101:LEU:HD22	2.05	0.80
12:O:681:GLN:HG3	12:O:725:LEU:CD2	2.04	0.80
12:O:702:GLU:CD	14:N:74:ARG:HD3	2.05	0.80
9:V:102:PRO:O	9:V:105:THR:HG22	1.81	0.80
12:O:688:MET:HG3	12:O:731:ILE:CD1	2.11	0.80
9:V:87:VAL:HB	9:V:118:LEU:CD1	2.12	0.80
9:V:90:ASN:HD21	9:V:92:ASP:HB2	1.44	0.79
9:V:163:LEU:CG	11:Q:104:LEU:CD1	2.57	0.79
9:V:178:LEU:HD13	10:P:103:MET:SD	2.21	0.79
12:O:612:LYS:HB3	12:O:657:MET:HE2	0.84	0.79
12:O:680:LEU:HD11	12:O:703:VAL:HG11	1.65	0.79
9:V:115:HIS:O	9:V:137:VAL:HG23	1.83	0.79
12:O:654:THR:C	12:O:655:THR:OG1	2.26	0.79
5:E:203:TYR:CD1	5:E:309:LYS:HB2	2.16	0.78
9:V:162:CYS:SG	11:Q:95:ILE:CD1	2.70	0.78
9:V:181:VAL:CG2	12:O:3:LEU:HB3	2.06	0.78
12:O:370:LYS:NZ	14:N:32:GLU:C	2.40	0.78
12:O:316:GLN:CG	14:N:32:GLU:OE1	2.32	0.78
9:V:178:LEU:CD2	10:P:100:PRO:HG2	2.15	0.77
9:V:177:ARG:H	10:P:102:VAL:CG1	1.98	0.77
9:V:178:LEU:CA	10:P:100:PRO:HG3	2.11	0.77
12:O:680:LEU:HD11	12:O:718:ILE:HD12	1.66	0.77
12:O:657:MET:SD	12:O:660:ASP:HB3	2.25	0.77
5:E:203:TYR:CZ	5:E:309:LYS:HB3	2.19	0.77
5:E:115:GLU:HG3	12:O:693:VAL:CG1	2.15	0.76
9:V:171:LYS:CD	10:P:106:GLN:CB	2.63	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:163:LEU:HD23	11:Q:104:LEU:HD22	1.65	0.76
12:O:700:ILE:HD11	12:O:715:ILE:HD12	1.67	0.76
9:V:134:GLU:OE1	9:V:201:LEU:HD21	1.85	0.76
12:O:661:THR:HG23	12:O:662:PRO:HD3	1.68	0.75
12:O:660:ASP:HA	12:O:663:GLN:CG	2.15	0.75
4:D:240:GLN:O	4:D:303:ALA:HB2	1.87	0.75
9:V:206:ILE:HD12	9:V:207:ALA:N	2.02	0.75
9:V:163:LEU:HG	11:Q:104:LEU:HD11	1.65	0.74
9:V:181:VAL:HG13	12:O:3:LEU:O	1.87	0.74
9:V:166:VAL:HG13	10:P:103:MET:HE2	1.66	0.74
12:O:370:LYS:NZ	14:N:35:GLY:H	1.85	0.73
9:V:77:CYS:HB3	9:V:79:ARG:NH1	2.04	0.73
9:V:181:VAL:CG2	12:O:3:LEU:C	2.62	0.73
5:E:235:ARG:H	6:F:46:LEU:H	1.35	0.73
9:V:184:LEU:HD23	11:Q:104:LEU:CD2	2.18	0.73
12:O:660:ASP:CA	12:O:663:GLN:HG2	2.19	0.73
9:V:177:ARG:HB2	10:P:102:VAL:N	2.03	0.72
12:O:697:ASN:O	12:O:700:ILE:HG22	1.89	0.72
9:V:62:VAL:CG1	9:V:205:ARG:HD2	2.18	0.72
9:V:163:LEU:HD22	11:Q:104:LEU:HD21	1.68	0.72
9:V:159:LYS:HE3	11:Q:104:LEU:HG	1.71	0.72
9:V:70:GLU:OE1	9:V:140:LEU:HD21	1.90	0.72
12:O:316:GLN:HG2	14:N:32:GLU:OE1	1.90	0.72
12:O:685:VAL:O	12:O:689:LYS:HG3	1.90	0.72
9:V:130:VAL:O	9:V:133:THR:HG22	1.91	0.71
5:E:203:TYR:CE2	5:E:309:LYS:C	2.68	0.71
9:V:171:LYS:HE3	10:P:106:GLN:OE1	1.91	0.71
9:V:163:LEU:CD2	11:Q:104:LEU:HD13	2.20	0.70
9:V:172:PRO:HA	9:V:175:TYR:CE2	2.26	0.70
9:V:75:ILE:HG21	9:V:148:PHE:CE2	2.26	0.70
9:V:181:VAL:HG22	12:O:3:LEU:C	2.15	0.70
9:V:61:PRO:O	9:V:64:ARG:HD3	1.91	0.70
9:V:184:LEU:HD23	11:Q:104:LEU:CG	2.22	0.70
5:E:98:LEU:HD22	5:E:113:ALA:HB1	1.74	0.70
9:V:163:LEU:HD23	11:Q:104:LEU:CG	2.20	0.69
12:O:700:ILE:CD1	12:O:715:ILE:HD12	2.22	0.69
12:O:731:ILE:HG23	12:O:742:SER:O	1.92	0.69
2:B:295:ASP:N	13:R:106:TYR:CE2	2.61	0.69
9:V:87:VAL:HB	9:V:118:LEU:HD11	1.74	0.69
9:V:177:ARG:HB3	10:P:102:VAL:N	2.00	0.69
9:V:180:ILE:HD13	11:Q:101:LEU:CG	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:203:TYR:CE1	5:E:309:LYS:HB3	2.24	0.69
9:V:158:LEU:HD23	11:Q:76:TYR:CD1	2.27	0.69
9:V:180:ILE:H	11:Q:101:LEU:HD22	1.53	0.69
12:O:680:LEU:CD1	12:O:703:VAL:HG11	2.22	0.69
9:V:184:LEU:HD22	11:Q:101:LEU:O	1.92	0.69
9:V:63:LEU:HD13	9:V:205:ARG:CZ	2.22	0.69
2:B:294:PHE:N	13:R:106:TYR:CE2	2.60	0.69
9:V:200:ARG:O	9:V:203:GLN:HG2	1.93	0.69
9:V:162:CYS:O	9:V:165:VAL:HG12	1.92	0.68
5:E:203:TYR:CE1	5:E:309:LYS:N	2.61	0.68
12:O:654:THR:OG1	12:O:655:THR:CB	2.41	0.68
12:O:684:ILE:HB	12:O:725:LEU:HD11	1.76	0.68
9:V:177:ARG:H	10:P:102:VAL:HG11	1.60	0.67
9:V:181:VAL:HG13	12:O:4:LYS:CA	2.25	0.67
12:O:685:VAL:CG1	12:O:689:LYS:HE3	2.15	0.67
9:V:62:VAL:HG12	9:V:205:ARG:HH11	1.58	0.67
9:V:163:LEU:HD22	9:V:188:LEU:HD23	1.76	0.67
12:O:657:MET:HG2	12:O:660:ASP:H	1.60	0.67
14:N:42:ARG:HD3	14:N:72:ALA:HA	1.76	0.67
9:V:63:LEU:HD21	9:V:202:THR:HA	1.76	0.67
5:E:112:ALA:CB	14:N:76:GLY:HA2	2.24	0.67
9:V:176:ARG:N	10:P:102:VAL:HG11	2.09	0.67
9:V:142:VAL:CG2	9:V:144:GLY:H	2.00	0.66
5:E:112:ALA:HB2	14:N:76:GLY:HA2	1.76	0.66
12:O:708:ARG:NH1	14:N:40:GLN:OE1	2.26	0.66
9:V:178:LEU:HB3	11:Q:101:LEU:HD11	1.77	0.66
9:V:182:ARG:H	12:O:5:PRO:HD3	0.57	0.66
9:V:163:LEU:HD23	11:Q:104:LEU:HD13	1.77	0.65
9:V:184:LEU:HD23	11:Q:104:LEU:HB3	1.77	0.65
12:O:662:PRO:O	12:O:666:GLU:HG3	1.97	0.65
9:V:74:VAL:HG22	9:V:147:ILE:HG22	1.76	0.65
12:O:680:LEU:HD11	12:O:718:ILE:CD1	2.24	0.65
9:V:170:VAL:CG1	10:P:103:MET:HA	2.26	0.65
9:V:159:LYS:HG2	11:Q:104:LEU:O	1.96	0.64
9:V:178:LEU:HD11	10:P:103:MET:CE	2.19	0.64
9:V:78:ASN:ND2	9:V:84:VAL:HG23	2.13	0.64
5:E:237:LEU:N	6:F:44:HIS:HB2	2.13	0.63
9:V:145:GLN:HB3	9:V:146:PRO:HD2	1.80	0.63
9:V:177:ARG:O	10:P:100:PRO:CB	2.43	0.63
9:V:182:ARG:N	12:O:5:PRO:CD	2.22	0.63
12:O:694:LEU:HD23	12:O:699:LEU:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:171:LYS:CE	10:P:106:GLN:CD	2.72	0.63
5:E:106:ARG:HH12	14:N:76:GLY:C	2.06	0.62
9:V:171:LYS:HD2	10:P:106:GLN:CB	2.29	0.62
5:E:203:TYR:CG	5:E:309:LYS:HB2	2.32	0.62
9:V:63:LEU:HD13	9:V:205:ARG:NH2	2.14	0.62
9:V:80:SER:HB2	9:V:81:PRO:HD2	1.82	0.62
2:B:294:PHE:CB	13:R:106:TYR:CD1	2.83	0.62
9:V:159:LYS:CD	11:Q:104:LEU:HD11	2.25	0.62
9:V:178:LEU:HB2	11:Q:101:LEU:HD21	1.81	0.62
2:B:294:PHE:CB	13:R:106:TYR:CE1	2.82	0.61
9:V:170:VAL:CG2	10:P:103:MET:HG2	2.16	0.61
12:O:684:ILE:HB	12:O:725:LEU:CD1	2.31	0.61
12:O:744:VAL:HG12	12:O:745:ALA:O	2.00	0.61
9:V:57:GLY:O	9:V:59:PRO:HD3	1.99	0.61
9:V:167:ARG:HD3	9:V:191:HIS:CD2	2.35	0.61
9:V:174:ASN:CB	10:P:102:VAL:C	2.46	0.61
12:O:393:LYS:NZ	12:O:661:THR:OG1	2.33	0.61
12:O:654:THR:OG1	12:O:655:THR:CA	2.47	0.61
12:O:694:LEU:CD1	14:N:74:ARG:NH1	2.62	0.61
2:B:294:PHE:HB3	13:R:106:TYR:CD1	2.35	0.61
9:V:178:LEU:HD21	10:P:103:MET:N	2.15	0.61
12:O:370:LYS:NZ	14:N:31:GLU:O	2.33	0.61
9:V:77:CYS:HB3	9:V:79:ARG:HH12	1.65	0.60
9:V:170:VAL:CG2	10:P:103:MET:HA	2.30	0.60
9:V:181:VAL:CG2	12:O:3:LEU:HB2	2.29	0.60
9:V:184:LEU:HD23	11:Q:104:LEU:CB	2.31	0.60
12:O:720:LYS:O	12:O:724:VAL:HG23	2.02	0.60
9:V:166:VAL:CG2	11:Q:100:ALA:HB1	2.31	0.60
9:V:69:ARG:O	9:V:71:PRO:HD3	2.00	0.60
9:V:145:GLN:HB3	9:V:146:PRO:CD	2.31	0.60
9:V:178:LEU:CD1	10:P:103:MET:SD	2.86	0.60
5:E:138:HIS:CE1	5:E:169:VAL:HG22	2.36	0.60
9:V:135:LEU:HD11	9:V:201:LEU:HD13	1.83	0.60
9:V:158:LEU:HD13	9:V:158:LEU:O	2.02	0.59
12:O:700:ILE:HD11	12:O:715:ILE:CD1	2.32	0.59
9:V:163:LEU:O	9:V:167:ARG:HG3	2.02	0.59
12:O:370:LYS:NZ	14:N:35:GLY:N	2.50	0.59
3:C:138:LEU:HD11	3:C:184:TYR:CE2	2.38	0.59
9:V:109:ILE:HD12	9:V:109:ILE:N	2.16	0.59
9:V:78:ASN:HD21	9:V:84:VAL:HG23	1.67	0.59
9:V:121:ASP:HB2	9:V:126:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:178:LEU:C	11:Q:101:LEU:HD21	2.28	0.59
9:V:171:LYS:HD3	10:P:106:GLN:HB3	1.82	0.59
12:O:500:VAL:HG21	12:O:539:MET:HE2	1.83	0.59
9:V:178:LEU:HD21	10:P:103:MET:HG3	0.95	0.59
12:O:680:LEU:HD21	12:O:718:ILE:CA	2.13	0.59
9:V:153:LEU:HD11	9:V:156:TYR:HE2	1.68	0.59
9:V:130:VAL:HG11	9:V:136:PHE:HB2	1.83	0.58
9:V:85:LEU:C	9:V:85:LEU:HD13	2.28	0.58
14:N:3:ILE:HG12	14:N:17:ILE:HD13	1.84	0.58
4:D:243:SER:HB2	4:D:303:ALA:HB3	1.85	0.58
9:V:90:ASN:ND2	9:V:92:ASP:H	2.01	0.58
9:V:159:LYS:HZ2	11:Q:108:ASN:CG	2.09	0.58
9:V:181:VAL:CA	12:O:4:LYS:HA	2.28	0.58
9:V:102:PRO:HD2	9:V:105:THR:HG21	1.85	0.58
9:V:178:LEU:C	10:P:100:PRO:HG3	2.27	0.58
9:V:184:LEU:CD2	11:Q:101:LEU:O	2.51	0.58
9:V:170:VAL:CG1	10:P:102:VAL:O	2.51	0.58
12:O:656:SER:HB2	12:O:660:ASP:OD2	2.03	0.58
5:E:63:LEU:HD22	6:F:46:LEU:HD13	1.85	0.58
9:V:184:LEU:CD2	11:Q:104:LEU:HB3	2.33	0.58
5:E:235:ARG:H	6:F:46:LEU:N	2.00	0.58
9:V:181:VAL:CG1	12:O:3:LEU:C	2.77	0.58
12:O:696:HIS:HB2	12:O:739:ASP:HB3	1.86	0.58
9:V:178:LEU:HB3	11:Q:101:LEU:CD2	2.27	0.57
6:F:230:MET:HE3	6:F:230:MET:HA	1.85	0.57
12:O:647:LYS:H	12:O:647:LYS:HD2	1.70	0.57
2:B:30:VAL:HG23	2:B:31:ASP:H	1.70	0.57
12:O:21:ILE:HD11	12:O:101:MET:HE3	1.86	0.57
9:V:80:SER:O	9:V:103:PRO:HB3	2.04	0.57
5:E:232:SER:HA	6:F:45:PRO:HB3	1.86	0.57
9:V:90:ASN:HD21	9:V:92:ASP:CB	2.16	0.56
9:V:159:LYS:HZ2	11:Q:108:ASN:CB	2.18	0.56
9:V:159:LYS:CE	11:Q:104:LEU:CD1	2.82	0.56
4:D:243:SER:CA	4:D:303:ALA:HB3	2.35	0.56
9:V:158:LEU:HD23	11:Q:76:TYR:CG	2.39	0.56
12:O:661:THR:CG2	12:O:662:PRO:HD3	2.35	0.56
5:E:203:TYR:CD2	5:E:309:LYS:CG	2.88	0.56
9:V:121:ASP:HB3	9:V:124:THR:OG1	2.05	0.56
9:V:178:LEU:CD2	10:P:103:MET:N	2.68	0.56
12:O:660:ASP:O	12:O:663:GLN:HG2	2.04	0.56
9:V:70:GLU:CD	9:V:113:ARG:HE	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:130:VAL:O	9:V:130:VAL:HG13	2.06	0.56
12:O:694:LEU:HD23	12:O:699:LEU:CA	2.35	0.56
4:D:316:TYR:HB2	4:D:365:GLU:HA	1.87	0.56
9:V:118:LEU:HD12	9:V:118:LEU:C	2.29	0.56
14:N:55:THR:OG1	14:N:58:ASP:OD1	2.23	0.56
9:V:144:GLY:O	9:V:145:GLN:HB2	2.06	0.56
9:V:170:VAL:HG13	10:P:102:VAL:O	2.06	0.56
5:E:233:LEU:O	6:F:44:HIS:CD2	2.59	0.56
9:V:184:LEU:HD21	11:Q:105:MET:H	1.65	0.56
9:V:206:ILE:HD12	9:V:206:ILE:C	2.30	0.55
12:O:723:GLU:O	12:O:726:ILE:HG12	2.06	0.55
12:O:685:VAL:HG12	12:O:689:LYS:CE	2.20	0.55
2:B:294:PHE:N	13:R:106:TYR:CZ	2.73	0.55
4:D:243:SER:H	4:D:303:ALA:H	1.53	0.55
5:E:106:ARG:NH1	14:N:76:GLY:H	2.04	0.55
9:V:159:LYS:HZ1	11:Q:108:ASN:CG	2.09	0.55
9:V:177:ARG:NE	10:P:102:VAL:N	2.54	0.55
12:O:660:ASP:C	12:O:663:GLN:HG2	2.31	0.55
12:O:694:LEU:HG	12:O:698:ALA:HB3	1.88	0.55
5:E:234:ASP:HA	6:F:44:HIS:CE1	2.42	0.55
9:V:155:VAL:HG23	9:V:155:VAL:O	2.06	0.55
9:V:166:VAL:HG22	11:Q:100:ALA:HB1	1.86	0.55
14:N:11:LYS:HG3	14:N:12:GLU:H	1.71	0.55
12:O:660:ASP:HA	12:O:663:GLN:CD	2.31	0.55
9:V:75:ILE:O	9:V:75:ILE:HG23	2.06	0.54
9:V:181:VAL:HG13	12:O:4:LYS:HA	1.89	0.54
4:D:316:TYR:HB2	4:D:365:GLU:H	1.72	0.54
5:E:237:LEU:HD22	6:F:190:LEU:HA	1.90	0.54
9:V:159:LYS:HG3	11:Q:108:ASN:HB2	1.88	0.54
9:V:181:VAL:HG13	12:O:3:LEU:C	2.32	0.54
14:N:5:VAL:HG22	14:N:67:LEU:HB2	1.88	0.54
9:V:166:VAL:CG1	10:P:103:MET:HE2	2.35	0.54
9:V:63:LEU:HD23	9:V:202:THR:OG1	2.08	0.54
12:O:708:ARG:NH1	14:N:40:GLN:CD	2.66	0.54
4:D:131:PRO:HG3	12:O:552:LYS:HZ2	1.72	0.54
9:V:159:LYS:CE	11:Q:104:LEU:HG	2.36	0.54
5:E:233:LEU:CB	6:F:47:VAL:HG22	2.38	0.54
9:V:87:VAL:HB	9:V:118:LEU:HD12	1.85	0.54
12:O:700:ILE:HG23	12:O:701:GLN:N	2.23	0.54
12:O:717:MET:HA	12:O:717:MET:CE	2.28	0.54
3:C:64:VAL:HG12	3:C:64:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:237:LEU:HG	6:F:44:HIS:CG	2.44	0.53
5:E:233:LEU:O	6:F:44:HIS:O	2.27	0.53
9:V:88:TRP:HB3	9:V:98:TYR:HE2	1.73	0.53
9:V:163:LEU:HG	11:Q:104:LEU:HD13	1.88	0.53
12:O:693:VAL:HG13	12:O:741:TYR:O	2.08	0.53
2:B:295:ASP:N	13:R:106:TYR:CZ	2.77	0.53
5:E:106:ARG:HH11	14:N:76:GLY:H	1.56	0.53
2:B:270:SER:HB2	2:B:271:PRO:HA	1.90	0.53
9:V:180:ILE:CD1	11:Q:101:LEU:CD2	2.77	0.53
12:O:72:LEU:O	12:O:76:VAL:HG23	2.08	0.53
9:V:67:ASN:HA	9:V:91:PHE:HE1	1.73	0.53
9:V:79:ARG:HB2	9:V:151:ILE:O	2.08	0.53
9:V:112:TYR:HB2	9:V:115:HIS:ND1	2.24	0.53
9:V:74:VAL:HG22	9:V:147:ILE:HG23	1.87	0.53
12:O:657:MET:HG2	12:O:660:ASP:N	2.23	0.53
12:O:726:ILE:HG22	12:O:731:ILE:O	2.09	0.53
7:H:80:ARG:HB2	7:H:89:ILE:HD13	1.90	0.53
12:O:675:ASP:O	12:O:679:TYR:HD1	1.92	0.53
5:E:112:ALA:HB2	14:N:76:GLY:CA	2.37	0.52
9:V:76:PHE:HE2	9:V:109:ILE:HG12	1.68	0.52
11:Q:59:GLU:HG2	12:O:32:ARG:HE	1.75	0.52
12:O:700:ILE:CD1	12:O:715:ILE:HG23	2.39	0.52
5:E:237:LEU:H	6:F:44:HIS:HB2	1.74	0.52
5:E:316:HIS:CE1	6:F:220:HIS:HB2	2.45	0.52
9:V:90:ASN:ND2	9:V:92:ASP:HB2	2.19	0.52
12:O:88:HIS:CG	12:O:183:GLY:HA3	2.44	0.52
5:E:237:LEU:HG	6:F:44:HIS:CB	2.40	0.52
12:O:699:LEU:O	12:O:703:VAL:HG23	2.10	0.52
2:B:180:GLN:HB2	2:B:181:THR:HG23	1.92	0.52
9:V:159:LYS:NZ	11:Q:108:ASN:ND2	2.58	0.52
9:V:159:LYS:HZ2	11:Q:108:ASN:HB2	1.68	0.51
9:V:165:VAL:HG13	9:V:166:VAL:N	2.25	0.51
14:N:44:ILE:HD11	14:N:70:VAL:HG12	1.92	0.51
9:V:62:VAL:HG11	9:V:205:ARG:HD2	1.91	0.51
5:E:239:GLU:HG3	6:F:200:VAL:HG11	1.91	0.51
9:V:158:LEU:HD13	9:V:158:LEU:C	2.35	0.51
2:B:294:PHE:O	13:R:106:TYR:CD1	2.62	0.51
5:E:235:ARG:N	6:F:46:LEU:H	2.07	0.51
12:O:654:THR:OG1	12:O:655:THR:OG1	2.26	0.51
12:O:654:THR:C	12:O:655:THR:CG2	2.84	0.51
9:V:76:PHE:HD1	9:V:149:ALA:HB3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:118:LEU:HD12	9:V:118:LEU:O	2.11	0.51
12:O:612:LYS:CB	12:O:657:MET:HE1	2.35	0.51
12:O:684:ILE:HG21	12:O:725:LEU:HD12	1.92	0.51
14:N:3:ILE:HD12	14:N:67:LEU:HD13	1.93	0.51
9:V:171:LYS:HE3	10:P:106:GLN:CD	2.36	0.50
12:O:77:LEU:HD22	12:O:155:LEU:HD13	1.93	0.50
11:Q:42:ILE:HG23	11:Q:60:VAL:HG21	1.93	0.50
9:V:76:PHE:CD2	9:V:109:ILE:CD1	2.95	0.50
9:V:159:LYS:HG3	11:Q:108:ASN:CA	2.41	0.50
4:D:168:ILE:HG21	4:D:194:VAL:HG21	1.93	0.50
9:V:59:PRO:O	9:V:60:ARG:HB2	2.10	0.50
9:V:176:ARG:HH21	9:V:185:TYR:HE2	1.56	0.50
12:O:667:GLN:HA	12:O:667:GLN:OE1	2.11	0.50
9:V:75:ILE:CG2	9:V:148:PHE:CD2	2.95	0.50
9:V:147:ILE:HG23	9:V:147:ILE:O	2.12	0.50
9:V:177:ARG:N	10:P:102:VAL:HG11	2.26	0.50
12:O:370:LYS:CG	14:N:33:LYS:CA	2.72	0.50
9:V:74:VAL:HG12	9:V:75:ILE:N	2.26	0.49
9:V:159:LYS:CE	11:Q:108:ASN:HB2	2.43	0.49
12:O:509:ILE:HG22	13:R:28:ASN:HB2	1.94	0.49
14:N:26:ILE:O	14:N:30:VAL:HG23	2.11	0.49
9:V:101:LEU:HB3	9:V:105:THR:CG2	2.41	0.49
12:O:687:ILE:HG21	12:O:702:GLU:OE1	2.11	0.49
12:O:312:ILE:HD13	12:O:363:HIS:CD2	2.47	0.49
4:D:243:SER:CB	4:D:303:ALA:HB3	2.43	0.49
9:V:120:ARG:HD2	9:V:127:GLY:HA2	1.94	0.49
9:V:178:LEU:CD2	10:P:103:MET:SD	2.84	0.49
5:E:233:LEU:HB2	6:F:47:VAL:HG22	1.93	0.49
9:V:178:LEU:HD13	10:P:103:MET:HE3	0.53	0.49
5:E:203:TYR:CE2	5:E:309:LYS:CG	2.95	0.49
9:V:174:ASN:CG	10:P:102:VAL:HA	2.37	0.49
12:O:661:THR:HG23	12:O:662:PRO:CD	2.42	0.49
12:O:661:THR:N	12:O:662:PRO:HD2	2.28	0.49
12:O:723:GLU:HA	12:O:726:ILE:HG12	1.95	0.48
12:O:700:ILE:HD11	12:O:715:ILE:HG23	1.95	0.48
2:B:72:LEU:HB3	2:B:95:LEU:HD21	1.94	0.48
3:C:305:LYS:HA	3:C:308:GLN:HG2	1.96	0.48
12:O:376:VAL:HG21	12:O:424:TYR:CD2	2.48	0.48
12:O:514:ALA:HA	13:R:32:LEU:HD22	1.95	0.48
12:O:659:LYS:C	12:O:662:PRO:HD2	2.39	0.48
14:N:50:MET:HE3	14:N:59:TYR:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:236:LYS:HB3	6:F:44:HIS:HA	1.96	0.48
5:E:234:ASP:H	6:F:47:VAL:H	1.60	0.48
6:F:314:ASP:CG	6:F:315:ARG:H	2.21	0.48
9:V:66:VAL:O	9:V:66:VAL:HG23	2.14	0.47
9:V:142:VAL:HG23	9:V:143:ASP:N	2.24	0.47
9:V:65:SER:HA	9:V:116:LEU:HD13	1.96	0.47
9:V:67:ASN:HA	9:V:91:PHE:CE1	2.49	0.47
9:V:154:PRO:HG2	9:V:156:TYR:CE1	2.49	0.47
9:V:158:LEU:HD13	9:V:162:CYS:SG	2.53	0.47
9:V:177:ARG:CZ	10:P:101:ASP:C	2.67	0.47
12:O:701:GLN:HE22	14:N:39:GLN:NE2	2.13	0.47
3:C:39:LEU:HB3	3:C:58:VAL:HG13	1.95	0.47
3:C:71:VAL:HB	3:C:72:PRO:HD2	1.95	0.47
9:V:76:PHE:O	9:V:106:GLY:HA2	2.15	0.47
9:V:170:VAL:HG13	10:P:103:MET:HA	1.95	0.47
9:V:172:PRO:HA	9:V:175:TYR:CD2	2.49	0.47
1:A:247:THR:HG23	1:A:274:SER:H	1.80	0.47
2:B:214:LEU:HD22	2:B:240:CYS:SG	2.55	0.47
2:B:294:PHE:O	13:R:106:TYR:CG	2.67	0.47
2:B:300:LYS:H	2:B:301:PRO:HD2	1.79	0.47
5:E:238:LEU:H	5:E:238:LEU:HG	1.43	0.47
12:O:694:LEU:CD2	12:O:699:LEU:HA	2.44	0.47
9:V:130:VAL:HA	9:V:150:ASN:O	2.15	0.47
3:C:205:TYR:CZ	3:C:226:LYS:HB3	2.50	0.47
14:N:54:LYS:NZ	14:N:58:ASP:OD2	2.31	0.47
9:V:208:HIS:O	9:V:210:ARG:HD2	2.15	0.47
9:V:159:LYS:O	9:V:163:LEU:HG	2.15	0.46
9:V:163:LEU:HD22	9:V:188:LEU:CD2	2.43	0.46
12:O:700:ILE:O	12:O:704:ILE:HD13	2.15	0.46
9:V:137:VAL:O	9:V:137:VAL:HG13	2.15	0.46
5:E:236:LYS:HB2	6:F:45:PRO:HD2	1.96	0.46
5:E:237:LEU:CA	6:F:44:HIS:HB2	2.44	0.46
12:O:503:LEU:H	13:R:25:LYS:HG3	1.79	0.46
5:E:92:ILE:HD13	5:E:134:ILE:HD13	1.98	0.46
12:O:711:PHE:O	12:O:713:PRO:HD3	2.16	0.46
3:C:180:HIS:HA	3:C:183:CYS:SG	2.56	0.46
9:V:163:LEU:CD2	11:Q:104:LEU:HD22	2.23	0.46
9:V:177:ARG:CB	10:P:102:VAL:CA	2.50	0.46
12:O:660:ASP:O	12:O:664:GLU:HG3	2.16	0.46
12:O:732:GLU:HG2	12:O:733:ARG:N	2.30	0.46
9:V:67:ASN:CA	9:V:91:PHE:HE1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:67:ASN:CA	9:V:91:PHE:CE1	2.99	0.46
9:V:178:LEU:HD23	10:P:103:MET:H	1.80	0.46
9:V:63:LEU:N	9:V:63:LEU:HD22	2.30	0.46
9:V:184:LEU:HB3	11:Q:104:LEU:HD23	1.98	0.46
2:B:282:LEU:HD11	2:B:346:HIS:CD2	2.52	0.45
9:V:62:VAL:HG12	9:V:205:ARG:HD2	1.95	0.45
12:O:680:LEU:CD1	12:O:703:VAL:CG1	2.94	0.45
12:O:681:GLN:HE22	12:O:728:LYS:NZ	2.14	0.45
9:V:109:ILE:HG22	9:V:110:HIS:N	2.30	0.45
9:V:162:CYS:O	9:V:166:VAL:HG23	2.15	0.45
12:O:509:ILE:O	12:O:510:TYR:CG	2.68	0.45
5:E:233:LEU:C	6:F:44:HIS:O	2.60	0.45
5:E:241:LEU:HG	6:F:192:THR:HA	1.99	0.45
11:Q:44:ALA:HB1	12:O:103:CYS:HB3	1.98	0.45
12:O:684:ILE:HG22	12:O:731:ILE:CD1	2.46	0.45
5:E:203:TYR:CD1	5:E:309:LYS:N	2.85	0.45
6:F:258:ARG:HB2	8:G:159:GLY:HA3	1.99	0.45
9:V:64:ARG:HG2	9:V:64:ARG:HH11	1.82	0.45
12:O:283:HIS:CE1	12:O:287:ARG:HH21	2.35	0.45
12:O:714:SER:HB2	12:O:717:MET:HG2	1.99	0.45
6:F:56:ILE:HG23	6:F:59:ARG:HH21	1.80	0.45
9:V:76:PHE:CD2	9:V:109:ILE:HD11	2.52	0.45
12:O:735:GLN:OE1	12:O:735:GLN:HA	2.15	0.45
9:V:70:GLU:HG3	9:V:113:ARG:HB3	1.99	0.45
9:V:159:LYS:HG3	11:Q:108:ASN:CB	2.46	0.45
4:D:55:GLU:CB	12:O:538:GLN:HE22	2.30	0.45
4:D:175:GLN:HG3	4:D:187:TYR:CD2	2.51	0.45
5:E:236:LYS:HB2	6:F:45:PRO:CD	2.46	0.45
9:V:181:VAL:HG22	12:O:3:LEU:HB2	1.98	0.45
14:N:51:ASN:OD1	14:N:52:ASP:N	2.44	0.45
9:V:84:VAL:HG22	9:V:128:LEU:CD1	2.47	0.44
12:O:717:MET:HE2	12:O:717:MET:CA	2.32	0.44
3:C:221:LEU:HD11	3:C:256:LEU:HD13	1.98	0.44
9:V:180:ILE:HB	11:Q:105:MET:HE2	1.99	0.44
12:O:717:MET:HE2	12:O:720:LYS:HD2	1.98	0.44
10:P:99:LEU:HD23	11:Q:98:GLU:HA	1.99	0.44
14:N:61:ILE:HD13	14:N:67:LEU:HD11	1.99	0.44
7:H:200:LEU:O	7:H:204:VAL:HG23	2.18	0.44
9:V:180:ILE:CG1	11:Q:101:LEU:CD2	1.87	0.44
2:B:314:LEU:HD11	2:B:326:PHE:CZ	2.52	0.44
3:C:112:VAL:HG22	3:C:151:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:62:VAL:HG12	9:V:205:ARG:NH1	2.28	0.44
3:C:138:LEU:HD11	3:C:184:TYR:CD2	2.52	0.44
9:V:88:TRP:HE1	9:V:115:HIS:CD2	2.35	0.44
9:V:163:LEU:CG	11:Q:104:LEU:HD13	2.41	0.44
9:V:177:ARG:CB	10:P:102:VAL:H	1.96	0.44
2:B:285:MET:HE1	2:B:315:VAL:HG22	1.99	0.44
3:C:12:VAL:HG21	3:C:54:HIS:HB2	2.00	0.44
5:E:261:TYR:CD1	5:E:261:TYR:C	2.96	0.44
5:E:236:LYS:H	6:F:44:HIS:C	2.26	0.43
9:V:60:ARG:HB3	9:V:61:PRO:HD2	1.99	0.43
3:C:263:LEU:HD12	3:C:275:LEU:HD11	2.00	0.43
9:V:178:LEU:CD2	10:P:103:MET:H	2.30	0.43
12:O:153:GLU:C	12:O:155:LEU:H	2.26	0.43
12:O:370:LYS:HE2	14:N:34:GLU:C	2.37	0.43
12:O:656:SER:HB3	12:O:657:MET:SD	2.58	0.43
3:C:153:LYS:H	3:C:153:LYS:HD2	1.83	0.43
8:G:45:GLU:CD	8:G:45:GLU:H	2.26	0.43
9:V:73:GLN:HG2	9:V:146:PRO:HG3	2.00	0.43
5:E:175:THR:OG1	6:F:198:ILE:HD13	2.19	0.43
5:E:233:LEU:HB3	6:F:47:VAL:HG22	2.00	0.43
4:D:309:LEU:HB3	4:D:348:MET:HE1	1.99	0.43
12:O:319:ILE:HD12	12:O:350:PHE:CG	2.52	0.43
14:N:37:PRO:HA	14:N:38:PRO:HD3	1.83	0.43
8:G:123:ARG:HG3	8:G:123:ARG:HH11	1.84	0.43
9:V:188:LEU:HD21	11:Q:104:LEU:HD22	2.00	0.43
12:O:654:THR:CB	12:O:655:THR:HB	2.44	0.43
12:O:684:ILE:CG2	12:O:725:LEU:CD1	2.97	0.43
9:V:124:THR:O	9:V:125:HIS:HB2	2.19	0.43
9:V:74:VAL:HG13	9:V:147:ILE:O	2.19	0.43
4:D:317:ASN:HB2	4:D:368:PRO:HD2	2.00	0.42
5:E:116:TYR:CE2	6:F:111:GLN:HB2	2.53	0.42
9:V:171:LYS:HD2	10:P:106:GLN:H	1.84	0.42
12:O:370:LYS:NZ	14:N:32:GLU:O	2.52	0.42
12:O:617:LEU:HG	12:O:623:ILE:HD13	2.01	0.42
12:O:659:LYS:O	12:O:662:PRO:HD2	2.19	0.42
1:A:141:LYS:HB3	1:A:141:LYS:HZ2	1.85	0.42
6:F:46:LEU:HD23	6:F:47:VAL:HA	2.01	0.42
2:B:101:SER:HB3	2:B:102:ALA:H	1.62	0.42
3:C:380:MET:HE1	6:F:290:ALA:HB3	2.00	0.42
9:V:159:LYS:CE	11:Q:104:LEU:HD11	2.49	0.42
12:O:654:THR:CA	12:O:655:THR:CB	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:680:LEU:CD1	12:O:718:ILE:CD1	2.94	0.42
9:V:170:VAL:HG12	9:V:171:LYS:O	2.19	0.42
9:V:185:TYR:HD2	9:V:186:GLU:OE2	2.03	0.42
5:E:234:ASP:HA	6:F:44:HIS:CG	2.55	0.42
5:E:334:SER:H	8:G:173:THR:HG22	1.85	0.42
2:B:93:LYS:HA	2:B:96:LEU:HD12	2.02	0.42
5:E:181:VAL:HG21	6:F:199:GLY:HA2	2.01	0.42
9:V:57:GLY:C	9:V:59:PRO:HD3	2.44	0.42
12:O:700:ILE:CG2	12:O:701:GLN:N	2.82	0.42
2:B:229:PRO:CB	12:O:474:HIS:CE1	3.03	0.42
9:V:119:PHE:CD1	9:V:119:PHE:N	2.87	0.42
9:V:158:LEU:CD1	9:V:162:CYS:SG	3.07	0.42
2:B:363:ILE:HG13	2:B:411:LEU:HD21	2.02	0.41
9:V:170:VAL:HG22	10:P:103:MET:O	2.20	0.41
9:V:177:ARG:HD3	10:P:102:VAL:HA	2.01	0.41
12:O:73:HIS:CE1	12:O:77:LEU:HD11	2.54	0.41
5:E:150:ILE:H	5:E:150:ILE:HD12	1.85	0.41
9:V:109:ILE:N	9:V:109:ILE:CD1	2.83	0.41
9:V:165:VAL:CG1	9:V:166:VAL:N	2.82	0.41
9:V:181:VAL:HG22	12:O:3:LEU:CB	2.43	0.41
12:O:475:ARG:HE	13:R:66:GLU:HA	1.85	0.41
1:A:442:MET:HE1	6:F:295:ILE:CD1	2.51	0.41
3:C:59:LEU:HD23	3:C:77:LEU:HD11	2.02	0.41
5:E:112:ALA:HB1	14:N:76:GLY:HA2	1.99	0.41
5:E:205:THR:HG21	5:E:261:TYR:CG	2.55	0.41
5:E:233:LEU:O	6:F:44:HIS:CG	2.73	0.41
5:E:300:LEU:HD23	5:E:300:LEU:HA	1.89	0.41
12:O:694:LEU:CG	12:O:698:ALA:HB3	2.50	0.41
9:V:111:SER:HB3	9:V:112:TYR:H	1.71	0.41
9:V:178:LEU:HA	10:P:100:PRO:CB	2.43	0.41
9:V:178:LEU:N	10:P:102:VAL:HB	2.34	0.41
10:P:44:LEU:HD23	10:P:44:LEU:HA	1.93	0.41
14:N:42:ARG:HG2	14:N:49:GLN:OE1	2.20	0.41
9:V:171:LYS:CE	10:P:106:GLN:OE1	2.63	0.41
12:O:680:LEU:HD12	12:O:703:VAL:CG1	2.51	0.41
12:O:731:ILE:HG22	12:O:732:GLU:N	2.36	0.41
14:N:48:LYS:HE3	14:N:48:LYS:HB2	1.87	0.41
13:R:53:CYS:SG	13:R:80:HIS:CD2	3.13	0.41
9:V:109:ILE:CG2	9:V:110:HIS:N	2.84	0.41
5:E:237:LEU:HG	6:F:44:HIS:HB2	2.02	0.41
9:V:130:VAL:CG2	9:V:149:ALA:HB1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:269:THR:O	3:C:270:ASN:HB2	2.20	0.41
4:D:316:TYR:CB	4:D:365:GLU:H	2.34	0.41
9:V:74:VAL:CG1	9:V:75:ILE:N	2.84	0.41
9:V:82:ARG:HD2	9:V:121:ASP:OD2	2.20	0.41
9:V:142:VAL:C	9:V:144:GLY:N	2.75	0.41
9:V:206:ILE:HD12	9:V:207:ALA:CA	2.51	0.41
12:O:473:LEU:N	12:O:473:LEU:HD22	2.36	0.41
9:V:158:LEU:C	9:V:158:LEU:CD1	2.94	0.41
9:V:170:VAL:HG12	9:V:171:LYS:N	2.35	0.41
12:O:512:LEU:HB2	13:R:32:LEU:HD23	2.01	0.41
12:O:725:LEU:HD23	12:O:725:LEU:HA	1.92	0.41
12:O:306:THR:CG2	14:N:2:LEU:HD21	2.51	0.40
2:B:418:GLY:O	2:B:422:THR:HG22	2.22	0.40
9:V:159:LYS:HZ1	11:Q:108:ASN:ND2	2.17	0.40
9:V:181:VAL:CG2	12:O:4:LYS:N	2.67	0.40
12:O:694:LEU:HD11	12:O:698:ALA:CB	2.51	0.40
2:B:171:ILE:HG13	2:B:172:LEU:N	2.37	0.40
6:F:200:VAL:O	6:F:200:VAL:HG12	2.22	0.40
9:V:107:ARG:HG2	9:V:108:ARG:N	2.37	0.40
14:N:55:THR:HG1	14:N:58:ASP:CG	2.30	0.40
12:O:513:GLN:HB2	12:O:516:ALA:HB3	2.03	0.40
5:E:233:LEU:C	6:F:45:PRO:HA	2.47	0.40
9:V:129:LEU:O	9:V:151:ILE:HA	2.21	0.40
12:O:654:THR:CB	12:O:655:THR:CB	2.99	0.40
12:O:657:MET:CG	12:O:660:ASP:HB3	2.51	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	431/433 (100%)	399 (93%)	26 (6%)	6 (1%)	9 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	412/443 (93%)	364 (88%)	33 (8%)	15 (4%)	2	20
3	C	401/403 (100%)	361 (90%)	26 (6%)	14 (4%)	3	20
4	D	404/406 (100%)	387 (96%)	8 (2%)	9 (2%)	5	29
5	E	309/311 (99%)	290 (94%)	15 (5%)	4 (1%)	9	42
6	F	286/288 (99%)	272 (95%)	8 (3%)	6 (2%)	5	30
7	H	164/209 (78%)	158 (96%)	5 (3%)	1 (1%)	21	59
8	G	206/208 (99%)	189 (92%)	13 (6%)	4 (2%)	6	32
9	V	158/160 (99%)	154 (98%)	1 (1%)	3 (2%)	6	32
10	P	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
11	Q	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
12	O	738/745 (99%)	691 (94%)	29 (4%)	18 (2%)	4	27
13	R	88/90 (98%)	70 (80%)	13 (15%)	5 (6%)	1	14
14	N	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
All	All	3897/4002 (97%)	3617 (93%)	195 (5%)	85 (2%)	7	29

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	ALA
1	A	426	ALA
2	B	61	GLU
2	B	141	ASP
2	B	186	ASP
2	B	411	LEU
3	C	51	VAL
3	C	70	SER
3	C	71	VAL
3	C	134	ASN
4	D	294	ALA
4	D	300	LEU
4	D	363	THR
4	D	364	ARG
6	F	192	THR
6	F	193	GLU
7	H	158	THR
9	V	145	GLN
12	O	234	GLN

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Mol	Chain	Res	Type
12	O	272	ALA
12	O	505	ILE
12	O	739	ASP
13	R	36	ASP
13	R	60	GLN
13	R	68	CYS
1	A	278	CYS
2	B	229	PRO
2	B	299	ALA
2	B	379	ASN
3	C	136	ASN
3	C	154	CYS
3	C	168	ASP
3	C	362	ASP
4	D	236	ALA
4	D	295	ASP
6	F	249	GLU
8	G	161	ASP
12	O	138	GLU
12	O	290	LYS
12	O	383	SER
12	O	522	ALA
12	O	525	SER
1	A	238	ARG
2	B	182	ASP
2	B	231	PRO
3	C	173	ASN
4	D	238	ALA
4	D	365	GLU
5	E	99	PRO
6	F	213	GLU
8	G	160	ARG
8	G	163	ARG
12	O	49	TYR
12	O	502	ASP
12	O	510	TYR
13	R	62	SER
1	A	86	PHE
2	B	163	GLU
2	B	185	GLU
2	B	270	SER
3	C	89	ASN

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Mol	Chain	Res	Type
3	C	172	GLU
4	D	299	ILE
6	F	95	GLU
8	G	24	GLY
12	O	171	ARG
12	O	529	ILE
12	O	536	SER
13	R	42	CYS
2	B	300	LYS
2	B	301	PRO
3	C	67	SER
3	C	270	ASN
5	E	102	GLY
5	E	196	PRO
2	B	84	ASN
3	C	48	ALA
12	O	173	GLY
12	O	191	VAL
6	F	164	PRO
9	V	142	VAL
12	O	154	PRO
1	A	117	PRO
9	V	60	ARG
5	E	172	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	377/377 (100%)	361 (96%)	16 (4%)	26	48
2	B	376/405 (93%)	353 (94%)	23 (6%)	17	38
3	C	359/359 (100%)	343 (96%)	16 (4%)	24	46
4	D	347/347 (100%)	340 (98%)	7 (2%)	48	66
5	E	267/267 (100%)	248 (93%)	19 (7%)	13	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	255/255 (100%)	235 (92%)	20 (8%)	11	32
7	H	139/173 (80%)	132 (95%)	7 (5%)	22	43
8	G	181/181 (100%)	172 (95%)	9 (5%)	22	43
9	V	147/147 (100%)	146 (99%)	1 (1%)	76	81
10	P	103/103 (100%)	99 (96%)	4 (4%)	28	49
11	Q	96/96 (100%)	93 (97%)	3 (3%)	35	56
12	O	680/681 (100%)	646 (95%)	34 (5%)	22	43
13	R	79/79 (100%)	73 (92%)	6 (8%)	12	33
14	N	64/66 (97%)	59 (92%)	5 (8%)	11	32
All	All	3470/3536 (98%)	3300 (95%)	170 (5%)	24	43

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	75	LEU
1	A	76	LYS
1	A	87	ASN
1	A	109	LEU
1	A	140	LEU
1	A	141	LYS
1	A	178	LEU
1	A	218	VAL
1	A	258	LEU
1	A	275	PHE
1	A	283	LEU
1	A	310	VAL
1	A	348	MET
1	A	400	LEU
1	A	468	SER
2	B	42	LEU
2	B	66	GLU
2	B	69	PHE
2	B	70	LYS
2	B	83	THR
2	B	87	GLU
2	B	115	ILE
2	B	124	GLN
2	B	146	ARG

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Mol	Chain	Res	Type
2	B	188	LEU
2	B	233	ILE
2	B	253	LYS
2	B	274	THR
2	B	291	ILE
2	B	303	LYS
2	B	320	ASN
2	B	330	LEU
2	B	337	ILE
2	B	363	ILE
2	B	380	ILE
2	B	384	ASP
2	B	391	GLN
2	B	409	LEU
3	C	5	LEU
3	C	15	LEU
3	C	29	ASN
3	C	35	LEU
3	C	51	VAL
3	C	85	ILE
3	C	124	LEU
3	C	125	LYS
3	C	153	LYS
3	C	217	SER
3	C	241	LEU
3	C	299	LEU
3	C	302	LEU
3	C	363	ASN
3	C	385	GLU
3	C	402	GLN
4	D	202	ILE
4	D	272	ILE
4	D	300	LEU
4	D	316	TYR
4	D	368	PRO
4	D	385	LEU
4	D	396	THR
5	E	77	VAL
5	E	80	LEU
5	E	85	VAL
5	E	130	LEU
5	E	131	GLU

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Mol	Chain	Res	Type
5	E	165	PHE
5	E	191	LYS
5	E	206	ILE
5	E	219	LYS
5	E	227	SER
5	E	229	PHE
5	E	238	LEU
5	E	240	LEU
5	E	241	LEU
5	E	261	TYR
5	E	282	ARG
5	E	305	ARG
5	E	312	ILE
5	E	315	ILE
6	F	30	VAL
6	F	44	HIS
6	F	45	PRO
6	F	46	LEU
6	F	47	VAL
6	F	49	LEU
6	F	50	ASN
6	F	64	ARG
6	F	67	GLN
6	F	73	ILE
6	F	90	LEU
6	F	132	ASP
6	F	154	LEU
6	F	163	LEU
6	F	172	ILE
6	F	197	ARG
6	F	214	ASN
6	F	259	GLU
6	F	269	VAL
6	F	289	MET
7	H	16	LEU
7	H	40	LEU
7	H	60	ILE
7	H	71	LEU
7	H	105	ILE
7	H	128	ILE
7	H	197	LEU
8	G	23	SER

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Mol	Chain	Res	Type
8	G	27	LEU
8	G	47	LEU
8	G	69	LEU
8	G	82	LYS
8	G	111	ILE
8	G	117	LEU
8	G	136	VAL
8	G	148	ARG
9	V	159	LYS
10	P	14	ILE
10	P	34	ILE
10	P	97	PRO
10	P	99	LEU
11	Q	51	GLN
11	Q	64	GLU
11	Q	101	LEU
12	O	21	ILE
12	O	50	PRO
12	O	108	LEU
12	O	115	LYS
12	O	148	ARG
12	O	155	LEU
12	O	168	LYS
12	O	175	ASP
12	O	184	VAL
12	O	206	ILE
12	O	255	HIS
12	O	257	SER
12	O	261	LYS
12	O	271	VAL
12	O	276	GLN
12	O	353	LEU
12	O	379	ARG
12	O	411	VAL
12	O	420	THR
12	O	439	LEU
12	O	473	LEU
12	O	477	TYR
12	O	501	ILE
12	O	531	GLN
12	O	537	VAL
12	O	565	LYS

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Mol	Chain	Res	Type
12	O	592	GLU
12	O	599	LEU
12	O	607	GLU
12	O	614	ILE
12	O	621	LYS
12	O	623	ILE
12	O	647	LYS
12	O	652	LYS
13	R	37	ILE
13	R	39	VAL
13	R	64	THR
13	R	75	CYS
13	R	82	HIS
13	R	99	ARG
14	N	2	LEU
14	N	17	ILE
14	N	66	VAL
14	N	68	HIS
14	N	70	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	61	GLN
1	A	66	HIS
1	A	95	HIS
1	A	110	GLN
1	A	155	ASN
1	A	171	HIS
1	A	217	HIS
1	A	371	ASN
2	B	90	ASN
2	B	106	ASN
2	B	129	GLN
2	B	180	GLN
2	B	210	ASN
2	B	297	GLN
2	B	313	ASN
2	B	319	GLN
2	B	333	ASN
2	B	346	HIS

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Mol	Chain	Res	Type
2	B	399	HIS
2	B	432	ASN
3	C	10	ASN
3	C	14	GLN
3	C	20	GLN
3	C	52	GLN
3	C	54	HIS
3	C	89	ASN
3	C	105	HIS
3	C	116	GLN
3	C	132	GLN
3	C	137	GLN
3	C	142	HIS
3	C	173	ASN
3	C	271	ASN
3	C	290	ASN
3	C	352	ASN
3	C	363	ASN
3	C	368	ASN
3	C	395	GLN
4	D	54	ASN
4	D	169	ASN
4	D	186	HIS
4	D	206	GLN
4	D	209	ASN
4	D	277	GLN
4	D	308	ASN
4	D	317	ASN
4	D	318	ASN
4	D	380	GLN
5	E	35	GLN
5	E	36	GLN
5	E	37	GLN
5	E	50	HIS
5	E	126	GLN
5	E	132	ASN
5	E	138	HIS
5	E	140	HIS
5	E	159	GLN
5	E	217	HIS
5	E	316	HIS
6	F	137	HIS

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Mol	Chain	Res	Type
6	F	202	HIS
6	F	214	ASN
6	F	225	HIS
6	F	300	ASN
6	F	310	ASN
7	H	19	GLN
7	H	39	GLN
8	G	33	GLN
8	G	60	ASN
8	G	124	ASN
8	G	169	ASN
8	G	196	ASN
8	G	203	ASN
9	V	115	HIS
9	V	145	GLN
11	Q	58	ASN
11	Q	108	ASN
12	O	15	ASN
12	O	68	HIS
12	O	73	HIS
12	O	88	HIS
12	O	111	GLN
12	O	156	GLN
12	O	182	HIS
12	O	190	HIS
12	O	267	GLN
12	O	276	GLN
12	O	283	HIS
12	O	310	HIS
12	O	317	ASN
12	O	318	HIS
12	O	352	GLN
12	O	363	HIS
12	O	377	ASN
12	O	474	HIS
12	O	487	ASN
12	O	488	ASN
12	O	491	ASN
12	O	538	GLN
12	O	643	ASN
12	O	658	GLN
12	O	663	GLN

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Mol	Chain	Res	Type
12	O	681	GLN
13	R	47	ASN
13	R	57	GLN
13	R	76	ASN
13	R	80	HIS
13	R	82	HIS
14	N	39	GLN
14	N	41	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	654:THR	C	655:THR	N	4.12

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4739. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit ⓘ

This section was not generated.